

Supplementary Materials

of

An ONIOM-based High-level Thermochemistry Study on
Hydrogen Abstraction Reactions of Large Straight-chain
Alkanes by Hydrogen, Hydroxyl, and Hydroperoxyl Radicals

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1. Figure

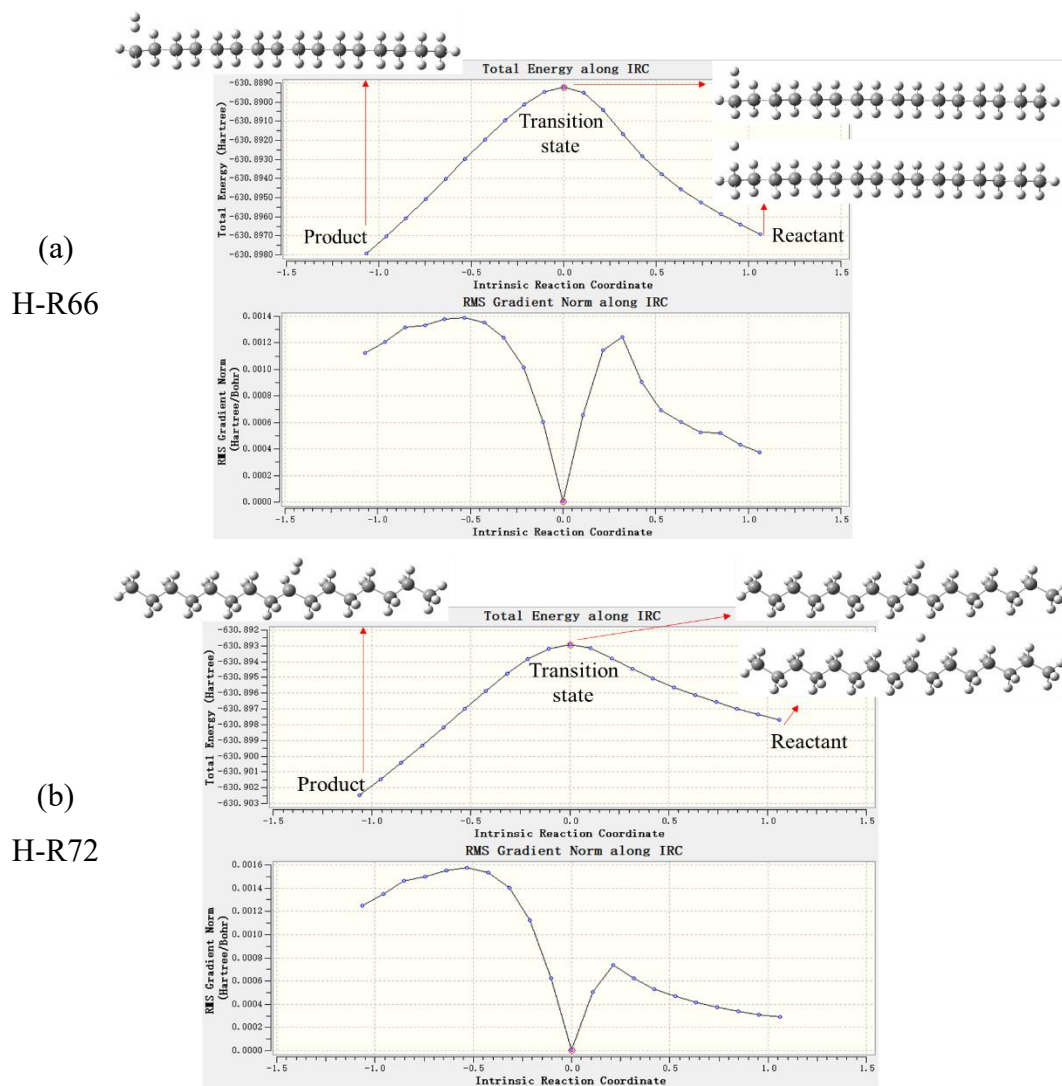


Figure S1 The IRC curves of the reactions (a) H-R66: $\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_{13}\text{CH}_3$ and (b) H-R72: $\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_6\text{CH}(\text{CH}_2)_7\text{CH}_3$.

2. Tables

Table S1 The calculated results (EB and ΔH) for the hydrogen abstraction reactions of $n\text{-C}_n\text{H}_{2n+2} + \text{H}$ ($n = 10\text{-}16$) using the ONIOM method (unit: kcal/mol).

	No.	Reactions	EB	ΔH
C10	H-R26	$\text{H} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_8\text{CH}_3$	9.82	-3.70
	H-R27	$\text{H} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_7\text{CH}_3$	7.15	-6.47
	H-R28	$\text{H} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_6\text{CH}_3$	7.05	-6.19
	H-R29	$\text{H} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_5\text{CH}_3$	7.04	-6.25
	H-R30	$\text{H} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_4\text{CH}_3$	7.02	-6.27
C11	H-R31	$\text{H} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_9\text{CH}_3$	9.78	-3.71
	H-R32	$\text{H} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_8\text{CH}_3$	7.12	-6.47
	H-R33	$\text{H} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_7\text{CH}_3$	7.06	-6.19
	H-R34	$\text{H} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_6\text{CH}_3$	6.96	-6.26
	H-R35	$\text{H} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_5\text{CH}_3$	6.99	-6.25
	H-R36	$\text{H} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_4\text{CH}_3$	6.98	-6.32
C12	H-R37	$\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_{10}\text{CH}_3$	9.79	-3.70
	H-R38	$\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_9\text{CH}_3$	7.13	-6.46
	H-R39	$\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_8\text{CH}_3$	7.11	-6.19
	H-R40	$\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_7\text{CH}_3$	7.05	-6.25
	H-R41	$\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_6\text{CH}_3$	7.05	-6.28
	H-R42	$\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_5\text{CH}_3$	7.01	-6.29
C13	H-R43	$\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_{11}\text{CH}_3$	9.79	-3.72
	H-R44	$\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_{10}\text{CH}_3$	7.16	-6.49
	H-R45	$\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_9\text{CH}_3$	7.09	-6.21
	H-R46	$\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_8\text{CH}_3$	7.05	-6.28
	H-R47	$\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_7\text{CH}_3$	7.00	-6.26
	H-R48	$\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_6\text{CH}_3$	7.00	-6.37
	H-R49	$\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_5\text{CH}_3$	6.97	-6.18
C14	H-R50	$\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_{12}\text{CH}_3$	9.81	-3.70
	H-R51	$\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_{11}\text{CH}_3$	7.21	-6.46
	H-R52	$\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_{10}\text{CH}_3$	7.12	-6.19
	H-R53	$\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_9\text{CH}_3$	7.08	-6.24
	H-R54	$\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_8\text{CH}_3$	7.05	-6.30

	H-R55	$\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_7\text{CH}_3$	7.03	-6.17
	H-R56	$\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_6\text{CH}_3$	6.98	-6.16
C15	H-R57	$\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_{13}\text{CH}_3$	9.82	-3.71
	H-R58	$\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_{12}\text{CH}_3$	7.19	-6.46
	H-R59	$\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_{11}\text{CH}_3$	7.11	-6.19
	H-R60	$\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_{10}\text{CH}_3$	7.08	-6.24
	H-R61	$\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_9\text{CH}_3$	7.01	-6.34
	H-R62	$\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_8\text{CH}_3$	7.01	-6.33
	H-R63	$\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_7\text{CH}_3$	6.95	-6.34
	H-R64	$\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_6\text{CH}(\text{CH}_2)_6\text{CH}_3$	6.93	-6.26
C16	H-R65	$\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_{14}\text{CH}_3$	9.82	-3.70
	H-R66	$\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_{13}\text{CH}_3$	7.21	-6.46
	H-R67	$\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_{12}\text{CH}_3$	7.12	-6.19
	H-R68	$\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_{11}\text{CH}_3$	7.08	-6.24
	H-R69	$\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_{10}\text{CH}_3$	7.00	-6.40
	H-R70	$\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_9\text{CH}_3$	7.02	-6.27
	H-R71	$\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_8\text{CH}_3$	6.93	-6.33
	H-R72	$\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_6\text{CH}(\text{CH}_2)_7\text{CH}_3$	6.98	-6.34

Table S2. The calculated results (EB and ΔH) for the hydrogen abstraction reactions of $n\text{-C}_n\text{H}_{2n+2} + \text{OH}$ ($n = 9\text{-}16$) using the ONIOM method (unit: kcal/mol).

	No.	Reactions	EB	ΔH
C9	OH-R21	$\text{OH} + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_2(\text{CH}_2)_7\text{CH}_3$	1.79	-18.52
	OH-R22	$\text{OH} + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}(\text{CH}_2)_6\text{CH}_3$	-0.32	-21.59
	OH-R23	$\text{OH} + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_5\text{CH}_3$	-0.43	-20.91
	OH-R24	$\text{OH} + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_4\text{CH}_3$	-0.39	-21.12
	OH-R25	$\text{OH} + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_3\text{CH}_3$	-0.67	-21.00
C10	OH-R26	$\text{OH} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_2(\text{CH}_2)_8\text{CH}_3$	2.24	-18.46
	OH-R27	$\text{OH} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}(\text{CH}_2)_7\text{CH}_3$	-0.50	-21.26
	OH-R28	$\text{OH} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_6\text{CH}_3$	-0.52	-21.06
	OH-R29	$\text{OH} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_5\text{CH}_3$	-1.13	-20.85
	OH-R30	$\text{OH} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_4\text{CH}_3$	-0.49	-21.12
C11	OH-R31	$\text{OH} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_2(\text{CH}_2)_9\text{CH}_3$	1.92	-18.50
	OH-R32	$\text{OH} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}(\text{CH}_2)_8\text{CH}_3$	-0.52	-21.52
	OH-R33	$\text{OH} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_7\text{CH}_3$	-0.59	-20.85
	OH-R34	$\text{OH} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_6\text{CH}_3$	-0.53	-21.31
	OH-R35	$\text{OH} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_5\text{CH}_3$	-1.20	-21.38
	OH-R36	$\text{OH} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_4\text{CH}_3$	-0.52	-21.47
C12	OH-R37	$\text{OH} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_2(\text{CH}_2)_{10}\text{CH}_3$	1.80	-18.47
	OH-R38	$\text{OH} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}(\text{CH}_2)_9\text{CH}_3$	-0.78	-21.29
	OH-R39	$\text{OH} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_8\text{CH}_3$	-0.91	-20.92
	OH-R40	$\text{OH} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_7\text{CH}_3$	-1.29	-20.84
	OH-R41	$\text{OH} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_6\text{CH}_3$	-0.56	-21.27
	OH-R42	$\text{OH} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_5\text{CH}_3$	-0.63	-21.20
C13	OH-R43	$\text{OH} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_2(\text{CH}_2)_{11}\text{CH}_3$	1.84	-18.48
	OH-R44	$\text{OH} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}(\text{CH}_2)_{10}\text{CH}_3$	-0.73	-21.46
	OH-R45	$\text{OH} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_9\text{CH}_3$	-1.33	-20.83
	OH-R46	$\text{OH} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_8\text{CH}_3$	-1.18	-21.04
	OH-R47	$\text{OH} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_7\text{CH}_3$	-1.41	-21.49
	OH-R48	$\text{OH} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_6\text{CH}_3$	-1.06	-21.36
	OH-R49	$\text{OH} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_5\text{CH}_3$	-1.00	-21.48
C14	OH-R50	$\text{OH} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_2(\text{CH}_2)_{12}\text{CH}_3$	2.17	-18.47
	OH-R51	$\text{OH} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}(\text{CH}_2)_{11}\text{CH}_3$	-1.06	-21.30
	OH-R52	$\text{OH} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_{10}\text{CH}_3$	-1.16	-20.87

	OH-R53	$\text{OH} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_9\text{CH}_3$	-1.36	-20.91
	OH-R54	$\text{OH} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_8\text{CH}_3$	-1.19	-21.43
	OH-R55	$\text{OH} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_7\text{CH}_3$	-1.27	-21.25
	OH-R56	$\text{OH} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_6\text{CH}_3$	-1.21	-21.48
C15	OH-R57	$\text{OH} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_2(\text{CH}_2)_{13}\text{CH}_3$	2.04	-18.47
	OH-R58	$\text{OH} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}(\text{CH}_2)_{12}\text{CH}_3$	-0.98	-21.40
	OH-R59	$\text{OH} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_{11}\text{CH}_3$	-1.57	-20.82
	OH-R60	$\text{OH} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_{10}\text{CH}_3$	-1.24	-20.94
	OH-R61	$\text{OH} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_9\text{CH}_3$	-1.53	-21.60
	OH-R62	$\text{OH} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_8\text{CH}_3$	-1.06	-21.59
	OH-R63	$\text{OH} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_7\text{CH}_3$	-1.45	-21.57
	OH-R64	$\text{OH} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_6\text{CH}(\text{CH}_2)_6\text{CH}_3$	-1.06	-21.57
C16	OH-R65	$\text{OH} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_2(\text{CH}_2)_{14}\text{CH}_3$	2.17	-19.35
	OH-R66	$\text{OH} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}(\text{CH}_2)_{13}\text{CH}_3$	-0.96	-21.29
	OH-R67	$\text{OH} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_{12}\text{CH}_3$	-1.40	-20.84
	OH-R68	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_{11}\text{CH}_3$	-1.48	-21.00
	OH-R69	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_{10}\text{CH}_3$	-1.31	-21.98
	OH-R70	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_9\text{CH}_3$	-1.26	-21.18
	OH-R71	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_8\text{CH}_3$	-1.24	-21.54
	OH-R72	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_6\text{CH}(\text{CH}_2)_7\text{CH}_3$	-1.31	-21.62

Table S3. The calculated results (EB and ΔH) for the hydrogen abstraction reactions of $n\text{-C}_n\text{H}_{2n+2} + \text{HO}_2$ ($n = 8\text{-}16$) using the ONIOM method (unit: kcal/mol).

	No.	Reactions	EB	ΔH
C8	HO ₂ -R17	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_2(\text{CH}_2)_6\text{CH}_3$	19.46	13.63
	HO ₂ -R18	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_5\text{CH}_3$	16.52	10.86
	HO ₂ -R19	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_4\text{CH}_3$	16.46	11.16
	HO ₂ -R20	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_3\text{CH}_3$	15.85	11.10
C9	HO ₂ -R21	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_2(\text{CH}_2)_7\text{CH}_3$	19.45	13.63
	HO ₂ -R22	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_6\text{CH}_3$	16.44	10.87
	HO ₂ -R23	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_5\text{CH}_3$	16.26	11.16
	HO ₂ -R24	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_4\text{CH}_3$	15.92	11.09
	HO ₂ -R25	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_3\text{CH}_3$	15.74	11.12
C10	HO ₂ -R26	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_2(\text{CH}_2)_8\text{CH}_3$	19.47	13.64
	HO ₂ -R27	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_7\text{CH}_3$	16.20	10.87
	HO ₂ -R28	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_6\text{CH}_3$	15.92	11.15
	HO ₂ -R29	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_5\text{CH}_3$	15.79	11.09
	HO ₂ -R30	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_4\text{CH}_3$	16.28	11.07
C11	HO ₂ -R31	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_2(\text{CH}_2)_9\text{CH}_3$	19.55	13.63
	HO ₂ -R32	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_8\text{CH}_3$	16.15	10.87
	HO ₂ -R33	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_7\text{CH}_3$	16.28	11.15
	HO ₂ -R34	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_6\text{CH}_3$	15.78	11.08
	HO ₂ -R35	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_5\text{CH}_3$	16.20	11.09
	HO ₂ -R36	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_4\text{CH}_3$	15.74	11.02
C12	HO ₂ -R37	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_2(\text{CH}_2)_{10}\text{CH}_3$	19.55	13.64
	HO ₂ -R38	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_9\text{CH}_3$	16.58	10.88
	HO ₂ -R39	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_8\text{CH}_3$	15.88	11.15
	HO ₂ -R40	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_7\text{CH}_3$	15.74	11.09
	HO ₂ -R41	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_6\text{CH}_3$	15.45	11.06
	HO ₂ -R42	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_5\text{CH}_3$	16.07	11.05
C13	HO ₂ -R43	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_2(\text{CH}_2)_{11}\text{CH}_3$	19.56	13.62
	HO ₂ -R44	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_{10}\text{CH}_3$	16.31	10.85
	HO ₂ -R45	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_9\text{CH}_3$	15.81	11.13
	HO ₂ -R46	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_8\text{CH}_3$	16.19	11.06
	HO ₂ -R47	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_7\text{CH}_3$	15.62	11.08
	HO ₂ -R48	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_6\text{CH}_3$	16.14	10.97
	HO ₂ -R49	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_5\text{CH}_3$	15.45	11.16

C14	HO ₂ -R50	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_2(\text{CH}_2)_{12}\text{CH}_3$	19.00	13.64
	HO ₂ -R51	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_{11}\text{CH}_3$	16.42	10.88
	HO ₂ -R52	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_{10}\text{CH}_3$	15.68	11.15
	HO ₂ -R53	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_9\text{CH}_3$	16.20	11.10
	HO ₂ -R54	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_8\text{CH}_3$	15.61	11.04
	HO ₂ -R55	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_7\text{CH}_3$	16.16	11.17
	HO ₂ -R56	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_6\text{CH}_3$	15.68	11.18
C15	HO ₂ -R57	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_2(\text{CH}_2)_{13}\text{CH}_3$	19.69	13.63
	HO ₂ -R58	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_{12}\text{CH}_3$	16.25	10.87
	HO ₂ -R59	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_{11}\text{CH}_3$	15.64	11.15
	HO ₂ -R60	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_{10}\text{CH}_3$	16.23	11.10
	HO ₂ -R61	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_9\text{CH}_3$	15.58	11.00
	HO ₂ -R62	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_8\text{CH}_3$	16.05	11.01
	HO ₂ -R63	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_7\text{CH}_3$	15.65	11.00
	HO ₂ -R64	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_6\text{CH}(\text{CH}_2)_6\text{CH}_3$	16.20	11.08
C16	HO ₂ -R65	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_2(\text{CH}_2)_{14}\text{CH}_3$	19.36	13.64
	HO ₂ -R66	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_{13}\text{CH}_3$	16.54	10.88
	HO ₂ -R67	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_{12}\text{CH}_3$	15.66	11.15
	HO ₂ -R68	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_{11}\text{CH}_3$	16.05	11.10
	HO ₂ -R69	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_{10}\text{CH}_3$	15.45	10.94
	HO ₂ -R70	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_9\text{CH}_3$	16.09	11.07
	HO ₂ -R71	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_8\text{CH}_3$	15.56	11.01
	HO ₂ -R72	$\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_6\text{CH}(\text{CH}_2)_7\text{CH}_3$	15.98	11.00

3. Cartesian coordinates for all optimized geometries at the B3LYP/6-311++G(d,p) level

2.1 Hydrogen abstraction reaction of n -C_nH_{2n+2} (n = 1-16) by H radical

2.1.1 C1 (CH₄)



H₂

H	0.00000000	0.00000000	0.37207600
H	0.00000000	0.00000000	-0.37207600

CH₄

C	0.00000000	0.00000000	0.00000000
H	0.62967300	0.62967300	0.62967300
H	-0.62967300	-0.62967300	0.62967300
H	-0.62967300	0.62967300	-0.62967300
H	0.62967300	-0.62967300	-0.62967300

CH₃

C	0.00000000	0.00000000	0.00001800
H	0.00000000	1.08065300	-0.00003700
H	-0.93587300	-0.54032600	-0.00003700
H	0.93587300	-0.54032600	-0.00003700



C	-0.27220900	-0.00001500	-0.00003000
H	-0.51369100	-0.71133900	-0.78411700
H	1.14354600	0.00045000	0.00080100
H	-0.51487100	1.03437400	-0.22422700
H	-0.51544100	-0.32336800	1.00763900
H	2.03371000	-0.00002700	0.00008400

2.1.2 C2 (C₂H₆)



C₂H₆

C	0.00000000	0.00000000	0.76536300
H	0.50903500	0.88239000	1.16386300
H	0.50965500	-0.88203200	1.16386300
H	-1.01869000	-0.00035800	1.16386300
C	0.00000000	0.00000000	-0.76536300
H	1.01869000	-0.00035800	-1.16386300
H	-0.50965500	-0.88203200	-1.16386300

H	-0.50903500	0.88239000	-1.16386300
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CH₂CH₃

C	-0.69339800	0.00000000	-0.00203400
H	-1.09320700	-0.00001300	1.02570600
H	-1.10669100	-0.88657600	-0.49273000
H	-1.10669100	0.88658800	-0.49270900
C	0.79402900	0.00000000	-0.01799900
H	1.35140100	-0.92666800	0.03996600
H	1.35140300	0.92666700	0.03996600

TS2: H + CH₃CH₃ → H₂ + CH₂CH₃

C	-0.83757200	0.13118800	0.00000100
H	-1.53770600	-0.71366500	-0.00136000
H	-1.05674800	0.73611200	-0.88401600
H	-1.05748800	0.73389400	0.88535600
C	0.59118000	-0.35114500	0.00000900
H	0.92251800	-0.86003800	-0.90454800
H	1.38656100	0.75505700	-0.00030000
H	0.92263800	-0.85955400	0.90479500
H	1.89857300	1.52793700	0.00001700

2.1.3 C3 (C₃H₈)

H-R3: H + CH₃CH₂CH₃ → H₂ + CH₂CH₂CH₃

C₃H₈

C	1.27718800	-0.25966800	0.00000100
H	1.32215700	-0.90561700	-0.88298000
H	1.32226900	-0.90542700	0.88311300
H	2.17408400	0.36654000	-0.00012500
C	0.00000000	0.58583200	0.00000000
H	0.00000000	1.24503000	0.87572500
H	0.00000100	1.24500600	-0.87574200
C	-1.27718800	-0.25966800	0.00000000
H	-1.32221900	-0.90550400	0.88305900
H	-2.17408400	0.36654000	-0.00001800
H	-1.32220700	-0.90553900	-0.88303400

CH₂CH₂CH₃

C	-1.22868000	-0.24244200	-0.03623100
H	-1.28758600	-0.98559200	0.76478900
H	-1.30416800	-0.77314700	-0.98929700
H	-2.09718200	0.41536300	0.05435700

C	0.08115200	0.55194800	0.04856200
H	0.10809800	1.31453500	-0.74028800
H	0.08546000	1.12545300	0.99248600
C	1.30479300	-0.29378200	-0.02818500
H	2.26467600	0.13528600	-0.28969800
H	1.28710700	-1.32624200	0.30277700

TS3: H + CH₃CH₂CH₃ → H₂ + CH₂CH₂CH₃

C	1.21194300	-0.04331500	0.24883100
C	-0.10598900	-0.58418200	-0.25145200
H	2.09709900	-0.61999000	-0.01814500
H	1.44128900	1.12700200	-0.41973600
H	1.22680600	0.28395200	1.28912200
C	-1.30525200	0.29968800	0.10632700
H	-0.05551100	-0.72195500	-1.33779700
H	-0.25824200	-1.59002800	0.16699400
H	-2.23947000	-0.13321600	-0.26070400
H	-1.39567400	0.41936200	1.19042800
H	-1.20287500	1.29686100	-0.33083800
H	1.58237000	1.90486300	-0.90155500

H-R4: H + CH₃CH₂CH₃ → H₂ + CH₃CHCH₃

CH₃CHCH₃

C	1.29700200	-0.19799900	0.00232700
H	1.31802000	-1.02272500	-0.72207300
H	1.47831500	-0.65750500	0.98902500
H	2.14582700	0.45760400	-0.20635700
C	0.00000000	0.53494500	-0.03998500
H	-0.00000100	1.61157700	0.09080500
C	-1.29700200	-0.19800000	0.00232600
H	-1.47833300	-0.65747300	0.98903700
H	-2.14582300	0.45759600	-0.20639300
H	-1.31800600	-1.02274900	-0.72204700

TS4: H + CH₃CH₂CH₃ → H₂ + CH₃CHCH₃

C	-1.28718800	-0.31316100	0.09263800
C	0.00000000	0.36119500	-0.32779900
H	-2.16214600	0.28252600	-0.18034200
H	-1.39014900	-1.29321500	-0.39083800
H	-1.31314500	-0.47858500	1.17419700
C	1.28717300	-0.31319000	0.09263200
H	0.00000100	0.67229900	-1.37527400
H	0.00001700	1.52553700	0.27375900

H	2.16214000	0.28252000	−0.18027200
H	1.31309200	−0.47869600	1.17418000
H	1.39015400	−1.29320700	−0.39091700
H	0.00012700	2.37175900	0.75067800

2.1.4 C4 (*n*-C₄H₁₀)



n-C₄H₁₀

C	1.96237900	−0.12089900	−0.00000100
H	2.11012200	−0.75099000	−0.88310500
H	2.11016900	−0.75087600	0.88317400
H	2.74857400	0.63959500	−0.00007400
C	0.56860800	0.51374700	0.00000200
H	0.46407900	1.16571000	0.87633500
H	0.46407600	1.16569900	−0.87633700
C	−0.56860800	−0.51374700	0.00000200
H	−0.46407800	−1.16570200	0.87634000
H	−0.46407700	−1.16570700	−0.87633100
C	−1.96237900	0.12089900	−0.00000200
H	−2.11013900	0.75094600	−0.88313300
H	−2.74857400	−0.63959500	−0.00002000
H	−2.11015200	0.75092000	0.88314600

CH₂(CH₂)₂CH₃

C	1.89065500	−0.13298000	0.01796600
H	2.03652800	−0.85347500	−0.79313500
H	2.01950800	−0.66948000	0.96344600
H	2.68875200	0.61101700	−0.05288000
C	0.50958400	0.52183700	−0.06432400
H	0.40401800	1.26027200	0.73940100
H	0.41882900	1.07740500	−1.00425200
C	−0.64479400	−0.48800600	0.03253100
H	−0.52452800	−1.06291900	0.96912500
H	−0.55129400	−1.23471300	−0.76737000
C	−1.99885700	0.13018100	−0.00809000
H	−2.86978100	−0.44772900	−0.29282800
H	−2.16155600	1.13342300	0.36999000



C	2.02529000	−0.04297600	0.09498100
H	2.25299100	−0.99578400	−0.39355900
H	2.13766000	−0.18941200	1.17386400
H	2.78105700	0.68095700	−0.22134400

C	0.61408900	0.43646200	-0.25422700
H	0.42567700	1.40507400	0.22223900
H	0.54114300	0.60799300	-1.33496800
C	-0.48037700	-0.55125600	0.17022000
H	-0.41128500	-0.73595800	1.24960700
H	-0.29010400	-1.52457400	-0.30812500
C	-1.87812100	-0.09940400	-0.17697800
H	-2.02115700	0.26551400	-1.19467500
H	-2.68557100	-0.75611600	0.14547700
H	-2.13166700	1.02020800	0.56430800
H	-2.28402800	1.76514200	1.09320000

H-R6: $\text{H} + \text{CH}_3(\text{CH}_2)_2\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CHCH}_2\text{CH}_3$
 $\text{CH}_3\text{CHCH}_2\text{CH}_3$

C	-1.93936300	0.16714600	-0.06931200
H	-2.01803200	0.69084600	-1.02618900
H	-2.10409100	0.90023900	0.72615300
H	-2.74863300	-0.56611000	-0.01877700
C	-0.56934200	-0.50448200	0.07821400
H	-0.55027300	-1.07417100	1.02541000
H	-0.44238400	-1.26679000	-0.70441400
C	0.58141500	0.44514500	0.03818600
H	0.40254800	1.48623900	0.29111800
C	1.98633600	-0.04327700	-0.05732100
H	2.09763400	-0.80211300	-0.84222100
H	2.68798200	0.76751100	-0.26816700
H	2.32097500	-0.52283700	0.87848600

TS6: $\text{H} + \text{CH}_3(\text{CH}_2)_2\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CHCH}_2\text{CH}_3$

C	-1.97191900	0.07469100	-0.08592600
H	-2.11538800	0.19957500	-1.16363300
H	-2.09074700	1.05626400	0.38127700
H	-2.77285600	-0.57089600	0.28366000
C	-0.59460500	-0.51996700	0.22207500
H	-0.48859700	-0.67561600	1.30280700
H	-0.51811600	-1.52004800	-0.23072400
C	0.56118400	0.32485500	-0.27412000
H	0.47343200	1.45810600	0.38709800
H	0.42681600	0.67133900	-1.30280100
C	1.95463700	-0.19329200	0.00443500
H	2.13909400	-1.12994400	-0.53703300
H	2.71960900	0.52279300	-0.30686100
H	2.09685300	-0.39818900	1.06999300

H	0.43411700	2.26889300	0.91743500
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2.1.5 C5 (*n*-C₅H₁₀)

H-R7: H + CH₃(CH₂)₃CH₃ → H₂ + CH₂(CH₂)₃CH₃

***n*-C₅H₁₀**

C	-2.56001500	0.32448200	0.00000100
H	-2.60551700	0.97009100	-0.88304800
H	-2.60552500	0.97007400	0.88306100
H	-3.45699100	-0.30156300	-0.00000900
C	-1.28414300	-0.52291400	-0.00000200
H	-1.28420500	-1.18280500	0.87636800
H	-1.28420500	-1.18280000	-0.87637500
C	0.00000000	0.31410100	0.00000000
H	-0.00000100	0.97529100	0.87691100
H	0.00000100	0.97529000	-0.87691200
C	1.28414300	-0.52291400	0.00000200
H	1.28420500	-1.18280500	-0.87636800
H	1.28420500	-1.18280000	0.87637500
C	2.56001500	0.32448200	-0.00000100
H	2.60552100	0.97008600	0.88305200
H	3.45699100	-0.30156300	0.00000200
H	2.60552200	0.97008000	-0.88305700

CH₂(CH₂)₃CH₃

C	-2.59979300	-0.34001800	-0.01596000
H	-2.60752600	-1.34842700	0.38253500
H	-3.54738000	0.08889400	-0.31886000
C	-1.35925600	0.48321500	0.01906600
H	-1.37319300	1.21235500	-0.80195100
H	-1.34407400	1.09610600	0.93885800
C	-0.06110100	-0.33667300	-0.03699200
H	-0.04951100	-0.92680500	-0.96128400
H	-0.05963500	-1.06036000	0.78810900
C	1.20699100	0.52024100	0.03782000
H	1.19066300	1.10902300	0.96323200
H	1.20067200	1.24638100	-0.78423600
C	2.49663200	-0.30357100	-0.02047300
H	2.55905800	-0.87499300	-0.95196600
H	3.38211000	0.33557200	0.03660800
H	2.54797500	-1.01691200	0.80819200

TS7: H + CH₃(CH₂)₃CH₃ → H₂ + CH₂(CH₂)₃CH₃

C	-2.61040100	0.35419500	-0.07328200
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H	-2.67690600	0.66321700	-1.12127900
H	-2.60496200	1.26189300	0.53839900
H	-3.52069400	-0.20205000	0.16688200
C	-1.35704200	-0.48926600	0.17686200
H	-1.33834600	-0.81318600	1.22459300
H	-1.40744300	-1.40579100	-0.42378000
C	-0.05518000	0.25295100	-0.14377400
H	-0.00010100	1.16743100	0.45929100
H	-0.07227700	0.57893500	-1.19190400
C	1.20393600	-0.58811200	0.10001800
H	1.14479100	-1.50698400	-0.50356200
H	1.22774800	-0.92372800	1.14429900
C	2.49084700	0.12922200	-0.22869800
H	2.61258800	1.16196400	0.65826900
H	3.40840800	-0.42588900	-0.03563500
H	2.51435200	0.64958000	-1.18681900
H	2.67988600	1.84066400	1.28449100

H-R8: $\text{H} + \text{CH}_3(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_2\text{CH}_3$
 $\text{CH}_3\text{CH}(\text{CH}_2)_2\text{CH}_3$

C	2.53691600	-0.29135500	-0.00753100
H	2.56519400	-1.05465800	-0.79171100
H	2.62825000	-0.80397800	0.95543200
H	3.41924000	0.34266300	-0.13080600
C	1.24616000	0.52854700	-0.07894100
H	1.26136100	1.30391700	0.69611800
H	1.19622200	1.05575000	-1.03826700
C	-0.02114900	-0.32113200	0.09001800
H	0.04936400	-0.87223700	1.04695900
H	-0.04257100	-1.10699000	-0.68023500
C	-1.29424100	0.45619300	0.04487800
H	-1.26731700	1.50922900	0.31006000
C	-2.61557100	-0.22477500	-0.06517300
H	-2.89124900	-0.74469000	0.86838100
H	-3.42156200	0.47920700	-0.28685700
H	-2.60962400	-0.99308300	-0.84858600

TS8: $\text{H} + \text{CH}_3(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_2\text{CH}_3$

C	2.59894100	-0.29149300	0.11327100
H	2.67495700	-1.21964200	-0.46207500
H	2.64545200	-0.55550800	1.17447800
H	3.47972200	0.31435400	-0.11610800
C	1.30536200	0.45963000	-0.21374400

H	1.27185000	1.39685900	0.35282000
H	1.30388500	0.74221600	-1.27335600
C	0.04295100	-0.35628800	0.08915600
H	0.03963500	-0.65180800	1.14675500
H	0.07611200	-1.29794100	-0.48130800
C	-1.25191300	0.36089700	-0.23293000
H	-1.23937000	0.85007100	-1.21095700
H	-1.28545500	1.40242300	0.57020800
C	-2.53446000	-0.39377400	0.03994000
H	-2.57354000	-0.75033700	1.07384700
H	-3.41413300	0.23089800	-0.13566900
H	-2.61686600	-1.27198500	-0.61300900
H	-1.32752900	2.13656800	1.20021700

H-R9: $\text{H} + \text{CH}_3(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CHCH}_2\text{CH}_3$

$\text{CH}_3\text{CH}_2\text{CHCH}_2\text{CH}_3$

C	-2.52091700	-0.40333900	0.07692800
H	-2.45671700	-1.05025200	0.95637500
H	-2.58977000	-1.04678900	-0.80538400
H	-3.45055000	0.16783100	0.14577700
C	-1.30323100	0.52378000	-0.01368500
H	-1.43520800	1.20304900	-0.87568000
H	-1.27716400	1.18973300	0.86096800
C	0.00000000	-0.19406900	-0.13277600
H	0.00000000	-1.20801900	-0.52637800
C	1.30323100	0.52378000	-0.01368500
H	1.27716400	1.18973300	0.86096800
H	1.43520800	1.20304900	-0.87568000
C	2.52091700	-0.40333900	0.07692800
H	2.58977000	-1.04678900	-0.80538400
H	3.45055000	0.16783100	0.14577700
H	2.45671700	-1.05025300	0.95637400

TS9: $\text{H} + \text{CH}_3(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CHCH}_2\text{CH}_3$

C	-2.55045800	0.27487600	-0.15823800
H	-2.58114500	0.57956800	-1.20888900
H	-2.58434300	1.18143700	0.45231000
H	-3.45634400	-0.30121500	0.04779900
C	-1.29222400	-0.54553500	0.14140000
H	-1.30305200	-0.87460100	1.18777200
H	-1.30481000	-1.46667100	-0.46015100
C	0.00000200	0.19554000	-0.13562000
H	0.00000000	1.21281700	0.70505700

H	0.00000100	0.71304500	-1.10033000
C	1.29223000	-0.54553400	0.14139700
H	1.30482200	-1.46666600	-0.46015900
H	1.30305600	-0.87460500	1.18776800
C	2.55046200	0.27488500	-0.15823100
H	2.58433700	1.18144500	0.45231800
H	3.45635000	-0.30120100	0.04781100
H	2.58115300	0.57957800	-1.20888200
H	-0.00009800	1.91168000	1.37333000

2.1.6 C6 (*n*-C₆H₁₄)



n-C₆H₁₄

C	-3.22383000	0.20850600	0.00000200
H	-3.31415500	0.84939500	-0.88305700
H	-3.31416000	0.84937700	0.88307500
H	-4.07532000	-0.47816400	-0.00000700
C	-1.89256500	-0.54887400	-0.00000200
H	-1.84760800	-1.20728600	0.87630600
H	-1.84761100	-1.20728000	-0.87631500
C	-0.66878800	0.37423000	-0.00000100
H	-0.71482800	1.03361900	0.87689900
H	-0.71482600	1.03361800	-0.87690100
C	0.66878800	-0.37423000	0.00000100
H	0.71482700	-1.03362100	-0.87689800
H	0.71482700	-1.03361600	0.87690200
C	1.89256500	0.54887400	-0.00000200
H	1.84760900	1.20728600	0.87630700
H	1.84761000	1.20728000	-0.87631400
C	3.22383000	-0.20850600	0.00000200
H	3.31415800	-0.84938900	-0.88306200
H	4.07532000	0.47816400	0.00000000
H	3.31415700	-0.84938300	0.88307000

CH₂(CH₂)₄CH₃

C	-3.14961200	-0.22281100	0.02044600
H	-3.23126700	-0.80292300	0.94515300
H	-3.23738200	-0.92269600	-0.81666300
H	-4.00688400	0.45478400	-0.02265900
C	-1.82564100	0.54488700	-0.03645300
H	-1.79005700	1.14385300	-0.95458100
H	-1.78234100	1.25990600	0.79412500
C	-0.59376800	-0.36581800	0.01853700

H	-0.63752300	-1.08125700	-0.81315600
H	-0.62970100	-0.96637300	0.93706000
C	0.73453000	0.39547300	-0.03771900
H	0.78221800	1.10694700	0.79640600
H	0.77431200	0.99578600	-0.95448500
C	1.96804600	-0.51925200	0.01555500
H	1.93361800	-1.23740300	-0.81447700
H	1.90192000	-1.14042600	0.92746400
C	3.26593900	0.21100800	-0.00187600
H	3.34421300	1.21199900	0.40754300
H	4.18190700	-0.28312800	-0.30266800

TS10: $\text{H} + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_4\text{CH}_3$

C	3.28971900	-0.15656400	0.10098400
H	3.41527800	-1.02502000	-0.55344600
H	3.36481200	-0.50882300	1.13467900
H	4.12949800	0.51991200	-0.08059100
C	1.94752700	0.53659200	-0.15117900
H	1.86563900	1.41987700	0.49371800
H	1.91737700	0.90977600	-1.18217000
C	0.73997800	-0.37645200	0.08973400
H	0.77114900	-0.74997000	1.12165800
H	0.82204000	-1.26107000	-0.55552300
C	-0.60757000	0.30908500	-0.15914100
H	-0.64093600	0.68211200	-1.19092500
H	-0.69330200	1.19077700	0.48731600
C	-1.81265300	-0.60927500	0.08086800
H	-1.78634600	-0.99244700	1.10854200
H	-1.72362500	-1.49531800	-0.56642900
C	-3.14494900	0.05188400	-0.17708300
H	-3.22669700	0.60956200	-1.11070400
H	-4.02587800	-0.55848100	0.01983800
H	-3.29017600	1.03930500	0.75661700
H	-3.37113800	1.68818700	1.41232200

H-R11: $\text{H} + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_3\text{CH}_3$
 $\text{CH}_3\text{CH}(\text{CH}_2)_3\text{CH}_3$

C	3.18193500	0.23363400	0.06760700
H	3.24206300	0.79021600	1.00824800
H	3.28691900	0.95472200	-0.74930300
H	4.04119600	-0.44158300	0.02630600
C	1.86096800	-0.53390200	-0.03774000
H	1.84618400	-1.10928400	-0.97158300

H	1.80152400	-1.27014700	0.77320700
C	0.62763900	0.37391800	0.01488000
H	0.68328100	1.10800600	-0.79909100
H	0.63904000	0.95072800	0.94775500
C	-0.70038300	-0.38854300	-0.08706300
H	-0.76157900	-1.13187300	0.72224100
H	-0.69271600	-0.98965500	-1.01586500
C	-1.91302600	0.48101900	-0.05682500
H	-1.81475500	1.51825500	-0.36385500
C	-3.27781200	-0.09721400	0.10061000
H	-3.31269300	-0.83396100	0.91304800
H	-4.02660900	0.67145800	0.30762100
H	-3.60777900	-0.63035600	-0.80754700

TS11: H + CH₃(CH₂)₄CH₃ → H₂ + CH₃CH(CH₂)₃CH₃

C	-3.25529300	0.21502000	-0.07079200
H	-3.34782500	0.51963700	-1.11811100
H	-3.31982100	1.11909900	0.54273000
H	-4.11841600	-0.41183400	0.16976600
C	-1.93872900	-0.52745300	0.17543400
H	-1.89189100	-0.84934400	1.22288500
H	-1.91914200	-1.44503600	-0.42548300
C	-0.70019200	0.31529100	-0.14810800
H	-0.71666300	1.23091200	0.45539300
H	-0.74665700	0.63921200	-1.19589800
C	0.62175800	-0.42303700	0.09218200
H	0.64066500	-1.33944200	-0.51846600
H	0.67193500	-0.76192200	1.13532500
C	1.85525100	0.39725700	-0.22516300
H	1.83359600	1.40388200	0.62050500
H	1.78548500	0.92450300	-1.18068300
C	3.19422800	-0.27339500	-0.01009100
H	3.32472200	-1.11562900	-0.70142800
H	4.02269900	0.42020800	-0.17589400
H	3.28195800	-0.66836900	1.00672100
H	1.83722800	2.11202100	1.28186100

H-R12: H + CH₃(CH₂)₄CH₃ → H₂ + CH₃CH₂CH(CH₂)₂CH₃
CH₃CH₂CH(CH₂)₂CH₃

C	-3.20624500	-0.13133400	0.08127500
H	-3.27656500	-0.80241400	0.94330900
H	-3.37895500	-0.73073300	-0.81837900
H	-4.02150700	0.59332300	0.15855800

C	-1.84376200	0.56467300	0.03074700
H	-1.81482000	1.25250900	-0.82260100
H	-1.71159400	1.18232900	0.92616600
C	-0.66683800	-0.41523900	-0.07813400
H	-0.82294500	-1.05498400	-0.96719900
H	-0.69017600	-1.11312700	0.77234800
C	0.67244600	0.23905700	-0.15365500
H	0.73144100	1.25751700	-0.53091800
C	1.93619200	-0.54305600	-0.01453300
H	2.05651100	-1.21584800	-0.88330300
H	1.85622000	-1.21917000	0.84897700
C	3.19499600	0.32162900	0.11988100
H	3.13985200	0.95932800	1.00667600
H	4.09347200	-0.29558800	0.20391800
H	3.31833100	0.97248000	-0.75104200

TS12: $\text{H} + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_2\text{CH}_3$

C	-3.23952300	-0.19863200	0.04134900
H	-3.33620300	-0.52417800	1.08189500
H	-3.34756000	-1.08390500	-0.59345300
H	-4.07713200	0.46978800	-0.17567700
C	-1.89587700	0.49531700	-0.19850200
H	-1.84227600	0.84052600	-1.23802100
H	-1.82996000	1.39333000	0.42582200
C	-0.69172400	-0.40885300	0.09244500
H	-0.75928200	-1.31162100	-0.53479700
H	-0.74161900	-0.76498700	1.12985900
C	0.65047800	0.25108500	-0.14708800
H	0.70400700	1.24631100	0.71711600
H	0.70223600	0.78905600	-1.09903500
C	1.88696800	-0.57870300	0.13292200
H	1.85220500	-1.48392900	-0.49155700
H	1.85732300	-0.93312300	1.17058100
C	3.20043300	0.16621000	-0.12444100
H	3.28078300	1.05309700	0.51013100
H	4.06377600	-0.47203100	0.08118500
H	3.26936900	0.49452200	-1.16613300
H	0.73980700	1.92860100	1.40197300

2.1.7 C7 (*n*-C₇H₁₆)

H-R13: $\text{H} + \text{CH}_3(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_5\text{CH}_3$

***n*-C₇H₁₆**

C	3.84318100	-0.35384700	0.00000200
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H	3.88847700	-0.99952200	-0.88303400
H	3.88848000	-0.99950900	0.88304900
H	4.74048100	0.27178600	-0.00000500
C	2.56763600	0.49398400	-0.00000300
H	2.56795800	1.15388300	0.87632600
H	2.56796000	1.15387500	-0.87633800
C	1.28319900	-0.34286400	0.00000000
H	1.28397200	-1.00382500	-0.87686000
H	1.28397400	-1.00382500	0.87686000
C	0.00000000	0.49570300	0.00000100
H	0.00000100	1.15639600	-0.87691900
H	-0.00000100	1.15639200	0.87692300
C	-1.28319900	-0.34286400	-0.00000200
H	-1.28397300	-1.00382800	0.87685500
H	-1.28397400	-1.00382100	-0.87686500
C	-2.56763600	0.49398400	0.00000200
H	-2.56796000	1.15388200	-0.87632800
H	-2.56795800	1.15387600	0.87633600
C	-3.84318100	-0.35384700	0.00000000
H	-3.88847800	-0.99951800	0.88304000
H	-4.74048100	0.27178600	0.00000300
H	-3.88847900	-0.99951300	-0.88304400

CH₂(CH₂)₅CH₃

C	3.77410400	-0.33403400	0.01418700
H	3.82298600	-1.02750600	-0.83138000
H	3.82906800	-0.92860000	0.93165800
H	4.66475700	0.29937800	-0.02440800
C	2.49053000	0.50034200	-0.02817500
H	2.48641000	1.20656600	0.81103500
H	2.48199500	1.11148400	-0.93899900
C	1.21446000	-0.34786300	0.02115200
H	1.21908900	-1.05479500	-0.81881300
H	1.22366200	-0.96019800	0.93232700
C	-0.07589800	0.47822400	-0.02021600
H	-0.08509400	1.08957900	-0.93207600
H	-0.07876300	1.18562500	0.81926900
C	-1.34961400	-0.37194600	0.03167100
H	-1.34591200	-0.98235500	0.94257300
H	-1.35191600	-1.07689000	-0.80929500
C	-2.64179200	0.45850300	-0.00962200
H	-2.62116800	1.08962900	-0.91683500
H	-2.65147700	1.17129500	0.82574500

C	-3.88820200	-0.35638700	0.00780400
H	-4.83388200	0.07452800	0.31386000
H	-3.90128300	-1.35877000	-0.40546100

TS13: $\text{H} + \text{CH}_3(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_5\text{CH}_3$

C	-3.90244100	0.37978800	-0.05125700
H	-3.95998900	0.77669200	-1.06982600
H	-3.92246200	1.23173300	0.63585900
H	-4.80597400	-0.21020800	0.12615300
C	-2.63734400	-0.46063100	0.14464500
H	-2.62474200	-0.86939700	1.16241100
H	-2.66632500	-1.32577700	-0.52919100
C	-1.34352000	0.32449200	-0.09867900
H	-1.35736800	0.73564900	-1.11661100
H	-1.31440800	1.18954300	0.57673000
C	-0.07215900	-0.50971600	0.09266100
H	-0.10006500	-1.37215900	-0.58629100
H	-0.06147300	-0.92414600	1.10908900
C	1.22009300	0.27904600	-0.14356100
H	1.25466500	1.13545800	0.54068700
H	1.21058300	0.69862400	-1.15775900
C	2.49059200	-0.56073600	0.03897300
H	2.45970400	-1.41559700	-0.65407100
H	2.50294800	-0.99855900	1.04488800
C	3.76842000	0.20931200	-0.19126300
H	3.85540100	1.14404700	0.80121300
H	4.69363200	-0.34651500	-0.04170600
H	3.79629000	0.82830300	-1.08868300
H	3.89773400	1.75298000	1.49798900

H-R14: $\text{H} + \text{CH}_3(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_4\text{CH}_3$

$\text{CH}_3\text{CH}(\text{CH}_2)_4\text{CH}_3$

C	3.80229900	-0.33135100	-0.00965000
H	3.83648800	-1.05700100	-0.82852700
H	3.87180100	-0.89015100	0.92909100
H	4.69291600	0.29851800	-0.08734800
C	2.51918100	0.50310700	-0.06326800
H	2.52981700	1.24131200	0.74788400
H	2.49646700	1.07846000	-0.99681400
C	1.24305400	-0.34001700	0.03956100
H	1.23458400	-1.07989500	-0.77162800
H	1.26553000	-0.91563700	0.97432600
C	-0.04577500	0.48644900	-0.01614400

H	-0.07176600	1.06037800	-0.95034200
H	-0.03953700	1.22414500	0.79618900
C	-1.32218800	-0.35988500	0.08672600
H	-1.27798100	-0.95514500	1.01820400
H	-1.33368000	-1.10919300	-0.71927400
C	-2.58808900	0.42984000	0.05012000
H	-2.55610200	1.47448300	0.34588300
C	-3.91330200	-0.23629100	-0.09765400
H	-4.20862300	-0.77617100	0.81842200
H	-4.70957100	0.48012900	-0.31480700
H	-3.90142400	-0.98534900	-0.89940500

TS14: $\text{H} + \text{CH}_3(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_4\text{CH}_3$

C	3.89225900	-0.31319300	0.10617400
H	3.96194700	-1.17608900	-0.56386300
H	3.93537400	-0.68901400	1.13338300
H	4.77853100	0.30612200	-0.05763200
C	2.60388600	0.47703200	-0.14037000
H	2.58198900	1.35393500	0.51808500
H	2.60568300	0.86755500	-1.16537000
C	1.33296500	-0.35071900	0.08117900
H	1.35542800	-1.22914900	-0.57739400
H	1.33179200	-0.74124600	1.10721100
C	0.03933200	0.43353700	-0.16267800
H	0.04072700	0.82599900	-1.18767200
H	0.01406500	1.30779200	0.49898300
C	-1.22974600	-0.39888400	0.05470000
H	-1.23461800	-0.80689700	1.07397800
H	-1.20851100	-1.27347800	-0.61442400
C	-2.51764600	0.36249400	-0.18342000
H	-2.50188300	0.95459100	-1.10273300
H	-2.53747800	1.31013900	0.72672400
C	-3.80801400	-0.40286100	0.01102400
H	-3.84887100	-0.86814100	1.00068400
H	-4.68085200	0.24691900	-0.09317800
H	-3.90240300	-1.20482900	-0.73221400
H	-2.56913200	1.97135500	1.43578200

H-R15: $\text{H} + \text{CH}_3(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_3\text{CH}_3$

C	-3.79129600	-0.42744300	0.07478200
H	-3.77572700	-1.08830800	0.94726800
H	-3.85272300	-1.05977300	-0.81662900

H	-4.70853800	0.16596100	0.12447100
C	-2.54774400	0.46544500	0.03474100
H	-2.60847700	1.13769400	-0.82998300
H	-2.53379400	1.11173700	0.92095500
C	-1.23736100	-0.32595900	-0.03273100
H	-1.17228600	-0.99739600	0.83212600
H	-1.24964300	-0.97140400	-0.92027400
C	0.01491900	0.56073400	-0.07485500
H	0.03298300	1.21464800	0.80995300
H	-0.07273900	1.25489500	-0.93170500
C	1.29882200	-0.19494400	-0.16528600
H	1.28344700	-1.19571300	-0.59079000
C	2.61809600	0.47547900	0.02987700
H	2.58190700	1.10125100	0.93354100
H	2.79984200	1.18948000	-0.79414200
C	3.80370900	-0.49248500	0.11702300
H	3.88308100	-1.09713600	-0.79147800
H	4.74718600	0.04541900	0.24237500
H	3.69060700	-1.17631500	0.96300100

TS15: $\text{H} + \text{CH}_3(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_3\text{CH}_3$

C	3.85604300	0.35178800	-0.10358500
H	3.88979200	1.19527700	0.59318900
H	3.89676600	0.76052000	-1.11826200
H	4.76091200	-0.24244600	0.05105100
C	2.59283200	-0.48835100	0.10459500
H	2.60828800	-1.34603600	-0.57930400
H	2.59677500	-0.90806800	1.11787900
C	1.29792900	0.30347100	-0.10725900
H	1.28007800	1.15969300	0.57801700
H	1.29285900	0.72382400	-1.12125100
C	0.02956800	-0.53327000	0.09738600
H	0.03164700	-0.96524400	1.10665100
H	0.04750500	-1.39128100	-0.59274900
C	-1.25891600	0.23437400	-0.11553900
H	-1.24994500	0.84748000	-1.02229700
H	-1.26868900	1.15924500	0.82308000
C	-2.55425800	-0.52920200	0.07152500
H	-2.57424600	-0.96612100	1.07743800
H	-2.56275000	-1.38237000	-0.62324200
C	-3.80934800	0.31989100	-0.15114000
H	-3.82952800	0.73558700	-1.16329700
H	-4.71724200	-0.27410700	-0.01732900

H	-3.85001600	1.15602000	0.55254300
H	-1.27531100	1.78581800	1.56199100

H-R16: $\text{H} + \text{CH}_3(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_2\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_2\text{CH}_3$

C	3.84900100	-0.24160100	0.11851900
H	4.01364700	-0.80718800	-0.80422900
H	3.86327500	-0.95434800	0.94929900
H	4.69775200	0.43546300	0.24848500
C	2.52513600	0.52553000	0.07016900
H	2.40303200	1.10869200	0.98980800
H	2.55165600	1.25114000	-0.75134500
C	1.30328000	-0.38669000	-0.10895800
H	1.44770600	-0.99187900	-1.02384100
H	1.27235900	-1.12359400	0.70774200
C	0.00000000	0.33709400	-0.18003600
H	0.00000000	1.37399300	-0.50838100
C	-1.30328000	-0.38669000	-0.10895800
H	-1.27235900	-1.12359400	0.70774200
H	-1.44770600	-0.99187900	-1.02384000
C	-2.52513600	0.52553000	0.07016900
H	-2.55165600	1.25114000	-0.75134500
H	-2.40303200	1.10869200	0.98980700
C	-3.84900100	-0.24160100	0.11851900
H	-3.86327500	-0.95434700	0.94929900
H	-4.69775200	0.43546300	0.24848500
H	-4.01364700	-0.80718900	-0.80422900

TS16: $\text{H} + \text{CH}_3(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_2\text{CH}_3$

C	-3.84859500	-0.34555000	0.05412300
H	-3.91006900	-0.71903900	1.08113000
H	-3.90643400	-1.20957200	-0.61565900
H	-4.73146900	0.27364200	-0.12642500
C	-2.55741800	0.44595400	-0.17037900
H	-2.53937600	0.83418400	-1.19582800
H	-2.54463900	1.32161400	0.48824400
C	-1.29179200	-0.38479900	0.07351500
H	-1.30519200	-0.78375100	1.09631000
H	-1.30548800	-1.26496700	-0.58834500
C	-0.00000300	0.37375000	-0.15218800
H	0.00000200	1.32942700	0.75483300
H	0.00001700	0.95592600	-1.07905300
C	1.29178600	-0.38478700	0.07355100

H	1.30545100	-1.26501600	-0.58822900
H	1.30521000	-0.78365200	1.09637900
C	2.55741300	0.44593200	-0.17045400
H	2.54463800	1.32167900	0.48805200
H	2.53937200	0.83402200	-1.19595600
C	3.84858600	-0.34555000	0.05414800
H	3.90638900	-1.20969500	-0.61547900
H	4.73146400	0.27359500	-0.12653900
H	3.91008800	-0.71885600	1.08122100
H	0.00017300	1.98076300	1.47144800

2.1.8 C8 (*n*-C₈H₁₈)



n-C₈H₁₈

C	4.49836200	-0.25644100	0.00002700
H	4.56897900	-0.89994900	-0.88294200
H	4.56905800	-0.89971100	0.88316000
H	5.37045300	0.40389200	-0.00010100
C	3.19068200	0.54093500	-0.00003200
H	3.16551000	1.20041200	0.87625200
H	3.16553100	1.20032700	-0.87637900
C	1.93965200	-0.34501000	-0.00000600
H	1.96588900	-1.00546800	0.87685600
H	1.96586200	-1.00546400	-0.87687100
C	0.62513200	0.44356800	0.00001300
H	0.59991500	1.10385100	-0.87682400
H	0.59991000	1.10380400	0.87688500
C	-0.62513200	-0.44356800	-0.00001400
H	-0.59991300	-1.10385400	0.87682100
H	-0.59991200	-1.10380100	-0.87688900
C	-1.93965200	0.34501000	0.00000900
H	-1.96587700	1.00548500	-0.87684000
H	-1.96587400	1.00544600	0.87688700
C	-3.19068200	-0.54093500	-0.00000800
H	-3.16552000	-1.20038800	0.87629300
H	-3.16552100	-1.20035100	-0.87633800
C	-4.49836200	0.25644100	0.00000900
H	-4.56901800	0.89985000	-0.88302700
H	-5.37045300	-0.40389200	-0.00000700
H	-4.56902000	0.89981000	0.88307500

CH₂(CH₂)₆CH₃

C	-4.42266500	-0.27035800	0.01656000
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H	-4.48942600	-0.86955900	0.93024600
H	-4.49047900	-0.95685000	-0.83340900
H	-5.29804900	0.38437900	-0.01531900
C	-3.11965100	0.53343300	-0.02403100
H	-3.09914200	1.15010900	-0.93091900
H	-3.09657200	1.23401100	0.81960100
C	-1.86376500	-0.34476600	0.01603300
H	-1.88744400	-1.04592000	-0.82849500
H	-1.88482600	-0.96281700	0.92325300
C	-0.55443100	0.45112700	-0.02401700
H	-0.53134200	1.15175200	0.82074000
H	-0.53488900	1.06921600	-0.93097700
C	0.70083000	-0.42785200	0.01484000
H	0.67663800	-1.12954300	-0.82905300
H	0.68289400	-1.04475100	0.92279400
C	2.00834100	0.36979200	-0.02905800
H	2.03759700	1.06858100	0.81653700
H	2.03149900	0.98582000	-0.93588800
C	3.26559800	-0.51276400	0.00906000
H	3.24840000	-1.21956900	-0.83122300
H	3.21748900	-1.14867100	0.91188700
C	4.54391700	0.25134200	0.00001200
H	4.59650200	1.24886400	0.42181400
H	5.47210400	-0.21478300	-0.30798500

TS17: $\text{H} + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_6\text{CH}_3$

C	-4.56650000	-0.21479800	0.09836000
H	-4.62773600	-0.63895400	1.10565800
H	-4.65978700	-1.04135800	-0.61335700
H	-5.43155800	0.44004000	-0.03876600
C	-3.25160700	0.54388600	-0.10353100
H	-3.23635900	0.98747500	-1.10661500
H	-3.20317300	1.38393000	0.60011100
C	-2.00953800	-0.33629200	0.07673100
H	-2.05768500	-1.17599900	-0.62910500
H	-2.02679500	-0.78266100	1.07967700
C	-0.68833000	0.41524900	-0.11958900
H	-0.63963700	1.25224400	0.58893800
H	-0.67323400	0.86467700	-1.12105100
C	0.55267700	-0.46726900	0.05614200
H	0.50678400	-1.30158500	-0.65604200
H	0.53523100	-0.92043800	1.05578100
C	1.87276300	0.28754800	-0.13227700

H	1.92481100	1.11618900	0.58422500
H	1.89173600	0.74470700	-1.12997800
C	3.11294100	-0.59951300	0.03563200
H	3.06205500	-1.42905400	-0.68635300
H	3.09882100	-1.07088900	1.02622400
C	4.41789000	0.13504000	-0.15480300
H	4.52081100	1.03846400	0.86490600
H	5.32262800	-0.45451400	-0.00915200
H	4.47829300	0.77790500	-1.03364900
H	4.57301900	1.62672000	1.57855700

H-R18: $\text{H} + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_5\text{CH}_3$
 $\text{CH}_3\text{CH}(\text{CH}_2)_5\text{CH}_3$

C	-4.44766400	0.27242000	0.05873600
H	-4.52858600	0.97652000	-0.77555800
H	-4.50173600	0.85229500	0.98564100
H	-5.32281400	-0.38261400	0.02587100
C	-3.14461300	-0.52868100	-0.01743000
H	-3.10903800	-1.24689900	0.81081000
H	-3.13633300	-1.12601600	-0.93739300
C	-1.88897400	0.34984400	0.02383200
H	-1.89818900	0.94877800	0.94391800
H	-1.92454400	1.06841500	-0.80550300
C	-0.57990000	-0.44384400	-0.05018800
H	-0.57106700	-1.04158300	-0.97104500
H	-0.54686900	-1.16328100	0.77840400
C	0.67442800	0.43512000	-0.00561400
H	0.67055700	1.03129500	0.91487800
H	0.64492100	1.15288200	-0.83511500
C	1.98398800	-0.36207400	-0.07996100
H	1.97028600	-0.98024100	-0.99737800
H	2.01875600	-1.09131900	0.74358200
C	3.21760700	0.47753800	-0.05348400
H	3.14771200	1.51209700	-0.37693800
C	4.56639300	-0.13174400	0.12366300
H	4.89230400	-0.68221300	-0.77559500
H	5.33158800	0.62081600	0.33009500
H	4.57545800	-0.86041300	0.94400300

TS18: $\text{H} + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_5\text{CH}_3$

C	-4.54176800	0.27471600	-0.05402700
H	-4.61375500	0.67566400	-1.07008500
H	-4.59735100	1.12059100	0.63860400

H	-5.42079100	-0.35276100	0.11785100
C	-3.24373500	-0.51467100	0.13871400
H	-3.21599600	-0.92920100	1.15384800
H	-3.23649000	-1.37595400	-0.54066600
C	-1.98267900	0.32408900	-0.09746600
H	-1.99121600	1.18690100	0.58139000
H	-2.01061000	0.73844400	-1.11381900
C	-0.67846700	-0.45742500	0.09471000
H	-0.67046600	-1.32005400	-0.58457500
H	-0.65182800	-0.87150200	1.11095400
C	0.58080100	0.38377700	-0.14043100
H	0.57732500	1.24247900	0.54173100
H	0.55482200	0.79997400	-1.15563500
C	1.88362900	-0.40241800	0.04694800
H	1.89050700	-1.26150900	-0.64230500
H	1.91398100	-0.83333800	1.05629500
C	3.13827200	0.41451900	-0.18393000
H	3.13017100	1.34033600	0.74773000
H	3.09060700	1.02703600	-1.08867400
C	4.45983700	-0.30316300	-0.01903800
H	4.58117600	-1.07963000	-0.78501500
H	5.30485000	0.38426500	-0.11052300
H	4.52681400	-0.79344900	0.95701200
H	3.14290900	1.98515400	1.47300100

H-R19: $\text{H} + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_4\text{CH}_3$
 $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_4\text{CH}_3$

C	4.46322000	-0.18594200	0.07441500
H	4.58271300	-0.81418700	-0.81404100
H	4.52325400	-0.83936500	0.95063300
H	5.31465600	0.49930600	0.11284100
C	3.13379400	0.57368000	0.04078000
H	3.06137900	1.22136100	0.92301900
H	3.11732000	1.24245600	-0.82844300
C	1.90969900	-0.34761600	-0.00963600
H	1.92624600	-1.01644600	0.86095800
H	1.98349000	-0.99719900	-0.89184900
C	0.57583500	0.40519000	-0.04519700
H	0.55843100	1.07132600	-0.91705100
H	0.49820000	1.05331900	0.83608400
C	-0.64941800	-0.51833400	-0.09675100
H	-0.63972200	-1.19212900	0.77307800
H	-0.54885200	-1.19011100	-0.96985200

C	-1.95627800	0.19993600	-0.15944900
H	-1.97471900	1.20985300	-0.56260300
C	-3.25277100	-0.51435400	0.03275000
H	-3.19087700	-1.15398100	0.92529500
H	-3.41800200	-1.21964400	-0.80215000
C	-4.46729300	0.41439800	0.14450800
H	-4.57284200	1.03091700	-0.75328400
H	-5.39246200	-0.15482200	0.26804500
H	-4.36894100	1.08759500	1.00080400

TS19: $\text{H} + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_4\text{CH}_3$

C	4.52791300	-0.22839500	0.05507700
H	4.61663100	-1.05220900	-0.66041100
H	4.59975800	-0.65574800	1.06029900
H	5.38987500	0.42920800	-0.08791400
C	3.20947200	0.52791200	-0.13164300
H	3.16628300	1.36629300	0.57416400
H	3.18276000	0.97341500	-1.13362900
C	1.97138600	-0.35535200	0.06018600
H	1.99888500	-0.80076900	1.06324700
H	2.01483700	-1.19536500	-0.64573000
C	0.64801800	0.39482700	-0.12392100
H	0.61884200	0.83800000	-1.12760800
H	0.60399800	1.23328600	0.58153700
C	-0.58843400	-0.49134900	0.07037800
H	-0.56312000	-0.94545500	1.06951500
H	-0.54563000	-1.33227900	-0.63930600
C	-1.90451100	0.23541500	-0.11574900
H	-1.92725700	0.86075800	-1.01393100
H	-1.93359600	1.14611000	0.83555900
C	-3.17142500	-0.57342100	0.07589200
H	-3.16497200	-1.02333400	1.07625200
H	-3.15996300	-1.41759400	-0.62970900
C	-4.45639500	0.23640600	-0.12132600
H	-4.50316900	0.66218600	-1.12839100
H	-5.34266700	-0.38835600	0.01723500
H	-4.51494700	1.06310500	0.59216900
H	-1.95270100	1.76249000	1.58329100

**H-R20: $\text{H} + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_3\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_3\text{CH}_3$**

C	-4.45410200	0.37618100	0.12745100
H	-4.54626100	1.01603700	-0.75591900

H	-4.43505300	1.02842000	1.00635300
H	-5.35773000	-0.23671800	0.18879700
C	-3.19342600	-0.49018100	0.05389700
H	-3.14965100	-1.14572200	0.93231200
H	-3.25683300	-1.15398900	-0.81713300
C	-1.90101700	0.32875200	-0.02907400
H	-1.83270500	0.99084300	0.84275000
H	-1.94389400	0.98457600	-0.90804500
C	-0.63196600	-0.53107200	-0.10691900
H	-0.72227700	-1.21667800	-0.97034800
H	-0.58297900	-1.19541900	0.76902500
C	0.63435800	0.25191900	-0.21279100
H	0.58780100	1.26251100	-0.61194400
C	1.97134600	-0.39656900	-0.07372100
H	2.15922600	-1.06051400	-0.93856400
H	1.96709500	-1.07073600	0.79609000
C	3.14215800	0.58917600	0.04783800
H	2.97982200	1.22933300	0.92224600
H	3.13932200	1.25468600	-0.82352200
C	4.50362300	-0.10154000	0.16003400
H	4.70633400	-0.72310100	-0.71806300
H	5.31468500	0.62693400	0.24508600
H	4.54726000	-0.75045900	1.04059300

TS20: $\text{H} + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_3\text{CH}_3$

C	4.49892800	0.25947100	-0.09472700
H	4.55958400	1.10119500	0.60235400
H	4.55823100	0.66654300	-1.10914200
H	5.38145700	-0.36655500	0.06348900
C	3.20575100	-0.53519400	0.10801900
H	3.19274700	-1.39188400	-0.57716700
H	3.19119700	-0.95626000	1.12064400
C	1.94086500	0.30299600	-0.10687500
H	1.95510300	0.72594900	-1.11969400
H	1.95086100	1.15748800	0.58071700
C	0.64243800	-0.48808500	0.09022300
H	0.62539900	-0.92403200	1.09760500
H	0.63146800	-1.34325400	-0.60349800
C	-0.61649000	0.32730100	-0.12340300
H	-0.58012900	0.94545900	-1.02592300
H	-0.59483600	1.24537300	0.82094800
C	-1.93941300	-0.38938200	0.05309300
H	-1.98039100	-0.83575500	1.05532900

H	-1.98033500	-1.23558700	-0.65060600
C	-3.16855900	0.50209000	-0.16248800
H	-3.12309400	0.93867800	-1.16744000
H	-3.12896400	1.34340800	0.53838200
C	-4.49233700	-0.24748200	0.01011700
H	-4.58120900	-0.66634200	1.01743400
H	-5.34813200	0.41386300	-0.15019100
H	-4.57514300	-1.07603200	-0.70063200
H	-0.58091200	1.86745700	1.56363500

2.1.9 C9 (*n*-C₉H₂₀)



n-C₉H₂₀

C	5.12585300	-0.37071200	0.00000200
H	5.17126900	-1.01633500	-0.88288000
H	5.17128300	-1.01630100	0.88290700
H	6.02293500	0.25485500	-0.00001800
C	3.85047700	0.47733900	-0.00000500
H	3.85066600	1.13718600	0.87623500
H	3.85066600	1.13717000	-0.87625700
C	2.56602500	-0.35945300	0.00000100
H	2.56666500	-1.02032000	0.87679700
H	2.56666000	-1.02032200	-0.87679400
C	1.28328800	0.47955800	0.00000300
H	1.28350100	1.14016400	-0.87681300
H	1.28349900	1.14015600	0.87682400
C	0.00000000	-0.35900300	-0.00000100
H	0.00000000	-1.01964100	0.87674700
H	0.00000000	-1.01963200	-0.87675700
C	-1.28328800	0.47955800	0.00000300
H	-1.28350100	1.14016300	-0.87681400
H	-1.28350000	1.14015700	0.87682400
C	-2.56602500	-0.35945300	0.00000000
H	-2.56666300	-1.02032200	0.87679500
H	-2.56666100	-1.02032000	-0.87679600
C	-3.85047700	0.47733900	0.00000000
H	-3.85066600	1.13717800	-0.87624600
H	-3.85066700	1.13717800	0.87624600
C	-5.12585300	-0.37071200	-0.00000100
H	-5.17127700	-1.01631800	0.88289200
H	-6.02293500	0.25485500	-0.00000300
H	-5.17127500	-1.01631800	-0.88289500

CH₂(CH₂)₇CH₃

C	-5.05426800	-0.35260200	0.01194800
H	-5.10541200	-0.95992900	0.92126400
H	-5.10241500	-1.03462700	-0.84293400
H	-5.94720800	0.27817300	-0.01625600
C	-3.77353600	0.48657400	-0.02140500
H	-3.76875700	1.11002600	-0.92388600
H	-3.77029800	1.18154000	0.82718200
C	-2.49441900	-0.35766500	0.01408600
H	-2.49821900	-1.05312100	-0.83546300
H	-2.50008700	-0.98267100	0.91674500
C	-1.20666800	0.47298100	-0.01797100
H	-1.20395800	1.16829100	0.83151400
H	-1.20175000	1.09757600	-0.92075900
C	0.07144400	-0.37272500	0.01815800
H	0.06878100	-1.06849000	-0.83087400
H	0.06659900	-0.99668500	0.92124300
C	1.35915400	0.45823600	-0.01431800
H	1.36006600	1.15610800	0.83309100
H	1.36605100	1.07994400	-0.91914000
C	2.63559500	-0.38833200	0.02762700
H	2.63974000	-1.08418400	-0.82088500
H	2.63436500	-1.00857500	0.93187400
C	3.92503400	0.44672100	-0.00525500
H	3.93236200	1.15108000	0.83726300
H	3.90234400	1.08694600	-0.90601500
C	5.17413600	-0.36416200	0.00397600
H	5.19050200	-1.36238700	-0.41912900
H	6.11846700	0.06683400	0.31408800

TS21: H + CH₃(CH₂)₇CH₃ → H₂ + CH₂(CH₂)₇CH₃

C	5.19112900	0.39180100	-0.04078800
H	5.22301700	1.20433100	0.69212300
H	5.24358100	0.84400400	-1.03634200
H	6.09160300	-0.21350700	0.09620400
C	3.92114000	-0.44900400	0.11883200
H	3.93818500	-1.27536500	-0.60240700
H	3.91374500	-0.91403100	1.11223000
C	2.63119800	0.35744700	-0.06917300
H	2.63973500	0.82447900	-1.06279600
H	2.61452400	1.18399000	0.65339900
C	1.35489700	-0.47669300	0.08670600
H	1.34885100	-0.94612600	1.07903300

H	1.37161400	-1.30107700	-0.63821200
C	0.06526400	0.33120000	-0.09699100
H	0.07322900	0.80523600	-1.08708100
H	0.04570200	1.15189700	0.63170700
C	-1.21022400	-0.50587900	0.05141900
H	-1.21594100	-0.98407400	1.03946400
H	-1.19310500	-1.32346700	-0.68119300
C	-2.49899800	0.30411400	-0.12424000
H	-2.49377500	0.78758200	-1.10961400
H	-2.52378700	1.11516600	0.61355700
C	-3.77341400	-0.53840800	0.01340000
H	-3.78463500	-1.03464600	0.99179400
H	-3.74920200	-1.35092200	-0.72906000
C	-5.04798900	0.24996300	-0.16717500
H	-5.07642800	0.91750200	-1.02908100
H	-5.97554000	-0.30850400	-0.04422700
H	-5.12628500	1.12963100	0.87484700
H	-5.16310900	1.70065200	1.60371700

H-R22: $\text{H} + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_6\text{CH}_3$
 $\text{CH}_3\text{CH}(\text{CH}_2)_6\text{CH}_3$

C	-5.07602300	-0.35362200	-0.01133800
H	-5.13743200	-0.93317200	0.91531900
H	-5.11273400	-1.06134900	-0.84565900
H	-5.96949000	0.27435700	-0.06956100
C	-3.79620500	0.48650700	-0.05463000
H	-3.78182600	1.08291400	-0.97510900
H	-3.80397400	1.20630600	0.77295600
C	-2.51633900	-0.35396900	0.02057600
H	-2.50975200	-1.07449000	-0.80781200
H	-2.53121000	-0.95167000	0.94146800
C	-1.22940100	0.47747100	-0.02243900
H	-1.23635400	1.19752100	0.80613600
H	-1.21582900	1.07505300	-0.94318800
C	0.04925700	-0.36479300	0.05161700
H	0.05411800	-1.08687700	-0.77525500
H	0.03721300	-0.96020400	0.97390400
C	1.33527300	0.46684600	0.00297000
H	1.33288200	1.18836600	0.82970400
H	1.35274100	1.05920200	-0.91983400
C	2.61475200	-0.37757400	0.07981000
H	2.62174800	-1.11174500	-0.74006900
H	2.57972300	-0.99021100	1.00034600

C	3.87809700	0.41641600	0.04773700
H	3.84525100	1.45576900	0.36152100
C	5.20418900	-0.24292300	-0.12114400
H	5.18803900	-0.97983500	-0.93397800
H	5.99628600	0.47940700	-0.33404200
H	5.50900400	-0.79549900	0.78420200

TS22: $\text{H} + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_6\text{CH}_3$

C	5.18161300	-0.33197700	0.09473100
H	5.24398900	-1.15590300	-0.62342500
H	5.22602500	-0.76609100	1.09867400
H	6.07115800	0.29039900	-0.03693300
C	3.89692900	0.47812200	-0.10153100
H	3.88259100	1.31606500	0.60619200
H	3.89769300	0.92690200	-1.10241300
C	2.62159300	-0.35344800	0.07647800
H	2.62147600	-0.80307200	1.07810500
H	2.63702700	-1.19245400	-0.63175400
C	1.33058700	0.44930900	-0.11774000
H	1.33275600	0.90090000	-1.11835000
H	1.31504100	1.28636100	0.59229800
C	0.05599200	-0.38397800	0.05700300
H	0.05503900	-0.83797000	1.05638200
H	0.06970200	-1.21922700	-0.65552100
C	-1.23370300	0.42194900	-0.13215000
H	-1.23184600	0.88100000	-1.12906600
H	-1.25330200	1.25087800	0.58561900
C	-2.50693200	-0.41629800	0.03232700
H	-2.51184100	-0.89171500	1.02195100
H	-2.49174500	-1.24412700	-0.69399600
C	-3.79106900	0.36617900	-0.15101600
H	-3.77340600	1.01984900	-1.02759500
H	-3.80528100	1.24917500	0.82145700
C	-5.08558600	-0.40345900	-0.00733100
H	-5.12597100	-0.93900900	0.94614000
H	-5.95450600	0.25771200	-0.06056700
H	-5.18804900	-1.14861000	-0.80648300
H	-3.83309700	1.86054100	1.57466000

H-R23: $\text{H} + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_5\text{CH}_3$
 $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_5\text{CH}_3$

C	-5.06856200	-0.43800800	0.06823700
H	-5.07345900	-1.10507500	0.93617400

H	-5.12525000	-1.06347600	-0.82835100
H	-5.97912200	0.16632300	0.10923800
C	-3.81337300	0.43935900	0.05209600
H	-3.85323600	1.11801100	-0.80872800
H	-3.80380000	1.07960700	0.94269300
C	-2.51078900	-0.36717000	-0.00215800
H	-2.52124000	-1.00916200	-0.89275600
H	-2.47152800	-1.04605000	0.85976800
C	-1.24825500	0.50160600	-0.01983400
H	-1.23915300	1.14369300	0.87062200
H	-1.28806000	1.17990300	-0.88218500
C	0.05181200	-0.30767800	-0.07290000
H	0.04485200	-0.94764500	-0.96428200
H	0.09659600	-0.98458000	0.78873200
C	1.31635300	0.56281300	-0.09194400
H	1.33139600	1.21017400	0.79756500
H	1.24913500	1.26368900	-0.94514200
C	2.59090400	-0.20975200	-0.17072600
H	2.56968500	-1.20177900	-0.61607800
C	3.91554700	0.43654100	0.06522500
H	3.87082700	1.04063400	0.98319300
H	4.12304200	1.16770200	-0.73735900
C	5.08553000	-0.55034500	0.15083000
H	5.17414000	-1.13342000	-0.77083300
H	6.03386700	-0.02951500	0.30769300
H	4.94630000	-1.25323700	0.97707700

TS23: $\text{H} + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_5\text{CH}_3$

C	-5.15326100	0.38496800	-0.06683200
H	-5.20026100	0.84560600	-1.05878100
H	-5.18603400	1.19136900	0.67273600
H	-6.05587900	-0.21906500	0.06128400
C	-3.88625100	-0.46059500	0.09129700
H	-3.88431000	-0.93350400	1.08097900
H	-3.90237600	-1.28106000	-0.63666900
C	-2.59356900	0.34418700	-0.08455700
H	-2.57876300	1.16599500	0.64326100
H	-2.59543000	0.81734500	-1.07530300
C	-1.32022800	-0.49394000	0.07374600
H	-1.33480700	-1.31484900	-0.65526700
H	-1.32056300	-0.96771100	1.06395200
C	-0.02910100	0.31352000	-0.09842900
H	-0.01120700	1.13112100	0.63218600

H	-0.02684500	0.78790600	-1.08812200
C	1.24267700	-0.52889800	0.05828200
H	1.22794500	-1.34637400	-0.67940400
H	1.24245300	-1.01730900	1.04144800
C	2.52790800	0.25500200	-0.11036600
H	2.53084100	1.12873900	0.87564400
H	2.51824800	0.91513900	-0.98350300
C	3.82681200	-0.51075000	0.03987600
H	3.84421600	-1.32296800	-0.70212500
H	3.84428700	-1.00377500	1.01955900
C	5.07786600	0.35706500	-0.12719800
H	5.10829300	1.15312600	0.62194700
H	5.98877400	-0.23778600	-0.02032300
H	5.10177400	0.82830700	-1.11464100
H	2.53252700	1.71640100	1.64622900

H-R24: $\text{H} + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_4\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_4\text{CH}_3$

C	5.11041800	-0.25792300	0.11837100
H	5.23054700	-0.86470600	-0.78479900
H	5.13876400	-0.93608500	0.97722400
H	5.97737800	0.40478500	0.19032400
C	3.80047000	0.53476200	0.08271800
H	3.72830700	1.16062300	0.98058600
H	3.81510500	1.22623500	-0.76857400
C	2.55573200	-0.35483700	-0.01262300
H	2.54175000	-1.04680500	0.83973200
H	2.62906000	-0.98221000	-0.91080400
C	1.24075600	0.43042500	-0.04942000
H	1.25417500	1.12066200	-0.90238300
H	1.16304600	1.05546400	0.84841200
C	-0.00461800	-0.46170600	-0.14771800
H	-0.02464900	-1.16109500	0.70162900
H	0.09454000	-1.10991200	-1.03858500
C	-1.29359000	0.28844600	-0.20900100
H	-1.27974400	1.31589900	-0.56526100
C	-2.60988400	-0.40391600	-0.08488400
H	-2.57761700	-1.11172400	0.75721400
H	-2.78648700	-1.03821000	-0.97400700
C	-3.80780600	0.54104800	0.08608700
H	-3.83336200	1.24014300	-0.75814600
H	-3.65567300	1.15071500	0.98381000
C	-5.14713400	-0.19389300	0.18298500

H	-5.16152500	-0.87978000	1.03608300
H	-5.97820800	0.50591600	0.30661800
H	-5.34147300	-0.78435200	-0.71816500

TS24: $\text{H} + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_4\text{CH}_3$

C	-5.14778900	-0.33746000	0.06016800
H	-5.20159700	-0.77482900	1.06222500
H	-5.20894800	-1.15846700	-0.66146900
H	-6.03325200	0.28976100	-0.07564800
C	-3.85807200	0.46748000	-0.12370800
H	-3.84934800	0.91987000	-1.12292400
H	-3.84473600	1.30256100	0.58725800
C	-2.58816500	-0.37091000	0.06070800
H	-2.60218400	-1.20749000	-0.65052800
H	-2.59742400	-0.82345200	1.06089700
C	-1.29333800	0.42809300	-0.12082500
H	-1.27674000	1.26082800	0.59263100
H	-1.28417100	0.88170200	-1.12022100
C	-0.02512500	-0.41475000	0.06002900
H	-0.03936100	-1.24830500	-0.65942500
H	-0.03093400	-0.88134700	1.05368400
C	1.26331800	0.36153900	-0.12087500
H	1.26513200	1.25379200	0.84806400
H	1.25661300	1.00470000	-1.00638600
C	2.55889200	-0.40548100	0.04661600
H	2.57488800	-1.23570200	-0.67689800
H	2.57700100	-0.87677100	1.03807600
C	3.82009400	0.44680300	-0.13990600
H	3.80486800	1.27263600	0.58013100
H	3.79736200	0.90787100	-1.13465800
C	5.11571700	-0.35227900	0.02389400
H	5.17583500	-1.16602500	-0.70604400
H	5.99507600	0.28266600	-0.11424900
H	5.18214100	-0.79795000	1.02142200
H	1.26658800	1.85574800	1.60745300

H-R25: $\text{H} + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_3\text{CH}_3$

C	5.07000100	-0.53507400	0.13068900
H	5.14134400	-1.11479100	-0.79510600
H	5.00587400	-1.24600500	0.96056700
H	6.00282300	0.02424900	0.24448000
C	3.85636100	0.39853400	0.10656500

H	3.83215200	0.98953500	1.03037800
H	3.96709800	1.12022800	-0.71216500
C	2.52529300	-0.34371100	-0.05201500
H	2.41050700	-1.06513500	0.76624500
H	2.54740200	-0.93287500	-0.97770900
C	1.30339400	0.58475000	-0.07738700
H	1.44086500	1.32779400	-0.88531700
H	1.27665800	1.18312000	0.84585200
C	0.00000000	-0.12073600	-0.25421900
H	0.00000000	-1.10181200	-0.72337400
C	-1.30339400	0.58475000	-0.07738600
H	-1.44086500	1.32779500	-0.88531400
H	-1.27665700	1.18311900	0.84585400
C	-2.52529300	-0.34371100	-0.05201500
H	-2.41050700	-1.06513600	0.76624400
H	-2.54740200	-0.93287400	-0.97771100
C	-3.85636100	0.39853400	0.10656600
H	-3.96709800	1.12022900	-0.71216300
H	-3.83215200	0.98953400	1.03038000
C	-5.07000100	-0.53507400	0.13068800
H	-5.00587500	-1.24600600	0.96056500
H	-6.00282300	0.02424900	0.24447900
H	-5.14134400	-1.11479000	-0.79510700

TS25: $\text{H} + \text{CH}_3(\text{CH}_2)_7\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_3\text{CH}_3$

C	-5.40808200	-0.14115900	0.79695700
H	-5.07412100	-1.18366400	0.79231600
H	-5.05015100	0.32380100	-0.12700100
H	-6.50116600	-0.14300900	0.76574000
C	-4.88462000	0.60239800	2.02915600
H	-5.26338800	1.63164400	2.02237500
H	-5.28845500	0.13593600	2.93619400
C	-3.35453700	0.62974700	2.11376800
H	-2.94938700	1.09933500	1.20926000
H	-2.97463000	-0.40008700	2.11970700
C	-2.82376400	1.36956700	3.34751400
H	-3.23184300	0.89772900	4.25492800
H	-3.20443500	2.39926400	3.35228800
C	-1.31230900	1.39369600	3.45023800
H	-0.90674400	2.07121200	2.39522100
H	-0.85420200	0.41650200	3.26799200
C	-0.71386600	2.11882000	4.63840600
H	-1.10362400	1.66488400	5.56280800

H	-1.06856000	3.15769000	4.64618500
C	0.81891700	2.09762500	4.67493700
H	1.20788700	2.54531000	3.75242700
H	1.16436100	1.05575900	4.67821700
C	1.41188700	2.83055600	5.88331500
H	1.01643200	2.38681300	6.80530600
H	1.06924100	3.87240400	5.87645100
C	2.94261700	2.79808200	5.91778800
H	3.36824600	3.26552700	5.02427200
H	3.33398900	3.33034900	6.78918700
H	3.31552500	1.76987300	5.96168900
H	-0.64348900	2.62464000	1.64572300

2.1.10 C10 (*n*-C₁₀H₂₂)



n-C₁₀H₂₂

C	5.77660500	-0.28684000	0.00000300
H	6.65746100	0.36138400	-0.00000300
H	5.83850900	-0.93107800	-0.88289300
H	5.83851000	-0.93106300	0.88291000
C	4.48011200	0.52857600	-0.00000500
H	4.46370600	1.18821300	-0.87624800
H	4.46370200	1.18822100	0.87623200
C	3.21714900	-0.34027500	-0.00000600
H	3.23430400	-1.00091900	-0.87680800
H	3.23430700	-1.00092200	0.87679300
C	1.91385500	0.46645500	0.00000000
H	1.89773400	1.12689100	-0.87680000
H	1.89773700	1.12688800	0.87680300
C	0.65167400	-0.40350500	0.00000200
H	0.66784000	-1.06394400	0.87676600
H	0.66783400	-1.06393800	-0.87676700
C	-0.65167400	0.40350500	0.00000700
H	-0.66783800	1.06394500	-0.87675600
H	-0.66783600	1.06393700	0.87677700
C	-1.91385600	-0.46645500	0.00000400
H	-1.89773700	-1.12689000	0.87680400
H	-1.89773400	-1.12688800	-0.87679800
C	-3.21714900	0.34027500	0.00000300
H	-3.23430300	1.00092300	-0.87679600
H	-3.23430700	1.00091900	0.87680500
C	-4.48011100	-0.52857700	-0.00000200
H	-4.46370600	-1.18821800	0.87623700

H	-4.46370100	-1.18821600	-0.87624400
C	-5.77660500	0.28683900	-0.00000500
H	-5.83850700	0.93107100	-0.88290600
H	-6.65746100	-0.36138500	-0.00000800
H	-5.83851200	0.93106900	0.88289700

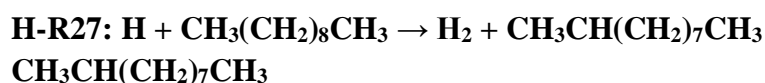
CH₂(CH₂)₈CH₃

C	-5.82494800	0.27545300	0.00054000
H	-6.75813200	-0.17783600	-0.31152300
H	-5.86667200	1.27047800	0.42941700
C	-4.55543900	-0.50319300	0.00508400
H	-4.54551200	-1.20390300	-0.84041000
H	-4.51547300	-1.14635500	0.90314900
C	-3.28805500	0.36504700	-0.02536000
H	-3.30359100	0.98862300	-0.92717400
H	-3.30958400	1.05729700	0.82582800
C	-1.98997800	-0.44814900	0.01252400
H	-1.97349600	-1.14283900	-0.83733900
H	-1.97991600	-1.07302300	0.91513100
C	-0.72442700	0.41623600	-0.01806200
H	-0.73913500	1.10892800	0.83337000
H	-0.73665400	1.04324700	-0.91897300
C	0.57531200	-0.39596100	0.01401400
H	0.58983400	-1.08818900	-0.83783300
H	0.58752900	-1.02360800	0.91457600
C	1.84104100	0.46830700	-0.01638700
H	1.82711900	1.15991600	0.83601200
H	1.82810300	1.09669500	-0.91645400
C	3.14090700	-0.34334900	0.01359600
H	3.15539500	-1.03574200	-0.83835300
H	3.15538700	-0.97137100	0.91408100
C	4.40739400	0.51983500	-0.01835600
H	4.39353600	1.21172600	0.83263200
H	4.39369200	1.14631900	-0.91863700
C	5.70051900	-0.30021900	0.01252300
H	5.75921300	-0.97836800	-0.84479200
H	6.58392700	0.34395600	-0.01306600
H	5.76047800	-0.90999100	0.91966700

TS26: H + CH₃(CH₂)₈CH₃ → H₂ + CH₂(CH₂)₈CH₃

C	5.69474000	0.18177200	-0.14575500
H	6.60969100	-0.39744500	-0.02445900
H	5.78476000	1.04676300	0.90808400

H	5.74245900	0.85966000	-0.99867700
C	4.40282800	-0.58196500	0.01647200
H	4.39963200	-1.09607000	0.98563800
H	4.36356800	-1.37997200	-0.74092300
C	3.14743000	0.29049500	-0.10990300
H	3.18428000	1.08343400	0.64676800
H	3.15941200	0.79669500	-1.08373700
C	1.84056700	-0.49578900	0.03784100
H	1.83012000	-0.99985000	1.01291200
H	1.80996600	-1.29311100	-0.71628200
C	0.58447200	0.37274200	-0.09505400
H	0.59476500	0.87595100	-1.07063600
H	0.61588700	1.17080800	0.65790400
C	-0.72373200	-0.41200300	0.05462200
H	-0.73608200	-0.91102300	1.03231900
H	-0.75260700	-1.21353400	-0.69500000
C	-1.98011800	0.45502000	-0.08571800
H	-1.96925400	0.95090100	-1.06509500
H	-1.94957600	1.25901200	0.66115800
C	-3.28856600	-0.32793600	0.06908000
H	-3.30233200	-0.82025800	1.05035600
H	-3.31847100	-1.13504700	-0.67475800
C	-4.54556000	0.53721500	-0.07745100
H	-4.53409200	1.02565500	-1.05953400
H	-4.51508900	1.34550900	0.66342000
C	-5.84763900	-0.25262500	0.08393800
H	-5.90551100	-0.72231500	1.07104500
H	-6.72366900	0.39236900	-0.02814300
H	-5.92352100	-1.04823000	-0.66422900
H	5.82912900	1.60853900	1.64344200



C	-5.85296100	-0.15480100	0.14178000
H	-6.62552300	0.59080300	0.34609800
H	-5.84908700	-0.87635100	0.96841400
H	-6.17778000	-0.71670700	-0.75078800
C	-4.51225400	0.46819700	-0.04841400
H	-4.45613400	1.50006800	-0.38295100
C	-3.26906100	-0.35720500	-0.07312000
H	-3.29108300	-1.07873000	0.75761200
H	-3.25262900	-0.98407800	-0.98456100
C	-1.96861500	0.45602600	-0.01325500

H	-1.96763600	1.06195300	0.90085500
H	-1.95135900	1.16525400	-0.85040800
C	-0.70420700	-0.40851000	-0.05425700
H	-0.71049900	-1.01694500	-0.96807200
H	-0.72450800	-1.11863600	0.78269800
C	0.59568900	0.40182500	0.00389000
H	0.60036500	1.01280400	0.91585200
H	0.61834900	1.10945600	-0.83501600
C	1.86080300	-0.46322700	-0.03075600
H	1.85579700	-1.07486900	-0.94239400
H	1.83789500	-1.17042400	0.80857500
C	3.16135100	0.34581100	0.02693800
H	3.16738000	0.95774500	0.93852400
H	3.18566900	1.05312400	-0.81243700
C	4.42681700	-0.51881600	-0.00708400
H	4.42182500	-1.12889900	-0.91866700
H	4.40271100	-1.22591400	0.83108200
C	5.72088400	0.29813300	0.05270400
H	5.77188400	0.89133900	0.97131900
H	6.60345400	-0.34713700	0.02522500
H	5.79023600	0.99154900	-0.79151300

TS27: $\text{H} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_7\text{CH}_3$

C	-5.73360200	-0.31946700	-0.02277100
H	-6.58554300	0.36393100	-0.06939400
H	-5.78970800	-0.86587600	0.92371700
H	-5.85278900	-1.05156600	-0.83158800
C	-4.41991000	0.41935800	-0.15381800
H	-4.41477200	1.29027800	0.82971800
H	-4.38389500	1.08336800	-1.02201900
C	-3.15619100	-0.39721900	0.02232900
H	-3.17712800	-0.88777600	1.00432300
H	-3.15834000	-1.21371400	-0.71688200
C	-1.86178800	0.41146300	-0.12384700
H	-1.86307800	1.22822200	0.60796000
H	-1.84465800	0.88722400	-1.11274300
C	-0.59359400	-0.43008500	0.05568800
H	-0.59808700	-1.25250600	-0.67171200
H	-0.61039600	-0.90175700	1.04671800
C	0.70250600	0.37340000	-0.09897200
H	0.70501200	1.19799700	0.62558800
H	0.72100900	0.84217300	-1.09144200
C	1.97161500	-0.46591400	0.08690300

H	1.96743200	-1.29267900	-0.63550200
H	1.95410600	-0.93204700	1.08065200
C	3.26828200	0.33560800	-0.07158800
H	3.27283900	1.16376200	0.64932700
H	3.28787100	0.80033800	-1.06613700
C	4.53788000	-0.50234300	0.11727200
H	4.53435200	-1.32966500	-0.60305100
H	4.51900000	-0.96596300	1.11118300
C	5.82825500	0.30661000	-0.04328300
H	5.87985000	1.11935600	0.68829500
H	6.71353200	-0.32043300	0.09501900
H	5.89210200	0.75578500	-1.03954100
H	-4.42943500	1.89308600	1.59004600

H-R28: $\text{H} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_6\text{CH}_3$

$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_6\text{CH}_3$

C	5.74192400	0.48050400	0.17446200
H	6.67886300	-0.06201200	0.32624800
H	5.61352400	1.17222900	1.01180900
H	5.84612700	1.07684900	-0.73701200
C	4.55258300	-0.48090800	0.06800200
H	4.49190200	-1.09899200	0.97568700
H	4.74857800	-1.20282700	-0.74576600
C	3.24230900	0.19595200	-0.16239100
H	3.24297300	1.19549600	-0.59111700
C	1.95204500	-0.55181900	-0.10181300
H	1.94937700	-1.21294300	0.77763400
H	1.87531700	-1.23805100	-0.96605600
C	0.70530700	0.34375200	-0.07559600
H	0.71601800	0.99738700	-0.95696200
H	0.75923300	1.00626700	0.79665300
C	-0.61117100	-0.43956100	-0.04170000
H	-0.61965500	-1.09589900	0.83826500
H	-0.66037800	-1.10301600	-0.91502600
C	-1.85583600	0.45478700	-0.01603500
H	-1.84675400	1.11197500	-0.89532300
H	-1.80693200	1.11741600	0.85780500
C	-3.17426000	-0.32628700	0.01637600
H	-3.18461800	-0.98369500	0.89567500
H	-3.22432900	-0.98908500	-0.85752900
C	-4.41926500	0.56774700	0.04189400
H	-4.40921800	1.22460400	-0.83649700
H	-4.37007000	1.22918100	0.91553400

C	-5.73160400	-0.22116100	0.07356500
H	-5.78581900	-0.86303000	0.95867000
H	-6.59873500	0.44497100	0.09335900
H	-5.82760200	-0.86486200	-0.80664300

TS28: $\text{H} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_6\text{CH}_3$

C	5.72315600	0.28669600	-0.10660200
H	6.62101300	-0.32633900	0.00765600
H	5.76416600	1.08289100	0.64192200
H	5.76390200	0.75620000	-1.09431200
C	4.45354500	-0.55534200	0.05193000
H	4.45450200	-1.04905200	1.03143800
H	4.45905700	-1.36745800	-0.69035900
C	3.17174700	0.23717200	-0.10598800
H	3.18437500	1.10622500	0.88475300
H	3.18296200	0.90197700	-0.97553300
C	1.86917600	-0.52077900	0.04743100
H	1.85417600	-1.02217800	1.02389300
H	1.83951500	-1.32761300	-0.70142300
C	0.61682700	0.35161800	-0.10246700
H	0.63676600	0.84460300	-1.08283600
H	0.64700500	1.15452000	0.64380100
C	-0.69281700	-0.43057500	0.04472900
H	-0.70849500	-0.92849300	1.02286300
H	-0.72295200	-1.23250300	-0.70452300
C	-1.94575200	0.44107200	-0.09742600
H	-1.92966100	0.94092800	-1.07469100
H	-1.91496700	1.24165200	0.65292100
C	-3.25726600	-0.33824900	0.04937700
H	-3.27309000	-0.84048300	1.02557000
H	-3.29068400	-1.13743900	-0.70280200
C	-4.51044100	0.53401000	-0.08775900
H	-4.49571000	1.03504200	-1.06343000
H	-4.47734700	1.33242200	0.66356900
C	-5.81598000	-0.25241000	0.06190800
H	-5.87664000	-0.73524600	1.04247900
H	-6.68911500	0.39784400	-0.04196200
H	-5.89468900	-1.03736300	-0.69713200
H	3.19274100	1.69058900	1.65734400

H-R29: $\text{H} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_5\text{CH}_3$

C	-5.79258700	-0.06974500	0.23036100
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H	-6.59837800	0.66452700	0.31567800
H	-5.81899800	-0.69657300	1.12745800
H	-6.01784900	-0.71176800	-0.62728100
C	-4.43105200	0.61131400	0.07031600
H	-4.24556500	1.27143300	0.92506000
H	-4.44538700	1.25573500	-0.81666100
C	-3.26776400	-0.38291300	-0.05448000
H	-3.24659300	-1.03638800	0.83076400
H	-3.47855000	-1.06615700	-0.89875400
C	-1.93145100	0.25553800	-0.23885500
H	-1.88978400	1.25706900	-0.66085400
C	-0.66611000	-0.53069000	-0.14639900
H	-0.59155500	-1.22407600	-1.00510000
H	-0.70270100	-1.18680300	0.73615700
C	0.60647300	0.32659300	-0.09726500
H	0.55395100	0.99534800	0.77031400
H	0.63467000	0.97530300	-0.98189600
C	1.89752200	-0.49596900	-0.03073000
H	1.94443800	-1.16702800	-0.89837800
H	1.86802900	-1.14572800	0.85370100
C	3.16804900	0.36006500	0.01461900
H	3.12179100	1.03180000	0.88179500
H	3.19874100	1.00964600	-0.86999600
C	4.46175100	-0.45961100	0.08214900
H	4.50829200	-1.13160400	-0.78355600
H	4.43238000	-1.10694200	0.96717100
C	5.72504800	0.40514600	0.12478900
H	5.72285600	1.06549700	0.99787200
H	6.62887300	-0.20850400	0.17537400
H	5.80205500	1.03684000	-0.76589800

TS29: $\text{H} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_5\text{CH}_3$

C	-5.75905200	-0.26264800	0.00306600
H	-6.62078500	0.40081400	-0.10971400
H	-5.83926300	-0.74667500	0.98150700
H	-5.83951400	-1.04402500	-0.75950700
C	-4.44201600	0.50710200	-0.12707300
H	-4.40419100	1.30034800	0.62774400
H	-4.40594100	1.00951200	-1.10118900
C	-3.20473300	-0.38688400	0.02234500
H	-3.23645200	-0.89881000	0.99307100
H	-3.24343700	-1.18485300	-0.73568300
C	-1.88859000	0.35082300	-0.11333500

H	-1.87260000	1.21049700	0.88466300
H	-1.86017500	1.02248800	-0.97708600
C	-0.62165500	-0.46392200	0.04938700
H	-0.62569400	-1.27666000	-0.69356400
H	-0.63254600	-0.95866400	1.02931900
C	0.66871000	0.35057900	-0.10227500
H	0.66551200	1.16899300	0.62767200
H	0.68082900	0.82412700	-1.09230600
C	1.94152900	-0.48412000	0.07626700
H	1.93835300	-1.31032100	-0.64689800
H	1.93070100	-0.95072400	1.06980100
C	3.23310200	0.32451500	-0.08727500
H	3.23376000	1.15512900	0.63066900
H	3.24826500	0.78567500	-1.08354600
C	4.50771200	-0.50548300	0.10266700
H	4.50656100	-1.33740000	-0.61239100
H	4.49446900	-0.96273900	1.09958800
C	5.79301100	0.30961700	-0.06711700
H	5.84206600	1.12766900	0.65866300
H	6.68210700	-0.31153700	0.07307600
H	5.85160300	0.75215900	-1.06665000
H	-1.86174000	1.78752500	1.66281700

H-R30: $\text{H} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_4\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_4\text{CH}_3$

C	5.72910600	0.48324200	0.16032400
H	6.65229600	-0.09238800	0.27130300
H	5.67280700	1.18518400	0.99837700
H	5.81379300	1.07266400	-0.75818700
C	4.50072000	-0.43031700	0.11990700
H	4.46329700	-1.03235500	1.03611400
H	4.60323100	-1.14338300	-0.70741700
C	3.18245900	0.33525200	-0.03456100
H	3.07505000	1.04660600	0.79350000
H	3.21886400	0.93720500	-0.95152500
C	1.94595900	-0.57259600	-0.07971200
H	1.90570800	-1.18532400	0.83383200
H	2.07425200	-1.30517700	-0.89850800
C	0.65490800	0.15674700	-0.25049900
H	0.67501800	1.15641200	-0.67802600
C	-0.65996600	-0.53856500	-0.12603300
H	-0.65567400	-1.17993800	0.76817200
H	-0.79388100	-1.24076100	-0.97025400

C	-1.86998500	0.40472600	-0.07585600
H	-1.86489300	1.04070200	-0.97013700
H	-1.76085200	1.08109300	0.78056400
C	-3.21328000	-0.32590500	0.01805300
H	-3.21761800	-0.96539100	0.91057300
H	-3.31861000	-1.00308500	-0.83989300
C	-4.42231900	0.61507200	0.06773400
H	-4.41695500	1.25570200	-0.82259400
H	-4.31941900	1.28926300	0.92680500
C	-5.76147100	-0.12261400	0.15686600
H	-5.81000000	-0.74731700	1.05448700
H	-6.60164800	0.57649300	0.19365400
H	-5.91155300	-0.77646200	-0.70818000

TS30: $\text{H} + \text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_4\text{CH}_3$

C	-5.75705500	0.31040700	-0.08908800
H	-6.65170100	-0.30533600	0.03855100
H	-5.80708400	0.76657200	-1.08291800
H	-5.80264200	1.11889300	0.64738700
C	-4.47963300	-0.51777000	0.07611500
H	-4.48132000	-1.33977400	-0.65038700
H	-4.47539400	-0.98827300	1.06684200
C	-3.19857400	0.30582400	-0.09507800
H	-3.20290400	0.78002400	-1.08503200
H	-3.19350100	1.12414100	0.63519900
C	-1.91572100	-0.51895000	0.06281500
H	-1.91682600	-1.33432700	-0.67730800
H	-1.91184500	-1.01028500	1.04453100
C	-0.64122900	0.28398500	-0.09944500
H	-0.65383300	1.14968500	0.89350000
H	-0.66058600	0.95097400	-0.96701000
C	0.66795100	-0.46458400	0.04562700
H	0.70160400	-1.26698000	-0.70775100
H	0.69031900	-0.97115200	1.01924500
C	1.91265400	0.41883700	-0.10368800
H	1.87852300	1.21725600	0.64720900
H	1.88523800	0.91711500	-1.08123000
C	3.22917100	-0.35299000	0.03447600
H	3.26399000	-1.15121200	-0.71875500
H	3.25398800	-0.85561300	1.01019500
C	4.47507300	0.52863900	-0.10855900
H	4.44033300	1.32526500	0.64442100
H	4.45102000	1.03119700	-1.08324300

C	5.78687100	-0.24889700	0.03208800
H	5.86692900	-1.03175000	-0.72897100
H	6.65457400	0.40791700	-0.07546200
H	5.85660600	-0.73301800	1.01139100
H	-0.66254200	1.73167100	1.66801400

2.1.11 C11 (*n*-C₁₁H₂₄)



n-C₁₁H₂₄

C	6.40891800	-0.38215800	0.00000500
H	6.45417800	-1.02780200	-0.88287800
H	6.45419100	-1.02776600	0.88291400
H	7.30617800	0.24317100	-0.00001500
C	5.13375500	0.46621600	-0.00000400
H	5.13411300	1.12607000	0.87623600
H	5.13411600	1.12605200	-0.87625800
C	3.84907600	-0.37023300	0.00000000
H	3.84955600	-1.03110800	0.87679600
H	3.84955300	-1.03111000	-0.87679500
C	2.56653900	0.46908700	0.00000000
H	2.56692600	1.12970500	-0.87681100
H	2.56692200	1.12969700	0.87681800
C	1.28301900	-0.36911700	-0.00000500
H	1.28285200	-1.02977300	0.87674500
H	1.28285100	-1.02975900	-0.87676600
C	0.00000000	0.46980800	0.00000200
H	-0.00000100	1.13043300	-0.87678200
H	0.00000100	1.13042400	0.87679200
C	-1.28301900	-0.36911700	0.00000000
H	-1.28285100	-1.02976800	0.87675400
H	-1.28285100	-1.02976400	-0.87675700
C	-2.56653900	0.46908700	0.00000200
H	-2.56692400	1.12970200	-0.87681200
H	-2.56692300	1.12970000	0.87681700
C	-3.84907600	-0.37023300	0.00000100
H	-3.84955500	-1.03110900	0.87679700
H	-3.84955400	-1.03111000	-0.87679400
C	-5.13375500	0.46621600	0.00000000
H	-5.13411400	1.12606100	-0.87624700
H	-5.13411500	1.12606200	0.87624700
C	-6.40891800	-0.38215800	-0.00000100
H	-6.45418600	-1.02778300	0.88289600
H	-7.30617800	0.24317100	-0.00000300

H	-6.45418400	-1.02778500	-0.88289600
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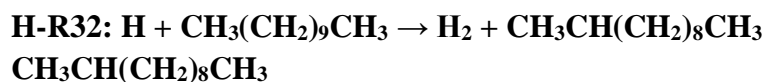
CH₂(CH₂)₉CH₃

C	-6.45896300	-0.36859000	0.00227300
H	-6.47743800	-1.36382800	-0.42776400
H	-7.40242400	0.06187600	0.31578400
C	-5.20843900	0.44012600	-0.00218900
H	-5.18484000	1.08584500	-0.89899100
H	-5.21435700	1.13926700	0.84465400
C	-3.92048500	-0.39739000	0.02526500
H	-3.92592000	-1.08789700	-0.82759500
H	-3.92028200	-1.02334500	0.92556400
C	-2.64255100	0.44715400	-0.01143000
H	-2.64208800	1.13951000	0.84049200
H	-2.64852700	1.07479000	-0.91215000
C	-1.35628100	-0.38623000	0.01537800
H	-1.35464300	-1.07599500	-0.83855000
H	-1.35271500	-1.01661700	0.91400000
C	-0.07677000	0.45754900	-0.01438700
H	-0.07835900	1.14641900	0.84030900
H	-0.08062000	1.08903400	-0.91234500
C	1.20964500	-0.37574000	0.01140200
H	1.21205600	-1.06346800	-0.84420600
H	1.21247000	-1.00850700	0.90844400
C	2.48944500	0.46771000	-0.01533100
H	2.48694400	1.15550900	0.84026700
H	2.48684400	1.10041700	-0.91247200
C	3.77571100	-0.36544700	0.01090800
H	3.77901100	-1.05384800	-0.84438500
H	3.77945100	-0.99802600	0.90830000
C	5.05646400	0.47660100	-0.01639200
H	5.05368100	1.16463400	0.83783800
H	5.05375100	1.10746700	-0.91371400
C	6.33559900	-0.36521900	0.01130700
H	6.38337600	-1.04016500	-0.84920100
H	7.22979100	0.26404500	-0.01065000
H	6.38459100	-0.98025900	0.91554700

TS31: H + CH₃(CH₂)₉CH₃ → H₂ + CH₂(CH₂)₉CH₃

C	6.32815500	0.27239900	-0.15908100
H	6.39708300	1.17320300	0.86586000
H	6.35737600	0.92341300	-1.03351400

H	7.25800900	-0.27863800	-0.02093100
C	5.05682500	-0.51914400	0.03004800
H	5.03747000	-1.34108100	-0.70221900
H	5.06875100	-1.00294400	1.01460700
C	3.77893300	0.31596200	-0.11970400
H	3.77900800	0.79785700	-1.10585000
H	3.79342900	1.12839000	0.61686700
C	2.49291000	-0.50055100	0.04585300
H	2.49959500	-0.99126800	1.02774100
H	2.47891400	-1.30874800	-0.69715200
C	1.21499100	0.33468300	-0.09174100
H	1.21471900	0.83751600	-1.06756200
H	1.22364400	1.13374100	0.66079500
C	-0.07301400	-0.48351300	0.05419300
H	-0.06767200	-0.99713100	1.02437800
H	-0.08681500	-1.27427400	-0.70720400
C	-1.35055500	0.35519400	-0.06540000
H	-1.35030900	0.87943900	-1.02991600
H	-1.34182000	1.13761100	0.70452800
C	-2.63938500	-0.46482000	0.06256200
H	-2.63535100	-0.99783100	1.02228600
H	-2.65287100	-1.24015800	-0.71453100
C	-3.91642900	0.37638800	-0.04162500
H	-3.91885200	0.91512200	-0.99832100
H	-3.90644300	1.14753300	0.73983100
C	-5.20638500	-0.44325400	0.07739000
H	-5.20245100	-0.98485600	1.03125100
H	-5.21986300	-1.21019200	-0.70667900
C	-6.47622200	0.40735500	-0.02052400
H	-6.52597800	0.93499100	-0.97838300
H	-7.37709700	-0.20648400	0.06705500
H	-6.50966800	1.16087800	0.77282300
H	6.42825200	1.75971800	1.58241100



C	-6.49200900	-0.24744000	-0.13929900
H	-6.80209500	-0.81060600	0.75769600
H	-6.47273300	-0.97439200	-0.96098200
H	-7.28210200	0.47850800	-0.34731100
C	-5.16593000	0.40801000	0.04422100
H	-5.13336300	1.44339900	0.37089500
C	-3.90369600	-0.38787100	0.07282800

H	-3.90826300	-1.11320700	-0.75487500
H	-3.87303800	-1.01034900	0.98689800
C	-2.62290800	0.45575100	0.01013600
H	-2.62282400	1.16825100	0.84466800
H	-2.63611300	1.05817500	-0.90619800
C	-1.33808600	-0.37796300	0.05460800
H	-1.34045200	-1.09065800	-0.78039700
H	-1.33053200	-0.98383900	0.97011200
C	-0.05815600	0.46349900	-0.00461000
H	-0.05328200	1.17337000	0.83269900
H	-0.06767500	1.07235800	-0.91796700
C	1.22757400	-0.37044000	0.03279400
H	1.22279400	-1.07930600	-0.80538300
H	1.23645900	-0.98056800	0.94538200
C	2.50818000	0.47023500	-0.02487900
H	2.51369900	1.17854900	0.81379100
H	2.49893100	1.08095300	-0.93709300
C	3.79347200	-0.36408600	0.01078700
H	3.78810300	-1.07357600	-0.82709000
H	3.80435600	-0.97406700	0.92365400
C	5.07521100	0.47476900	-0.04921500
H	5.08132900	1.18407700	0.78740700
H	5.06529900	1.08280400	-0.96212400
C	6.35326900	-0.36832900	-0.01193200
H	6.39158600	-1.06562700	-0.85492400
H	7.24817900	0.25854100	-0.05907800
H	6.41019900	-0.95959900	0.90758200

TS32: $\text{H} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_8\text{CH}_3$

C	-6.36520400	-0.40027900	0.00999600
H	-6.40576400	-0.90745800	0.97885900
H	-6.47206200	-1.16827400	-0.76666500
H	-7.23169900	0.26237600	-0.06098700
C	-5.06803700	0.35981200	-0.15821500
H	-5.05141800	0.99213700	-1.05034000
H	-5.07445600	1.26721700	0.79251700
C	-3.78656800	-0.42403300	0.03708600
H	-3.77070200	-1.25738900	-0.68300000
H	-3.79659200	-0.89181600	1.03024700
C	-2.51038000	0.40966500	-0.12788200
H	-2.52168100	1.23129100	0.59836600
H	-2.51250100	0.87894000	-1.12000700
C	-1.22317800	-0.40421800	0.04373800

H	-1.20698400	-1.21642900	-0.69484300
H	-1.23017500	-0.88964200	1.02823000
C	0.05353900	0.43244500	-0.09632800
H	0.04523000	1.23116200	0.65656300
H	0.05144500	0.93575700	-1.07191700
C	1.34288000	-0.38416900	0.04662100
H	1.35924900	-1.17020300	-0.71959000
H	1.33728200	-0.90371700	1.01363400
C	2.61903400	0.45770700	-0.06601600
H	2.60990800	1.23230600	0.71178300
H	2.61690900	0.99161500	-1.02525300
C	3.90920500	-0.36127700	0.05203400
H	3.92403600	-1.12846300	-0.73327100
H	3.90816200	-0.90470600	1.00606400
C	5.18563700	0.48219500	-0.04496600
H	5.17507300	1.24356000	0.74448900
H	5.18396500	1.03042900	-0.99504200
C	6.46931400	-0.34603000	0.06335600
H	6.52670900	-1.09300300	-0.73484900
H	7.35993500	0.28462100	-0.00813900
H	6.51637200	-0.87974100	1.01797300
H	-5.09770300	1.89851800	1.52863500

H-R33: $\text{H} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_7\text{CH}_3$
 $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_7\text{CH}_3$

C	6.36693400	-0.59181300	0.18093600
H	6.46241900	-1.16536300	-0.74600600
H	6.21083700	-1.30260400	0.99735100
H	7.31764400	-0.08114400	0.35582500
C	5.20671700	0.40622800	0.09137000
H	5.15568800	1.00087800	1.01513500
H	5.43070800	1.14394100	-0.70071000
C	3.87961200	-0.22597000	-0.16776200
H	3.85551000	-1.21251000	-0.62504200
C	2.61047100	0.55602300	-0.09513500
H	2.55501100	1.26143700	-0.94544000
H	2.62352900	1.19880700	0.79764800
C	1.33922100	-0.30495700	-0.09022100
H	1.37202500	-0.98606400	0.76862400
H	1.33464100	-0.94086600	-0.98454000
C	0.04492100	0.51389000	-0.04389900
H	0.01666800	1.19569200	-0.90390100
H	0.05209400	1.15256000	0.84901000

C	-1.22414400	-0.34585300	-0.03898900
H	-1.19549600	-1.02770100	0.82078500
H	-1.23136200	-0.98448700	-0.93183700
C	-2.52054600	0.47098100	0.00783600
H	-2.54886800	1.15376800	-0.85132700
H	-2.51403100	1.10866200	0.90142400
C	-3.78911400	-0.38924800	0.01089900
H	-3.76099800	-1.07326700	0.86925900
H	-3.79705200	-1.02625400	-0.88332700
C	-5.08677700	0.42550100	0.05979700
H	-5.11551400	1.10936200	-0.79733300
H	-5.07991300	1.06056800	0.95413200
C	-6.34784400	-0.44357900	0.06116000
H	-6.36371900	-1.11574700	0.92502600
H	-7.25473800	0.16647300	0.09885200
H	-6.40179000	-1.06335700	-0.83955200

TS33: $\text{H} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_7\text{CH}_3$

C	-6.35172600	0.37513300	-0.13126600
H	-6.37569400	0.82322000	-1.12942600
H	-6.37941900	1.18858000	0.59912400
H	-7.26398700	-0.21476200	-0.00944900
C	-5.10269300	-0.49169000	0.05432400
H	-5.12126500	-0.96375000	1.04428300
H	-5.12197200	-1.31962400	-0.67007800
C	-3.80203500	0.26781500	-0.11159500
H	-3.79763000	1.15310200	0.86509000
H	-3.79472700	0.91884800	-0.99154100
C	-2.51875200	-0.51913100	0.05706500
H	-2.50347300	-1.33148900	-0.68633300
H	-2.52257400	-1.01427000	1.03679200
C	-1.24444100	0.32139600	-0.08940000
H	-1.25249100	1.11979900	0.66222900
H	-1.25265600	0.82129600	-1.06641100
C	0.04428400	-0.49634700	0.04960400
H	0.05725700	-1.28453800	-0.71457200
H	0.04256100	-1.01289700	1.01816900
C	1.31993700	0.34513000	-0.07007200
H	1.31333400	1.12170900	0.70558300
H	1.31480100	0.87627400	-1.03077100
C	2.61008100	-0.47457300	0.04623800
H	2.62322400	-1.24102700	-0.73962100
H	2.60856900	-1.01830600	0.99992100

C	3.88571300	0.36965900	-0.05049300
H	3.87691300	1.13017400	0.74126000
H	3.88484100	0.92112600	-0.99990200
C	5.17692000	-0.45004500	0.05398300
H	5.18985600	-1.20522300	-0.74141800
H	5.17542600	-1.00570100	0.99973100
C	6.44542200	0.40368800	-0.03353700
H	6.47928400	1.14511400	0.77108400
H	7.34727700	-0.21017500	0.04304200
H	6.49260500	0.94584100	-0.98337900
H	-3.79631500	1.75046600	1.62749000

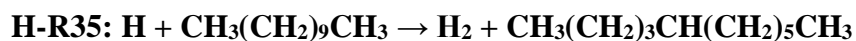
H-R34: $\text{H} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_6\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_6\text{CH}_3$

C	6.43518600	-0.14824000	0.25276700
H	6.65681000	-0.75892400	-0.62838800
H	6.44219100	-0.81141500	1.12373500
H	7.25305700	0.56725500	0.37472000
C	5.08734900	0.56311000	0.10931500
H	4.90696400	1.19313100	0.98753400
H	5.12001200	1.24067400	-0.75207700
C	3.90759300	-0.40459600	-0.06177600
H	3.86735000	-1.08999400	0.79823600
H	4.11341800	-1.05940900	-0.92949200
C	2.58445200	0.26435700	-0.23251100
H	2.56381100	1.27913800	-0.62326700
C	1.30412800	-0.50037800	-0.17068600
H	1.32210500	-1.18107600	0.69363300
H	1.22328500	-1.16841800	-1.04869900
C	0.04726000	0.37877500	-0.10659100
H	0.03655900	1.05081500	-0.97400500
H	0.10653900	1.02348700	0.77860300
C	-1.25905300	-0.42117800	-0.06930900
H	-1.24684100	-1.09472700	0.79750200
H	-1.31302300	-1.06789200	-0.95483900
C	-2.51396500	0.45701200	-0.00808800
H	-2.52570700	1.13111200	-0.87443900
H	-2.46025200	1.10317700	0.87773400
C	-3.82217500	-0.34084500	0.02812800
H	-3.81181000	-1.01491500	0.89471500
H	-3.87678800	-0.98748500	-0.85754400
C	-5.07762600	0.53677300	0.08861800
H	-5.08837000	1.21046100	-0.77691200

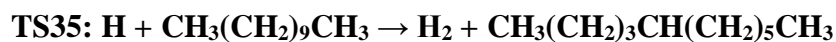
H	-5.02403500	1.18185400	0.97416100
C	-6.37946000	-0.26920300	0.12363400
H	-6.41214800	-0.92963300	0.99605800
H	-7.25442100	0.38526100	0.17012300
H	-6.48083300	-0.89600800	-0.76809100

TS34: H + CH₃(CH₂)₉CH₃ → H₂ + CH₃(CH₂)₂CH(CH₂)₆CH₃

C	-6.38918900	-0.34259300	0.02529100
H	-6.45097200	-0.84585100	0.99532900
H	-6.46044000	-1.11143600	-0.75080300
H	-7.26519200	0.30502100	-0.06805600
C	-5.08927400	0.45626600	-0.10164100
H	-5.07219700	0.97763000	-1.06626400
H	-5.06083900	1.23567100	0.66785800
C	-3.83276900	-0.41482200	0.01995800
H	-3.86072000	-1.19735100	-0.75443800
H	-3.84649700	-0.94754200	0.97986100
C	-2.53325500	0.35291800	-0.10932100
H	-2.52628600	1.18850400	0.90935500
H	-2.52625600	1.04569800	-0.95664500
C	-1.24821600	-0.43870800	0.02296800
H	-1.23851100	-1.22860500	-0.74412300
H	-1.24305300	-0.96260800	0.98765700
C	0.02331300	0.40823700	-0.10998500
H	0.00611600	1.20323100	0.64513500
H	0.01947100	0.91243500	-1.08484200
C	1.31522100	-0.40307500	0.03636900
H	1.32770000	-1.20498800	-0.71341200
H	1.31936400	-0.90186800	1.01416100
C	2.58728400	0.44044300	-0.10526300
H	2.56892800	1.24855900	0.63742100
H	2.58800200	0.93133500	-1.08718900
C	3.88100300	-0.36492700	0.05783000
H	3.89868400	-1.17718000	-0.68081500
H	3.88317300	-0.85103100	1.04226800
C	5.15342500	0.47702400	-0.09030800
H	5.13403600	1.29162100	0.64399800
H	5.15451900	0.95773300	-1.07625200
C	6.44093800	-0.33383400	0.08305900
H	6.50673600	-1.13629400	-0.65871000
H	7.32834000	0.29528700	-0.02972900
H	6.48624700	-0.79682200	1.07397800
H	-2.52122400	1.74727900	1.70051400

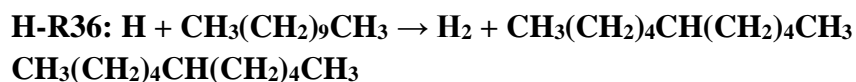


C	6.34317300	-0.62897100	0.18435700
H	6.42894000	-1.15472100	-0.77194900
H	6.24117300	-1.38594000	0.96848000
H	7.28357300	-0.09789700	0.35627500
C	5.14979200	0.33071700	0.18306400
H	5.11193900	0.86708500	1.13918600
H	5.29758200	1.09636600	-0.58848400
C	3.80887500	-0.37185400	-0.05401500
H	3.65686200	-1.13681400	0.71727200
H	3.84472000	-0.90667500	-1.01172700
C	2.60747800	0.58331400	-0.05756700
H	2.78268000	1.36836500	-0.81703400
H	2.56758400	1.12805600	0.89785400
C	1.29487700	-0.08133700	-0.30866700
H	1.28738500	-1.03555900	-0.83035200
C	0.00210600	0.64351300	-0.13221700
H	-0.10967700	1.41057000	-0.92142500
H	0.02511000	1.21508000	0.80767900
C	-1.23673200	-0.26310000	-0.15187500
H	-1.14720700	-1.00781500	0.64818200
H	-1.25286600	-0.82652500	-1.09340600
C	-2.55621800	0.49981700	0.00535000
H	-2.64280200	1.24353900	-0.79760500
H	-2.53583700	1.06858900	0.94416500
C	-3.79330400	-0.40488400	-0.00886600
H	-3.70740800	-1.14847300	0.79429000
H	-3.81528500	-0.97433000	-0.94730800
C	-5.11473600	0.35595400	0.14915000
H	-5.20232300	1.09733100	-0.65455000
H	-5.09241100	0.92594600	1.08606100
C	-6.34456100	-0.55666000	0.13692700
H	-6.30332400	-1.28657700	0.95165100
H	-7.26922200	0.01602600	0.25119800
H	-6.41368400	-1.11468400	-0.80229800



C	-6.38068900	0.41110600	-0.09588200
H	-6.41741500	0.87171200	-1.08825200
H	-6.40593300	1.21799600	0.64328200
H	-7.29139300	-0.18131700	0.02859100
C	-5.12571000	-0.45098400	0.06813000

H	-5.13543100	-0.92495600	1.05716100
H	-5.14792000	-1.27005000	-0.66134500
C	-3.82319900	0.33930600	-0.09800300
H	-3.79690900	1.15333700	0.63657500
H	-3.81414100	0.81857500	-1.08548800
C	-2.56275300	-0.52007200	0.05630400
H	-2.58325700	-1.32907500	-0.69046300
H	-2.57449000	-1.01932400	1.03397100
C	-1.26728600	0.25074200	-0.09555700
H	-1.25894600	1.10518700	0.90752800
H	-1.26784800	0.92810800	-0.95524300
C	0.02137100	-0.53393000	0.04203600
H	0.03845500	-1.32195300	-0.72695900
H	0.02492000	-1.05995900	1.00552100
C	1.28960900	0.31929100	-0.08274700
H	1.27511500	1.09859800	0.68850100
H	1.27818700	0.84323300	-1.04705200
C	2.58454700	-0.49158500	0.03775800
H	2.60247200	-1.26452600	-0.74172800
H	2.58812200	-1.02687200	0.99611600
C	3.85346900	0.36164300	-0.06729500
H	3.83767200	1.13049400	0.71611000
H	3.84907000	0.90263000	-1.02268200
C	5.15081300	-0.44685600	0.04733700
H	5.17052200	-1.21093700	-0.73939900
H	5.15283900	-0.99157500	0.99940200
C	6.41254600	0.41591100	-0.04878200
H	6.43977400	1.16656400	0.74744900
H	7.31907500	-0.18996600	0.03552200
H	6.45638500	0.94762700	-1.00465800
H	-1.25524000	1.67901900	1.68774900



C	6.41107800	-0.18732500	0.16022300
H	6.54848900	-0.82340700	-0.72004400
H	6.45017800	-0.83345200	1.04302000
H	7.26322300	0.49620300	0.21154300
C	5.08461400	0.57504000	0.09087800
H	4.99489600	1.23121500	0.96522600
H	5.08848200	1.23560500	-0.78475200
C	3.85957800	-0.34384800	0.02257900
H	3.85445000	-1.00330800	0.90042400

H	3.95197600	-1.00309200	-0.85069200
C	2.52882500	0.41150400	-0.05234900
H	2.53456300	1.06939000	-0.93060500
H	2.43142500	1.06816600	0.82070300
C	1.30298300	-0.50920300	-0.12573500
H	1.28832300	-1.17349700	0.75184100
H	1.42383300	-1.19212900	-0.98737600
C	0.00000000	0.21120000	-0.23150700
H	0.00000000	1.23539400	-0.59668400
C	-1.30298300	-0.50920300	-0.12573300
H	-1.28832300	-1.17349400	0.75184500
H	-1.42383200	-1.19213100	-0.98737200
C	-2.52882500	0.41150400	-0.05235100
H	-2.53456300	1.06938800	-0.93060900
H	-2.43142500	1.06816900	0.82069900
C	-3.85957800	-0.34384800	0.02257900
H	-3.85445000	-1.00330600	0.90042700
H	-3.95197600	-1.00309400	-0.85068900
C	-5.08461400	0.57504000	0.09087600
H	-5.08848300	1.23560200	-0.78475700
H	-4.99489600	1.23121900	0.96522100
C	-6.41107800	-0.18732500	0.16022500
H	-6.45017700	-0.83344900	1.04302400
H	-7.26322300	0.49620200	0.21154300
H	-6.54848900	-0.82341000	-0.72004000

TS36: $\text{H} + \text{CH}_3(\text{CH}_2)_9\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_4\text{CH}_3$

C	-6.41451400	-0.32769600	0.06247000
H	-6.46764300	-0.77535900	1.05998700
H	-6.48308300	-1.14057200	-0.66761600
H	-7.29656000	0.30632300	-0.06365900
C	-5.12043800	0.47120000	-0.11701600
H	-5.11368100	0.93747200	-1.10983400
H	-5.09783900	1.29605400	0.60551700
C	-3.85519900	-0.37812200	0.04893100
H	-3.87465100	-1.19970700	-0.67940200
H	-3.86620000	-0.85109300	1.03959200
C	-2.55606300	0.41738300	-0.11646200
H	-2.53171300	1.23017000	0.61936900
H	-2.54762500	0.89796300	-1.10317200
C	-1.29225900	-0.43763000	0.03668300
H	-1.30706700	-1.24270700	-0.71437800
H	-1.30420500	-0.94207800	1.01164700

C	-0.00017200	0.34030000	-0.10763100
H	0.00194100	1.18776700	0.90101400
H	-0.00234900	1.02324600	-0.96290500
C	1.29227300	-0.43858200	0.02746200
H	1.31445200	-1.22250500	-0.74553300
H	1.29749800	-0.96948100	0.98825500
C	2.55604300	0.42211600	-0.09173800
H	2.53548900	1.19900600	0.68184100
H	2.54363000	0.94889000	-1.05452800
C	3.85528700	-0.38134800	0.02897800
H	3.87770200	-1.15575600	-0.74913600
H	3.86372200	-0.91510200	0.98830500
C	5.12026300	0.47778500	-0.07939500
H	5.09918700	1.24898600	0.70005700
H	5.11130300	1.01339300	-1.03657700
C	6.41458700	-0.33202300	0.03978900
H	6.48170700	-1.08962200	-0.74759100
H	7.29655100	0.30942600	-0.04135600
H	6.46922600	-0.85100800	1.00205100
H	0.00136700	1.75598700	1.68562300

2.1.12 C12 (*n*-C₁₂H₂₆)



n-C₁₂H₂₆

C	-7.05725600	0.30807300	-0.00000700
H	-7.11424600	0.95278200	-0.88290500
H	-7.11426400	0.95275200	0.88291000
H	-7.94303000	-0.33343800	-0.00002700
C	-5.76696100	-0.51712000	-0.00000900
H	-5.75549700	-1.17688000	0.87623400
H	-5.75549300	-1.17686500	-0.87626100
C	-4.49748800	0.34222000	-0.00000200
H	-4.50973000	1.00298200	0.87680400
H	-4.50972200	1.00298300	-0.87680700
C	-3.20024300	-0.47419500	0.00000300
H	-3.18902200	-1.13474400	-0.87679900
H	-3.18902400	-1.13473600	0.87681200
C	-1.93160900	0.38635000	0.00000100
H	-1.94288800	1.04690600	0.87676500
H	-1.94288300	1.04689300	-0.87677100
C	-0.63428400	-0.43029200	0.00001100
H	-0.62301100	-1.09085200	-0.87676100
H	-0.62301600	-1.09084300	0.87678900

C	0.63428400	0.43029200	0.00001000
H	0.62301400	1.09084900	0.87678400
H	0.62301400	1.09084700	-0.87676600
C	1.93160900	-0.38634900	0.00001000
H	1.94288400	-1.04690100	-0.87675800
H	1.94288600	-1.04689800	0.87677800
C	3.20024300	0.47419500	0.00000600
H	3.18902600	1.13473900	0.87681300
H	3.18902000	1.13474100	-0.87679800
C	4.49748800	-0.34222000	0.00000000
H	4.50972200	-1.00298300	-0.87680600
H	4.50973000	-1.00298300	0.87680600
C	5.76696100	0.51712000	-0.00000600
H	5.75549900	1.17687300	0.87624100
H	5.75549000	1.17687300	-0.87625400
C	7.05725600	-0.30807300	-0.00001300
H	7.11425000	-0.95276700	-0.88292100
H	7.94303000	0.33343800	-0.00001800
H	7.11426000	-0.95276700	0.88289400

CH₂(CH₂)₁₀CH₃

C	-7.10711300	0.29134300	0.00036200
H	-7.14352600	1.28426000	0.43462400
H	-8.04271400	-0.15463100	-0.31503800
C	-5.84225500	-0.49481800	0.00201000
H	-5.80668400	-1.14236300	0.89709800
H	-5.83598800	-1.19161000	-0.84672700
C	-4.56968700	0.36595100	-0.02366500
H	-4.58740700	1.05418100	0.83086300
H	-4.58108300	0.99400200	-0.92242500
C	-3.27659100	-0.45528500	0.01074800
H	-3.26389900	-1.14573300	-0.84262900
H	-3.27082300	-1.08483300	0.91013100
C	-2.00572000	0.40143000	-0.01477800
H	-2.01633100	1.08946300	0.84048200
H	-2.01386900	1.03352400	-0.91216800
C	-0.71107800	-0.41901600	0.01297600
H	-0.70054300	-1.10623100	-0.84299000
H	-0.70319100	-1.05215100	0.90974100
C	0.56006700	0.43740700	-0.01170900
H	0.55056500	1.12335100	0.84529000
H	0.55107400	1.07193800	-0.90747400
C	1.85475200	-0.38304600	0.01264000

H	1.86401400	-1.06899100	-0.84436300
H	1.86387700	-1.01761300	0.90838700
C	3.12609000	0.47313500	-0.01253100
H	3.11709000	1.15900700	0.84456900
H	3.11681200	1.10778400	-0.90825000
C	4.42067600	-0.34711900	0.01123200
H	4.43014300	-1.03398100	-0.84525800
H	4.43155100	-0.98119000	0.90751800
C	5.69284700	0.50783700	-0.01576400
H	5.68397100	1.19428400	0.83969400
H	5.68289300	1.14025300	-0.91193700
C	6.98049400	-0.32099900	0.00913100
H	7.03428000	-0.99385500	-0.85266500
H	7.86821400	0.31737600	-0.01257700
H	7.03668400	-0.93715900	0.91219200

TS37: $\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_{10}\text{CH}_3$

C	6.97328500	0.20806000	-0.15780500
H	7.05767500	1.09884600	0.87498100
H	7.01184400	0.86624400	-1.02648600
H	7.89439000	-0.35893800	-0.02578600
C	5.68962400	-0.56472100	0.02568400
H	5.65456500	-1.37731000	-0.71633300
H	5.69612100	-1.06035000	1.00438100
C	4.42524700	0.29312100	-0.11058300
H	4.43221900	0.78886500	-1.08981800
H	4.45374700	1.09461100	0.63741600
C	3.12635500	-0.50485200	0.04462100
H	3.12574000	-1.00973300	1.01932300
H	3.09871400	-1.30183000	-0.70999100
C	1.86198400	0.35284200	-0.07999600
H	1.87076900	0.87150700	-1.04745900
H	1.88256700	1.13916900	0.68555600
C	0.56105100	-0.44724200	0.05104800
H	0.55611100	-0.97563400	1.01326400
H	0.53663700	-1.22591700	-0.72241700
C	-0.70301300	0.41301700	-0.05875500
H	-0.69079100	0.95338000	-1.01427400
H	-0.68540300	1.18207000	0.72434700
C	-2.00466500	-0.38931800	0.04994700
H	-2.01401200	-0.93706700	1.00126300
H	-2.02547500	-1.15223900	-0.73912400
C	-3.26837800	0.47290600	-0.04844200

H	-3.25474800	1.02753600	-0.99576600
H	-3.25160400	1.23014200	0.74616200
C	-4.57044800	-0.33006900	0.04698600
H	-4.58420600	-0.88777500	0.99264700
H	-4.58956800	-1.08506500	-0.74993800
C	-5.83454800	0.53212000	-0.04712000
H	-5.82045000	1.09014900	-0.99137600
H	-5.81735000	1.28498800	0.75033400
C	-7.13013400	-0.27922400	0.04627200
H	-7.19052600	-0.82002300	0.99613400
H	-8.01158400	0.36415100	-0.02556500
H	-7.19264800	-1.01881000	-0.75840500
H	7.09909700	1.67919300	1.59579700

H-R38: $\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_9\text{CH}_3$

$\text{CH}_3\text{CH}(\text{CH}_2)_9\text{CH}_3$

C	7.13846000	-0.17110000	0.15681900
H	7.46296200	-0.74240400	-0.72988200
H	7.12699800	-0.88577700	0.98934200
H	7.91499700	0.57125800	0.35786400
C	5.80245500	0.45879500	-0.04342900
H	5.75417000	1.48831400	-0.38634700
C	4.55411100	-0.35883300	-0.06668800
H	4.56896000	-1.07516200	0.76866400
H	4.53635100	-0.99134100	-0.97420500
C	3.25879000	0.46318700	-0.01597300
H	3.24859600	1.16700700	-0.85779300
H	3.25913500	1.07511700	0.89412600
C	1.98882500	-0.39326300	-0.05497100
H	2.00188800	-1.09774900	0.78687900
H	1.99383300	-1.00799300	-0.96456700
C	0.69417200	0.42606100	-0.00635500
H	0.67835600	1.12742000	-0.85067700
H	0.69126700	1.04402200	0.90090700
C	-0.57654600	-0.43083000	-0.03758000
H	-0.56079700	-1.13110000	0.80767500
H	-0.57294600	-1.05014900	-0.94400100
C	-1.87188600	0.38759500	0.00942900
H	-1.88860400	1.08680100	-0.83667300
H	-1.87485400	1.00801900	0.91507000
C	-3.14223700	-0.46997100	-0.01916800
H	-3.12520500	-1.16937500	0.82681300
H	-3.13934000	-1.09024900	-0.92496500

C	-4.43789800	0.34754200	0.02840300
H	-4.45575400	1.04780400	-0.81703300
H	-4.44230300	0.96731100	0.93469800
C	-5.70875200	-0.50931400	-0.00138700
H	-5.69113200	-1.20951600	0.84271600
H	-5.70549400	-1.12704300	-0.90781100
C	-6.99769500	0.31637500	0.04839400
H	-7.06044500	1.00317000	-0.80172900
H	-7.88435600	-0.32339600	0.02406000
H	-7.04708700	0.91753000	0.96191700

TS38: $\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_9\text{CH}_3$

C	-7.01075500	-0.32997300	-0.04097700
H	-7.06134100	-0.94483400	0.86288700
H	-7.12820800	-1.00125700	-0.90117500
H	-7.86642900	0.35032500	-0.03526100
C	-5.70131600	0.42370400	-0.12016800
H	-5.67134000	1.15089700	-0.93637900
H	-5.69776900	1.21851400	0.92671600
C	-4.43281200	-0.39692600	-0.00860000
H	-4.43188800	-1.15478700	-0.80770900
H	-4.44895500	-0.96076000	0.93334500
C	-3.14301400	0.42780200	-0.09511100
H	-3.14924900	1.18937300	0.69379400
H	-3.12831100	0.97373900	-1.04712000
C	-1.87016200	-0.41751500	0.02453000
H	-1.87387500	-1.19116600	-0.75442200
H	-1.88068000	-0.95212700	0.98316600
C	-0.57840700	0.40058900	-0.08382100
H	-0.58207300	1.18555200	0.68340400
H	-0.56076800	0.92128400	-1.05009500
C	0.69512400	-0.44019900	0.06102900
H	0.68903900	-1.23918600	-0.69187700
H	0.68620500	-0.94335700	1.03665000
C	1.98767000	0.37214900	-0.07720600
H	1.98567300	1.18422400	0.66150600
H	2.00488700	0.85821500	-1.06136700
C	3.26088500	-0.46368600	0.09617700
H	3.25423500	-1.28794200	-0.62906900
H	3.25178900	-0.93348800	1.08833300
C	4.55397700	0.34221000	-0.06929300
H	4.55657600	1.17522700	0.64608700
H	4.56969400	0.80043800	-1.06693000

C	5.82745200	-0.48907200	0.12283600
H	5.82207700	-1.32635700	-0.58590800
H	5.81628700	-0.93895800	1.12315800
C	7.11423600	0.32148000	-0.05725800
H	7.16685400	1.14620100	0.66074900
H	8.00236700	-0.30027200	0.08660200
H	7.17145000	0.75462800	-1.06098900
H	-5.71351600	1.76249000	1.72907700

H-R39: $\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_8\text{CH}_3$
 $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_8\text{CH}_3$

C	-7.01868000	0.52955400	0.20356000
H	-7.12510300	1.11659800	-0.71368200
H	-6.86946100	1.22911200	1.03088000
H	-7.96173600	0.00316000	0.37320700
C	-5.84525700	-0.45098900	0.09417100
H	-5.78261700	-1.05925000	1.00828400
H	-6.06218500	-1.17916500	-0.70864100
C	-4.52801500	0.20351200	-0.15984400
H	-4.51936600	1.19607200	-0.60449100
C	-3.24748700	-0.56088200	-0.10075100
H	-3.18500000	-1.25560000	-0.95934200
H	-3.24800200	-1.21404500	0.78456200
C	-1.98887200	0.31839300	-0.09030200
H	-2.02889100	0.98963800	0.77597900
H	-1.99630700	0.96392200	-0.97767000
C	-0.68261000	-0.48186100	-0.05670400
H	-0.64698600	-1.15373400	-0.92422600
H	-0.67779600	-1.13032000	0.82913100
C	0.57373900	0.39629600	-0.04589700
H	0.53783800	1.06796100	0.82160900
H	0.56880200	1.04499200	-0.93148400
C	1.88206000	-0.40193000	-0.01227200
H	1.91785700	-1.07397200	-0.87956700
H	1.88742700	-1.05024000	0.87359900
C	3.13798300	0.47697900	-0.00239000
H	3.10221500	1.14883900	0.86507500
H	3.13215800	1.12558500	-0.88808300
C	4.44682900	-0.31999700	0.03061600
H	4.48365700	-0.99223900	-0.83670000
H	4.45408800	-0.96854900	0.91651300
C	5.70307400	0.55854800	0.03995500
H	5.66692300	1.22978600	0.90672200

H	5.69641100	1.20612200	-0.84535000
C	7.00555500	-0.24648400	0.07300100
H	7.08799200	-0.90144100	-0.80025100
H	7.88117300	0.40873000	0.07995800
H	7.05699700	-0.87880000	0.96512300

TS39: $\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_8\text{CH}_3$

C	-6.99606400	0.30766700	-0.13556300
H	-7.02639100	0.74133400	-1.13989300
H	-7.03707500	1.13075300	0.58334700
H	-7.89904000	-0.29471000	-0.00591700
C	-5.73372100	-0.53671300	0.06259000
H	-5.74597800	-0.99612400	1.05859100
H	-5.73896300	-1.37426700	-0.65092900
C	-4.44508900	0.24117000	-0.11173200
H	-4.45348200	1.13513200	0.85716100
H	-4.44871300	0.88460200	-0.99727700
C	-3.14960600	-0.52449200	0.06153300
H	-3.11964900	-1.33804100	-0.68012700
H	-3.14729500	-1.01748700	1.04232400
C	-1.88876400	0.33633900	-0.08425300
H	-1.90771800	1.13142000	0.67066000
H	-1.90693700	0.84009100	-1.05915100
C	-0.58709700	-0.46176000	0.04813000
H	-0.56112300	-1.24250700	-0.72330400
H	-0.58061400	-0.98721300	1.01187600
C	0.67475400	0.40146700	-0.06324000
H	0.65893200	1.16582400	0.72430900
H	0.65744600	0.94719100	-1.01560600
C	1.97803600	-0.39956300	0.03504800
H	2.00131000	-1.15074800	-0.76513600
H	1.98777800	-0.96113000	0.97825900
C	3.23982100	0.46699400	-0.04893400
H	3.22337600	1.20768500	0.76106200
H	3.22307500	1.04090800	-0.98464500
C	4.54351000	-0.33546100	0.02699200
H	4.56450700	-1.07002100	-0.78875300
H	4.55800000	-0.91687000	0.95825900
C	5.80583900	0.53148600	-0.04446400
H	5.78820200	1.26150800	0.77392300
H	5.78953600	1.11591700	-0.97257500
C	7.10298600	-0.27984800	0.02434400
H	7.16626200	-0.99525500	-0.80182800

H	7.98319000	0.36701300	-0.02902500
H	7.16494300	-0.84826500	0.95783700
H	-4.46121000	1.73954000	1.61385400

H-R40: $\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_7\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_7\text{CH}_3$

C	-7.07784600	0.04041900	0.28980800
H	-7.31936100	0.69948000	-0.55030400
H	-7.09192500	0.64807000	1.20027800
H	-7.87947400	-0.69868100	0.37263300
C	-5.71662900	-0.63169700	0.09337100
H	-5.51438100	-1.30822800	0.93131400
H	-5.74334400	-1.25806700	-0.80616800
C	-4.55934500	0.36961500	-0.03054100
H	-4.52676300	1.00611200	0.86667600
H	-4.78614200	1.06803300	-0.85807500
C	-3.22361300	-0.25960900	-0.24773800
H	-3.18472000	-1.25378200	-0.68710100
C	-1.95991800	0.53012800	-0.16319400
H	-1.98935000	1.18015900	0.72400900
H	-1.89607600	1.22921300	-1.01814700
C	-0.68429100	-0.32367700	-0.13298700
H	-0.66369100	-0.96691000	-1.02183900
H	-0.72566100	-0.99790100	0.73093900
C	0.60501400	0.50225400	-0.07519300
H	0.58252800	1.14750600	0.81271500
H	0.64146300	1.17776400	-0.93984700
C	1.87821000	-0.35091000	-0.04674500
H	1.90038900	-0.99623600	-0.93452300
H	1.84153600	-1.02639500	0.81774500
C	3.16988100	0.47267600	0.01092900
H	3.14902400	1.11633500	0.89999600
H	3.20570200	1.14977500	-0.85245200
C	4.44248100	-0.38122300	0.03576100
H	4.46459400	-1.02426000	-0.85389700
H	4.40701400	-1.05951700	0.89839300
C	5.73549700	0.44017100	0.09515300
H	5.71467000	1.08105100	0.98510900
H	5.77144700	1.11852200	-0.76607900
C	7.00065500	-0.42265600	0.11772300
H	7.06891700	-1.04776400	-0.77831600
H	7.90401600	0.19211400	0.16290500
H	7.00902000	-1.08933700	0.98594800

TS40: $\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_7\text{CH}_3$

C	-7.03084000	-0.27306700	0.02980200
H	-7.10513100	-0.69522100	1.03692800
H	-7.10865700	-1.10120400	-0.68201800
H	-7.89697900	0.37684400	-0.12152600
C	-5.71897100	0.49493100	-0.15239500
H	-5.68969400	0.93766400	-1.15526500
H	-5.68340200	1.33283000	0.55284200
C	-4.47591100	-0.38114500	0.04515500
H	-4.50724400	-1.21768500	-0.67048400
H	-4.50606100	-0.84272500	1.04091700
C	-3.16451900	0.35807100	-0.12457200
H	-3.14519000	1.24700300	0.84820900
H	-3.14661300	1.00515500	-1.00716000
C	-1.89311000	-0.44764800	0.04696300
H	-1.88728200	-1.25855000	-0.69814300
H	-1.90732700	-0.94476200	1.02554700
C	-0.60620200	0.37449000	-0.09346700
H	-0.60243100	1.16770600	0.66364600
H	-0.60629900	0.88120200	-1.06700500
C	0.66987200	-0.46378900	0.04020900
H	0.67339300	-1.24342500	-0.73277100
H	0.65752100	-0.99114200	1.00286300
C	1.95828900	0.35984400	-0.06612700
H	1.96261700	1.12514600	0.72065200
H	1.96246600	0.90479600	-1.01906900
C	3.23562100	-0.48114300	0.03958100
H	3.23883800	-1.23484100	-0.75860000
H	3.22366800	-1.04019900	0.98429300
C	4.52416600	0.34498100	-0.04083200
H	4.52592000	1.09162500	0.76405100
H	4.53320100	0.91285000	-0.98048200
C	5.80246700	-0.49625200	0.05090100
H	5.80491000	-1.23741400	-0.75765500
H	5.79093700	-1.06836000	0.98672300
C	7.08405800	0.33927200	-0.01998000
H	7.12773400	1.06625900	0.79725500
H	7.97627200	-0.28956000	0.04754200
H	7.14128400	0.89678600	-0.96032700
H	-3.13597000	1.84795100	1.60760700

**H-R41: $\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_6\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_6\text{CH}_3$**

C	-7.00202100	0.57341400	0.20026600
H	-7.09114400	1.11742800	-0.74545100
H	-6.91456200	1.31542600	1.00026800
H	-7.93533200	0.02533700	0.35675600
C	-5.79482700	-0.36871200	0.18478100
H	-5.75299500	-0.92386300	1.12994800
H	-5.92848500	-1.12057600	-0.60277100
C	-4.46334900	0.35779100	-0.03238100
H	-4.32473400	1.10797800	0.75581600
H	-4.50388200	0.91264400	-0.97842200
C	-3.24845900	-0.57961200	-0.05259600
H	-3.40834400	-1.34956400	-0.83052300
H	-3.20512600	-1.14618700	0.89018700
C	-1.94450500	0.10953100	-0.28195100
H	-1.95002300	1.08982800	-0.75265900
C	-0.64386600	-0.61121000	-0.15303100
H	-0.53463100	-1.33861000	-0.97929300
H	-0.65181200	-1.22760200	0.75841700
C	0.58700800	0.30619100	-0.14214100
H	0.50307700	1.00718800	0.69707500
H	0.58484300	0.91831600	-1.05291800
C	1.91507900	-0.45176400	-0.04447600
H	1.99496900	-1.15178900	-0.88644500
H	1.91434200	-1.06890300	0.86346500
C	3.14408900	0.46418100	-0.03087100
H	3.06623800	1.16110000	0.81372000
H	3.14241500	1.08464500	-0.93650500
C	4.47419800	-0.29205700	0.05991800
H	4.55348800	-0.98827100	-0.78539600
H	4.47700300	-0.91363000	0.96496700
C	5.70346100	0.62368100	0.07455200
H	5.62566600	1.31784300	0.92029200
H	5.70030600	1.24546600	-0.82907400
C	7.02785800	-0.14030100	0.16301400
H	7.15281000	-0.81579500	-0.68930800
H	7.88311100	0.54122300	0.17396600
H	7.07480800	-0.74642600	1.07338000

TS41: $\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_6\text{CH}_3$

C	-7.02371000	0.34240500	-0.11062800
H	-7.06466300	0.77894900	-1.11364700
H	-7.06482400	1.16593900	0.60925900
H	-7.92495200	-0.26191300	0.02500100

C	-5.75533400	-0.49477800	0.07715300
H	-5.76100300	-0.94678900	1.07643300
H	-5.76122600	-1.33015200	-0.63395900
C	-4.46530700	0.31294000	-0.10197600
H	-4.45293400	1.14040000	0.61790700
H	-4.46269200	0.77456900	-1.09786500
C	-3.19166400	-0.52345800	0.06831100
H	-3.19614600	-1.34256700	-0.66762900
H	-3.19875700	-1.00999200	1.05244200
C	-1.90836200	0.26646200	-0.08895900
H	-1.91091300	1.12309100	0.91214800
H	-1.92127800	0.94194100	-0.95004200
C	-0.60774300	-0.49878000	0.04550800
H	-0.57720100	-1.28025100	-0.72974800
H	-0.59735800	-1.03228200	1.00478800
C	0.64738200	0.37491900	-0.07068000
H	0.62600300	1.13988100	0.71458900
H	0.62293900	0.91598100	-1.02525500
C	1.95442600	-0.41941300	0.02721300
H	1.98093000	-1.17325400	-0.77046000
H	1.96925900	-0.97721100	0.97251000
C	3.21035600	0.45504400	-0.06162500
H	3.18937200	1.19887800	0.74522800
H	3.18917500	1.02478000	-0.99977300
C	4.51915200	-0.33875300	0.01687400
H	4.54493700	-1.07626600	-0.79607200
H	4.53767500	-0.91635700	0.95041300
C	5.77554700	0.53648200	-0.05804600
H	5.75275000	1.26962400	0.75738100
H	5.75539800	1.11701600	-0.98851700
C	7.07814500	-0.26572500	0.01424000
H	7.14653800	-0.98405500	-0.80898900
H	7.95385100	0.38697500	-0.04163800
H	7.14386800	-0.82982600	0.95008000
H	-1.91607400	1.69881800	1.69110400

H-R42: $\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_5\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_5\text{CH}_3$

C	-7.04605800	0.04896900	0.27359200
H	-7.22877700	0.77162300	-0.52810200
H	-7.07336400	0.59497100	1.22198500
H	-7.87784600	-0.66105300	0.27582500
C	-5.70314500	-0.66198800	0.08252500

H	-5.56622500	-1.40388200	0.87877800
H	-5.71965600	-1.22642200	-0.85784600
C	-4.50570800	0.29499300	0.07430000
H	-4.48999100	0.86023100	1.01548400
H	-4.64346600	1.03789600	-0.72246300
C	-3.15832600	-0.40874300	-0.11632600
H	-3.17316200	-0.97235800	-1.05779000
H	-3.01660400	-1.14884900	0.68057700
C	-1.96068600	0.55129100	-0.12681900
H	-1.94127200	1.12597700	0.81160800
H	-2.12374600	1.31163000	-0.91356200
C	-0.64117500	-0.11543800	-0.33202800
H	-0.62081600	-1.08937000	-0.81548400
C	0.64500300	0.62281200	-0.16307000
H	0.60902400	1.22035900	0.76023500
H	0.75911000	1.36857500	-0.97209900
C	1.88983600	-0.27540400	-0.14546700
H	1.91826400	-0.86538700	-1.07029100
H	1.79794800	-0.99756500	0.67477500
C	3.20293500	0.50048100	0.00152600
H	3.17127300	1.09439000	0.92431600
H	3.29091200	1.22269900	-0.82069700
C	4.44606000	-0.39574900	0.02135200
H	4.47889700	-0.99048200	-0.90094500
H	4.35916400	-1.11768400	0.84394500
C	5.76123200	0.37810000	0.16815300
H	5.72856400	0.97259200	1.08940000
H	5.84937400	1.09847700	-0.65437500
C	6.99723700	-0.52596000	0.18835800
H	7.07677900	-1.10776600	-0.73547400
H	7.91716000	0.05593100	0.29405500
H	6.95523400	-1.23470900	1.02155400

TS42: $\text{H} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_5\text{CH}_3$

C	-7.05455100	-0.25239700	0.01318500
H	-7.12361100	-0.80141300	0.95768600
H	-7.13228400	-0.98238600	-0.79889400
H	-7.92373400	0.40818300	-0.05051700
C	-5.74446800	0.53588000	-0.07416300
H	-5.72097900	1.10240100	-1.01313500
H	-5.71202300	1.28045100	0.73036200
C	-4.49665000	-0.35059400	0.01070900
H	-4.53049900	-1.09872100	-0.79227500

H	-4.51937800	-0.91495300	0.95212900
C	-3.18189200	0.43142700	-0.07911300
H	-3.15019800	1.18294800	0.71870800
H	-3.15506800	0.98799000	-1.02470200
C	-1.93512600	-0.45651800	0.01790100
H	-1.96982300	-1.21663100	-0.77805200
H	-1.95355100	-1.01535200	0.96255200
C	-0.62774700	0.30130600	-0.09081100
H	-0.61913400	1.12211900	0.93992300
H	-0.60873600	1.00608500	-0.92796000
C	0.64910500	-0.50376600	0.03972300
H	0.65102200	-1.29266800	-0.72842000
H	0.64875000	-1.02918000	1.00365500
C	1.92909400	0.33046900	-0.09204200
H	1.91516800	1.13153300	0.65674400
H	1.93535900	0.82696100	-1.07082400
C	3.21247000	-0.49167400	0.06827000
H	3.21650300	-1.30638600	-0.66777700
H	3.21100200	-0.97384900	1.05439300
C	4.49363700	0.33490100	-0.08760100
H	4.48397800	1.15866700	0.63811500
H	4.50253900	0.80551600	-1.07951600
C	5.77873500	-0.48056100	0.09441000
H	5.78570300	-1.30886300	-0.62479300
H	5.77383900	-0.94286300	1.08907000
C	7.05359000	0.35087300	-0.07495600
H	7.09406000	1.16701700	0.65349100
H	7.95052200	-0.25978500	0.06141600
H	7.10479300	0.79744500	-1.07310600
H	-0.61140600	1.66965400	1.73866000

2.1.13 C13 (*n*-C₁₃H₂₈)



n-C₁₃H₂₈

C	7.69200200	-0.39093400	0.00002100
H	7.73708200	-1.03665200	-0.88285500
H	7.73706300	-1.03654200	0.88297900
H	8.58950700	0.23409600	-0.00000800
C	6.41710900	0.45786700	-0.00005100
H	6.41768000	1.11779400	0.87617100
H	6.41770000	1.11768500	-0.87635500
C	5.13211900	-0.37811100	-0.00001300
H	5.13237300	-1.03897700	0.87682700

H	5.13236700	-1.03904500	-0.87680300
C	3.84985100	0.46163800	-0.00003400
H	3.85045800	1.12224600	-0.87689100
H	3.85047100	1.12231700	0.87676800
C	2.56603700	-0.37612000	0.00001200
H	2.56567800	-1.03678100	0.87679800
H	2.56564600	-1.03682500	-0.87674100
C	1.28326600	0.46318100	0.00001300
H	1.28345800	1.12382200	-0.87679600
H	1.28347000	1.12383900	0.87681000
C	0.00000000	-0.37535500	0.00002900
H	0.00000800	-1.03603700	0.87680900
H	-0.00000800	-1.03604500	-0.87674500
C	-1.28326600	0.46318100	0.00003600
H	-1.28346100	1.12384100	-0.87675900
H	-1.28346700	1.12382000	0.87684800
C	-2.56603700	-0.37612000	0.00002100
H	-2.56566300	-1.03681900	0.87677800
H	-2.56566100	-1.03678700	-0.87676100
C	-3.84985100	0.46163900	0.00003300
H	-3.85045400	1.12231100	-0.87677400
H	-3.85047500	1.12225200	0.87688500
C	-5.13211900	-0.37811100	-0.00001100
H	-5.13238000	-1.03904400	0.87677900
H	-5.13236000	-1.03897800	-0.87685100
C	-6.41710900	0.45786700	0.00000500
H	-6.41767500	1.11777900	-0.87622900
H	-6.41770500	1.11770000	0.87629700
C	-7.69200200	-0.39093400	-0.00005500
H	-7.73708800	-1.03663700	0.88283200
H	-8.58950700	0.23409600	-0.00004300
H	-7.73705700	-1.03655700	-0.88300300

CH₂(CH₂)₁₁CH₃

C	-7.74322800	-0.37133100	0.00186200
H	-7.76295900	-1.36466000	-0.43250900
H	-8.68608500	0.05866700	0.31782800
C	-6.49178700	0.43601000	0.00063800
H	-6.46787100	1.08588400	-0.89313200
H	-6.49654700	1.13116800	0.85075200
C	-5.20477700	-0.40308000	0.02363800
H	-5.21121900	-1.08945700	-0.83253300
H	-5.20499700	-1.03335200	0.92091100

C	-3.92595200	0.44026500	-0.00935000
H	-3.92457600	1.12858300	0.84583100
H	-3.93146800	1.07216800	-0.90707400
C	-2.64054700	-0.39458000	0.01322700
H	-2.63976300	-1.08027000	-0.84397000
H	-2.63746800	-1.02924000	0.90882600
C	-1.36020200	0.44806400	-0.01270900
H	-1.36099600	1.13283600	0.84526800
H	-1.36357300	1.08384700	-0.90761900
C	-0.07458400	-0.38657500	0.00889300
H	-0.07281100	-1.06999500	-0.85016300
H	-0.07239600	-1.02385500	0.90273500
C	1.20596000	0.45582900	-0.01349400
H	1.20412300	1.13907000	0.84572000
H	1.20388400	1.09331400	-0.90721000
C	2.49150000	-0.37894400	0.00825700
H	2.49365000	-1.06179000	-0.85125800
H	2.49313100	-1.01687500	0.90164200
C	3.77231200	0.46313200	-0.01295200
H	3.77002000	1.14630600	0.84634300
H	3.77107900	1.10070000	-0.90664000
C	5.05759400	-0.37165900	0.00965000
H	5.06057700	-1.05558300	-0.84922600
H	5.06008400	-1.00892900	0.90371500
C	6.33936100	0.46899400	-0.01250200
H	6.33690300	1.15252500	0.84533100
H	6.33790300	1.10457300	-0.90648300
C	7.61748300	-0.37448400	0.01146000
H	7.66501400	-1.04478400	-0.85267800
H	8.51244500	0.25380700	-0.00647000
H	7.66511000	-0.99450400	0.91235900

TS43: $\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_{11}\text{CH}_3$

C	7.60883100	0.28730100	-0.16639300
H	7.67815000	1.19629700	0.85145400
H	7.63470700	0.93174100	-1.04579300
H	8.54018000	-0.26070200	-0.02625700
C	6.33961800	-0.50559700	0.03118700
H	6.31890800	-1.33064100	-0.69756700
H	6.35613600	-0.98516800	1.01772500
C	5.05969600	0.32668500	-0.11711800
H	5.05786400	0.80914600	-1.10298300
H	5.07302900	1.13873200	0.61988700

C	3.77555500	-0.49279400	0.04850900
H	3.78627400	-0.98926200	1.02746300
H	3.76030700	-1.29661000	-0.69920100
C	2.49593600	0.34137800	-0.07975500
H	2.49608900	0.85757400	-1.04857400
H	2.50158500	1.13000900	0.68369400
C	1.20947100	-0.48167900	0.05205900
H	1.21639500	-1.01386800	1.01216700
H	1.19649300	-1.25760000	-0.72444100
C	-0.06959200	0.35702700	-0.05052700
H	-0.06623400	0.90733900	-1.00042100
H	-0.06632700	1.11816700	0.74044800
C	-1.35696900	-0.46930500	0.04835900
H	-1.35462500	-1.03227200	0.99080500
H	-1.36639700	-1.21975600	-0.75279000
C	-2.63549400	0.37254300	-0.03329700
H	-2.63124300	0.94702300	-0.96877100
H	-2.63233200	1.11318500	0.77691600
C	-3.92349200	-0.45516400	0.04426100
H	-3.92440300	-1.03676900	0.97536100
H	-3.93046800	-1.18955600	-0.77167100
C	-5.20152300	0.38818000	-0.02499100
H	-5.19933000	0.97425700	-0.95345000
H	-5.19771600	1.11912200	0.79422200
C	-6.49059900	-0.43857200	0.04494400
H	-6.49227000	-1.02561000	0.97154900
H	-6.49670200	-1.16671900	-0.77533200
C	-7.76134900	0.41377800	-0.02096800
H	-7.80600900	0.98561000	-0.95337100
H	-8.66172300	-0.20473400	0.03216800
H	-7.80081700	1.12929200	0.80654900
H	7.70994000	1.78907600	1.56260900

H-R44: $\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_{10}\text{CH}_3$

$\text{CH}_3\text{CH}(\text{CH}_2)_{10}\text{CH}_3$

C	-7.77827000	-0.25149900	-0.15329800
H	-8.09144700	-0.82223100	0.73782500
H	-7.75667700	-0.97137100	-0.98113800
H	-8.56740600	0.47654600	-0.35758100
C	-6.45251400	0.40177000	0.04002400
H	-6.42058400	1.43423200	0.37590800
C	-5.19069500	-0.39485000	0.06586400
H	-5.19321900	-1.11361200	-0.76755500

H	-5.16279100	-1.02454800	0.97506500
C	-3.90939500	0.44871400	0.01338900
H	-3.91112400	1.15438300	0.85370600
H	-3.92000500	1.05861700	-0.89801800
C	-2.62507200	-0.38596400	0.05423600
H	-2.62589000	-1.09207500	-0.78635000
H	-2.61991500	-0.99905400	0.96494100
C	-1.34457200	0.45525100	0.00457400
H	-1.34118100	1.15845300	0.84750000
H	-1.35174000	1.07136700	-0.90392200
C	-0.05937500	-0.37968000	0.03816600
H	-0.06262600	-1.08172300	-0.80575600
H	-0.05296900	-0.99724100	0.94577000
C	1.22182800	0.46067000	-0.00961800
H	1.22600500	1.16174200	0.83510300
H	1.21489200	1.07924600	-0.91651400
C	2.50651700	-0.37513000	0.02159100
H	2.50207100	-1.07615800	-0.82316600
H	2.51328100	-0.99384500	0.92840100
C	3.78836000	0.46429300	-0.02628500
H	3.79299300	1.16559700	0.81827200
H	3.78191200	1.08264300	-0.93337500
C	5.07249000	-0.37199700	0.00524900
H	5.06792500	-1.07472100	-0.83832100
H	5.08065600	-0.98934400	0.91317900
C	6.35547600	0.46557600	-0.04527500
H	6.36061900	1.16828600	0.79690900
H	6.34843800	1.08078700	-0.95339100
C	7.63232700	-0.37951100	-0.01173500
H	7.67166800	-1.07013600	-0.86015600
H	8.52819700	0.24648200	-0.05179300
H	7.68628300	-0.97816700	0.90316900

TS44: $\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_{10}\text{CH}_3$

C	7.64549400	-0.39776900	0.01809300
H	7.75341300	-1.18001200	-0.74407200
H	7.68741300	-0.88665400	0.99626200
H	8.51071800	0.26504000	-0.06566600
C	6.34681300	0.35659200	-0.16359800
H	6.35078500	1.28014600	0.77186100
H	6.32937500	0.97390400	-1.06615900
C	5.06699400	-0.42688700	0.04350400
H	5.07960900	-0.88305300	1.04200900

H	5.05130200	-1.26862100	-0.66683500
C	3.78902400	0.40264200	-0.12858100
H	3.79190800	0.86681900	-1.12309400
H	3.79683000	1.22807600	0.59338400
C	2.50350200	-0.41366800	0.04421100
H	2.51343300	-0.90176200	1.02736100
H	2.48694400	-1.22391800	-0.69650800
C	1.22514900	0.42145400	-0.09026100
H	1.22870900	0.93591500	-1.06001100
H	1.22944600	1.21150800	0.67172300
C	-0.06264200	-0.39990900	0.03915000
H	-0.05473200	-0.93831900	0.99578500
H	-0.07881700	-1.17078300	-0.74230100
C	-1.34035500	0.44191300	-0.05473000
H	-1.33625300	1.00244700	-0.99862900
H	-1.33575400	1.19445900	0.74440300
C	-2.62896500	-0.38350000	0.03540400
H	-2.62532500	-0.96013200	0.96954200
H	-2.64162000	-1.12222200	-0.77651400
C	-3.90639300	0.46142900	-0.03077800
H	-3.90269200	1.05103500	-0.95683100
H	-3.90107400	1.18879500	0.79139000
C	-5.19520000	-0.36561400	0.03504300
H	-5.19668000	-0.96249500	0.95658600
H	-5.20494500	-1.08690300	-0.79265700
C	-6.47329500	0.47919600	-0.01920500
H	-6.46972200	1.07946300	-0.93729100
H	-6.46720200	1.19550200	0.81140000
C	-7.75519900	-0.35689400	0.03826000
H	-7.80439300	-0.94243700	0.96187600
H	-8.64729300	0.27444700	-0.00205500
H	-7.80719500	-1.05892000	-0.80006500
H	6.37426000	1.92475900	1.49603700

H-R45: $\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_9\text{CH}_3$
 $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_9\text{CH}_3$

C	7.64846800	-0.62368200	0.20604900
H	7.74845500	-1.19330600	-0.72283700
H	7.48101000	-1.33745300	1.01759100
H	8.60070000	-0.11964100	0.39157300
C	6.49503900	0.38178000	0.11145200
H	6.43989700	0.97253800	1.03745100
H	6.73007000	1.12161400	-0.67542800

C	5.16639700	-0.24136700	-0.16136900
H	5.14033600	-1.22486300	-0.62509400
C	3.90089700	0.54691900	-0.09337500
H	3.85310200	1.25445300	-0.94238500
H	3.91270100	1.18753500	0.80093800
C	2.62537300	-0.30780200	-0.09681800
H	2.65056400	-0.99098300	0.76062500
H	2.62219300	-0.94169900	-0.99257800
C	1.33483300	0.51720600	-0.05510800
H	1.31388700	1.20075000	-0.91392600
H	1.34084500	1.15415300	0.83904200
C	0.06168000	-0.33649900	-0.05776800
H	0.08315600	-1.02011500	0.80081500
H	0.05564300	-0.97341900	-0.95186300
C	-1.23107900	0.48629100	-0.01545300
H	-1.25233100	1.17062800	-0.87355600
H	-1.22571200	1.12245300	0.87920000
C	-2.50358000	-0.36847200	-0.01968500
H	-2.48184500	-1.05325100	0.83803300
H	-2.50877600	-1.00430600	-0.91456700
C	-3.79720700	0.45294000	0.02327800
H	-3.81864500	1.13864300	-0.83375900
H	-3.79291300	1.08771300	0.91895600
C	-5.06898700	-0.40254400	0.01703900
H	-5.04774500	-1.08953200	0.87322900
H	-5.07474600	-1.03654700	-0.87934600
C	-6.36389900	0.41679200	0.06208700
H	-6.38576900	1.10364000	-0.79284600
H	-6.35927500	1.04880700	0.95860100
C	-7.62813500	-0.44765000	0.05407100
H	-7.65087200	-1.12267300	0.91555500
H	-8.53299200	0.16558200	0.08919800
H	-7.67973300	-1.06418900	-0.84900600

TS45: H + CH₃(CH₂)₁₁CH₃ → H₂ + CH₃CH₂CH(CH₂)₉CH₃

C	-7.62835500	0.38547000	-0.14555600
H	-7.64819100	0.82189700	-1.14895900
H	-7.65894000	1.20739200	0.57519200
H	-8.54122700	-0.20282400	-0.02060000
C	-6.38029600	-0.47932200	0.05509700
H	-6.40342600	-0.94070800	1.04999100
H	-6.39633800	-1.31508800	-0.66035200
C	-5.07875400	0.27822200	-0.11293500

H	-5.07593600	1.16986400	0.85831200
H	-5.06915200	0.92388000	-0.99681200
C	-3.79659300	-0.50906100	0.06225200
H	-3.77832100	-1.32126400	-0.68129300
H	-3.80527200	-1.00443500	1.04180700
C	-2.52091500	0.33049400	-0.07814800
H	-2.52652000	1.12201900	0.68070700
H	-2.52932000	0.83930200	-1.05054500
C	-1.23369000	-0.49126000	0.05109600
H	-1.22090600	-1.26776700	-0.72493300
H	-1.23774200	-1.02248800	1.01168400
C	0.04367900	0.34961900	-0.05390500
H	0.04218300	1.10789800	0.73964900
H	0.03627400	0.90303000	-1.00194900
C	1.33193900	-0.47620100	0.03754600
H	1.34158300	-1.22029400	-0.76952100
H	1.33074800	-1.04655000	0.97553300
C	2.60966400	0.36740900	-0.03794800
H	2.60757900	1.09939900	0.78004700
H	2.60333800	0.95171600	-0.96729500
C	3.89811300	-0.46058700	0.02844500
H	3.90534100	-1.18406900	-0.79718300
H	3.89939600	-1.05454000	0.95171400
C	5.17576800	0.38415200	-0.02954800
H	5.17254700	1.10275000	0.80050100
H	5.17252200	0.98405800	-0.94912500
C	6.46509300	-0.44327500	0.02674100
H	6.47118700	-1.15801000	-0.80525800
H	6.46707500	-1.04531300	0.94367100
C	7.73557100	0.41041200	-0.02546000
H	7.77517900	1.11191500	0.81395300
H	8.63613400	-0.20865500	0.01687400
H	7.77962300	0.99785700	-0.94813100
H	-5.07676800	1.77260200	1.61625900

H-R46: $\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_8\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_8\text{CH}_3$

C	7.71891700	-0.10691700	0.31672000
H	7.96170000	-0.73645400	-0.54538100
H	7.71770000	-0.74864500	1.20363700
H	8.52736100	0.61983800	0.43493800
C	6.36665300	0.58658000	0.13318600
H	6.16424100	1.23501500	0.99299700

H	6.40751300	1.24411700	-0.74325900
C	5.19999500	-0.39739200	-0.03553300
H	5.15200400	-1.06331100	0.83921300
H	5.42764300	-1.06949200	-0.88437500
C	3.87331300	0.25367300	-0.24363900
H	3.84937500	1.25756100	-0.66152000
C	2.59893500	-0.52087700	-0.18160800
H	2.61508200	-1.18871800	0.69259500
H	2.53055300	-1.20195400	-1.05063800
C	1.33457400	0.34906400	-0.14078100
H	1.32581400	1.00833300	-1.01798100
H	1.38153500	1.00708900	0.73528200
C	0.03422600	-0.46050800	-0.10230300
H	0.04507100	-1.12194600	0.77382500
H	-0.00816000	-1.11976700	-0.97916200
C	-1.22761000	0.40891900	-0.06241900
H	-1.23839100	1.07026300	-0.93854500
H	-1.18473100	1.06832500	0.81414600
C	-2.53022900	-0.39829800	-0.02335400
H	-2.52029800	-1.05873200	0.85346900
H	-2.57265700	-1.05859400	-0.89934300
C	-3.79155700	0.47208800	0.01440400
H	-3.80079400	1.13307000	-0.86205400
H	-3.74939200	1.13194700	0.89076400
C	-5.09475100	-0.33386300	0.05219500
H	-5.08685500	-0.99501300	0.92871900
H	-5.13802500	-0.99390700	-0.82415700
C	-6.35645400	0.53606800	0.08973800
H	-6.36474100	1.19675200	-0.78580300
H	-6.31415200	1.19459500	0.96594400
C	-7.65316900	-0.27804900	0.12649300
H	-7.68885600	-0.92503100	1.00882200
H	-8.53285100	0.37109100	0.15541900
H	-7.74275100	-0.91935500	-0.75613600

TS46: $\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_8\text{CH}_3$

C	-7.66388800	-0.34659900	0.03492900
H	-7.73070800	-0.76124100	1.04569200
H	-7.72938600	-1.18190000	-0.66972700
H	-8.54025400	0.28832400	-0.12108800
C	-6.36444300	0.44038900	-0.15498800
H	-6.34263600	0.87444700	-1.16182600
H	-6.34212000	1.28517800	0.54258900

C	-5.10749400	-0.41380000	0.04977200
H	-5.12458100	-1.25604000	-0.65965700
H	-5.13081500	-0.86853400	1.04887300
C	-3.80817800	0.34547700	-0.12429600
H	-3.80167500	1.23729400	0.84599100
H	-3.80179100	0.99046600	-1.00857200
C	-2.52396100	-0.43977200	0.04678500
H	-2.50390500	-1.24813100	-0.70083500
H	-2.53120500	-0.94003000	1.02382400
C	-1.25042900	0.40374400	-0.08940800
H	-1.25810500	1.19106700	0.67376900
H	-1.26018100	0.91786400	-1.05900500
C	0.03900400	-0.41520600	0.03556000
H	0.05520900	-1.18606100	-0.74600400
H	0.03524200	-0.95331600	0.99231400
C	1.31394700	0.43033300	-0.06144500
H	1.30813600	1.18374700	0.73670400
H	1.30698800	0.98948600	-1.00612000
C	2.60461300	-0.39190000	0.02817600
H	2.61815800	-1.13181800	-0.78265000
H	2.60344700	-0.96704000	0.96322300
C	3.87989900	0.45602100	-0.04065200
H	3.87328700	1.18507200	0.77997500
H	3.87428600	1.04360900	-0.96796800
C	5.17058600	-0.36799800	0.02628500
H	5.18160800	-1.09103200	-0.79988300
H	5.17379400	-0.96288400	0.94911000
C	6.44675600	0.47955500	-0.03027400
H	6.43925700	1.19776100	0.79866700
H	6.44163600	1.07766300	-0.94975900
C	7.73050600	-0.35357500	0.02886300
H	7.78386100	-1.05752000	-0.80777100
H	8.62117700	0.27964700	-0.01321000
H	7.78124100	-0.93675100	0.95389300
H	-3.80147900	1.84066100	1.60359400

H-R47: $\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_7\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_7\text{CH}_3$

C	7.57907700	-0.79398300	0.25312600
H	7.71579800	-1.13645400	-0.77758200
H	7.40248500	-1.67827400	0.87361900
H	8.51973100	-0.34197500	0.57995500
C	6.41566300	0.19644700	0.35762500

H	6.32619200	0.54516400	1.39380400
H	6.63877200	1.08643400	-0.24365800
C	5.07574200	-0.39483400	-0.09234900
H	4.85019700	-1.28450300	0.50833100
H	5.16291400	-0.74128700	-1.13007500
C	3.90247400	0.58952700	0.01111500
H	4.14423300	1.49059100	-0.58352800
H	3.81885300	0.95507700	1.04554200
C	2.59072700	0.02711900	-0.42616300
H	2.59177200	-0.79942800	-1.13333300
C	1.30282100	0.73779500	-0.17265100
H	1.19265100	1.58321800	-0.87761200
H	1.32932400	1.20461200	0.82238200
C	0.05883900	-0.15635800	-0.28803200
H	0.14105700	-0.97621900	0.43552000
H	0.04556400	-0.62492000	-1.28025300
C	-1.25791800	0.59425400	-0.06317900
H	-1.34491300	1.40361000	-0.79976000
H	-1.23342300	1.08106900	0.92055000
C	-2.49711000	-0.30410800	-0.14898900
H	-2.40945300	-1.11036200	0.59072900
H	-2.52125500	-0.79503800	-1.13056000
C	-3.81627600	0.44420700	0.07407700
H	-3.91057700	1.24281200	-0.67321300
H	-3.78683400	0.94502500	1.05056300
C	-5.05344000	-0.45834300	0.00793200
H	-4.96028700	-1.25506700	0.75756800
H	-5.08319400	-0.96234600	-0.96704600
C	-6.37387900	0.28844100	0.22865800
H	-6.47094800	1.07979000	-0.52467300
H	-6.34223500	0.79695600	1.20005600
C	-7.60278400	-0.62382800	0.17124500
H	-7.55245600	-1.40308900	0.93834000
H	-8.52701700	-0.06114900	0.33012600
H	-7.68056700	-1.12226000	-0.80028900

TS47: $\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_7\text{CH}_3$

C	-7.65218600	0.43118300	-0.10349700
H	-7.68581200	0.88468900	-1.09924200
H	-7.67692000	1.24345900	0.62976800
H	-8.56460500	-0.15807700	0.02342300
C	-6.39970600	-0.43283800	0.06911900
H	-6.41299900	-0.90061800	1.06104500

H	-6.42212100	-1.25639700	-0.65529100
C	-5.09481800	0.35316900	-0.09866300
H	-5.06648000	1.16925300	0.63357900
H	-5.08386700	0.82954300	-1.08753300
C	-3.83703400	-0.50957000	0.05837200
H	-3.85806400	-1.31834900	-0.68860500
H	-3.85227600	-1.00912900	1.03585500
C	-2.53914900	0.25788700	-0.09012300
H	-2.52683900	1.10551000	0.91888800
H	-2.53857100	0.94123800	-0.94506000
C	-1.25313300	-0.53247300	0.03927800
H	-1.23725300	-1.30951600	-0.74085500
H	-1.25295500	-1.07215000	0.99517000
C	0.01824700	0.31809300	-0.07125600
H	0.00957800	1.08042800	0.71681800
H	0.00591300	0.86301200	-1.02386200
C	1.31007000	-0.50081400	0.02656400
H	1.32411900	-1.25249100	-0.77347100
H	1.31244400	-1.06179000	0.97010200
C	2.58223900	0.35034400	-0.05670800
H	2.57275400	1.09246300	0.75191300
H	2.57438700	0.92269100	-0.99343200
C	3.87599100	-0.46800900	0.02381300
H	3.89071000	-1.20225100	-0.79217000
H	3.87880900	-1.04953800	0.95493200
C	5.14767900	0.38515800	-0.04166400
H	5.13567900	1.11579600	0.77769000
H	5.14379600	0.97142100	-0.96998800
C	6.44280400	-0.43172100	0.03213700
H	6.45779600	-1.15875200	-0.78903500
H	6.44545200	-1.01990100	0.95800900
C	7.70706000	0.43067000	-0.02761100
H	7.73777300	1.14498100	0.80129100
H	8.61201500	-0.18089300	0.02787000
H	7.75073500	1.00446100	-0.95884900
H	-2.52157600	1.67443200	1.70247400

H-R48: $\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_6\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_6\text{CH}_3$

C	7.69904300	-0.11580500	0.24635700
H	7.86207900	-0.81185900	-0.58267300
H	7.72997100	-0.69563100	1.17434900
H	8.54071400	0.58227000	0.26341300

C	6.36406600	0.61973700	0.09741100
H	6.24765600	1.33511600	0.92071900
H	6.37680800	1.21639600	-0.82290400
C	5.15312600	-0.31976100	0.07126400
H	5.14022400	-0.91669700	0.99270100
H	5.27103100	-1.03669700	-0.75205100
C	3.81397800	0.40888400	-0.07953600
H	3.82759700	1.00576600	-1.00026800
H	3.69090500	1.12174900	0.74488200
C	2.60258800	-0.53281900	-0.11228100
H	2.58388600	-1.14069700	0.80538300
H	2.74613200	-1.26729400	-0.92670800
C	1.29117000	0.15974700	-0.28105700
H	1.28320000	1.16606400	-0.69298100
C	-0.00263400	-0.57650800	-0.17252400
H	0.01553600	-1.22778700	0.71438900
H	-0.10974500	-1.27267700	-1.02547400
C	-1.24108500	0.32893600	-0.11985500
H	-1.24720700	0.97773500	-1.00484600
H	-1.16027700	0.99574100	0.74710300
C	-2.56253200	-0.44348400	-0.04959100
H	-2.55494800	-1.09584400	0.83333000
H	-2.63803900	-1.11044800	-0.91839000
C	-3.79922800	0.46073500	0.00153200
H	-3.80298100	1.11759300	-0.87804400
H	-3.72715100	1.12322700	0.87389400
C	-5.12286300	-0.30984700	0.06096100
H	-5.12065800	-0.96750700	0.94012300
H	-5.19580700	-0.97192400	-0.81191100
C	-6.36006100	0.59386000	0.11165700
H	-6.36128900	1.25249200	-0.76545700
H	-6.28938900	1.25305000	0.98553800
C	-7.67777700	-0.18474300	0.16637300
H	-7.71971800	-0.82945500	1.05008600
H	-8.53901500	0.48814400	0.20557100
H	-7.79626700	-0.82441500	-0.71404200

TS48: $\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_6\text{CH}_3$

C	-7.68604900	-0.31618100	0.06854600
H	-7.74003800	-0.75160400	1.07141600
H	-7.75809800	-1.13753200	-0.65165400
H	-8.56587400	0.31948600	-0.06457800
C	-6.38918600	0.47575100	-0.12139600

H	-6.38202600	0.93119900	-1.11922300
H	-6.36241600	1.30830700	0.59211700
C	-5.12702400	-0.37666400	0.05186300
H	-5.14911900	-1.20386300	-0.67002300
H	-5.14009600	-0.84184000	1.04617900
C	-3.82493600	0.41288100	-0.11880400
H	-3.79558600	1.22759900	0.61471800
H	-3.81654300	0.89065800	-1.10687900
C	-2.56449200	-0.44716800	0.03375900
H	-2.58100400	-1.24982800	-0.71980900
H	-2.57989200	-0.95474000	1.00707900
C	-1.26934700	0.32670000	-0.10522900
H	-1.26205500	1.16297600	0.91298700
H	-1.27032200	1.01932700	-0.95267200
C	0.01992100	-0.45941100	0.01763400
H	0.04204600	-1.22580400	-0.77278600
H	0.01974200	-1.01177400	0.96624300
C	1.28742600	0.39885900	-0.07744600
H	1.27199400	1.15101100	0.72022400
H	1.27572700	0.95581300	-1.02307900
C	2.58307300	-0.41461200	0.01479400
H	2.60330000	-1.15703300	-0.79368800
H	2.58561200	-0.98627400	0.95188200
C	3.85113800	0.44389700	-0.05523800
H	3.83496500	1.17790400	0.76067900
H	3.84363900	1.02544700	-0.98631600
C	5.14866000	-0.36836100	0.02174100
H	5.16918100	-1.09716200	-0.79917000
H	5.15397300	-0.95640500	0.94890500
C	6.41714100	0.49056700	-0.03640700
H	6.39915800	1.21551500	0.78643800
H	6.41053900	1.08087900	-0.96089900
C	7.70834100	-0.32990100	0.03550600
H	7.77216700	-1.04058100	-0.79468500
H	8.59311000	0.31140700	-0.00821900
H	7.76053800	-0.90442400	0.96584300
H	-1.26061700	1.72319000	1.70303200

H-R49: $\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_5\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_5\text{CH}_3$

C	7.54733400	0.84722100	-0.19186900
H	7.66413900	1.11755600	0.86248400
H	7.40147100	1.77418200	-0.75555100

H	8.48806800	0.40058400	-0.52590400
C	6.36986600	-0.11192400	-0.39023800
H	6.29873700	-0.38759300	-1.44953600
H	6.56356400	-1.04477000	0.15338300
C	5.02890300	0.47115100	0.06947600
H	4.83950000	1.40773100	-0.47124000
H	5.09899500	0.74350400	1.13079300
C	3.84130800	-0.47659600	-0.13242400
H	4.02748200	-1.41185700	0.41162300
H	3.77549600	-0.75092800	-1.19344800
C	2.50283300	0.11617200	0.31977700
H	2.31870300	1.05421700	-0.21764000
H	2.56264400	0.38035700	1.38317000
C	1.30716600	-0.82378400	0.10369300
H	1.50687100	-1.77364200	0.63455200
H	1.24636600	-1.10408300	-0.95778000
C	0.00000000	-0.25452700	0.54569800
H	0.00000100	0.44979600	1.37493300
C	-1.30716700	-0.82378800	0.10370100
H	-1.50687300	-1.77363800	0.63457200
H	-1.24636900	-1.10410000	-0.95776900
C	-2.50283200	0.11617200	0.31977600
H	-2.31870200	1.05421100	-0.21765400
H	-2.56264100	0.38037100	1.38316500
C	-3.84130900	-0.47659900	-0.13241700
H	-4.02748300	-1.41185300	0.41164200
H	-3.77549800	-0.75094400	-1.19343800
C	-5.02890200	0.47115200	0.06947400
H	-4.83949800	1.40772500	-0.47125300
H	-5.09899300	0.74351700	1.13078800
C	-6.36986600	-0.11192600	-0.39023400
H	-6.56356600	-1.04476600	0.15339800
H	-6.29873800	-0.38760600	-1.44952900
C	-7.54733300	0.84722400	-0.19187500
H	-7.40146800	1.77417800	-0.75556700
H	-8.48806800	0.40058500	-0.52590500
H	-7.66413700	1.11757000	0.86247500

TS49: $\text{H} + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_5\text{CH}_3$

C	7.67839600	-0.44664500	-0.06006000
H	7.72278300	-0.91952900	-1.04635200
H	7.69944800	-1.24449900	0.68911600
H	8.58771600	0.14819900	0.06360200

C	6.42092400	0.41556200	0.08412800
H	6.42311900	0.90264100	1.06690600
H	6.44732000	1.22514900	-0.65558700
C	5.11949300	-0.37720000	-0.08150100
H	5.09198000	-1.18404300	0.66246900
H	5.11970200	-0.86997000	-1.06263900
C	3.85532600	0.47872300	0.05432300
H	3.87790500	1.27853700	-0.69749300
H	3.86160000	0.97999200	1.03087000
C	2.55585600	-0.32017600	-0.09342900
H	2.52720300	-1.11070600	0.66599800
H	2.55109500	-0.82969800	-1.06550100
C	1.29244100	0.54045300	0.02908500
H	1.31080000	1.32232700	-0.74599100
H	1.30152000	1.07414000	0.98839700
C	0.00012800	-0.24044500	-0.09600800
H	-0.00398900	-1.05975900	0.93603400
H	0.00336600	-0.94679100	-0.93203300
C	-1.29237800	0.54204400	0.01587300
H	-1.31483200	1.30275800	-0.77995800
H	-1.29762900	1.10108000	0.96058900
C	-2.55588500	-0.32227100	-0.07739000
H	-2.53439900	-1.07603000	0.71863400
H	-2.54394300	-0.87713000	-1.02424300
C	-3.85560100	0.48398600	0.02083400
H	-3.87977800	1.23283900	-0.78162300
H	-3.86095600	1.04793400	0.96260500
C	-5.11906400	-0.38031700	-0.05609000
H	-5.09571000	-1.12671700	0.74852800
H	-5.11378200	-0.94789900	-0.99592000
C	-6.42162900	0.42221600	0.03997400
H	-6.44808600	1.16517600	-0.76653200
H	-6.42543200	0.99175300	0.97740200
C	-7.67748300	-0.45154900	-0.03064400
H	-7.69674400	-1.18234300	0.78406500
H	-8.58809700	0.14974300	0.04152900
H	-7.72034400	-1.00714700	-0.97287800
H	-0.00497600	-1.60630400	1.73543800

2.1.14 C14 (*n*-C₁₄H₃₀)



n-C₁₄H₃₀

C	-8.33887800	0.32393900	0.00001500
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H	-8.39288300	0.96900900	-0.88284300
H	-8.39286200	0.96882300	0.88301100
H	-9.22768300	-0.31341800	-0.00004100
C	-7.05242900	-0.50726000	-0.00008800
H	-7.04400100	-1.16717600	0.87610700
H	-7.04402300	-1.16699300	-0.87642100
C	-5.77895700	0.34615700	-0.00001500
H	-5.78815700	1.00692000	0.87686300
H	-5.78814700	1.00706300	-0.87678600
C	-4.48545200	-0.47619200	-0.00007600
H	-4.47722900	-1.13672900	-0.87695600
H	-4.47724400	-1.13687300	0.87669500
C	-3.21291400	0.37858800	0.00000900
H	-3.22126700	1.03916700	0.87682400
H	-3.22121400	1.03925800	-0.87673900
C	-1.91923300	-0.44381300	0.00001100
H	-1.91086400	-1.10440500	-0.87680500
H	-1.91090000	-1.10446300	0.87678400
C	-0.64686400	0.41115500	0.00006600
H	-0.65526900	1.07176800	0.87686700
H	-0.65521400	1.07179100	-0.87671800
C	0.64686400	-0.41115400	0.00009200
H	0.65524000	-1.07180700	-0.87667900
H	0.65524300	-1.07175100	0.87690700
C	1.91923300	0.44381300	0.00006000
H	1.91088200	1.10447000	0.87682700
H	1.91088200	1.10439800	-0.87676200
C	3.21291400	-0.37858800	0.00009200
H	3.22121700	-1.03928400	-0.87663500
H	3.22126400	-1.03914100	0.87692700
C	4.48545200	0.47619200	-0.00001500
H	4.47725800	1.13688200	0.87675100
H	4.47721600	1.13672100	-0.87690100
C	5.77895700	-0.34615700	0.00002800
H	5.78811900	-1.00709100	-0.87672100
H	5.78818500	-1.00689200	0.87692700
C	7.05242900	0.50726000	-0.00011700
H	7.04404100	1.16719100	0.87606800
H	7.04398400	1.16697800	-0.87646000
C	8.33887800	-0.32394000	-0.00005800
H	8.39284600	-0.96901900	-0.88291200
H	9.22768300	0.31341700	-0.00015800
H	8.39289800	-0.96881300	0.88294300

CH₂(CH₂)₁₂CH₃

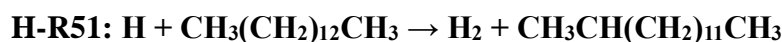
C	-8.38989800	0.30209400	-0.00007700
H	-8.42302000	1.29382800	0.43708800
H	-9.32672600	-0.13989900	-0.31738200
C	-7.12765300	-0.48825700	-0.00042800
H	-7.09461500	-1.13903100	0.89241900
H	-7.12321700	-1.18217300	-0.85156900
C	-5.85215700	0.36831700	-0.02248800
H	-5.86784500	1.05340300	0.83461800
H	-5.86111500	0.99973500	-0.91892300
C	-4.56190000	-0.45748900	0.00923800
H	-4.55138400	-1.14484800	-0.84667100
H	-4.55853700	-1.09034600	0.90631700
C	-3.28802100	0.39485700	-0.01284300
H	-3.29635400	1.07967700	0.84502800
H	-3.29380200	1.03036700	-0.90784300
C	-1.99629800	-0.43028200	0.01196800
H	-1.98805300	-1.11421400	-0.84666100
H	-1.99084800	-1.06691000	0.90628300
C	-0.72205600	0.42164000	-0.00915600
H	-0.72918900	1.10417400	0.85059700
H	-0.72863800	1.05977600	-0.90238400
C	0.56962800	-0.40362300	0.01204600
H	0.57664300	-1.08585800	-0.84796000
H	0.57609700	-1.04213900	0.90502300
C	1.84413800	0.44791500	-0.00892800
H	1.83768800	1.12959200	0.85152200
H	1.83727200	1.08699500	-0.90149500
C	3.13561500	-0.37771000	0.01079500
H	3.14179300	-1.05953800	-0.84953400
H	3.14258600	-1.01666900	0.90344500
C	4.41043400	0.47339500	-0.01073100
H	4.40441300	1.15535800	0.84952400
H	4.40359400	1.11218000	-0.90354000
C	5.70163000	-0.35230000	0.00902600
H	5.70815100	-1.03519900	-0.85066800
H	5.70995600	-0.99058100	0.90235600
C	6.97738400	0.49742800	-0.01410500
H	6.97146300	1.17988700	0.84457900
H	6.97001300	1.13406800	-0.90731500
C	8.26152200	-0.33695100	0.00676100
H	8.31240600	-1.00591000	-0.85824500
H	9.15195600	0.29773800	-0.01193800

H	8.31510200	-0.95766000	0.90686700
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TS50: $\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_{12}\text{CH}_3$

C	8.25325400	0.22478700	-0.17429500
H	8.33979100	1.11527300	0.85855500
H	8.28426300	0.88377400	-1.04267600
H	9.17738700	-0.33855700	-0.04790100
C	6.97382200	-0.55348700	0.01539800
H	6.93735300	-1.36427800	-0.72852900
H	6.98838800	-1.05159500	0.99273400
C	5.70517800	0.29960900	-0.11079700
H	5.70574700	0.80060300	-1.08738100
H	5.73344000	1.09719500	0.64136100
C	4.41047500	-0.50497700	0.04536300
H	4.41682200	-1.01689100	1.01636900
H	4.38259200	-1.29660700	-0.71484900
C	3.14173100	0.34797500	-0.06697700
H	3.14594100	0.87744400	-1.02860300
H	3.16003300	1.12576800	0.70727900
C	1.84509000	-0.46014800	0.05727600
H	1.84514200	-1.00090700	1.01261000
H	1.82284100	-1.22893900	-0.72607400
C	0.57625000	0.39474500	-0.03870300
H	0.58595200	0.95133300	-0.98489600
H	0.58879900	1.15042400	0.75738500
C	-0.72065600	-0.41717300	0.05485100
H	-0.72693200	-0.98269200	0.99575000
H	-0.73642700	-1.16535600	-0.74832800
C	-1.98974500	0.43871500	-0.02811400
H	-1.97688700	1.01483300	-0.96251700
H	-1.98080700	1.17776200	0.78351600
C	-3.28646400	-0.37569700	0.04422200
H	-3.29731800	-0.95699200	0.97541700
H	-3.29723700	-1.11027600	-0.77147500
C	-4.55587500	0.48043600	-0.03125600
H	-4.54182900	1.06677900	-0.95928700
H	-4.54860100	1.21055300	0.78847500
C	-5.85232500	-0.33489500	0.03052800
H	-5.86720800	-0.92264100	0.95780900
H	-5.86083600	-1.06419500	-0.79014300
C	-7.12261200	0.52009000	-0.04378900
H	-7.10772000	1.10748800	-0.97005300
H	-7.11581900	1.24777400	0.77686900

C	-8.41215300	-0.30396500	0.01663500
H	-8.47363100	-0.87436800	0.94895000
H	-9.29838300	0.33428800	-0.04066400
H	-8.46379400	-1.01872300	-0.81089800
H	8.38310700	1.69564500	1.57913100



C	8.42344200	-0.18393100	0.16843400
H	8.74719500	-0.76126900	-0.71461600
H	8.40752200	-0.89412000	1.00472300
H	9.20265700	0.55628300	0.36700100
C	7.09040700	0.45037800	-0.03761700
H	7.04693600	1.47853900	-0.38520700
C	5.83882500	-0.36232700	-0.05960300
H	5.84857300	-1.07404800	0.77976100
H	5.82088900	-0.99982000	-0.96361400
C	4.54673900	0.46520400	-0.01684500
H	4.54133600	1.16408700	-0.86281400
H	4.54746000	1.08251300	0.88962400
C	3.27339500	-0.38630800	-0.05368900
H	3.28189100	-1.08612100	0.79211400
H	3.27778300	-1.00617100	-0.95980100
C	1.98197000	0.43848300	-0.01233000
H	1.97068400	1.13518600	-0.86057600
H	1.97975700	1.06153200	0.89145000
C	0.70784300	-0.41340900	-0.04129000
H	0.71921900	-1.10916200	0.80776500
H	0.71059200	-1.03765700	-0.94432800
C	-0.58426800	0.41046300	-0.00109000
H	-0.59677700	1.10491600	-0.85118800
H	-0.58618400	1.03607700	0.90098900
C	-1.85799000	-0.44213300	-0.02682400
H	-1.84532600	-1.13637400	0.82345700
H	-1.85591200	-1.06803800	-0.92871900
C	-3.15048100	0.38115900	0.01326000
H	-3.16346500	1.07519400	-0.83716800
H	-3.15249000	1.00723900	0.91501600
C	-4.42398600	-0.47182600	-0.01189900
H	-4.41071200	-1.16628100	0.83822400
H	-4.42222400	-1.09748300	-0.91399300
C	-5.71659600	0.35086500	0.02905100
H	-5.73048400	1.04637700	-0.82037800

H	-5.71997000	0.97582100	0.93178900
C	-6.99073500	-0.50118500	0.00220900
H	-6.97716300	-1.19659100	0.85035000
H	-6.98848400	-1.12415000	-0.90063100
C	-8.27649200	0.32984000	0.04516100
H	-8.33516800	1.01192000	-0.80904000
H	-9.16565400	-0.30653700	0.02314300
H	-8.32491300	0.93650200	0.95509100

TS51: $\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_{11}\text{CH}_3$

C	8.29019200	-0.33309900	0.01706000
H	8.40625800	-1.11871600	-0.74041700
H	8.33975000	-0.81529700	0.99818800
H	9.14713900	0.33963900	-0.07240800
C	6.98209100	0.40427300	-0.16700600
H	6.97659300	1.33384600	0.76247800
H	6.95552300	1.01545800	-1.07350700
C	5.71236600	-0.39345200	0.04753800
H	5.73183400	-0.84201100	1.04937600
H	5.70647500	-1.24061100	-0.65650000
C	4.42383100	0.41850200	-0.12924600
H	4.42053900	0.87657900	-1.12658200
H	4.42097000	1.24837100	0.58766600
C	3.14913300	-0.41356800	0.04856400
H	3.16572700	-0.89610700	1.03436200
H	3.14325800	-1.22806900	-0.68766300
C	1.85971900	0.40360600	-0.09015500
H	1.85747300	0.91508400	-1.06148500
H	1.85206800	1.19598100	0.66939500
C	0.58319400	-0.43510400	0.03994500
H	0.59837000	-0.97257700	0.99702200
H	0.57774000	-1.20678300	-0.74085700
C	-0.70592400	0.38903300	-0.05461300
H	-0.70840000	0.95088000	-0.99773400
H	-0.71281200	1.14046900	0.74555000
C	-1.98314000	-0.45424000	0.03269500
H	-1.97121700	-1.03456800	0.96448800
H	-1.98609400	-1.18976000	-0.78222200
C	-3.27184600	0.37365200	-0.02923700
H	-3.27592500	0.96859500	-0.95183300
H	-3.27646900	1.09630000	0.79705500
C	-4.54958100	-0.47119000	0.03161300
H	-4.54031500	-1.07598600	0.94777700

H	-4.55057100	-1.18492300	-0.80248000
C	-5.83786300	0.35813900	-0.01217100
H	-5.84503700	0.96912000	-0.92440700
H	-5.84088400	1.06668100	0.82649900
C	-7.11664200	-0.48587200	0.03803400
H	-7.10823000	-1.09901300	0.94753900
H	-7.11654300	-1.19045500	-0.80259800
C	-8.39776100	0.35254900	0.00020500
H	-8.45199700	0.95072000	-0.91499900
H	-9.29046300	-0.27811700	0.03762100
H	-8.44337200	1.04313500	0.84833500
H	6.99200500	1.98277200	1.48298900

H-R52: $\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_{10}\text{CH}_3$

$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_{10}\text{CH}_3$

C	-8.29678700	0.56802800	0.23020000
H	-8.40532000	1.15308300	-0.68806700
H	-8.13264600	1.26873300	1.05369500
H	-9.24374300	0.05214200	0.41012100
C	-7.13466900	-0.42517400	0.11361200
H	-7.07014900	-1.03105600	1.02910900
H	-7.36652300	-1.15345400	-0.68492400
C	-5.81309400	0.21494800	-0.15413000
H	-5.79845200	1.20338700	-0.60776600
C	-4.53898600	-0.56020300	-0.09650300
H	-4.48639000	-1.26061800	-0.95111500
H	-4.54091500	-1.20784000	0.79282600
C	-3.27286800	0.30836500	-0.09736400
H	-3.30355600	0.98573600	0.76451000
H	-3.27863400	0.94796700	-0.98903200
C	-1.97325600	-0.50264700	-0.06370700
H	-1.94651300	-1.18024000	-0.92707700
H	-1.97048400	-1.14551800	0.82620500
C	-0.70962700	0.36509300	-0.06309100
H	-0.73699100	1.04269800	0.80008700
H	-0.71234500	1.00800300	-0.95290100
C	0.59224900	-0.44356900	-0.02867900
H	0.61977200	-1.12132400	-0.89182100
H	0.59523900	-1.08631300	0.86126500
C	1.85522600	0.42521300	-0.02836200
H	1.82754700	1.10290800	0.83481200
H	1.85180100	1.06814800	-0.91817400
C	3.15780000	-0.38231700	0.00572500

H	3.18534900	-1.06039600	-0.85715700
H	3.16178000	-1.02477500	0.89586900
C	4.42031300	0.48719600	0.00497500
H	4.39271100	1.16535400	0.86782500
H	4.41614300	1.12963200	-0.88522400
C	5.72325100	-0.31937100	0.03892400
H	5.75172700	-0.99820600	-0.82354800
H	5.72896000	-0.96146100	0.92953500
C	6.98617500	0.54960900	0.03708000
H	6.95820600	1.22777900	0.89873200
H	6.98127500	1.19034500	-0.85320600
C	8.28257000	-0.26512100	0.07179700
H	8.35639800	-0.92804800	-0.79619600
H	9.16324900	0.38331100	0.06973400
H	8.33272200	-0.89027700	0.96902400

TS52: $\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_{10}\text{CH}_3$

C	-8.27203600	0.32631700	-0.14615300
H	-8.29719100	0.76088200	-1.15023900
H	-8.31168900	1.14901800	0.57327300
H	-9.17811800	-0.27210600	-0.01989900
C	-7.01414500	-0.52387900	0.05538700
H	-7.03193200	-0.98443400	1.05077900
H	-7.02061600	-1.36055300	-0.65915300
C	-5.72143700	0.24844800	-0.11343200
H	-5.72858200	1.14026600	0.85762100
H	-5.71953700	0.89402000	-0.99742000
C	-4.43011600	-0.52382800	0.06140800
H	-4.40154000	-1.33454800	-0.68341200
H	-4.43346600	-1.02075900	1.04020200
C	-3.16457100	0.33136700	-0.07675700
H	-3.18022400	1.12124900	0.68365200
H	-3.17874100	0.84196700	-1.04815100
C	-1.86749300	-0.47487500	0.05144500
H	-1.84462300	-1.24933500	-0.72639300
H	-1.86559800	-1.00836000	1.01078900
C	-0.60048900	0.38193100	-0.05074500
H	-0.61145100	1.13775800	0.74506200
H	-0.61453500	0.93803400	-0.99714100
C	0.69772600	-0.42838500	0.03833000
H	0.71630800	-1.16996100	-0.77090000
H	0.70355700	-1.00145600	0.97463800
C	1.96521400	0.43074800	-0.03488900

H	1.95534000	1.15927000	0.78614500
H	1.95092400	1.01877500	-0.96181200
C	3.26330700	-0.38238700	0.02640100
H	3.27773400	-1.10216500	-0.80233300
H	3.27277100	-0.98031000	0.94701900
C	4.53120100	0.47745500	-0.02981900
H	4.52151600	1.19031400	0.80492700
H	4.51731600	1.08300700	-0.94542700
C	5.82902900	-0.33670600	0.01665900
H	5.84141100	-1.04636700	-0.82100800
H	5.84223800	-0.94624100	0.92979000
C	7.09784100	0.52222200	-0.03330300
H	7.08780200	1.22894200	0.80544700
H	7.08391200	1.13282700	-0.94444600
C	8.38875700	-0.30080500	0.00915600
H	8.44398100	-0.99350000	-0.83670000
H	9.27393600	0.34033500	-0.02888700
H	8.44869300	-0.89536300	0.92635500
H	-5.73632200	1.74305400	1.61549200

H-R53: $\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_9\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_9\text{CH}_3$

C	-8.36193600	0.01451600	0.33672200
H	-8.61511200	0.68296800	-0.49246300
H	-8.36783000	0.61088800	1.25470900
H	-9.16006900	-0.72837000	0.41944000
C	-7.00074500	-0.65035200	0.11682800
H	-6.78651400	-1.33587400	0.94441500
H	-7.03563900	-1.26627100	-0.78962300
C	-5.84842900	0.35649300	-0.00863000
H	-5.80857400	0.98348200	0.89496700
H	-6.08651400	1.06282000	-0.82620700
C	-4.51286600	-0.26555600	-0.24648300
H	-4.47513000	-1.25506300	-0.69638100
C	-3.25093300	0.52751300	-0.16701800
H	-3.27553200	1.17226900	0.72412200
H	-3.19544200	1.23160500	-1.01844000
C	-1.97265900	-0.32280100	-0.15138500
H	-1.95682500	-0.96070500	-1.04417100
H	-2.00577100	-1.00225400	0.70878200
C	-0.68525600	0.50641900	-0.09814500
H	-0.70341400	1.14695600	0.79327000
H	-0.65654300	1.18653400	-0.95946800

C	0.59035500	-0.34347500	-0.08281000
H	0.60806400	-0.98431400	-0.97394500
H	0.56131100	-1.02339000	0.77849600
C	1.88033800	0.48304000	-0.02990200
H	1.86364300	1.12296800	0.86191900
H	1.90906800	1.16378000	-0.89065100
C	3.15500500	-0.36840600	-0.01677500
H	3.17104200	-1.00844400	-0.90852700
H	3.12610500	-1.04920200	0.84390400
C	4.44611700	0.45640200	0.03562300
H	4.43136300	1.09503600	0.92844000
H	4.47446100	1.13843900	-0.82413900
C	5.71993800	-0.39600800	0.04578500
H	5.73597100	-1.03399200	-0.84764400
H	5.69192800	-1.07922300	0.90480400
C	7.01241400	0.42660600	0.09985800
H	6.99764700	1.06245700	0.99354100
H	7.04095600	1.10982300	-0.75778900
C	8.27871700	-0.43481100	0.10784900
H	8.34071000	-1.05488900	-0.79213900
H	9.18171700	0.18074800	0.14940800
H	8.29455800	-1.10626700	0.97227800

TS53: $\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_9\text{CH}_3$

C	-8.30623600	-0.27956200	0.03309600
H	-8.37921700	-0.69498000	1.04311400
H	-8.38161500	-1.11281000	-0.67299800
H	-9.17432100	0.36669800	-0.12265200
C	-6.99666900	0.49108100	-0.15443300
H	-6.96878500	0.92709800	-1.16028000
H	-6.96362800	1.33386900	0.54510500
C	-5.75101500	-0.37990800	0.04886900
H	-5.77922200	-1.22061200	-0.66201400
H	-5.78036400	-0.83598800	1.04719600
C	-4.44178300	0.36243900	-0.12397800
H	-4.42407800	1.25378300	0.84677800
H	-4.42645500	1.00766300	-1.00797500
C	-3.16819100	-0.43980100	0.04752300
H	-3.15921600	-1.24890800	-0.69952200
H	-3.18211900	-0.93928300	1.02489000
C	-1.88330700	0.38613700	-0.08940900
H	-1.87974500	1.17372500	0.67352900
H	-1.88631600	0.90003900	-1.05916500

C	-0.60527900	-0.45059300	0.03525900
H	-0.59998300	-1.22149500	-0.74640600
H	-0.61639200	-0.98874300	0.99193600
C	0.68129600	0.37710000	-0.06173400
H	0.68635500	1.12995800	0.73695000
H	0.68181200	0.93697300	-1.00600600
C	1.96042800	-0.46311200	0.02686900
H	1.96432300	-1.20132200	-0.78562100
H	1.95062200	-1.04028500	0.96062500
C	3.24723400	0.36740600	-0.03888900
H	3.25008000	1.09399300	0.78390900
H	3.25022500	0.95785000	-0.96436500
C	4.52666600	-0.47453600	0.02644000
H	4.52913000	-1.19275900	-0.80379100
H	4.51855200	-1.07436400	0.94586900
C	5.81330400	0.35708400	-0.02174200
H	5.81446200	1.07072100	0.81258600
H	5.81980000	0.96247200	-0.93770100
C	7.09367500	-0.48414200	0.03439400
H	7.09530500	-1.19412900	-0.80167700
H	7.08602400	-1.09140700	0.94784100
C	8.37320900	0.35645400	-0.00829600
H	8.41700300	1.05277800	0.83521900
H	9.26707300	-0.27225900	0.03387100
H	8.42687100	0.94858000	-0.92745600
H	-4.41616600	1.85686100	1.60440700

H-R54: $\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_8\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_8\text{CH}_3$

C	-8.28146800	0.63886700	0.21595800
H	-8.36947300	1.15580600	-0.74494400
H	-8.17992100	1.40304600	0.99310400
H	-9.22059800	0.10751100	0.39382600
C	-7.08617000	-0.31843800	0.22171300
H	-7.04639500	-0.84674300	1.18223100
H	-7.23315400	-1.09074800	-0.54332000
C	-5.74691100	0.38479800	-0.02251300
H	-5.59463100	1.15471500	0.74384000
H	-5.78578300	0.91367200	-0.98338900
C	-4.54408300	-0.56808500	-0.02324400
H	-4.71742400	-1.35688300	-0.77900400
H	-4.50311600	-1.10956900	0.93443900
C	-3.23254500	0.09759100	-0.27729900

H	-3.22814000	1.07240800	-0.75919500
C	-1.94186200	-0.64168900	-0.15359200
H	-1.85074500	-1.37713700	-0.97487400
H	-1.95104400	-1.25052600	0.76289200
C	-0.69717500	0.25700700	-0.16099000
H	-0.76206000	0.96469400	0.67426700
H	-0.69926300	0.86307900	-1.07581800
C	0.62019000	-0.52044600	-0.07166300
H	0.68103900	-1.22665300	-0.91003900
H	0.61916500	-1.13200200	0.84006600
C	1.86305300	0.37670800	-0.07599200
H	1.80494400	1.07901200	0.76566600
H	1.86101400	0.99246200	-0.98481900
C	3.18242800	-0.39971100	0.00428300
H	3.24043400	-1.10136800	-0.83801200
H	3.18483200	-1.01619100	0.91261300
C	4.42499100	0.49798800	-0.00016300
H	4.36853100	1.19762100	0.84393400
H	4.42051500	1.11673000	-0.90699100
C	5.74504000	-0.27738300	0.07475700
H	5.80268100	-0.97691000	-0.76955500
H	5.75103900	-0.89653800	0.98145900
C	6.98773600	0.62022200	0.07009400
H	6.93114000	1.31835800	0.91422300
H	6.98188600	1.23881300	-0.83572200
C	8.30180900	-0.16291000	0.14413000
H	8.40487200	-0.84423300	-0.70648000
H	9.16717100	0.50582100	0.13998300
H	8.35229200	-0.76536500	1.05674200

TS54: $\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_8\text{CH}_3$

C	-8.29525800	0.36887700	-0.11631700
H	-8.33147400	0.81156000	-1.11682800
H	-8.33284300	1.18838100	0.60834000
H	-9.20045300	-0.23071000	0.01389900
C	-7.03241000	-0.47715900	0.06906700
H	-7.04308700	-0.93537600	1.06547500
H	-7.04178700	-1.30800500	-0.64728700
C	-5.73705800	0.32374700	-0.10208800
H	-5.72063600	1.14584600	0.62381400
H	-5.72986400	0.79253700	-1.09460600
C	-4.46903800	-0.52200000	0.06411500
H	-4.47730800	-1.33524100	-0.67825900

H	-4.48119300	-1.01622900	1.04436100
C	-3.18037500	0.26087300	-0.08441800
H	-3.17897100	1.10913700	0.92403700
H	-3.18745400	0.94369000	-0.93975400
C	-1.88514000	-0.51419800	0.04549300
H	-1.85858900	-1.28877700	-0.73680400
H	-1.88012300	-1.05652400	0.99985700
C	-0.62369300	0.35165200	-0.06058900
H	-0.63990500	1.10822900	0.73287400
H	-0.64353600	0.90312800	-1.00929100
C	0.67730900	-0.45351900	0.02924900
H	0.69885900	-1.19795400	-0.77736700
H	0.68684900	-1.02274300	0.96779000
C	1.94004800	0.41215300	-0.04782400
H	1.92559000	1.14431800	0.76974400
H	1.92292600	0.99564300	-0.97753900
C	3.24240000	-0.39374500	0.01798700
H	3.26184000	-1.11684300	-0.80775700
H	3.25421800	-0.98765900	0.94115000
C	4.50531300	0.47325000	-0.04028100
H	4.49008900	1.18968500	0.79127700
H	4.48925300	1.07465200	-0.95857900
C	5.80785500	-0.33298400	0.01184200
H	5.82616500	-1.04588300	-0.82296600
H	5.82299300	-0.93874500	0.92744600
C	7.07146400	0.53352500	-0.03906700
H	7.05532900	1.24352000	0.79680100
H	7.05564400	1.14036300	-0.95269100
C	8.36736000	-0.28129000	0.00937500
H	8.42875400	-0.97699900	-0.83358100
H	9.24857600	0.36523400	-0.02936700
H	8.42908400	-0.87177200	0.92908300
H	-3.18161800	1.67844300	1.70745800

H-R55: $\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_7\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_7\text{CH}_3$

C	-8.28516700	-0.19681600	0.51687300
H	-8.54355600	0.71990600	-0.02276600
H	-8.25096000	0.04721100	1.58345700
H	-9.09962300	-0.91094300	0.36623400
C	-6.94642000	-0.76400300	0.03585900
H	-6.73210900	-1.69704000	0.57117600
H	-7.02394800	-1.03374000	-1.02452200

C	-5.77363100	0.20504500	0.22424200
H	-5.70049500	0.47938400	1.28491700
H	-5.98617500	1.13721800	-0.31568700
C	-4.42970600	-0.35986400	-0.24631600
H	-4.50259500	-0.63601100	-1.30585700
H	-4.21361800	-1.28780900	0.29693300
C	-3.25478200	0.61082400	-0.06228100
H	-3.18795100	0.91206800	0.99401700
H	-3.48169800	1.54794100	-0.60442600
C	-1.93828100	0.06801900	-0.51005900
H	-1.93150000	-0.73111000	-1.24802700
C	-0.65252700	0.76627200	-0.21468700
H	-0.69545900	1.20848900	0.79082200
H	-0.52498500	1.62779700	-0.89677500
C	0.58907700	-0.13163300	-0.32911400
H	0.61533500	-0.57985200	-1.33044300
H	0.49173300	-0.96571400	0.37601400
C	1.90611800	0.60705000	-0.06896200
H	1.86875700	1.07506200	0.92345400
H	2.00928800	1.42974700	-0.78843200
C	3.14115400	-0.29727300	-0.15257000
H	3.17693500	-0.77059600	-1.14241400
H	3.03766700	-1.11614000	0.57104100
C	4.46151800	0.43835200	0.10327700
H	4.42098500	0.92153600	1.08821500
H	4.57172300	1.24968300	-0.62791800
C	5.69366100	-0.47117900	0.03852200
H	5.73390300	-0.95801700	-0.94477800
H	5.58479000	-1.28040800	0.77246000
C	7.01575500	0.26258600	0.29085300
H	6.97413200	0.75348400	1.27090000
H	7.12819200	1.06680100	-0.44650800
C	8.23925200	-0.65693700	0.23342700
H	8.32761300	-1.13727700	-0.74628600
H	9.16490200	-0.10394000	0.41622200
H	8.17258800	-1.45037600	0.98458700

TS55: $\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_7\text{CH}_3$

C	-8.32617600	-0.24032800	0.07326700
H	-8.38555200	-0.67884300	1.07448200
H	-8.41130000	-1.05765500	-0.65006800
H	-9.19648700	0.40901800	-0.05630300
C	-7.01770100	0.53265800	-0.11520300

H	-7.00540300	0.99290700	-1.11078000
H	-6.97662700	1.36107200	0.60240000
C	-5.76845500	-0.33996900	0.05137600
H	-5.80466100	-1.16321600	-0.67440800
H	-5.78680500	-0.80962500	1.04350500
C	-4.45480500	0.43044800	-0.11814700
H	-4.41231700	1.24221900	0.61795500
H	-4.44026900	0.91120800	-1.10470700
C	-3.20723700	-0.44896200	0.03030300
H	-3.23742400	-1.24987800	-0.72468400
H	-3.22846200	-0.95797400	1.00275400
C	-1.90087200	0.30558200	-0.10983900
H	-1.88045300	1.14246600	0.90786200
H	-1.89226000	0.99763800	-0.95771000
C	-0.62324300	-0.49934200	0.01286900
H	-0.61287200	-1.26668000	-0.77688000
H	-0.63104500	-1.05080800	0.96197300
C	0.65664000	0.34017200	-0.08350300
H	0.65181900	1.09403200	0.71269600
H	0.65337200	0.89540900	-1.03020800
C	1.94046400	-0.49161000	0.01102500
H	1.95130200	-1.23486100	-0.79688000
H	1.93357600	-1.06251200	0.94856800
C	3.22047500	0.34904200	-0.05757500
H	3.21296100	1.08385600	0.75771000
H	3.22272700	0.92993400	-0.98905400
C	4.50672600	-0.48107400	0.02265200
H	4.51951600	-1.20852400	-0.79941600
H	4.49970400	-1.07039600	0.94883500
C	5.78586700	0.36184300	-0.02898700
H	5.77524400	1.08629100	0.79586700
H	5.79220300	0.95518900	-0.95278200
C	7.07373600	-0.46632900	0.04598300
H	7.08728300	-1.18748400	-0.78037000
H	7.06634300	-1.06120100	0.96754300
C	8.34537600	0.38597500	-0.00046300
H	8.37707200	1.09430800	0.83352200
H	9.24493400	-0.23340000	0.05606100
H	8.39921500	0.96576200	-0.92744000
H	-1.87010800	1.70311900	1.69740900

H-R56: $\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_6\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_6\text{CH}_3$

C	8.18605600	-0.86678500	0.25185600
H	8.31307400	-1.13812100	-0.80105900
H	8.03106000	-1.79291000	0.81445900
H	9.12473800	-0.42318400	0.59557200
C	7.00986900	0.09649900	0.43730300
H	6.92834100	0.37272700	1.49570500
H	7.21257800	1.02850300	-0.10445600
C	5.67183000	-0.48195800	-0.03662800
H	5.47384100	-1.41832500	0.50135300
H	5.75196400	-0.75371000	-1.09738700
C	4.48543200	0.46961100	0.15393200
H	4.68137100	1.40562300	-0.38535400
H	4.40832800	0.74136600	1.21486100
C	3.15002100	-0.11666900	-0.31553800
H	2.95716100	-1.05691200	0.21489700
H	3.22034000	-0.37543800	-1.37961700
C	1.95522100	0.82624300	-0.10715300
H	2.16593700	1.77977500	-0.62703300
H	1.88139000	1.09732500	0.95581600
C	0.65176900	0.26671500	-0.57199100
H	0.65907300	-0.42235600	-1.41388300
C	-0.65853600	0.83020000	-0.13190300
H	-0.84086400	1.80117700	-0.62980200
H	-0.61401200	1.07050800	0.94028400
C	-1.85771400	-0.09028600	-0.40343300
H	-1.68988700	-1.05012000	0.09987500
H	-1.90240700	-0.31240800	-1.47715900
C	-3.19858000	0.49579700	0.05036700
H	-3.36750300	1.45422700	-0.45778900
H	-3.14840600	0.72588300	1.12267200
C	-4.39043900	-0.43238600	-0.21011500
H	-4.21526500	-1.39282900	0.29191700
H	-4.44577100	-0.65742000	-1.28318300
C	-5.73303700	0.14158800	0.25553900
H	-5.91321700	1.09989000	-0.24920300
H	-5.67693000	0.37027500	1.32797000
C	-6.92235500	-0.79198900	0.00247000
H	-6.74131700	-1.74971000	0.50564000
H	-6.98102400	-1.01891300	-1.06908700
C	-8.25919200	-0.21334600	0.47507500
H	-8.48662600	0.72719700	-0.03683200
H	-9.08499100	-0.90385900	0.28198100
H	-8.24305600	-0.00766500	1.55015400

TS56: $\text{H} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_6\text{CH}_3$

C	-8.31680500	0.41121500	0.00392300
H	-8.37076400	0.97168100	-0.93484900
H	-8.33498700	1.13735900	0.82281100
H	-9.22258300	-0.19690000	0.07967000
C	-7.05430900	-0.45398600	0.06011900
H	-7.04701900	-1.02885700	0.99426300
H	-7.08155700	-1.19251500	-0.75042200
C	-5.75827600	0.35842900	-0.04101400
H	-5.73400500	1.09987800	0.76815200
H	-5.76441500	0.93199000	-0.97719900
C	-4.48798800	-0.49707100	0.02051500
H	-4.51201500	-1.23971300	-0.78769500
H	-4.48270300	-1.06843700	0.95780100
C	-3.19516000	0.31990500	-0.07987400
H	-3.17366900	1.06643200	0.72294000
H	-3.19442600	0.88359100	-1.02157900
C	-1.92418500	-0.53513200	-0.00379300
H	-1.94466000	-1.28648500	-0.80850000
H	-1.91956700	-1.10531900	0.93424300
C	-0.63913700	0.25988600	-0.11305400
H	-0.64485600	1.06581600	0.92952200
H	-0.64677800	0.97681400	-0.93999700
C	0.66111400	-0.51034500	-0.00487700
H	0.68485000	-1.27923700	-0.79266500
H	0.67869800	-1.05933400	0.94563500
C	1.91509900	0.36542800	-0.11704600
H	1.87914100	1.14416600	0.65413800
H	1.90286200	0.88935200	-1.08138200
C	3.22385000	-0.42064600	0.01693300
H	3.25590000	-1.20765000	-0.74785300
H	3.23660400	-0.93761300	0.98517000
C	4.47715100	0.45364500	-0.10487800
H	4.43524300	1.25084600	0.64853000
H	4.47265400	0.95782000	-1.08004800
C	5.78825500	-0.32349600	0.05629600
H	5.82946200	-1.12634800	-0.69158000
H	5.79612800	-0.82084300	1.03507800
C	7.04128400	0.55003500	-0.07421300
H	6.99574300	1.35794000	0.66626200
H	7.03903600	1.03850000	-1.05634200
C	8.34645300	-0.23100400	0.10398300
H	8.43604200	-1.02805100	-0.64112200

H	9.21948800	0.41941200	0.00022800
H	8.39606700	-0.69766100	1.09296700
H	-0.64798900	1.60219200	1.73570200

2.1.15 C15 (*n*-C₁₅H₃₂)



n-C₁₅H₃₂

C	8.97511000	-0.39797300	0.00000900
H	9.01999200	-1.04376800	-0.88283700
H	9.01997600	-1.04355200	0.88301300
H	9.87283200	0.22677200	-0.00005900
C	7.70047200	0.45122700	-0.00011300
H	7.70125000	1.11121600	0.87607500
H	7.70126600	1.11100100	-0.87646400
C	6.41519900	-0.38433100	-0.00002100
H	6.41524100	-1.04532000	-0.87678200
H	6.41526100	-1.04515600	0.87686300
C	5.13317300	0.45580200	-0.00007600
H	5.13397700	1.11636600	-0.87697800
H	5.13400700	1.11653600	0.87669800
C	3.84908400	-0.38154700	0.00002900
H	3.84853600	-1.04217300	0.87685400
H	3.84847900	-1.04230100	-0.87669900
C	2.56655500	0.45813500	0.00001000
H	2.56694200	1.11875200	-0.87683200
H	2.56697000	1.11883800	0.87678600
C	1.28302300	-0.38000000	0.00007000
H	1.28284500	-1.04066500	0.87687800
H	1.28280600	-1.04073000	-0.87669000
C	0.00000000	0.45890900	0.00006600
H	-0.00000100	1.11956200	-0.87675000
H	0.00000100	1.11957500	0.87687300
C	-1.28302300	-0.38000000	0.00007200
H	-1.28282000	-1.04070300	0.87685200
H	-1.28283100	-1.04069300	-0.87671600
C	-2.56655500	0.45813500	0.00008400
H	-2.56694300	1.11882800	-0.87670100
H	-2.56696900	1.11876300	0.87691700
C	-3.84908400	-0.38154700	0.00003100
H	-3.84851800	-1.04227900	0.87677600
H	-3.84849700	-1.04219600	-0.87677700
C	-5.13317300	0.45580300	0.00005300
H	-5.13396700	1.11651300	-0.87673800

H	-5.13401700	1.11638900	0.87693800
C	-6.41519900	-0.38433100	-0.00004400
H	-6.41527400	-1.04530500	0.87672800
H	-6.41522700	-1.04517100	-0.87691700
C	-7.70047200	0.45122700	-0.00001600
H	-7.70122700	1.11118500	-0.87622800
H	-7.70128800	1.11103200	0.87631100
C	-8.97511000	-0.39797300	-0.00013400
H	-9.02001500	-1.04373700	0.88273200
H	-9.87283200	0.22677200	-0.00011100
H	-9.01995300	-1.04358200	-0.88311800

CH₂(CH₂)₁₃CH₃

C	9.02728400	-0.37307300	-0.00266800
H	9.04805700	-1.36482900	0.43521500
H	9.96950400	0.05667500	-0.32084000
C	7.77523700	0.43329900	-0.00310500
H	7.75115400	1.08564000	0.88887900
H	7.77905000	1.12611700	-0.85515200
C	6.48882700	-0.40683600	-0.02316200
H	6.48914500	-1.03967000	-0.91864100
H	6.49617500	-1.09077500	0.83497200
C	5.20937700	0.43563400	0.00796900
H	5.20716800	1.12156800	-0.84914000
H	5.21477300	1.07005500	0.90392900
C	3.92455500	-0.40018400	-0.01178300
H	3.92446700	-1.08331600	0.84746900
H	3.92170400	-1.03753100	-0.90548700
C	2.64362100	0.44163300	0.01191900
H	2.64370200	1.12374000	-0.84819600
H	2.64683400	1.08022300	0.90484300
C	1.35852800	-0.39389100	-0.00669000
H	1.35726500	-1.07437700	0.85471200
H	1.35665700	-1.03424300	-0.89834900
C	0.07745900	0.44779000	0.01288900
H	0.07873800	1.12789400	-0.84883000
H	0.07934800	1.08856500	0.90426400
C	-1.20764600	-0.38773600	-0.00554400
H	-1.20951800	-1.06705500	0.85679100
H	-1.20883300	-1.02935800	-0.89630700
C	-2.48885500	0.45378200	0.01199000
H	-2.48691200	1.13309700	-0.85035300
H	-2.48786600	1.09539400	0.90276800

C	-3.77380000	-0.38198300	-0.00679300
H	-3.77583100	-1.06119200	0.85562100
H	-3.77457000	-1.02372400	-0.89746400
C	-5.05528000	0.45917400	0.01029400
H	-5.05317600	1.13869800	-0.85190900
H	-5.05488400	1.10055100	0.90126600
C	-6.33992400	-0.37667300	-0.00922700
H	-6.34265000	-1.05701600	0.85250800
H	-6.34164300	-1.01768900	-0.90062800
C	-7.62237100	0.46304500	0.00900600
H	-7.62023300	1.14290700	-0.85175800
H	-7.62164500	1.10245800	0.90026200
C	-8.89982600	-0.38153100	-0.01164300
H	-8.94711300	-1.04805700	0.85543700
H	-9.79530400	0.24612300	0.00322300
H	-8.94667000	-1.00557500	-0.90981400

TS57: $\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_{13}\text{CH}_3$

C	8.89017800	0.29212900	-0.18983600
H	8.97279600	1.17170400	0.85266200
H	8.90889800	0.96147600	-1.05061800
H	9.82127600	-0.26218200	-0.07513900
C	7.62069400	-0.50278600	-0.00248900
H	7.58887500	-1.30419100	-0.75673700
H	7.64671900	-1.01331700	0.96816100
C	6.34173100	0.33735500	-0.11023300
H	6.36394300	1.12359500	0.65394800
H	6.33218000	0.85315600	-1.07903100
C	5.05723600	-0.48480600	0.03875900
H	5.07352100	-1.01137700	1.00177500
H	5.03584800	-1.26498900	-0.73338800
C	3.77789700	0.35434000	-0.05600200
H	3.77259300	0.89906400	-1.00906600
H	3.78901700	1.11980800	0.73054900
C	2.49172300	-0.47173000	0.05896800
H	2.50031400	-1.02595500	1.00651200
H	2.47791000	-1.22953100	-0.73519600
C	1.21192200	0.36812100	-0.02316200
H	1.21282900	0.93755100	-0.96173200
H	1.21606500	1.11302000	0.78309800
C	-0.07422400	-0.46174700	0.06126900
H	-0.07282300	-1.03806100	0.99561300
H	-0.08028800	-1.20081000	-0.75043500

C	-1.35451500	0.37817900	-0.01199500
H	-1.34959500	0.96446900	-0.94012200
H	-1.35511700	1.10847900	0.80756000
C	-2.64031400	-0.45409500	0.05172900
H	-2.64398500	-1.04422700	0.97741300
H	-2.64071900	-1.18105400	-0.77084300
C	-3.92092900	0.38573000	-0.01674800
H	-3.91413900	0.98072700	-0.93929600
H	-3.92389200	1.10832100	0.80961500
C	-5.20654500	-0.44759500	0.03662800
H	-5.21306400	-1.04380500	0.95842300
H	-5.20388600	-1.16911600	-0.79073700
C	-6.48721000	0.39189400	-0.03049700
H	-6.48130400	0.98894500	-0.95192000
H	-6.49143100	1.11308700	0.79731700
C	-7.77351300	-0.44051400	0.02133400
H	-7.78037100	-1.03588200	0.94258400
H	-7.76991600	-1.16127100	-0.80545900
C	-9.04714000	0.40729000	-0.04747600
H	-9.08690600	0.98644700	-0.97557100
H	-9.94539800	-0.21520700	-0.00631000
H	-9.09590000	1.11596000	0.78542600
H	9.01398600	1.74457700	1.57944300

H-R58: $\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_{12}\text{CH}_3$

$\text{CH}_3\text{CH}(\text{CH}_2)_{12}\text{CH}_3$

C	-9.06353900	-0.25490900	-0.16559200
H	-9.37898000	-0.83298700	0.71997900
H	-9.03989300	-0.96792300	-0.99929900
H	-9.85212500	0.47484700	-0.36584600
C	-7.73824200	0.39665800	0.03642700
H	-7.70711400	1.42660700	0.38001900
C	-6.47660200	-0.40030900	0.06018400
H	-6.45027400	-1.03476800	0.96612100
H	-6.47780700	-1.11463900	-0.77701600
C	-5.19510300	0.44336500	0.01433300
H	-5.19822400	1.14471200	0.85826100
H	-5.20405000	1.05796100	-0.89392900
C	-3.91095200	-0.39167100	0.05312100
H	-3.91049500	-1.09358100	-0.79097900
H	-3.90734600	-1.00931400	0.96074900
C	-2.63026700	0.44961000	0.00971800
H	-2.62796000	1.14837500	0.85633200

H	-2.63607800	1.07051100	-0.89552200
C	-1.34524500	-0.38569000	0.04067300
H	-1.34737900	-1.08315700	-0.80704200
H	-1.34026400	-1.00818200	0.94491100
C	-0.06382300	0.45466900	-0.00065200
H	-0.06056100	1.15083700	0.84812400
H	-0.06952000	1.07851200	-0.90394000
C	1.22066400	-0.38155600	0.02727100
H	1.21737500	-1.07724700	-0.82190800
H	1.22586400	-1.00601900	0.93015300
C	2.50273800	0.45785900	-0.01319900
H	2.50645300	1.15329800	0.83617800
H	2.49761100	1.08250900	-0.91594300
C	3.78661100	-0.37933100	0.01419200
H	3.78251500	-1.07503500	-0.83496300
H	3.79169100	-1.00377400	0.91707700
C	5.06932400	0.45912000	-0.02681400
H	5.07336000	1.15544600	0.82186000
H	5.06483100	1.08281600	-0.93025000
C	6.35261300	-0.37856300	0.00173700
H	6.34863200	-1.07640700	-0.84588000
H	6.35885200	-1.00116400	0.90608700
C	7.63647300	0.45805200	-0.04201200
H	7.64094200	1.15596000	0.80416500
H	7.63145500	1.07843600	-0.94661500
C	8.91245700	-0.38844900	-0.01126900
H	8.95254700	-1.07417000	-0.86362400
H	9.80900000	0.23689200	-0.04618700
H	8.96429500	-0.99247500	0.90022100

TS58: $\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_{12}\text{CH}_3$

C	8.92655100	-0.39546100	0.02059500
H	9.03577700	-1.17918800	-0.73986100
H	8.96890500	-0.88218600	0.99982400
H	9.79086000	0.26838800	-0.06436600
C	7.62684300	0.35667600	-0.16303600
H	7.62934000	1.28222800	0.77051400
H	7.60874900	0.97212600	-1.06685600
C	6.34806000	-0.42813700	0.04537300
H	6.33335900	-1.27083900	-0.66385000
H	6.36142700	-0.88295300	1.04448200
C	5.06897000	0.39947300	-0.12758300
H	5.07175100	0.86357700	-1.12212900

H	5.07511100	1.22497300	0.59432400
C	3.78457500	-0.41878900	0.04437500
H	3.79536400	-0.90834700	1.02678900
H	3.76896800	-1.22795600	-0.69754800
C	2.50505000	0.41479600	-0.08851400
H	2.50869100	0.93255800	-1.05650600
H	2.50740200	1.20225600	0.67615200
C	1.21842700	-0.40905000	0.03679500
H	1.22709000	-0.95230100	0.99068500
H	1.20340100	-1.17597200	-0.74855200
C	-0.06051300	0.43138600	-0.05277900
H	-0.05629600	0.99835200	-0.99282800
H	-0.05795300	1.17847400	0.75146300
C	-1.34792200	-0.39665600	0.03024500
H	-1.34342400	-0.98137000	0.95935500
H	-1.35945100	-1.12835500	-0.78803600
C	-2.62656000	0.44695200	-0.02851200
H	-2.62259400	1.04663200	-0.94804800
H	-2.62343500	1.16535300	0.80149000
C	-3.91417100	-0.38311300	0.02650800
H	-3.91329300	-0.99253100	0.93961200
H	-3.92219100	-1.09267100	-0.81107200
C	-5.19285500	0.46145600	-0.01520700
H	-5.18936800	1.07841800	-0.92326600
H	-5.18939900	1.16405100	0.82826400
C	-6.48033700	-0.36927900	0.02509400
H	-6.48315700	-0.99009800	0.93068300
H	-6.48650800	-1.06873100	-0.82118300
C	-7.75987700	0.47432500	-0.01051600
H	-7.75628600	1.09632500	-0.91401700
H	-7.75606000	1.17069000	0.83692100
C	-9.04028400	-0.36525900	0.02540900
H	-9.08969200	-0.97227400	0.93504600
H	-9.93353900	0.26515800	-0.00156200
H	-9.08960900	-1.04765700	-0.82912800
H	7.65031300	1.92794500	1.49372000

H-R59: $\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_{11}\text{CH}_3$
 $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_{11}\text{CH}_3$

C	8.92962100	-0.65025800	0.22916400
H	9.03235400	-1.22229600	-0.69793900
H	8.75319100	-1.36144400	1.04105400
H	9.88334900	-0.15090000	0.41961400

C	7.78212600	0.36115700	0.12531900
H	7.72429800	0.95405200	1.04973600
H	8.02611100	1.09799400	-0.66165200
C	6.45202700	-0.25574300	-0.15446000
H	6.42402100	-1.23768400	-0.62139600
C	5.18930800	0.53724800	-0.08954700
H	5.14725300	1.24678200	-0.93719200
H	5.20019600	1.17583400	0.80621300
C	3.91064300	-0.31275000	-0.09959000
H	3.93050900	-0.99829900	0.75609900
H	3.90815000	-0.94424400	-0.99704800
C	2.62294900	0.51679700	-0.05987300
H	2.60694800	1.20234900	-0.91719100
H	2.62857100	1.15168600	0.83574400
C	1.34684400	-0.33246200	-0.06817900
H	1.36345900	-1.01798200	0.78899100
H	1.34129500	-0.96746100	-0.96364400
C	0.05671100	0.49454800	-0.02793800
H	0.04000000	1.18039400	-0.88493400
H	0.06174100	1.12916900	0.86781400
C	-1.21852400	-0.35610900	-0.03704700
H	-1.20153100	-1.04197600	0.81991600
H	-1.22296600	-0.99089100	-0.93269500
C	-2.50971600	0.46924200	0.00284300
H	-2.52648900	1.15580600	-0.85358000
H	-2.50621800	1.10316600	0.89910300
C	-3.78401700	-0.38280500	-0.00811900
H	-3.76677800	-1.06982700	0.84791500
H	-3.78732100	-1.01636200	-0.90463200
C	-5.07613900	0.44110500	0.03230600
H	-5.09311700	1.12909300	-0.82299300
H	-5.07380600	1.07352600	0.92965900
C	-6.34960900	-0.41179900	0.01922800
H	-6.33268900	-1.10125000	0.87353200
H	-6.35352300	-1.04324800	-0.87897300
C	-7.64304500	0.40997500	0.06212600
H	-7.66053300	1.09940200	-0.79082500
H	-7.64034100	1.03930000	0.96054000
C	-8.90896800	-0.45191200	0.04703800
H	-8.93608100	-1.12949000	0.90638700
H	-9.81273100	0.16300700	0.08082300
H	-8.95859500	-1.06561900	-0.85808000

TS59: $\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2)_{11}\text{CH}_3$

C	-8.90647800	0.39693000	-0.14971300
H	-8.92463300	0.84078700	-1.14988300
H	-8.93712800	1.21352000	0.57705900
H	-9.82008000	-0.19137400	-0.03025000
C	-7.65950200	-0.47055100	0.04609600
H	-7.68465400	-0.93978400	1.03726500
H	-7.67515000	-1.30059400	-0.67598600
C	-6.35704400	0.28718800	-0.11375700
H	-6.34539800	0.93994300	-0.99237600
H	-6.35526100	1.17112300	0.86464700
C	-5.07577700	-0.50243900	0.05732800
H	-5.05628300	-1.30786800	-0.69350800
H	-5.08698700	-1.00663700	1.03234200
C	-3.79922500	0.33751600	-0.07261600
H	-3.80564900	1.12168800	0.69380300
H	-3.80544200	0.85563000	-1.04010500
C	-2.51291100	-0.48653900	0.05099900
H	-2.49996900	-1.25615600	-0.73185200
H	-2.51861900	-1.02624300	1.00684300
C	-1.23455100	0.35390100	-0.04522200
H	-1.23589000	1.10509600	0.75503200
H	-1.24048400	0.91571000	-0.98832800
C	0.05263300	-0.47428200	0.03985400
H	0.06121200	-1.21204300	-0.77301800
H	0.05066400	-1.05198900	0.97332600
C	1.33159800	0.36800300	-0.02921100
H	1.33123300	1.09306200	0.79494500
H	1.32555100	0.96016500	-0.95358700
C	2.61867400	-0.46270100	0.02900300
H	2.62371700	-1.17919500	-0.80269000
H	2.61987700	-1.06448000	0.94716300
C	3.89783700	0.38048400	-0.02330500
H	3.89717000	1.09003600	0.81427700
H	3.89233200	0.98989400	-0.93640100
C	5.18496800	-0.45105800	0.02046900
H	5.18818400	-1.15631700	-0.82080500
H	5.18809600	-1.06513400	0.93047700
C	6.46399800	0.39244600	-0.02334900
H	6.46307800	1.09568200	0.81978300
H	6.46059400	1.00920800	-0.93170600
C	7.75200600	-0.43801100	0.01599700
H	7.75460300	-1.13917800	-0.82749100

H	7.75533200	-1.05487100	0.92301600
C	9.02383200	0.41424700	-0.02575600
H	9.06660400	1.10240600	0.82448800
H	9.92344900	-0.20690000	0.00466900
H	9.06666900	1.01607000	-0.93917200
H	-6.35708200	1.76793400	1.62712400

H-R60: $\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_{10}\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_{10}\text{CH}_3$

C	9.00225400	-0.07298300	0.36525400
H	9.25839600	-0.71613600	-0.48281500
H	8.99564300	-0.69878800	1.26345500
H	9.80466600	0.66112900	0.47909400
C	7.64760700	0.60815000	0.15495300
H	7.43127400	1.26967500	1.00129700
H	7.69399600	1.25103300	-0.73203400
C	6.48935300	-0.38633600	-0.00997900
H	6.73018700	-1.07017300	-0.84568900
H	6.43681200	-1.03864900	0.87470600
C	5.16058500	0.25238800	-0.24167200
H	5.13432700	1.24971700	-0.67487100
C	3.89059900	-0.52943200	-0.18077400
H	3.90460900	-1.18813500	0.70032500
H	3.83235500	-1.21964900	-1.04330100
C	2.62076400	0.33322400	-0.15772500
H	2.61404300	0.98324200	-1.04183600
H	2.65789200	1.00067700	0.71164600
C	1.32497500	-0.48364800	-0.11937800
H	1.33425300	-1.13639200	0.76327600
H	1.29182100	-1.15171500	-0.98993700
C	0.05796300	0.37881600	-0.09567400
H	0.04849000	1.03117700	-0.97853600
H	0.09211600	1.04734800	0.77433300
C	-1.24037600	-0.43522500	-0.05569500
H	-1.23144600	-1.08716500	0.82749300
H	-1.27461900	-1.10412400	-0.92549700
C	-2.50648100	0.42868700	-0.03284700
H	-2.51472600	1.08099900	-0.91577800
H	-2.47219700	1.09736500	0.83711500
C	-3.80571500	-0.38395000	0.00630000
H	-3.79819300	-1.03573600	0.88961400
H	-3.83978800	-1.05305200	-0.86334800
C	-5.07125600	0.48087800	0.02777400

H	-5.07818500	1.13314900	-0.85522500
H	-5.03748600	1.14956500	0.89778600
C	-6.37093900	-0.33072800	0.06564100
H	-6.36539700	-0.98302800	0.94880400
H	-6.40574600	-0.99974000	-0.80425800
C	-7.63688200	0.53358300	0.08663800
H	-7.64298500	1.18506200	-0.79580800
H	-7.60285500	1.20141200	0.95613400
C	-8.92998500	-0.28622300	0.12418400
H	-8.96843000	-0.92339100	1.01351400
H	-9.81290100	0.35897500	0.14003800
H	-9.01072500	-0.93787000	-0.75170000

TS60: $\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_{10}\text{CH}_3$

C	-8.94144600	-0.34408300	0.03677500
H	-9.00839400	-0.75822800	1.04773300
H	-9.00827200	-1.17958700	-0.66751500
H	-9.81706200	0.29189500	-0.11916000
C	-7.64105900	0.44115500	-0.15396300
H	-7.61921700	0.87504700	-1.16087300
H	-7.61720600	1.28599400	0.54350000
C	-6.38516500	-0.41472800	0.05019900
H	-6.40888400	-0.86983900	1.04912100
H	-6.40348100	-1.25666000	-0.65956000
C	-5.08488800	0.34294200	-0.12374100
H	-5.07669900	1.23369200	0.84763500
H	-5.07807700	0.98898800	-1.00724000
C	-3.80172500	-0.44438000	0.04561700
H	-3.78244500	-1.25054500	-0.70439700
H	-3.81000800	-0.94752300	1.02116000
C	-2.52694700	0.39775900	-0.08755100
H	-2.53284600	1.18151700	0.67928700
H	-2.53647000	0.91640300	-1.05473600
C	-1.23882500	-0.42397500	0.03269600
H	-1.22377800	-1.19010500	-0.75351500
H	-1.24361700	-0.96788300	0.98616600
C	0.03757900	0.41997200	-0.05890200
H	0.03378100	1.16728800	0.74496600
H	0.03095600	0.98632300	-0.99928200
C	1.32673800	-0.40540000	0.02340800
H	1.33913200	-1.13769400	-0.79433900
H	1.32417400	-0.98934500	0.95299100
C	2.60363800	0.44069600	-0.03689300

H	2.59911300	1.16045400	0.79188500
H	2.59856200	1.03875600	-0.95746900
C	3.89266000	-0.38707800	0.01967100
H	3.90199500	-1.09810500	-0.81665500
H	3.89265500	-0.99486200	0.93385800
C	5.16997100	0.45948700	-0.02329500
H	5.16484800	1.16408800	0.81847700
H	5.16610400	1.07423200	-0.93285000
C	6.45869100	-0.36919200	0.01988700
H	6.46652800	-1.07066600	-0.82470200
H	6.46179300	-0.98781600	0.92697400
C	7.73698400	0.47624500	-0.01682500
H	7.73135500	1.17484500	0.82875100
H	7.73329000	1.09581900	-0.92198900
C	9.01860600	-0.36133000	0.02253100
H	9.06972000	-1.04601900	-0.83006700
H	9.91093600	0.27035000	-0.00540000
H	9.06813000	-0.96574200	0.93389300
H	-5.07549900	1.83638900	1.60566200

H-R61: $\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_9\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_9\text{CH}_3$

C	-8.85727300	0.85845000	0.30129200
H	-8.99669000	1.19704100	-0.73033500
H	-8.67030900	1.74427300	0.91654000
H	-9.79980500	0.41565800	0.63525600
C	-7.70144500	-0.14090200	0.40451100
H	-7.60889100	-0.48483200	1.44201800
H	-7.93523300	-1.03223900	-0.19068900
C	-6.35919500	0.43659100	-0.05642100
H	-6.44941300	0.77765300	-1.09567200
H	-6.12275600	1.32781500	0.53771900
C	-5.19406600	-0.55737900	0.04617500
H	-5.44848300	-1.46111600	-0.53903700
H	-5.10590100	-0.91520500	1.08294900
C	-3.88043600	-0.01145400	-0.40609600
H	-3.87848900	0.80965500	-1.11947500
C	-2.59908500	-0.73525100	-0.15654000
H	-2.52055900	-1.60711900	-0.83305400
H	-2.61122600	-1.16723300	0.85464900
C	-1.34283400	0.13122800	-0.32992200
H	-1.39711800	0.97979700	0.36263600
H	-1.34045000	0.56083500	-1.33969600

C	-0.03500300	-0.63322700	-0.09994700
H	0.02488500	-1.47120800	-0.80668000
H	-0.05006000	-1.08224200	0.90179300
C	1.21759100	0.23911900	-0.24056200
H	1.15624900	1.07403600	0.46951200
H	1.23334600	0.69246800	-1.24021600
C	2.52757000	-0.52301300	-0.01047200
H	2.60025300	-1.34556200	-0.73380400
H	2.50233500	-0.99313100	0.98126600
C	3.77758500	0.35788700	-0.11803400
H	3.70448600	1.17688300	0.60928900
H	3.80211000	0.83300100	-1.10736400
C	5.08867800	-0.40312000	0.10947900
H	5.17072300	-1.21198100	-0.62817300
H	5.05703700	-0.89149500	1.09218700
C	6.33620800	0.48378100	0.02798000
H	6.25553800	1.28991000	0.76898000
H	6.36789200	0.97647100	-0.95270900
C	7.64868000	-0.27594300	0.25192800
H	7.73455100	-1.07536400	-0.49420400
H	7.61411900	-0.77496500	1.22814300
C	8.88780500	0.62155900	0.18253500
H	8.84934000	1.40764800	0.94332500
H	9.80606500	0.04956100	0.34278000
H	8.96777500	1.11103000	-0.79337000

TS61: $\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_9\text{CH}_3$

C	-8.92595400	0.45415400	-0.09777000
H	-8.95862400	0.91926300	-1.08818100
H	-8.94715000	1.25794300	0.64487600
H	-9.84041500	-0.13323000	0.02300700
C	-7.67645300	-0.41630600	0.06395800
H	-7.69094100	-0.89566900	1.05032500
H	-7.70208800	-1.23115000	-0.67010600
C	-6.36893600	0.36715000	-0.09517300
H	-6.35645400	0.85448100	-1.07867000
H	-6.33777100	1.17485400	0.64614800
C	-5.11398500	-0.50146300	0.05220700
H	-5.13807400	-1.30226300	-0.70320600
H	-5.13050000	-1.01111700	1.02443700
C	-3.81367900	0.26326700	-0.08890900
H	-3.79954600	1.10242100	0.92739100
H	-3.81048400	0.95385800	-0.93799300

C	-2.52995500	-0.53170400	0.03495900
H	-2.51582600	-1.30277400	-0.75110300
H	-2.53172500	-1.07868400	0.98669200
C	-1.25622700	0.31624900	-0.06850900
H	-1.26334000	1.07278900	0.72513800
H	-1.26655700	0.86819000	-1.01709000
C	0.03341400	-0.50672900	0.02392900
H	0.04551000	-1.25304800	-0.78113400
H	0.03425800	-1.07401900	0.96368500
C	1.30778500	0.34166600	-0.05368600
H	1.30079000	1.07771200	0.76049900
H	1.30077200	0.92108300	-0.98607300
C	2.59946700	-0.48060600	0.01954600
H	2.61175100	-1.20830600	-0.80228600
H	2.60144700	-1.06959800	0.94593700
C	3.87321600	0.37026800	-0.04004700
H	3.86400100	1.09210300	0.78688400
H	3.86752500	0.96600100	-0.96211600
C	5.16587600	-0.45146600	0.02178400
H	5.17808600	-1.16905100	-0.80891300
H	5.16916600	-1.05186400	0.94086700
C	6.43890100	0.40073000	-0.02866900
H	6.42824500	1.11699300	0.80334000
H	6.43573800	1.00318100	-0.94657900
C	7.73286400	-0.41919700	0.03053100
H	7.74532200	-1.13364900	-0.80164400
H	7.73602900	-1.02146400	0.94730500
C	8.99839300	0.44203100	-0.01816900
H	9.03104900	1.14437600	0.82083900
H	9.90251300	-0.17158500	0.02755100
H	9.04190100	1.02905100	-0.94113600
H	-3.79295600	1.66490800	1.71541500

H-R62: $\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_8\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_8\text{CH}_3$

C	8.98291700	-0.05342000	0.31948900
H	9.16458700	-0.79009900	-0.46957900
H	9.00462200	-0.58379900	1.27684300
H	9.81813700	0.65253000	0.31263600
C	7.64407600	0.66069700	0.11234800
H	7.50771800	1.41575900	0.89620800
H	7.66663500	1.21000800	-0.83681400
C	6.44218600	-0.29074300	0.11475500

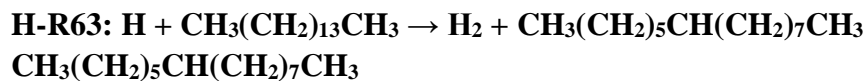
H	6.57922800	-1.04631500	-0.67011700
H	6.42059100	-0.84146800	1.06438300
C	5.09880500	0.41624400	-0.09131000
H	5.12064000	0.96764500	-1.03982100
H	4.95667000	1.16711700	0.69544400
C	3.89722600	-0.53842900	-0.09564700
H	3.87296500	-1.10376100	0.84879500
H	4.05842100	-1.30807600	-0.87341400
C	2.58096100	0.13150800	-0.31129000
H	2.56784900	1.12208300	-0.75965800
C	1.29402600	-0.61552500	-0.19543000
H	1.31324800	-1.24793100	0.70487800
H	1.19887200	-1.33003500	-1.03454500
C	0.04599900	0.27805300	-0.16906800
H	0.03916500	0.90899100	-1.06689500
H	0.11415300	0.96282200	0.68483900
C	-1.26773500	-0.50680500	-0.09191300
H	-1.25830700	-1.14266900	0.80297100
H	-1.33126100	-1.19046500	-0.94859500
C	-2.51418000	0.38492800	-0.06422400
H	-2.51987300	1.02559800	-0.95563600
H	-2.45418400	1.06391600	0.79623600
C	-3.82983900	-0.39910600	0.00177600
H	-3.82476900	-1.04029000	0.89281300
H	-3.88926700	-1.07765700	-0.85916100
C	-5.07631800	0.49274700	0.02837000
H	-5.07856200	1.13714200	-0.86040400
H	-5.01936500	1.16824000	0.89188700
C	-6.39249100	-0.29062000	0.08655100
H	-6.39158900	-0.93589200	0.97486400
H	-6.45059000	-0.96559200	-0.77749700
C	-7.63940500	0.60070700	0.11339500
H	-7.63985100	1.24640500	-0.77329900
H	-7.58309200	1.27329700	0.97804900
C	-8.94940300	-0.19081600	0.16833100
H	-8.99276100	-0.82214100	1.06159000
H	-9.81796400	0.47343200	0.18921300
H	-9.05302100	-0.84531800	-0.70300900

TS62: $\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_8\text{CH}_3$

C	-8.96090100	-0.29861900	0.08057500
H	-9.01326200	-0.74647200	1.07804200
H	-9.03987300	-1.11039100	-0.64968800

H	-9.83799000	0.34311000	-0.04103500
C	-7.66074300	0.48909100	-0.10436300
H	-7.65559400	0.95817600	-1.09586400
H	-7.62627900	1.31153700	0.62042100
C	-6.40229800	-0.37221900	0.05147600
H	-6.41377500	-0.85144500	1.03911700
H	-6.43155400	-1.18885300	-0.68205200
C	-5.09698000	0.41327300	-0.11317000
H	-5.06132000	1.21807300	0.63090300
H	-5.08949900	0.90395400	-1.09490900
C	-3.84005100	-0.45454500	0.02412400
H	-3.86276300	-1.24743600	-0.73953900
H	-3.85460200	-0.97430900	0.99099300
C	-2.54194200	0.31530900	-0.10933700
H	-2.52964000	1.14165800	0.91714500
H	-2.54147600	1.01615400	-0.94999300
C	-1.25549400	-0.47682400	0.00416200
H	-1.23723600	-1.23589800	-0.79337900
H	-1.25641500	-1.03797700	0.94760400
C	0.01491700	0.37783900	-0.08453500
H	0.00198600	1.12390700	0.71887200
H	0.00498900	0.94209100	-1.02585300
C	1.30803300	-0.44034000	0.00151200
H	1.32640600	-1.17627100	-0.81293300
H	1.30844400	-1.01954300	0.93397300
C	2.57849900	0.41516500	-0.06084800
H	2.56368900	1.14262200	0.76091800
H	2.57319900	1.00427700	-0.98715200
C	3.87395200	-0.40128700	0.01052400
H	3.89344700	-1.12157000	-0.81766900
H	3.87492100	-0.99850400	0.93162400
C	5.14372100	0.45637800	-0.03602000
H	5.12640700	1.17235300	0.79590000
H	5.14004900	1.05852200	-0.95396000
C	6.43995800	-0.35915300	0.02713400
H	6.45996700	-1.07286600	-0.80693600
H	6.44339800	-0.96420500	0.94331900
C	7.71001300	0.49842300	-0.01419700
H	7.69135400	1.21023300	0.82007600
H	7.70652800	1.10347000	-0.92913400
C	8.99973700	-0.32521900	0.04756600
H	9.06390500	-1.02319200	-0.79330400
H	9.88572100	0.31512400	0.01538500

H	9.04910400	-0.91408300	0.96905800
H	-2.52475400	1.69412000	1.71242700



C	8.87520200	-0.81168900	0.22327300
H	8.96003800	-1.23965000	-0.78074500
H	8.76434900	-1.64258000	0.92726900
H	9.81929600	-0.30839700	0.44997800
C	7.68902800	0.15280200	0.31559500
H	7.65433900	0.59312400	1.31963000
H	7.84331900	0.98894600	-0.37727000
C	6.34202200	-0.51244800	0.01050900
H	6.37767400	-0.95359500	-0.99431000
H	6.18883900	-1.34999000	0.70352100
C	5.14732800	0.44355300	0.10076400
H	5.30177000	1.28189900	-0.59096900
H	5.11154000	0.88269800	1.10636500
C	3.80344300	-0.22512800	-0.20700800
H	3.64665600	-1.06474800	0.48067900
H	3.83585700	-0.65760700	-1.21505200
C	2.60533000	0.73044400	-0.11150100
H	2.78913100	1.59302700	-0.77943000
H	2.56036700	1.16577200	0.89777100
C	1.29306300	0.10168300	-0.44402000
H	1.28574300	-0.75454000	-1.11478800
C	-0.00287900	0.77999500	-0.14665300
H	-0.13625200	1.64835900	-0.81896000
H	0.03139500	1.21400900	0.86359600
C	-1.23325000	-0.12973400	-0.27476600
H	-1.12741900	-0.97387100	0.41713700
H	-1.25427100	-0.56188700	-1.28326600
C	-2.55859600	0.59012500	-0.00440500
H	-2.66164400	1.43312800	-0.70000100
H	-2.53405800	1.02855500	1.00181800
C	-3.78591100	-0.32007700	-0.12808500
H	-3.68349300	-1.16145000	0.56935400
H	-3.80878500	-0.76084600	-1.13324700
C	-5.11396800	0.39782200	0.13815700
H	-5.21684900	1.23883600	-0.55980100
H	-5.09136000	0.83903300	1.14316700
C	-6.34033000	-0.51345900	0.01468300
H	-6.23848000	-1.35452100	0.71293100

H	-6.36335700	-0.95543800	-0.99014500
C	-7.66976100	0.20242100	0.27960200
H	-7.77212400	1.04238800	-0.41827800
H	-7.64788700	0.64331100	1.28375600
C	-8.88833300	-0.71681800	0.15355100
H	-8.83096100	-1.54855800	0.86289800
H	-9.81914600	-0.17719400	0.34965100
H	-8.95855100	-1.14516400	-0.85143300

TS63: $\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_7\text{CH}_3$

C	8.94715700	-0.48265700	-0.04473000
H	8.99083400	-0.97034400	-1.02381800
H	8.96076400	-1.26942500	0.71621900
H	9.86016400	0.10781400	0.07255700
C	7.69511100	0.38996600	0.08350400
H	7.69819800	0.89147600	1.05899800
H	7.72856400	1.18830100	-0.66803400
C	6.38897500	-0.39679600	-0.07357500
H	6.38754600	-0.90254900	-1.04808500
H	6.35535100	-1.19347400	0.68099400
C	5.12981300	0.46848800	0.04912500
H	5.15887200	1.25917800	-0.71203400
H	5.13700800	0.98116900	1.01972400
C	3.82603700	-0.32455200	-0.09216900
H	3.79251900	-1.10784200	0.67450500
H	3.81924400	-0.84303400	-1.05948100
C	2.56703600	0.54376800	0.02150900
H	2.59088600	1.31968300	-0.75938200
H	2.57720800	1.08453500	0.97683000
C	1.27103100	-0.23152400	-0.10018500
H	1.26228000	-1.04547200	0.93614800
H	1.27158100	-0.94229900	-0.93245600
C	-0.01805500	0.55730700	0.00665400
H	-0.03655600	1.31410200	-0.79300400
H	-0.02166400	1.12106900	0.94856500
C	-1.28505800	-0.30222200	-0.08333600
H	-1.26730300	-1.05195000	0.71659200
H	-1.27439600	-0.86207900	-1.02727000
C	-2.58183000	0.50939000	0.00934500
H	-2.60293900	1.25343900	-0.79762300
H	-2.58572800	1.07902200	0.94767100
C	-3.84805200	-0.35160900	-0.06302500
H	-3.82721700	-1.09165900	0.74728900

H	-3.84197200	-0.92622800	-0.99837300
C	-5.14787300	0.45627200	0.02466900
H	-5.17237700	1.19202800	-0.78970900
H	-5.15120700	1.03579900	0.95702900
C	-6.41264700	-0.40743400	-0.03688800
H	-6.38852900	-1.14275200	0.77800800
H	-6.41012300	-0.98819200	-0.96866700
C	-7.71437200	0.39743700	0.05090400
H	-7.74079200	1.13072500	-0.76440100
H	-7.71661800	0.97829000	0.98138900
C	-8.97130000	-0.47567800	-0.00806800
H	-8.99019000	-1.19733100	0.81480100
H	-9.88127300	0.12725700	0.05859800
H	-9.01600100	-1.04180000	-0.94394000
H	1.25802500	-1.58839500	1.73794900

H-R64: $\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_6\text{CH}(\text{CH}_2)_6\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_6\text{CH}(\text{CH}_2)_6\text{CH}_3$

C	8.93968500	-0.01366500	0.41737600
H	9.11870400	-0.80394400	-0.31862100
H	8.94508800	-0.47884900	1.40828700
H	9.78446300	0.67940000	0.37192100
C	7.61249200	0.70184400	0.14874000
H	7.47730100	1.50788500	0.88026600
H	7.65256600	1.18783100	-0.83382100
C	6.39828900	-0.23270300	0.19915000
H	6.53400500	-1.03958300	-0.53290700
H	6.35905700	-0.71964300	1.18244000
C	5.06509700	0.47470800	-0.06830900
H	5.10480600	0.96071100	-1.05187500
H	4.93105100	1.28198500	0.66331000
C	3.85157500	-0.46048100	-0.01573000
H	3.81275600	-0.94616200	0.96808500
H	3.98509200	-1.26808600	-0.74723200
C	2.51931900	0.24818200	-0.28175500
H	2.55256900	0.72588000	-1.26914500
H	2.38422900	1.05810400	0.44508600
C	1.30410000	-0.68837900	-0.21933700
H	1.26157800	-1.17106300	0.76822600
H	1.46497500	-1.52088700	-0.92995800
C	0.00000000	-0.02101800	-0.50550800
H	0.00000000	0.86487300	-1.13664200
C	-1.30410000	-0.68838000	-0.21934000

H	-1.26157900	-1.17106600	0.76822200
H	-1.46497400	-1.52088600	-0.92996300
C	-2.51931900	0.24818200	-0.28175600
H	-2.55256700	0.72588400	-1.26914400
H	-2.38423000	1.05810100	0.44508700
C	-3.85157500	-0.46048200	-0.01573600
H	-3.81275700	-0.94616900	0.96807600
H	-3.98509300	-1.26808300	-0.74724300
C	-5.06509700	0.47470800	-0.06830900
H	-5.10480500	0.96071800	-1.05187200
H	-4.93105000	1.28198000	0.66331500
C	-6.39828900	-0.23270400	0.19914600
H	-6.35905600	-0.71965300	1.18243200
H	-6.53400700	-1.03957700	-0.53291800
C	-7.61249200	0.70184600	0.14874700
H	-7.65256600	1.18784200	-0.83381000
H	-7.47729900	1.50787900	0.88028000
C	-8.93968500	-0.01366400	0.41737700
H	-8.94508800	-0.47885700	1.40828400
H	-9.78446200	0.67940100	0.37192900
H	-9.11870600	-0.80393700	-0.31862700

TS64: $\text{H} + \text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_6\text{CH}(\text{CH}_2)_6\text{CH}_3$

C	-8.98085000	-0.28299300	0.09901000
H	-9.02598600	-0.80896500	1.05799000
H	-9.06544400	-1.03406900	-0.69292900
H	-9.85869500	0.36612700	0.03537800
C	-7.68156800	0.51694600	-0.03254900
H	-7.68323500	1.06259600	-0.98409900
H	-7.64181200	1.27988600	0.75443500
C	-6.42198400	-0.35338700	0.04642200
H	-6.42348000	-0.90402100	0.99628200
H	-6.45939800	-1.11391300	-0.74458500
C	-5.11709700	0.44129100	-0.07532400
H	-5.08171500	1.20061800	0.71650900
H	-5.11673800	0.99299100	-1.02442300
C	-3.85661900	-0.42755000	0.00418500
H	-3.88670400	-1.18320900	-0.79162100
H	-3.86009600	-0.98322600	0.95082300
C	-2.55488700	0.37388200	-0.10540500
H	-2.52536300	1.12874800	0.68936500
H	-2.54804400	0.92741800	-1.05310200
C	-1.29291800	-0.49349900	-0.02023800

H	-1.31580600	-1.24617200	-0.82359900
H	-1.29925200	-1.06193800	0.91887800
C	-0.00000900	0.28973800	-0.12231500
H	-0.00004100	1.08676300	0.92712600
H	-0.00000300	1.01381300	-0.94303700
C	1.29292900	-0.49345400	-0.02025300
H	1.31610800	-1.24566100	-0.82404400
H	1.29902300	-1.06243300	0.91853600
C	2.55487500	0.37405000	-0.10454200
H	2.52539700	1.12801900	0.69107700
H	2.54795900	0.92865400	-1.05161400
C	3.85662300	-0.42749900	0.00400500
H	3.88681400	-1.18193500	-0.79295700
H	3.86001900	-0.98463000	0.94978900
C	5.11708200	0.44150200	-0.07402900
H	5.08188800	1.19921400	0.71935500
H	5.11651200	0.99513200	-1.02200400
C	6.42199200	-0.35344000	0.04576600
H	6.45930800	-1.11213400	-0.74700400
H	6.42360400	-0.90626900	0.99435000
C	7.68156100	0.51708100	-0.03134300
H	7.64206500	1.27797600	0.75762900
H	7.68294400	1.06519500	-0.98147600
C	8.98087100	-0.28322500	0.09773100
H	9.06526000	-1.03213400	-0.69627700
H	9.85870500	0.36606100	0.03565700
H	9.02623100	-0.81180900	1.05526300
H	-0.00002300	1.61664800	1.73758500

2.1.16 C16 (*n*-C₁₆H₃₄)



n-C₁₆H₃₄

C	-9.62090800	0.33619200	-0.00000600
H	-9.67291100	0.98132900	-0.88292200
H	-9.67291500	0.98132800	0.88291000
H	-10.51166600	-0.29841800	-0.00000900
C	-8.33700800	-0.49893100	-0.00000400
H	-8.33058100	-1.15877000	0.87625200
H	-8.33057900	-1.15877000	-0.87626000
C	-7.06095300	0.35062700	-0.00000300
H	-7.06817000	1.01147600	0.87681100
H	-7.06816700	1.01147500	-0.87681900
C	-5.76992600	-0.47560500	-0.00000100

H	-5.76367800	-1.13622500	-0.87681800
H	-5.76368000	-1.13622300	0.87681800
C	-4.49484600	0.37538400	0.00000000
H	-4.50122300	1.03602300	0.87677100
H	-4.50122000	1.03602000	-0.87677300
C	-3.20360300	-0.45083400	0.00000300
H	-3.19718800	-1.11146900	-0.87678200
H	-3.19719000	-1.11146700	0.87679000
C	-1.92873500	0.40040500	0.00000400
H	-1.93519700	1.06104700	0.87678600
H	-1.93519500	1.06104600	-0.87677800
C	-0.63740500	-0.42565700	0.00000600
H	-0.63092800	-1.08629500	-0.87678000
H	-0.63093000	-1.08629400	0.87679200
C	0.63740500	0.42565700	0.00000600
H	0.63092900	1.08629400	0.87679200
H	0.63092900	1.08629500	-0.87677900
C	1.92873500	-0.40040500	0.00000600
H	1.93519500	-1.06104600	-0.87677600
H	1.93519600	-1.06104600	0.87678800
C	3.20360300	0.45083400	0.00000500
H	3.19719000	1.11146800	0.87679100
H	3.19718800	1.11146900	-0.87678000
C	4.49484600	-0.37538400	0.00000300
H	4.50122000	-1.03602100	-0.87676800
H	4.50122300	-1.03602100	0.87677500
C	5.76992600	0.47560500	0.00000100
H	5.76368100	1.13622400	0.87681900
H	5.76367700	1.13622500	-0.87681700
C	7.06095300	-0.35062700	-0.00000200
H	7.06816600	-1.01147500	-0.87681800
H	7.06817100	-1.01147600	0.87681200
C	8.33700800	0.49893100	-0.00000600
H	8.33058200	1.15876900	0.87625100
H	8.33057700	1.15877000	-0.87626100
C	9.62090800	-0.33619200	-0.00000900
H	9.67291100	-0.98132800	-0.88292600
H	10.51166600	0.29841800	-0.00001200
H	9.67291500	-0.98132900	0.88290600

CH₂(CH₂)₁₄CH₃

C	-9.67282200	0.30986100	-0.00058200
H	-9.70410700	1.30046500	0.43928400

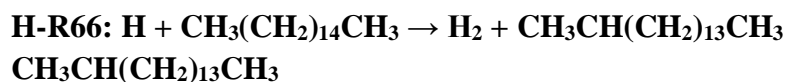
H	-10.61045200	-0.12927500	-0.31949000
C	-8.41223700	-0.48312200	-0.00254200
H	-8.38078700	-1.13611900	0.88873200
H	-8.40904400	-1.17497400	-0.85535900
C	-7.13493800	0.37081800	-0.02222200
H	-7.14936500	1.05384800	0.83654200
H	-7.14235000	1.00443800	-0.91711100
C	-5.84646100	-0.45782000	0.00778100
H	-5.83718900	-1.14305600	-0.84984000
H	-5.84469900	-1.09292800	0.90326700
C	-4.57074300	0.39182800	-0.01181700
H	-4.57778500	1.07445200	0.84781000
H	-4.57494400	1.02965100	-0.90517400
C	-3.28084200	-0.43620200	0.01114600
H	-3.27384900	-1.11783700	-0.84931700
H	-3.27705600	-1.07525700	0.90373300
C	-2.00470600	0.41293900	-0.00729600
H	-2.01048100	1.09302900	0.85439900
H	-2.00969400	1.05364300	-0.89869000
C	-0.71489400	-0.41529400	0.01176500
H	-0.70920400	-1.09496500	-0.85027800
H	-0.71010200	-1.05650700	0.90281400
C	0.56156700	0.43338300	-0.00631900
H	0.55659100	1.11227400	0.85634100
H	0.55624800	1.07538200	-0.89679500
C	1.85114100	-0.39526800	0.01080800
H	1.85592800	-1.07409300	-0.85191100
H	1.85640800	-1.03739000	0.90120200
C	3.12791000	0.45294400	-0.00740200
H	3.12346400	1.13154600	0.85549100
H	3.12255500	1.09525800	-0.89765400
C	4.41718800	-0.37618100	0.00908900
H	4.42133800	-1.05503600	-0.85359900
H	4.42265400	-1.01826400	0.89949900
C	5.69430700	0.47153500	-0.00976200
H	5.69020800	1.15067200	0.85273600
H	5.68912200	1.11328100	-0.90045100
C	6.98324900	-0.35773600	0.00716100
H	6.98785700	-1.03780900	-0.85478000
H	6.98988000	-0.99899100	0.89836600
C	8.26134300	0.48853800	-0.01322000
H	8.25733900	1.16815000	0.84773000
H	8.25569100	1.12817300	-0.90429700

C	9.54315600	-0.34947700	0.00479100
H	9.59218100	-1.01559800	-0.86250500
H	10.43536300	0.28277700	-0.01171200
H	9.59496900	-0.97342800	0.90275300

TS65: $\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_2)_{14}\text{CH}_3$

C	9.53419300	0.23291300	-0.19244200
H	9.62639400	1.10982800	0.85167200
H	9.55955400	0.90355200	-1.05203800
H	10.45946100	-0.33132800	-0.07904400
C	8.25642100	-0.54876800	-0.00571300
H	8.21542700	-1.34847900	-0.76129900
H	8.27757300	-1.06121100	0.96405300
C	6.98647200	0.30527200	-0.11121100
H	6.98141500	0.82198300	-1.07955900
H	7.01810200	1.09055000	0.65361800
C	5.69341100	-0.50316800	0.03859500
H	5.70468200	-1.02976600	1.00167000
H	5.66323400	-1.28318500	-0.73342500
C	4.42292200	0.34941900	-0.05555300
H	4.42245600	0.89341600	-1.00904600
H	4.44287400	1.11533600	0.73038400
C	3.12835700	-0.46314700	0.06125000
H	3.13174100	-1.01605300	1.00959700
H	3.10637600	-1.22195800	-0.73177200
C	1.85703800	0.38944600	-0.02155900
H	1.86321300	0.95740500	-0.96100100
H	1.86895500	1.13547100	0.78357800
C	0.56288900	-0.42768900	0.06457900
H	0.55896900	-1.00244300	0.99987700
H	0.54955400	-1.16805000	-0.74586200
C	-0.70948300	0.42409400	-0.00988400
H	-0.69907000	1.00909700	-0.93878100
H	-0.70347400	1.15540500	0.80874500
C	-2.00270900	-0.39652300	0.05462200
H	-2.01165100	-0.98569600	0.98088300
H	-2.00940200	-1.12431000	-0.76719900
C	-3.27609600	0.45414100	-0.01490100
H	-3.26365100	1.04890200	-0.93755800
H	-3.27368700	1.17684700	0.81137100
C	-4.56840400	-0.36879000	0.03742500
H	-4.58028800	-0.96526700	0.95895900
H	-4.57081200	-1.09006200	-0.79012600

C	-5.84262400	0.48079000	-0.03048900
H	-5.82956800	1.07909600	-0.95086500
H	-5.84201600	1.20033400	0.79857700
C	-7.13423600	-0.34313200	0.01728800
H	-7.14894500	-0.94096400	0.93810100
H	-7.13501800	-1.06357800	-0.81120900
C	-8.40963000	0.50456800	-0.05277100
H	-8.39567500	1.10078900	-0.97339300
H	-8.40991300	1.22449600	0.77473700
C	-9.69406300	-0.32821400	-0.00408700
H	-9.75499300	-0.90722600	0.92294000
H	-10.58419700	0.30481300	-0.05881600
H	-9.73822000	-1.03593300	-0.83807100
H	9.67383300	1.68091400	1.57939900



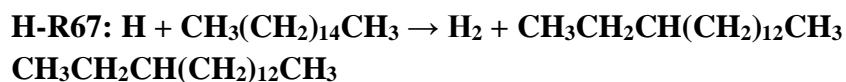
C	9.70781000	-0.19378000	0.17998500
H	10.03190900	-0.77763800	-0.69864000
H	9.68812100	-0.89859000	1.02074200
H	10.48860900	0.54555300	0.37556400
C	8.37697500	0.44284000	-0.03301400
H	8.33708900	1.46914400	-0.38647500
C	7.12329600	-0.36665100	-0.05392500
H	7.12985200	-1.07529400	0.78804600
H	7.10497700	-1.00736500	-0.95565400
C	5.83338500	0.46454400	-0.01619300
H	5.83125600	1.16043700	-0.86463800
H	5.83434500	1.08506300	0.88807400
C	4.55776200	-0.38359000	-0.05207500
H	4.56302100	-1.08048200	0.79616200
H	4.56182800	-1.00660300	-0.95602100
C	3.26857400	0.44492400	-0.01556100
H	3.26040300	1.13855500	-0.86635500
H	3.26683300	1.07127500	0.88593200
C	1.99212400	-0.40353100	-0.04316900
H	2.00037400	-1.09612900	0.80849600
H	1.99442400	-1.03116900	-0.94385200
C	0.70223700	0.42405000	-0.00790200
H	0.69268600	1.11512400	-0.86078800
H	0.70092200	1.05327700	0.89165900
C	-0.57378200	-0.42516300	-0.03177400
H	-0.56410900	-1.11586600	0.82142400

H	-0.57220900	-1.05486000	-0.93102600
C	-1.86412300	0.40173500	0.00313400
H	-1.87439000	1.09184900	-0.85052800
H	-1.86537900	1.03201300	0.90197000
C	-3.13979500	-0.44804200	-0.01930700
H	-3.12933000	-1.13821800	0.83430700
H	-3.13854400	-1.07828900	-0.91817300
C	-4.43038200	0.37845700	0.01587700
H	-4.44086000	1.06881700	-0.83757400
H	-4.43179800	1.00847100	0.91489000
C	-5.70593300	-0.47153400	-0.00687300
H	-5.69514100	-1.16247200	0.84614500
H	-5.70487900	-1.10094300	-0.90635000
C	-6.99653500	0.35451900	0.02943700
H	-7.00780400	1.04666000	-0.82277900
H	-6.99927600	0.98309200	0.92965900
C	-8.27280000	-0.49441000	0.00467400
H	-8.26189400	-1.18642700	0.85562100
H	-8.27118500	-1.12100900	-0.89564400
C	-9.55646100	0.34008400	0.04288300
H	-9.61245300	1.01882300	-0.81415200
H	-10.44724000	-0.29408100	0.02250700
H	-9.60425900	0.95057300	0.95028000

TS66: $\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}(\text{CH}_2)_{13}\text{CH}_3$

C	9.57065100	-0.33598000	0.01882200
H	9.68612700	-1.12152700	-0.73881600
H	9.61931200	-0.81849000	0.99984100
H	10.42838000	0.33582900	-0.07015000
C	8.26344900	0.40292300	-0.16550900
H	8.25869700	1.33222000	0.76428900
H	8.23793800	1.01448400	-1.07179000
C	6.99269400	-0.39339900	0.04818000
H	7.01175000	-0.84342600	1.04936400
H	6.98553300	-1.23952100	-0.65709500
C	5.70521800	0.42055700	-0.12715000
H	5.70285300	0.88104000	-1.12337900
H	5.70314800	1.24870000	0.59175200
C	4.42938500	-0.41031600	0.04814200
H	4.44542800	-0.89617600	1.03231500
H	4.42222700	-1.22232200	-0.69081800
C	3.14114800	0.40922300	-0.08762700
H	3.14007000	0.92493400	-1.05672000

H	3.13426600	1.19828900	0.67536000
C	1.86335400	-0.42821900	0.03817100
H	1.87749300	-0.97036900	0.99262300
H	1.85691200	-1.19606900	-0.74638500
C	0.57552900	0.39836500	-0.05269600
H	0.57461300	0.96547100	-0.99267100
H	0.56919400	1.14534600	0.75162900
C	-0.70306200	-0.44340200	0.02887300
H	-0.69271500	-1.02918400	0.95726600
H	-0.70659000	-1.17415400	-0.79032300
C	-1.99041000	0.38688900	-0.02917000
H	-1.99219400	0.98818200	-0.94766000
H	-1.99508300	1.10387500	0.80205400
C	-3.26954000	-0.45632600	0.02383700
H	-3.26225200	-1.06831400	0.93520400
H	-3.27077300	-1.16352000	-0.81578700
C	-4.55642900	0.37578700	-0.01484700
H	-4.55914800	0.99586500	-0.92074600
H	-4.55949000	1.07553900	0.83095700
C	-5.83604500	-0.46753400	0.02305100
H	-5.83069000	-1.09272100	0.92545200
H	-5.83604500	-1.16245100	-0.82679200
C	-7.12249100	0.36527700	-0.00604000
H	-7.12729500	0.99359600	-0.90643500
H	-7.12494200	1.05771800	0.84599200
C	-8.40315800	-0.47672700	0.02662600
H	-8.39817800	-1.10541200	0.92547900
H	-8.40253000	-1.16681100	-0.82596200
C	-9.68239200	0.36499900	0.00020200
H	-9.73329300	0.97862000	-0.90491000
H	-10.57653900	-0.26424300	0.02505100
H	-9.72836400	1.04131600	0.85974000
H	8.27477000	1.98098100	1.48489000



C	-9.57611700	0.59998800	0.25199800
H	-9.68605000	1.18428400	-0.66658900
H	-9.40147600	1.30083800	1.07319600
H	-10.52575900	0.09151800	0.43876400
C	-8.42215100	-0.40207600	0.12985700
H	-8.35644300	-1.00694800	1.04588500
H	-8.66441700	-1.12973300	-0.66614800

C	-7.09759000	0.22795200	-0.14695600
H	-7.07865700	1.21395400	-0.60573600
C	-5.82819100	-0.55504500	-0.09129300
H	-5.78275100	-1.25834300	-0.94394000
H	-5.83119000	-1.19987600	0.80004500
C	-4.55675400	0.30570600	-0.09902100
H	-4.58060500	0.98603100	0.76073700
H	-4.56145500	0.94247900	-0.99272500
C	-3.26195200	-0.51301500	-0.06676800
H	-3.24176400	-1.19338200	-0.92812600
H	-3.26037800	-1.15317400	0.82510600
C	-1.99324900	0.34727100	-0.07245100
H	-2.01448900	1.02801900	0.78842300
H	-1.99454400	0.98711800	-0.96447500
C	-0.69593800	-0.46870000	-0.03849600
H	-0.67435600	-1.14956200	-0.89935700
H	-0.69436300	-1.10838900	0.85365600
C	0.57185700	0.39302200	-0.04425800
H	0.54985900	1.07399700	0.81649400
H	0.56987600	1.03275500	-0.93638600
C	1.87014600	-0.42136900	-0.01021500
H	1.89212200	-1.10271000	-0.87069200
H	1.87274800	-1.06061800	0.88225800
C	3.13714800	0.44152600	-0.01699400
H	3.11492400	1.12303300	0.84334200
H	3.13427300	1.08069200	-0.90953000
C	4.43609600	-0.37181200	0.01706600
H	4.45815900	-1.05382700	-0.84286300
H	4.43958800	-1.01035400	0.91003200
C	5.70260400	0.49183800	0.00899100
H	5.68029100	1.17422700	0.86865400
H	5.69915000	1.13003900	-0.88425700
C	7.00188900	-0.32056000	0.04356500
H	7.02495100	-1.00385800	-0.81553600
H	7.00698900	-0.95818600	0.93738600
C	8.26883700	0.54249500	0.03398300
H	8.24619200	1.22534200	0.89208700
H	8.26466300	1.17853100	-0.85967900
C	9.56148800	-0.27810700	0.06976700
H	9.62972000	-0.94636400	-0.79459000
H	10.44520800	0.36612800	0.06149100
H	9.61124500	-0.89833000	0.97043400

TS67: H + CH₃(CH₂)₁₄CH₃ → H₂ + CH₃CH₂CH(CH₂)₁₂CH₃

C	-9.54997800	0.34000400	-0.15401500
H	-9.57184100	0.77981300	-1.15589400
H	-9.58891200	1.15908100	0.56956900
H	-10.45794400	-0.25659900	-0.03276000
C	-8.29482100	-0.51464200	0.04578100
H	-8.31620600	-0.98066000	1.03855700
H	-8.30181400	-1.34731700	-0.67340500
C	-6.99966000	0.25516700	-0.11565900
H	-7.00671800	1.14147000	0.86046100
H	-6.99397800	0.90576700	-0.99593600
C	-5.71086000	-0.52162500	0.05769700
H	-5.68267200	-1.32785600	-0.69199200
H	-5.71797100	-1.02451800	1.03341900
C	-4.44256700	0.33080600	-0.07223800
H	-4.45727400	1.11551900	0.69350800
H	-4.45338100	0.84803000	-1.04016500
C	-3.14823500	-0.48033800	0.05280100
H	-3.12686100	-1.25002800	-0.72979700
H	-3.14941600	-1.01979500	1.00880200
C	-1.87818600	0.37275200	-0.04249300
H	-1.88723900	1.12346800	0.75815400
H	-1.88930300	0.93497400	-0.98530800
C	-0.58304200	-0.44290200	0.04255600
H	-0.56695600	-1.17989200	-0.77090800
H	-0.57986500	-1.02139800	0.97553700
C	0.68788600	0.41158200	-0.02524100
H	0.68093200	1.13514000	0.80020200
H	0.67610600	1.00528400	-0.94857700
C	1.98254400	-0.40737100	0.03111900
H	1.99383500	-1.12216100	-0.80198500
H	1.98938200	-1.01097700	0.94805700
C	3.25421000	0.44716500	-0.01984800
H	3.24834100	1.15409700	0.81993600
H	3.24248400	1.05930800	-0.93106900
C	4.54828500	-0.37369100	0.01982200
H	4.55629400	-1.07609100	-0.82377900
H	4.55748500	-0.99082300	0.92768400
C	5.82054800	0.48044700	-0.02269800
H	5.81514200	1.17928100	0.82388700
H	5.80919800	1.10135000	-0.92800000
C	7.11414800	-0.34110900	0.00930200
H	7.12103900	-1.03890700	-0.83833900

H	7.12593400	-0.96361600	0.91366000
C	8.38745600	0.51163700	-0.03115500
H	8.38209300	1.20773800	0.81649000
H	8.37580100	1.13382300	-0.93445900
C	9.67397800	-0.31877300	-0.00061300
H	9.72431200	-1.00130200	-0.85499300
H	10.56257500	0.31799300	-0.03198200
H	9.73185600	-0.92489100	0.90912100
H	-7.01468600	1.74003800	1.62160300

H-R68: $\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_{11}\text{CH}_3$

$\text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_{11}\text{CH}_3$

C	9.64562800	-0.00946700	0.37366600
H	9.64627600	0.57805200	1.29736300
H	9.90710100	0.66612600	-0.44711300
H	10.44091700	-0.75551700	0.45532200
C	8.28421700	-0.66812200	0.13707900
H	8.32439900	-1.27591300	-0.77462600
H	8.06146000	-1.36045300	0.95670700
C	7.13591200	0.34329700	0.01175000
H	7.38196100	1.05565000	-0.79819400
H	7.09146400	0.96288200	0.92023900
C	5.80021500	-0.27267500	-0.24070000
H	5.76270400	-1.25889800	-0.69778700
C	4.54009900	0.52364400	-0.16498800
H	4.49097000	1.23103800	-1.01405900
H	4.56168400	1.16488400	0.72872700
C	3.25950200	-0.32334600	-0.15941900
H	3.28631500	-1.00611700	0.69832900
H	3.24677400	-0.95786000	-1.05467200
C	1.97392300	0.50893100	-0.10983500
H	1.95100600	1.19182700	-0.96912200
H	1.98933300	1.14660100	0.78368900
C	0.69625700	-0.33799000	-0.10327000
H	0.71973100	-1.02073700	0.75596100
H	0.68127300	-0.97594500	-0.99652900
C	-0.59214700	0.49119500	-0.05374400
H	-0.61559700	1.17446800	-0.91264300
H	-0.57808300	1.12851100	0.83999300
C	-1.86860400	-0.35766000	-0.04877400
H	-1.84506500	-1.04069000	0.81030500
H	-1.88165600	-0.99544900	-0.94220100
C	-3.15838700	0.46943500	-0.00049900

H	-3.18151300	1.15339800	-0.85885900
H	-3.14666300	1.10608700	0.89375300
C	-4.43368800	-0.38118100	0.00176200
H	-4.41027700	-1.06539200	0.85990500
H	-4.44488700	-1.01771600	-0.89257600
C	-5.72460700	0.44419100	0.04983400
H	-5.74760400	1.12955100	-0.80743700
H	-5.71463800	1.07937900	0.94517600
C	-6.99895400	-0.40750000	0.04936000
H	-6.97611400	-1.09422200	0.90573100
H	-7.01035000	-1.04184200	-0.84673400
C	-8.29127600	0.41560300	0.09956400
H	-8.31467700	1.10233800	-0.75541900
H	-8.28115200	1.04778100	0.99591700
C	-9.55804900	-0.44516100	0.09693600
H	-9.57908300	-1.12011600	0.95852200
H	-10.46096700	0.17069200	0.13590500
H	-9.61528000	-1.06155200	-0.80590100

TS68: $\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_{11}\text{CH}_3$

C	-9.58376700	-0.28241100	0.03568300
H	-9.65556100	-0.69845900	1.04552700
H	-9.65855700	-1.11538100	-0.67080200
H	-10.45277700	0.36282600	-0.11915500
C	-8.27531000	0.49000800	-0.15226500
H	-8.24871300	0.92679100	-1.15781500
H	-8.24282500	1.33233100	0.54786200
C	-7.02840100	-0.37954000	0.04948000
H	-7.05568800	-1.21935900	-0.66248100
H	-7.05679500	-0.83697000	1.04721900
C	-5.72026000	0.36486600	-0.12274200
H	-5.70305000	1.25404200	0.85010700
H	-5.70645000	1.01217300	-1.00523800
C	-4.44549900	-0.43612600	0.04583600
H	-4.43519400	-1.24220300	-0.70445900
H	-4.45882200	-0.93953100	1.02119200
C	-3.16180000	0.39226100	-0.08757200
H	-3.15899200	1.17600800	0.67930000
H	-3.16594800	0.91101600	-1.05473600
C	-1.88257900	-0.44335300	0.03228900
H	-1.87626000	-1.20978900	-0.75374300
H	-1.89284200	-0.98695600	0.98589000
C	-0.59716800	0.38668800	-0.06010500

H	-0.59273900	1.13452700	0.74328000
H	-0.59787200	0.95248200	-1.00084400
C	0.68312300	-0.45236800	0.02252000
H	0.68764600	-1.18522500	-0.79480100
H	0.67446000	-1.03569700	0.95245600
C	1.96884500	0.38021000	-0.03831100
H	1.97174200	1.10052000	0.79000100
H	1.97004100	0.97772200	-0.95925500
C	3.24931000	-0.46070500	0.01893900
H	3.25197000	-1.17176000	-0.81741900
H	3.24260300	-1.06848000	0.93312100
C	4.53497400	0.37312400	-0.02303900
H	4.53626000	1.07734300	0.81903700
H	4.53764900	0.98835700	-0.93223200
C	5.81568900	-0.46826000	0.02058500
H	5.81722500	-1.16803300	-0.82526300
H	5.81046500	-1.08826500	0.92655500
C	7.10109500	0.36600500	-0.01232000
H	7.10174400	1.06374000	0.83537600
H	7.10610900	0.98867900	-0.91662400
C	8.38276000	-0.47419900	0.02706900
H	8.38383300	-1.16982700	-0.82099800
H	8.37763900	-1.09700300	0.93000600
C	9.66100300	0.36888700	-0.00358700
H	9.70511700	1.05113000	0.85134800
H	10.55587100	-0.25908900	0.02665800
H	9.71227300	0.97634200	-0.91282700
H	-5.69564900	1.85547700	1.60899100

H-R69: $\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_{10}\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_{10}\text{CH}_3$

C	-9.49889100	0.83019800	0.37143800
H	-9.65122300	1.18721700	-0.65210900
H	-9.30807900	1.70525800	1.00076500
H	-10.43603100	0.37788400	0.70781100
C	-8.33857600	-0.16667000	0.44310600
H	-8.23288100	-0.52927700	1.47297400
H	-8.57619400	-1.04779800	-0.16565100
C	-7.00355700	0.42381600	-0.02241200
H	-6.76318700	1.30477300	0.58532600
H	-7.10672700	0.78363300	-1.05410900
C	-5.83431500	-0.56809700	0.04886800
H	-6.09246300	-1.46143300	-0.55056300

H	-5.73383700	-0.94511900	1.07764900
C	-4.52717400	-0.00973600	-0.40694300
H	-4.53523900	0.82206100	-1.10781100
C	-3.24063300	-0.73191300	-0.18049700
H	-3.16243800	-1.59004800	-0.87438200
H	-3.24359500	-1.18335500	0.82219300
C	-1.98966500	0.14388200	-0.34571300
H	-2.04355300	0.97907000	0.36294300
H	-1.99587000	0.59230200	-1.34725900
C	-0.67684300	-0.61849200	-0.13839200
H	-0.61783200	-1.44322500	-0.86060900
H	-0.68313900	-1.08567000	0.85510200
C	0.57089100	0.26199100	-0.27148900
H	0.50988900	1.08451300	0.45293000
H	0.57866400	0.73218100	-1.26343100
C	1.88559600	-0.49789100	-0.06182200
H	1.95650500	-1.30956200	-0.79751700
H	1.86932000	-0.98244900	0.92313100
C	3.13127500	0.38958000	-0.16557700
H	3.05887400	1.19938000	0.57205700
H	3.14814000	0.87676400	-1.14919200
C	4.44677200	-0.36853800	0.04544200
H	4.52652500	-1.17039800	-0.70002400
H	4.42405400	-0.86586200	1.02387000
C	5.69035000	0.52415300	-0.03721900
H	5.60901500	1.32552200	0.70866800
H	5.71402300	1.02220000	-1.01526900
C	7.00645300	-0.23179600	0.17631900
H	7.09262000	-1.02963500	-0.57299600
H	6.98118400	-0.73460300	1.15205700
C	8.24923100	0.66294300	0.10383800
H	8.16259000	1.46033900	0.85201500
H	8.27613900	1.16406200	-0.87153400
C	9.55926500	-0.09997400	0.32105800
H	9.69009400	-0.88378900	-0.43188900
H	10.42500500	0.56554500	0.26073600
H	9.57856000	-0.58122900	1.30409900

TS69: $\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_{10}\text{CH}_3$

C	-9.56859800	0.40476800	-0.08933700
H	-9.60636500	0.87882300	-1.07531200
H	-9.59557400	1.20138300	0.66081800
H	-10.47797000	-0.19134700	0.02699900

C	-8.31164700	-0.45665300	0.06279200
H	-8.32092600	-0.94545600	1.04458200
H	-8.33127800	-1.26466700	-0.67895600
C	-7.01095000	0.33928200	-0.09030800
H	-6.98617300	1.14063900	0.65810200
H	-7.00335200	0.83537200	-1.06946300
C	-5.74851100	-0.51980400	0.04873100
H	-5.76643500	-1.31446300	-0.71331200
H	-5.75979800	-1.03763300	1.01670500
C	-4.45487900	0.25709300	-0.08721300
H	-4.44776600	1.08924100	0.93483900
H	-4.45776200	0.95341100	-0.93160500
C	-3.16428800	-0.52754400	0.03117000
H	-3.14408600	-1.29415000	-0.75910100
H	-3.16055600	-1.07972000	0.97989700
C	-1.89804100	0.33200500	-0.06863100
H	-1.91183300	1.08512800	0.72816800
H	-1.91323700	0.88778800	-1.01490300
C	-0.60122800	-0.47997900	0.02047300
H	-0.58311000	-1.22373300	-0.78685000
H	-0.59487600	-1.05009200	0.95849900
C	0.66569600	0.37967200	-0.05537300
H	0.65240500	1.11386700	0.76040400
H	0.65352600	0.96101600	-0.98651000
C	1.96443300	-0.43156900	0.01594000
H	1.98240900	-1.15806900	-0.80685600
H	1.97200900	-1.02176700	0.94153600
C	3.23090900	0.43011800	-0.04335700
H	3.21611800	1.15092100	0.78440500
H	3.21964300	1.02683300	-0.96475300
C	4.53035800	-0.38092000	0.01666000
H	4.54772700	-1.09764900	-0.81465300
H	4.53940200	-0.98212300	0.93514300
C	5.79642500	0.48195100	-0.03424900
H	5.78038300	1.19636600	0.79907800
H	5.78583300	1.08576600	-0.95104700
C	7.09624000	-0.32845300	0.02105200
H	7.11389700	-1.04231000	-0.81294600
H	7.10762500	-0.93328400	0.93732900
C	8.36273800	0.53393400	-0.02836700
H	8.34588100	1.24695100	0.80492800
H	8.35196600	1.13757100	-0.94418300
C	9.65596200	-0.28463000	0.02760000

H	9.71778100	-0.98430400	-0.81203800
H	10.53931000	0.35898500	-0.01132100
H	9.71304700	-0.87119200	0.95011600
H	-4.44559800	1.64627200	1.72675500

H-R70: $\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_9\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_9\text{CH}_3$

C	9.57033600	-0.25874800	0.56016100
H	9.53623300	-0.01074100	1.62583100
H	9.83634100	0.65413300	0.01772700
H	10.37969800	-0.97943000	0.41333100
C	8.22815700	-0.81757800	0.07886800
H	8.30540400	-1.09129600	-0.98051300
H	8.00600900	-1.74725800	0.61681700
C	7.06245300	0.16091100	0.26218600
H	7.28374600	1.09031700	-0.27897600
H	6.98859100	0.43792600	1.32211600
C	5.71533900	-0.39406000	-0.21117000
H	5.49044400	-1.31963200	0.33251800
H	5.78890100	-0.67192400	-1.27022000
C	4.54798400	0.58648100	-0.03152000
H	4.78631600	1.52289800	-0.56995300
H	4.47779200	0.88572700	1.02514400
C	3.22918700	0.05745200	-0.48890100
H	3.21902400	-0.73909600	-1.22953800
C	1.94984100	0.76952100	-0.19877400
H	1.85650200	1.65805800	-0.85122200
H	1.97709500	1.17505100	0.82294000
C	0.69456800	-0.09815800	-0.37427500
H	0.76126600	-0.96137700	0.29877100
H	0.68077100	-0.50568500	-1.39308500
C	-0.61360700	0.65500400	-0.11113200
H	-0.68621900	1.50773200	-0.79872800
H	-0.58814900	1.08218800	0.89990200
C	-1.86333900	-0.22088800	-0.25547200
H	-1.78973800	-1.06986400	0.43649900
H	-1.88787800	-0.65369000	-1.26403200
C	-3.17492100	0.52882300	0.00446200
H	-3.25947700	1.36633000	-0.70013200
H	-3.14221200	0.97746400	1.00588500
C	-4.42084400	-0.35706700	-0.10986900
H	-4.33606600	-1.19094600	0.59901000
H	-4.45199800	-0.81107000	-1.10889100

C	-5.73428500	0.39078900	0.14600100
H	-5.82727400	1.21567300	-0.57231900
H	-5.69715700	0.85681200	1.13931900
C	-6.97716700	-0.50170100	0.05456200
H	-6.88555600	-1.32410000	0.77612900
H	-7.01404500	-0.97192200	-0.93693000
C	-8.29230500	0.24455500	0.30652500
H	-8.38840000	1.06109900	-0.41951000
H	-8.25330800	0.72011500	1.29421700
C	-9.52657100	-0.65860700	0.22474500
H	-9.47706200	-1.46319700	0.96529300
H	-10.44694400	-0.09656100	0.40663000
H	-9.61160500	-1.12410500	-0.76240400

TS70: H + CH₃(CH₂)₁₄CH₃ → H₂ + CH₃(CH₂)₄CH(CH₂)₉CH₃

C	-9.60127700	-0.22813500	0.08520000
H	-9.65861800	-0.67259900	1.08390700
H	-9.69013400	-1.04089400	-0.64281800
H	-10.47066900	0.42370300	-0.03788400
C	-8.29181800	0.54339100	-0.10240100
H	-8.28172900	1.01013700	-1.09497400
H	-8.24668400	1.36695900	0.62049900
C	-7.04381500	-0.33285300	0.05445700
H	-7.08382100	-1.15105100	-0.67679700
H	-7.06012700	-0.80918800	1.04343300
C	-5.72924700	0.43629100	-0.11371500
H	-5.68347500	1.24340500	0.62727500
H	-5.71638700	0.92311000	-1.09732400
C	-4.48271800	-0.44603100	0.02619900
H	-4.51595200	-1.24215100	-0.73370500
H	-4.50238100	-0.96102700	0.99552200
C	-3.17565900	0.30759700	-0.11236400
H	-3.15256000	1.13933200	0.90960200
H	-3.16770000	1.00394300	-0.95671800
C	-1.89856000	-0.49908600	0.00428300
H	-1.88991700	-1.26238600	-0.78938600
H	-1.90538800	-1.05536100	0.95058500
C	-0.61829200	0.34013500	-0.08961600
H	-0.62185700	1.09021800	0.71014600
H	-0.62239600	0.89988600	-1.03366000
C	0.66539000	-0.49247500	-0.00054300
H	0.67537600	-1.23154900	-0.81227900
H	0.65927400	-1.06817700	0.93406600

C	1.94534700	0.34852100	-0.06594100
H	1.93880300	1.07861800	0.75359200
H	1.94629900	0.93484200	-0.99402800
C	3.23188300	-0.48173200	0.00764900
H	3.24429700	-1.20350300	-0.81939000
H	3.22587100	-1.07741200	0.92973700
C	4.51051300	0.36260500	-0.03921200
H	4.50016100	1.07943500	0.79205300
H	4.51340600	0.96401000	-0.95760300
C	5.79855100	-0.46613200	0.02531300
H	5.81196800	-1.17902300	-0.80939700
H	5.79348900	-1.07176200	0.94094800
C	7.07606400	0.37997300	-0.01286000
H	7.06382700	1.09191600	0.82283400
H	7.08144900	0.98725900	-0.92756600
C	8.36565000	-0.44655000	0.04993200
H	8.37970900	-1.15678900	-0.78581700
H	8.36035200	-1.05351500	0.96359200
C	9.63556700	0.40880200	0.01335800
H	9.66638400	1.10676600	0.85608900
H	10.53644500	-0.20937400	0.06155000
H	9.68757000	1.00023300	-0.90634300
H	-3.14034900	1.69605200	1.70182400

H-R71: $\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_8\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_8\text{CH}_3$

C	-9.52115300	0.79045100	0.28233500
H	-9.61612500	1.23211600	-0.71481100
H	-9.40781300	1.61185300	0.99699900
H	-10.46125500	0.28007000	0.50977700
C	-8.33032900	-0.17023100	0.35114100
H	-8.28500100	-0.62415400	1.34867700
H	-8.48725500	-0.99745900	-0.35177300
C	-6.98868700	0.50464800	0.04348100
H	-6.83287800	1.33353100	0.74626400
H	-7.03469300	0.95895800	-0.95502400
C	-5.78971800	-0.44783300	0.11099000
H	-5.94714200	-1.27779200	-0.59013300
H	-5.74365400	-0.89981600	1.11046300
C	-4.45075600	0.22939900	-0.19960500
H	-4.29121700	1.06120700	0.49689000
H	-4.49277300	0.67383800	-1.20207300
C	-3.24906800	-0.72353400	-0.12498700

H	-3.43587800	-1.57888000	-0.80135600
H	-3.19482300	-1.17041200	0.87875500
C	-1.94103100	-0.08767700	-0.46060600
H	-1.94073600	0.77532700	-1.12264400
C	-0.64155800	-0.76589700	-0.17885100
H	-0.51321600	-1.63028700	-0.85721800
H	-0.66645800	-1.20586300	0.82914100
C	0.58679500	0.14571500	-0.31226000
H	0.48514300	0.98692700	0.38383800
H	0.60014000	0.58195300	-1.31912900
C	1.91458800	-0.57411900	-0.05416200
H	2.01304900	-1.41472800	-0.75332500
H	1.89758300	-1.01602200	0.95070000
C	3.14064700	0.33696800	-0.18351000
H	3.04226000	1.17670800	0.51649800
H	3.15703500	0.78004600	-1.18779000
C	4.47048000	-0.38116000	0.07290800
H	4.56906600	-1.22086400	-0.62721400
H	4.45424600	-0.82430100	1.07716100
C	5.69607300	0.53067800	-0.05658600
H	5.59724400	1.37051100	0.64337200
H	5.71220300	0.97371000	-1.06092800
C	7.02632300	-0.18623400	0.19981200
H	7.12601500	-1.02657900	-0.49965000
H	7.01171000	-0.62880400	1.20453000
C	8.25236200	0.72492900	0.06940900
H	8.15279700	1.56495600	0.76761100
H	8.26836000	1.16570800	-0.93492700
C	9.57642200	0.00018800	0.32863400
H	9.71838900	-0.82683700	-0.37434900
H	10.43005500	0.67560400	0.22297400
H	9.60728100	-0.41796800	1.33983700

TS71: $\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_8\text{CH}_3$

C	-9.58460200	0.46274000	0.02046300
H	-9.63648600	1.01277200	-0.92457800
H	-9.59168100	1.19851000	0.83087600
H	-10.49647400	-0.13474400	0.10693500
C	-8.33115600	-0.41520200	0.08168200
H	-8.32629100	-0.97943800	1.02229900
H	-8.36953500	-1.16261200	-0.72023700
C	-7.02702300	0.38217800	-0.03359600
H	-6.99092300	1.13121200	0.76811900

H	-7.03154500	0.94661800	-0.97531700
C	-5.76554500	-0.48612800	0.03015300
H	-5.79971200	-1.23392600	-0.77292300
H	-5.76333600	-1.05114900	0.97128100
C	-4.46480100	0.31695600	-0.07926700
H	-4.43146800	1.06526000	0.72151500
H	-4.46315000	0.87826700	-1.02239200
C	-3.20208800	-0.55062300	-0.00789100
H	-3.23112600	-1.29944900	-0.81465000
H	-3.20113000	-1.12352600	0.92852100
C	-1.91012200	0.23322600	-0.11661700
H	-1.90282600	1.02753200	0.93480000
H	-1.91605200	0.95935300	-0.93550300
C	-0.61613300	-0.54962800	-0.02526300
H	-0.59960100	-1.30258500	-0.82849900
H	-0.60171700	-1.11769600	0.91399900
C	0.64446100	0.31857900	-0.12127800
H	0.61915700	1.07598800	0.67122500
H	0.63091300	0.86908200	-1.07067100
C	1.94805900	-0.48057000	-0.01715500
H	1.97375000	-1.24026100	-0.80927200
H	1.95913000	-1.03129300	0.93232900
C	3.20616100	0.39034400	-0.10997000
H	3.17200800	1.15679100	0.67501800
H	3.20035300	0.93344800	-1.06397600
C	4.51402000	-0.39946200	0.01411900
H	4.54994900	-1.16762000	-0.76929600
H	4.52005800	-0.94017900	0.96945600
C	5.76920400	0.47584300	-0.07841600
H	5.72587000	1.25137900	0.69732700
H	5.76877100	1.00784300	-1.03871500
C	7.07913800	-0.30683000	0.06486500
H	7.12368000	-1.08554300	-0.70787500
H	7.08192900	-0.83503400	1.02739800
C	8.33317000	0.56975700	-0.03160200
H	8.28493500	1.35267500	0.73508600
H	8.33507400	1.09053200	-0.99699400
C	9.63737400	-0.21736600	0.12587400
H	9.72980200	-0.98909700	-0.64507400
H	10.51109000	0.43572900	0.04756300
H	9.68270700	-0.71688500	1.09889400
H	-1.89683600	1.55516800	1.74673800

H-R72: $\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_6\text{CH}(\text{CH}_2)_7\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_6\text{CH}(\text{CH}_2)_7\text{CH}_3$

C	9.58515100	-0.12337600	0.38909600
H	9.61056700	0.29399000	1.40077200
H	9.77373200	0.69697900	-0.31069400
H	10.41430300	-0.83112500	0.30158000
C	8.24022900	-0.79728900	0.10169100
H	8.26029900	-1.23746100	-0.90284700
H	8.09500400	-1.63361200	0.79632100
C	7.04682800	0.15912500	0.20851100
H	7.19316100	0.99676400	-0.48594200
H	7.02693200	0.59940700	1.21414200
C	5.69664200	-0.50682500	-0.07921300
H	5.55157100	-1.34455900	0.61506600
H	5.71816500	-0.94686500	-1.08476600
C	4.50304000	0.44927400	0.02723600
H	4.64927100	1.28901000	-0.66454000
H	4.47906900	0.88636900	1.03404600
C	3.15581700	-0.21904300	-0.26625600
H	3.00712400	-1.06017200	0.42138600
H	3.17675000	-0.64939500	-1.27552600
C	1.95848000	0.73584200	-0.15530100
H	2.13520200	1.60069100	-0.82218900
H	1.92353200	1.16781000	0.85582100
C	0.64331600	0.10741100	-0.47681400
H	0.63005200	-0.74720100	-1.14954300
C	-0.65024600	0.78411200	-0.16574200
H	-0.79025500	1.65425100	-0.83439300
H	-0.60724400	1.21529800	0.84538200
C	-1.88093700	-0.12633600	-0.28553700
H	-1.76888900	-0.97159400	0.40399600
H	-1.90960100	-0.55674900	-1.29459400
C	-3.20484700	0.59170300	-0.00351800
H	-3.31435600	1.43562800	-0.69698900
H	-3.17290000	1.02857600	1.00317200
C	-4.43191500	-0.31992500	-0.11906200
H	-4.32321900	-1.16192200	0.57665600
H	-4.46161100	-0.75962100	-1.12451800
C	-5.75902000	0.39576700	0.15767700
H	-5.86815700	1.23747100	-0.53848200
H	-5.72985300	0.83573500	1.16306000
C	-6.98481100	-0.51729700	0.04178700
H	-6.87669400	-1.35902300	0.73827800

H	-7.01420400	-0.95810700	-0.96339000
C	-8.31353700	0.19605600	0.31690300
H	-8.42210500	1.03679500	-0.37908800
H	-8.28545200	0.63556800	1.32150500
C	-9.53137200	-0.72512400	0.19796000
H	-9.46726800	-1.55811900	0.90525200
H	-10.46171200	-0.18759200	0.40187400
H	-9.60811400	-1.15167300	-0.80731100

TS72: $\text{H} + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_6\text{CH}(\text{CH}_2)_7\text{CH}_3$

C	9.61879800	-0.21032200	0.11547200
H	9.71184600	-1.00817100	-0.62834500
H	9.66826400	-0.67540800	1.10520000
H	10.49006900	0.44251500	0.01211100
C	8.31160300	0.56659400	-0.06585900
H	8.26224700	1.37512200	0.67368800
H	8.30964000	1.05404800	-1.04849100
C	7.06099100	-0.31061700	0.06324700
H	7.06886700	-0.80740600	1.04230800
H	7.10573400	-1.11375500	-0.68411200
C	5.74785700	0.46258700	-0.10027100
H	5.74384200	0.96728400	-1.07517300
H	5.70195900	1.25925600	0.65346200
C	4.49692200	-0.41553800	0.01837700
H	4.50962700	-0.93385200	0.98589000
H	4.53246700	-1.20134300	-0.74747700
C	3.18620900	0.36709100	-0.11648300
H	3.17476300	0.89380900	-1.07930900
H	3.14619500	1.14347900	0.65686300
C	1.93435100	-0.51243300	-0.00997800
H	1.95154400	-1.06503700	0.93844800
H	1.96154100	-1.27822900	-0.80065000
C	0.63248900	0.25515100	-0.11754000
H	0.62554100	0.97693600	-0.94024700
H	0.62181500	1.05495100	0.92963200
C	-0.65115200	-0.54331900	-0.01694300
H	-0.64723800	-1.12103200	0.91647100
H	-0.66863100	-1.28819500	-0.82773000
C	-1.92351700	0.31003700	-0.08858300
H	-1.92032800	0.88383400	-1.02416800
H	-1.90630700	1.04799700	0.72221200
C	-3.21540600	-0.50998900	-0.00199900
H	-3.21196600	-1.09334700	0.92785500

H	-3.23626600	-1.24220200	-0.81972100
C	-4.48637000	0.34536100	-0.05597500
H	-4.48763000	0.93342700	-0.98294600
H	-4.46544700	1.07379500	0.76479300
C	-5.78174100	-0.47021600	0.02614800
H	-5.77809400	-1.06266600	0.95034600
H	-5.80620500	-1.19469200	-0.79828000
C	-7.05093800	0.38804800	-0.01788800
H	-7.05531200	0.98165000	-0.94153000
H	-7.02678300	1.11216600	0.80697900
C	-8.34842300	-0.42422700	0.06441200
H	-8.34396400	-1.01765600	0.98691700
H	-8.37475500	-1.14651900	-0.76065300
C	-9.60967900	0.44361400	0.02253400
H	-9.66111000	1.02192900	-0.90549900
H	-10.51652500	-0.16444600	0.08510700
H	-9.62829900	1.15416200	0.85502300
H	0.61693300	1.58666600	1.73899900

2.2 Hydrogen abstraction reaction of n -C_nH_{2n+2} (n = 1-16) by HO₂ radical

2.2.1 C1 (CH₄)



HO₂

O	0.05528300	0.71892300	0.00000000
O	0.05528300	-0.60935400	0.00000000
H	-0.88453600	-0.87655400	0.00000000

H₂O₂

O	0.71704600	0.11962300	-0.05193700
H	1.02700100	-0.66834300	0.41527900
O	-0.71712100	-0.11966100	-0.05186800
H	-1.02640600	0.66865000	0.41516300



C	-2.88344700	0.65332700	-0.08987500
H	-2.85876200	-0.34755400	0.33008700
H	-2.51556000	1.44594600	0.55514500
H	-2.60730100	0.73043500	-1.13734600
H	-4.26643500	0.97018900	-0.12740200
O	-5.37311300	1.18560400	-0.15080800
O	-5.67089200	1.73592000	1.12046800
H	-6.09269300	0.99186800	1.57527100

2.2.2 C2 (C₂H₆)



C	-2.87442600	1.61357800	-0.36349700
H	-2.61465600	2.41482500	0.32814300
H	-2.38626700	1.71329900	-1.33269000
H	-4.16962900	1.94657800	-0.69675300
C	-2.94859200	0.22913000	0.21556600
H	-3.29174200	-0.49929900	-0.52262000
H	-1.95728900	-0.09613200	0.56292200
H	-3.62214300	0.18797800	1.07544500
O	-5.27330500	2.20320600	-0.95172500
O	-6.00721300	1.88298200	0.21720100
H	-6.14849700	2.75233500	0.62049100

2.2.3 C3 (C₃H₈)



TS3: HO₂ + CH₃CH₂CH₃ → H₂O₂ + CH₂CH₂CH₃

C	0.53663500	1.24751900	-0.09684400
H	0.89144800	1.58233900	-1.07276500
H	-0.63814300	0.61813200	-0.45091000
H	0.16479300	2.06204200	0.52491700
C	1.36643300	0.20121500	0.59693500
H	0.80258000	-0.21087300	1.44160600
H	2.24191200	0.69979800	1.04408100
C	1.83603900	-0.93031000	-0.32227500
H	2.45003300	-1.65017100	0.22462200
H	0.98338500	-1.46661800	-0.74573100
H	2.43494800	-0.54104300	-1.15140000
O	-1.62704000	0.06280700	-0.70795200
O	-2.00712200	-0.58834200	0.49247000
H	-2.69230000	0.00013000	0.84253700

HO₂-R4: HO₂ + CH₃CH₂CH₃ → H₂O₂ + CH₃CHCH₃**TS4: HO₂ + CH₃CH₂CH₃ → H₂O₂ + CH₃CHCH₃**

C	-3.48885600	1.89379900	0.07289100
H	-3.11090400	2.41174000	0.95975800
H	-3.22929100	2.51390700	-0.79725800
H	-4.57959000	1.85491600	0.13056500
C	-2.88311300	0.51879800	-0.05781500
H	-3.36693400	-0.11087100	-0.80885600
H	-3.26651800	-0.13895800	1.05904800
C	-1.37791700	0.42351800	-0.04884900
H	-1.03771100	-0.61427100	-0.05636900
H	-0.95695500	0.91723600	-0.93674200
H	-0.95387300	0.91720500	0.83028300
O	-3.59628900	-0.68613700	2.06078200
O	-3.28720700	0.22362700	3.10088600
H	-4.15142400	0.61007000	3.30618500

2.2.4 C4 (*n*-C₄H₁₀)**HO₂-R5: HO₂ + CH₃(CH₂)₂CH₃ → H₂O₂ + CH₂(CH₂)₂CH₃****TS5: HO₂ + CH₃(CH₂)₂CH₃ → H₂O₂ + CH₂(CH₂)₂CH₃**

C	0.42269200	1.54623300	-0.03433400
H	0.25995900	2.08722100	0.89900500
H	1.36662600	0.62363700	0.36241900
H	0.98307000	2.12353200	-0.76977600
C	-0.73716700	0.74340400	-0.55721500
H	-1.44696000	1.43538400	-1.04151100
H	-0.39066700	0.07583500	-1.35590900

C	-1.47500800	-0.06912500	0.51408000
H	-0.76501300	-0.75216600	0.99113500
H	-1.82719400	0.61010600	1.29989700
C	-2.65757500	-0.86218500	-0.04738000
H	-2.32818100	-1.57358100	-0.81100900
H	-3.16203100	-1.43052700	0.73846000
H	-3.39923900	-0.20090700	-0.50723700
O	2.14829200	-0.18685400	0.65752200
O	2.15695400	-1.10179200	-0.42512600
H	2.95000900	-0.83933300	-0.91554900

HO₂-R6: HO₂ + CH₃(CH₂)₂CH₃ → H₂O₂ + CH₃CHCH₂CH₃

TS6: HO₂ + CH₃(CH₂)₂CH₃ → H₂O₂ + CH₃CHCH₂CH₃

C	-3.92949300	1.73325200	-0.13823800
H	-3.71676400	2.24274200	0.80668100
H	-3.52029100	2.36209800	-0.94177400
H	-5.01296000	1.69429500	-0.27609200
C	-3.30915900	0.35890500	-0.17421100
H	-3.90170400	-0.31830600	0.83549200
H	-3.63637400	-0.25570900	-1.01834700
C	-1.83158300	0.25506400	0.12481200
H	-1.29076000	0.87740400	-0.60681200
H	-1.62968900	0.70805600	1.10289100
C	-1.28294700	-1.17418800	0.08526700
H	-1.43644700	-1.62935900	-0.89812200
H	-0.21027000	-1.18755900	0.29414200
H	-1.77956300	-1.80255900	0.82847400
O	-4.41807100	-0.87168700	1.75301300
O	-4.18441200	-0.03356300	2.87113200
H	-5.02972200	0.42958400	2.96753000

2.2.5 C5 (*n*-C₅H₁₀)

HO₂-R7: HO₂ + CH₃(CH₂)₃CH₃ → H₂O₂ + CH₂(CH₂)₃CH₃

TS7: HO₂ + CH₃(CH₂)₃CH₃ → H₂O₂ + CH₂(CH₂)₃CH₃

C	1.26056500	1.48997700	0.40831700
H	1.36901800	1.25192800	1.46787200
H	1.95761300	0.44260100	-0.15469200
H	1.87016300	2.33780700	0.09595200
C	-0.13642900	1.42825900	-0.14866100
H	-0.68223700	2.32368700	0.19391800
H	-0.10088500	1.51016100	-1.24172500
C	-0.92141200	0.17460700	0.25676700
H	-0.37242100	-0.71382700	-0.07368700

H	-0.96694300	0.11703700	1.35196300
C	-2.34361900	0.14012000	-0.31299900
H	-2.29402600	0.19735100	-1.40715300
H	-2.88856400	1.03445600	0.01432800
C	-3.12498900	-1.11151100	0.09632600
H	-4.13297300	-1.10879400	-0.32758900
H	-2.62174800	-2.02056400	-0.24688700
H	-3.22234600	-1.17892900	1.18452200
O	2.55141500	-0.42113500	-0.66066300
O	2.48892400	-1.50942600	0.24483800
H	3.35793600	-1.47714200	0.67127800

HO₂-R8: HO₂ + CH₃(CH₂)₃CH₃ → H₂O₂ + CH₃CH(CH₂)₂CH₃

TS8: HO₂ + CH₃(CH₂)₃CH₃ → H₂O₂ + CH₃CH(CH₂)₂CH₃

C	-3.99555300	2.89315900	0.07412600
H	-3.68448000	3.50449800	0.93325700
H	-3.68280500	3.42676600	-0.82863800
H	-5.08731600	2.84405600	0.08875800
C	-3.37101500	1.52192000	0.14678700
H	-3.78546600	0.88550100	0.93437900
H	-3.84387600	0.86779300	-0.93795500
C	-1.86891400	1.43460300	0.01205800
H	-1.56140400	1.90619400	-0.93009600
H	-1.41565000	2.04692700	0.81015400
C	-1.30518000	0.01021400	0.08846200
H	-1.75529000	-0.59328000	-0.70620200
H	-1.61246100	-0.44669200	1.03691200
C	0.22040300	-0.03385600	-0.03091400
H	0.59304700	-1.06001900	0.02622900
H	0.55345200	0.38692700	-0.98470900
H	0.69969300	0.53902700	0.76961500
O	-4.25673600	0.33598700	-1.91890000
O	-3.94115300	1.21876300	-2.98095300
H	-4.78500800	1.66695100	-3.14029400

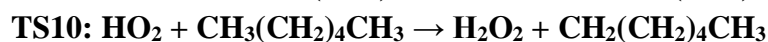
HO₂-R9: HO₂ + CH₃(CH₂)₃CH₃ → H₂O₂ + CH₃CH₂CHCH₂CH₃

TS9: HO₂ + CH₃(CH₂)₃CH₃ → H₂O₂ + CH₃CH₂CHCH₂CH₃

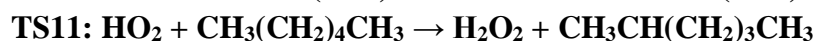
C	-3.96262100	3.02364500	0.52308400
H	-3.72982300	3.19953400	1.57789200
H	-3.51969200	3.83472700	-0.05960100
H	-5.04809000	3.07873700	0.40794700
C	-3.43044300	1.66438600	0.05918700
H	-3.91852800	0.86184100	0.63557300

H	-3.71150900	1.48996100	-0.98629900
C	-1.93480400	1.50450900	0.20579200
H	-1.42781500	2.42410500	-0.64884800
H	-1.53539800	1.89446900	1.14837300
C	-1.32479900	0.18800400	-0.21638000
H	-1.60815800	-0.02806500	-1.25426400
H	-1.78845400	-0.61245800	0.38200400
C	0.19737800	0.12021000	-0.05729100
H	0.58293200	-0.85388600	-0.36913200
H	0.69216200	0.88846900	-0.65747600
H	0.49107800	0.27576800	0.98515900
O	-1.01880500	3.20576700	-1.44841400
O	-1.61074500	2.82083700	-2.67731600
H	-0.89071300	2.34669300	-3.11892900

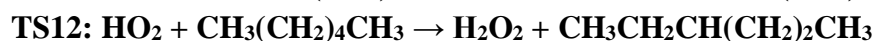
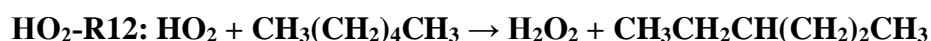
2.2.6 C6 (*n*-C₆H₁₄)



C	-1.98870100	1.42727500	-0.33561800
H	-2.12100900	1.20046700	-1.39494500
H	-2.55019300	0.29985000	0.22506200
H	-2.66566700	2.20194500	0.02425700
C	-0.56863900	1.49791000	0.15758100
H	-0.13204900	2.44906600	-0.19161200
H	-0.56060200	1.55962200	1.25254400
C	0.31978500	0.33695100	-0.30773300
H	-0.11115900	-0.60664200	0.04395900
H	0.30476000	0.29142000	-1.40418700
C	1.76835800	0.45366200	0.17730200
H	2.19498000	1.40346600	-0.17195600
H	1.78071100	0.50024600	1.27410700
C	2.66342700	-0.70122300	-0.28629300
H	2.23787900	-1.64901100	0.06427100
H	2.65051600	-0.74955400	-1.38200600
C	4.10980000	-0.57851000	0.20157800
H	4.15882600	-0.56408100	1.29504600
H	4.72120000	-1.41574800	-0.14634600
H	4.57315200	0.34440800	-0.16165600
O	-3.03092000	-0.63500400	0.72317800
O	-3.01608000	-1.64571800	-0.27010400
H	-3.92952000	-1.63607000	-0.59202800



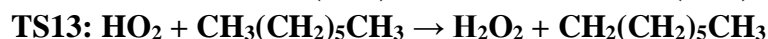
C	-3.63919900	2.58704400	-0.31661700
H	-3.53408100	3.02248600	0.68120700
H	-3.18655400	3.28924600	-1.03138600
H	-4.70419200	2.52024200	-0.54929400
C	-2.96470300	1.24052300	-0.40219500
H	-3.63847500	0.48636600	0.49462000
H	-3.19484100	0.68276100	-1.31495800
C	-1.51404800	1.16196700	0.01236000
H	-0.94083400	1.87493800	-0.60357000
H	-1.41038700	1.52578500	1.04351500
C	-0.88712500	-0.23094800	-0.12009500
H	-1.46034200	-0.94593700	0.48234100
H	-0.97989700	-0.56938400	-1.15992100
C	0.58721000	-0.27750800	0.29654900
H	1.15623600	0.44009200	-0.30711700
H	0.68021600	0.06070400	1.33601900
C	1.21029400	-1.66917700	0.15592700
H	1.16728700	-2.01886300	-0.88030800
H	2.25974600	-1.66915300	0.46284200
H	0.68338400	-2.40326200	0.77356900
O	-4.22872300	-0.13467800	1.32076500
O	-3.93074900	0.50651800	2.54861600
H	-3.26159200	-0.07790700	2.93457900



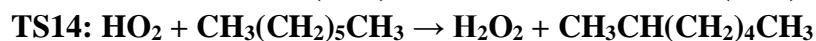
C	-3.44998600	2.82622200	0.42267500
H	-3.15391000	3.14644000	1.42654400
H	-3.04182700	3.54326900	-0.29338700
H	-4.54037300	2.87521200	0.36595900
C	-2.94863400	1.41025700	0.12347700
H	-3.40250300	0.70121400	0.83462100
H	-3.29195000	1.09392700	-0.86867400
C	-1.44699300	1.25657700	0.20200500
H	-0.99171300	2.05512800	-0.79090900
H	-0.99311100	1.76044000	1.06217600
C	-0.86780800	-0.10977500	-0.08156900
H	-1.29961800	-0.82398900	0.63924200
H	-1.20933300	-0.45489100	-1.06678800
C	0.66213600	-0.18546300	-0.00202000
H	1.09561700	0.52612900	-0.71311000

H	0.98528500	0.14446700	0.99233900
C	1.20724300	-1.58960500	-0.27662800
H	0.92572800	-1.93636500	-1.27618700
H	2.29842200	-1.61180200	-0.21373200
H	0.81825500	-2.31499100	0.44497900
O	-0.63240100	2.72817000	-1.70603400
O	-1.28662900	2.18781700	-2.84114800
H	-0.58796500	1.66104500	-3.25666900

2.2.7 C7 (*n*-C₇H₁₆)



C	-2.74081800	-1.27969300	0.39427900
H	-2.81939400	-1.02728900	1.45310600
H	-3.15161500	-0.09533300	-0.17796400
H	-3.52536000	-1.95683800	0.05668200
C	-1.35426400	-1.54874100	-0.12588600
H	-1.04758300	-2.55216400	0.21497400
H	-1.37710600	-1.60855200	-1.22079100
C	-0.30457700	-0.52265600	0.31995100
H	-0.62260000	0.47563800	0.00064800
H	-0.27083500	-0.49759000	1.41665400
C	1.09657100	-0.81515500	-0.22656700
H	1.05887500	-0.83452800	-1.32342400
H	1.40780400	-1.82124100	0.08480900
C	2.15130300	0.20175600	0.22322800
H	2.19513200	0.21763400	1.32016200
H	1.83595400	1.20784000	-0.08180000
C	3.55198300	-0.07814100	-0.33285000
H	3.50780400	-0.09338600	-1.42868000
H	3.86746700	-1.08359500	-0.02789000
C	4.59877300	0.94364400	0.12062000
H	4.68896700	0.95997300	1.21147500
H	5.58595000	0.71440400	-0.29038900
H	4.33087800	1.95439600	-0.20308000
O	-3.50742600	0.88549100	-0.69419400
O	-3.19358100	1.92971500	0.21100300
H	-4.05011400	2.11290600	0.62438300



C	-4.31894100	3.05553700	0.20225900
H	-3.93443900	3.74952500	0.96323100

H	-4.11811800	3.50729800	-0.77401200
H	-5.40132100	2.99028600	0.33945600
C	-3.65455100	1.70748100	0.33213400
H	-3.96573400	1.14177800	1.21547600
H	-4.22214500	0.94599600	-0.62973500
C	-2.17362400	1.63168300	0.04250800
H	-1.98380600	2.00739000	-0.97097700
H	-1.65463900	2.33178900	0.71885300
C	-1.56700700	0.23229100	0.20153700
H	-2.08557500	-0.46009900	-0.47069800
H	-1.75384200	-0.12737100	1.22159300
C	-0.06196900	0.19082700	-0.08299100
H	0.45562300	0.89351700	0.58367900
H	0.12254300	0.54856100	-1.10417200
C	0.55359200	-1.20364400	0.08002500
H	0.03612500	-1.90497700	-0.58534600
H	0.37060600	-1.56151600	1.10054800
C	2.05677400	-1.23809900	-0.21077900
H	2.60587400	-0.57360800	0.46408700
H	2.46478200	-2.24535300	-0.08911800
H	2.26816300	-0.91567600	-1.23526200
O	-4.72068400	0.31607700	-1.50780800
O	-4.53141900	1.09312800	-2.67705700
H	-5.39535200	1.51613800	-2.79132200

HO₂-R15: HO₂ + CH₃(CH₂)₅CH₃ → H₂O₂ + CH₃CH₂CH(CH₂)₃CH₃

TS15: HO₂ + CH₃(CH₂)₅CH₃ → H₂O₂ + CH₃CH₂CH(CH₂)₃CH₃

C	-4.24807300	3.13116100	0.09807700
H	-3.90834000	3.65651400	0.99592400
H	-3.91981500	3.70763000	-0.76949200
H	-5.34103400	3.12568300	0.10891400
C	-3.69497300	1.70319900	0.05315700
H	-4.06891700	1.13826500	0.92248500
H	-4.08364700	1.17782800	-0.82734100
C	-2.18517700	1.62075600	0.05812900
H	-1.80941800	2.23615500	-1.08818400
H	-1.70972300	2.29327600	0.78086000
C	-1.56050300	0.24541000	0.00085200
H	-1.93754400	-0.29260100	-0.87838900
H	-1.91866000	-0.32933800	0.87121800
C	-0.02698500	0.23942400	-0.00441000
H	0.33838800	0.77648800	0.88061900
H	0.33119500	0.79928300	-0.87600600

C	0.57484900	-1.17005900	-0.02375100
H	0.20663200	-1.70641400	-0.90657600
H	0.21195600	-1.73099000	0.84629200
C	2.10614900	-1.17087900	-0.02902100
H	2.50504500	-0.67057600	0.85918400
H	2.50520600	-2.18876300	-0.04364900
H	2.49816100	-0.64778500	-0.90689900
O	-1.48768700	2.72674100	-2.12428500
O	-1.29280900	4.10345300	-1.85353900
H	-0.32980900	4.16938400	-1.77384200

HO₂-R16: HO₂ + CH₃(CH₂)₅CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₂CH₃

TS16: HO₂ + CH₃(CH₂)₅CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₂CH₃

C	-4.19561700	3.12376400	-0.00694500
H	-3.80046300	3.76890900	0.78459700
H	-3.94275500	3.58401600	-0.96708300
H	-5.28532300	3.11999400	0.08126100
C	-3.62548000	1.70627500	0.09180200
H	-3.92279000	1.25653000	1.04684400
H	-4.05793200	1.07901500	-0.69386800
C	-2.09693300	1.66981000	-0.02610000
H	-1.78869000	2.13025100	-0.97341500
H	-1.65711800	2.29924200	0.76579700
C	-1.49306300	0.28834700	0.07790300
H	-1.95999200	-0.34838300	-1.02030200
H	-1.94383200	-0.33806500	0.85499700
C	0.01177200	0.17545300	0.00055800
H	0.44474000	0.77442300	0.81896500
H	0.36827100	0.65147400	-0.92282400
C	0.55071400	-1.25800100	0.09285400
H	0.11852600	-1.85797600	-0.71523600
H	0.20143200	-1.71095900	1.02821300
C	2.07879700	-1.32864900	0.03024200
H	2.53649200	-0.76443700	0.84902100
H	2.43186100	-2.36089300	0.10066900
H	2.45740700	-0.91229500	-0.90873500
O	-2.35435400	-0.85456200	-2.02488100
O	-2.00418200	0.05135200	-3.05709400
H	-1.21094100	-0.35581200	-3.43553300

2.2.8 C8 (*n*-C₈H₁₈)

HO₂-R17: HO₂ + CH₃(CH₂)₆CH₃ → H₂O₂ + CH₂(CH₂)₆CH₃

TS17: HO₂ + CH₃(CH₂)₆CH₃ → H₂O₂ + CH₂(CH₂)₆CH₃

C	-3.38401900	-1.23271300	0.33778700
H	-3.47816500	-0.99451500	1.39864400
H	-3.74886700	-0.02795200	-0.22288800
H	-4.18041700	-1.88122100	-0.02717700
C	-1.99507300	-1.53495400	-0.15673700
H	-1.99504900	-1.57616800	-1.25273500
H	-1.72672900	-2.55283900	0.17351200
C	-0.92454700	-0.54977000	0.32972300
H	-1.19927700	0.46227500	0.01339700
H	-0.92067900	-0.53773500	1.42718200
C	0.48064500	-0.88449100	-0.18113200
H	0.47374200	-0.88897500	-1.27876900
H	0.74738400	-1.90470600	0.12540500
C	1.55683600	0.08908600	0.31223000
H	1.56936800	0.08834500	1.40995700
H	1.28434500	1.10919700	0.01294600
C	2.96150800	-0.23279900	-0.20938800
H	2.94941100	-0.22996800	-1.30722100
H	3.23434100	-1.25410400	0.08782900
C	4.03877600	0.73969900	0.28418100
H	4.05326300	0.73510100	1.38099100
H	3.76498300	1.76000000	-0.01096100
C	5.43812800	0.41403200	-0.24583100
H	5.46383100	0.44569600	-1.33975400
H	6.18185200	1.12550800	0.12389000
H	5.75517200	-0.58750600	0.06227400
O	-4.06647000	0.97035100	-0.73056400
O	-3.76266800	1.98951100	0.20610600
H	-4.62893400	2.18213100	0.59414600

HO₂-R18: HO₂ + CH₃(CH₂)₆CH₃ → H₂O₂ + CH₃CH(CH₂)₅CH₃

TS18: HO₂ + CH₃(CH₂)₆CH₃ → H₂O₂ + CH₃CH(CH₂)₅CH₃

C	-4.82744100	3.05965600	-0.00626400
H	-4.42296100	3.64336100	0.82658900
H	-4.62288900	3.62454100	-0.92708100
H	-5.91315800	3.00257400	0.10452000
C	-4.20316100	1.68883600	-0.07674300
H	-4.65306600	1.03837200	-0.83234300
H	-4.64660600	1.05099600	1.03234100
C	-2.69623100	1.59914400	-0.01251400
H	-2.28176200	2.15438500	-0.87082000
H	-2.33671000	2.12813600	0.87948000
C	-2.14441400	0.16764500	-0.02778500

H	-2.50830900	-0.34809300	-0.92533500
H	-2.54905800	-0.38524400	0.82766500
C	-0.61356100	0.10981800	0.00528300
H	-0.25182700	0.62563200	0.90422200
H	-0.21037900	0.66948700	-0.84904100
C	-0.05505900	-1.31744800	-0.01675600
H	-0.41509900	-1.83374800	-0.91624100
H	-0.45935100	-1.87773900	0.83610600
C	1.47596900	-1.37922100	0.01997700
H	1.83564700	-0.86572100	0.91999500
H	1.88016600	-0.81811000	-0.83152700
C	2.02462300	-2.80894500	-0.00502200
H	1.71079400	-3.33729700	-0.91094100
H	3.11781700	-2.81868600	0.02269900
H	1.66559200	-3.38545600	0.85342900
O	-5.01902200	0.52780100	2.03314300
O	-6.32508200	1.02755400	2.25717700
H	-6.17831600	1.70546400	2.93337800

HO₂-R19: HO₂ + CH₃(CH₂)₆CH₃ → H₂O₂ + CH₃CH₂CH(CH₂)₄CH₃

TS19: HO₂ + CH₃(CH₂)₆CH₃ → H₂O₂ + CH₃CH₂CH(CH₂)₄CH₃

C	-4.94768600	3.01020700	-0.06919700
H	-4.63279700	3.56991700	0.81415100
H	-4.60225900	3.55736800	-0.95172400
H	-6.04041200	2.99741100	-0.09190200
C	-4.38506400	1.58544900	-0.04933100
H	-4.74561300	1.03705900	-0.93475800
H	-4.77959000	1.03837100	0.81522500
C	-2.87471500	1.51309300	-0.03949300
H	-2.39596000	2.20443800	-0.74200500
H	-2.51560200	2.10529400	1.12405800
C	-2.24176600	0.14085300	-0.00539000
H	-2.58929400	-0.41804500	-0.89023600
H	-2.62265000	-0.41752300	0.85937200
C	-0.70808400	0.14373000	0.01234800
H	-0.36089700	0.68744400	0.89833200
H	-0.33948800	0.70149100	-0.85826100
C	-0.09994000	-1.26278500	0.00690100
H	-0.45314700	-1.80893300	-0.87776100
H	-0.47109300	-1.82084900	0.87626300
C	1.43284400	-1.26801900	0.02301400
H	1.78510900	-0.72350700	0.90748500
H	1.80433700	-0.71008000	-0.84532100

C	2.03331600	-2.67670900	0.01868600
H	1.72685500	-3.23507300	-0.87160700
H	3.12631400	-2.64515500	0.03027900
H	1.70856000	-3.24785900	0.89416000
O	-2.20786200	2.57536400	2.17400000
O	-2.02053200	3.95908700	1.93561500
H	-1.05739400	4.03345900	1.86561200

HO₂-R20: HO₂ + CH₃(CH₂)₆CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₃CH₃

TS20: HO₂ + CH₃(CH₂)₆CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₃CH₃

C	-4.92659600	3.08351600	-0.18763200
H	-4.74730800	3.53453400	0.79324500
H	-4.47598700	3.73788900	-0.94106400
H	-6.00675800	3.07805800	-0.35643800
C	-4.34658000	1.66848600	-0.25886400
H	-4.57370700	1.22785300	-1.23719600
H	-4.83240400	1.03242400	0.48757900
C	-2.83020600	1.63392900	-0.03249700
H	-2.33710700	2.27392100	-0.78349200
H	-2.59163100	2.08360000	0.93982700
C	-2.21617200	0.25525700	-0.11049400
H	-2.60725700	-0.36115800	-0.92685400
H	-2.75946000	-0.39759800	0.94192200
C	-0.72041900	0.14513500	0.07452700
H	-0.43574900	0.60040400	1.03256600
H	-0.23230500	0.76563400	-0.69519600
C	-0.16981800	-1.28381900	-0.01245100
H	-0.44670200	-1.71677200	-0.98206600
H	-0.65576900	-1.90670300	0.74780000
C	1.35114500	-1.36055100	0.15889300
H	1.62782700	-0.92665800	1.12769000
H	1.83305800	-0.73433700	-0.60192000
C	1.89744000	-2.78821600	0.06486900
H	1.66815900	-3.23594300	-0.90720000
H	2.98325300	-2.80956900	0.19201400
H	1.45983500	-3.43110700	0.83503900
O	-3.22221200	-0.91834400	1.90928500
O	-2.93765900	-0.03161400	2.97766900
H	-2.17252500	-0.44867600	3.40059400

2.2.9 C9 (*n*-C₉H₂₀)

HO₂-R21: HO₂ + CH₃(CH₂)₇CH₃ → H₂O₂ + CH₂(CH₂)₇CH₃

TS21: HO₂ + CH₃(CH₂)₇CH₃ → H₂O₂ + CH₂(CH₂)₇CH₃

C	-4.03199800	-1.10234100	0.39667000
H	-4.09371300	-0.81756300	1.44842000
H	-4.34054100	0.10024000	-0.20192900
H	-4.86937400	-1.71923000	0.07067500
C	-2.67107800	-1.50259200	-0.10586500
H	-2.69367900	-1.59503600	-1.19844000
H	-2.45310700	-2.51727500	0.26838800
C	-1.53851600	-0.55794500	0.31640200
H	-1.75284600	0.44848100	-0.05873300
H	-1.52541600	-0.48116800	1.41112700
C	-0.16045400	-1.01005100	-0.17823200
H	-0.17578400	-1.08296700	-1.27338400
H	0.04421400	-2.02365100	0.19114400
C	0.97837000	-0.07737200	0.24918200
H	0.99225400	-0.00208400	1.34426500
H	0.77453300	0.93499100	-0.12181400
C	2.35799000	-0.52930800	-0.24323400
H	2.34411500	-0.60376100	-1.33839100
H	2.55974700	-1.54293300	0.12706400
C	3.49881500	0.40048500	0.18471100
H	3.51267300	0.47700700	1.27991900
H	3.29933100	1.41397400	-0.18699300
C	4.87902600	-0.05263000	-0.30527300
H	4.86578300	-0.12825300	-1.39947200
H	5.07857800	-1.06517200	0.06634600
C	6.01272900	0.88183300	0.12714100
H	6.07529700	0.94963000	1.21793500
H	6.98188000	0.53194800	-0.23943600
H	5.85851400	1.89499500	-0.25752300
O	-4.61179900	1.09844800	-0.73522300
O	-4.29656200	2.12360400	0.19107200
H	-5.16486900	2.35093200	0.55502500

HO₂-R22: HO₂ + CH₃(CH₂)₇CH₃ → H₂O₂ + CH₃CH(CH₂)₆CH₃

TS22: HO₂ + CH₃(CH₂)₇CH₃ → H₂O₂ + CH₃CH(CH₂)₆CH₃

C	-2.17925600	4.47884200	1.45667100
H	-1.32040500	4.68601800	2.10271400
H	-2.03364700	5.05284800	0.53034400
H	-3.07922400	4.86675700	1.94028700
C	-2.30194500	3.00672700	1.15358900
H	-3.20781400	2.74547100	0.59892100
H	-2.61818800	2.43648600	2.33981700
C	-1.06491100	2.28146800	0.67741700

H	-0.74238500	2.74012000	-0.27259800
H	-0.24267900	2.45883000	1.38244300
C	-1.25457200	0.77382500	0.46639600
H	-2.08722500	0.61042100	-0.22937100
H	-1.55286000	0.31095800	1.41400000
C	-0.00011100	0.07684400	-0.07128500
H	0.83452600	0.24893900	0.62065800
H	0.29317400	0.54085800	-1.02221000
C	-0.17963700	-1.43116000	-0.27943500
H	-1.02131700	-1.60415200	-0.96257400
H	-0.46227600	-1.89612000	0.67363300
C	1.06942700	-2.12688000	-0.83167200
H	1.91294100	-1.95185400	-0.15097600
H	1.34984900	-1.66355000	-1.78680600
C	0.89370700	-3.63583500	-1.03718200
H	0.04824100	-3.81125600	-1.71360800
H	0.61919400	-4.10003300	-0.08215300
C	2.14423300	-4.32064800	-1.59636700
H	2.99922400	-4.19254600	-0.92485600
H	1.98618400	-5.39439900	-1.73067300
H	2.42304300	-3.90202000	-2.56867300
O	-2.85726200	1.95549600	3.40157300
O	-3.66371500	2.90576000	4.07395600
H	-3.03049300	3.33879800	4.66542500

HO₂-R23: HO₂ + CH₃(CH₂)₇CH₃ → H₂O₂ + CH₃CH₂CH(CH₂)₅CH₃

TS23: HO₂ + CH₃(CH₂)₇CH₃ → H₂O₂ + CH₃CH₂CH(CH₂)₅CH₃

C	-2.39962900	4.42264900	1.48483300
H	-1.66747900	4.58289000	2.27924200
H	-2.04802200	4.95369400	0.59489800
H	-3.34296700	4.87983600	1.79441200
C	-2.58489100	2.92936700	1.19725000
H	-3.35114400	2.79968800	0.41571100
H	-2.98257300	2.42300600	2.08487000
C	-1.32810400	2.22399100	0.73966200
H	-0.75555300	2.78550900	-0.00711600
H	-0.47734600	2.32903100	1.78827500
C	-1.42262700	0.74361200	0.44874500
H	-2.17401000	0.59844600	-0.34524300
H	-1.82290400	0.22198900	1.32755100
C	-0.10334200	0.09306500	0.01367800
H	0.63944000	0.22462100	0.80855800
H	0.28593600	0.62307800	-0.86524700

C	-0.24114800	-1.39759100	-0.31439800
H	-0.98441700	-1.52720400	-1.11196500
H	-0.64045200	-1.92470000	0.56166100
C	1.07667800	-2.05425300	-0.74011200
H	1.81801400	-1.92859700	0.05972900
H	1.48019900	-1.52521400	-1.61356300
C	0.94259600	-3.54463300	-1.07257200
H	0.20483300	-3.67034500	-1.87447600
H	0.53668000	-4.07286200	-0.20122000
C	2.26530900	-4.19332800	-1.49070800
H	3.01285500	-4.11589300	-0.69485500
H	2.13512700	-5.25444200	-1.72086100
H	2.68000200	-3.70937100	-2.38078700
O	0.25868300	2.36518300	2.72354800
O	0.97109300	3.58380200	2.60638800
H	1.81594800	3.29993700	2.22728500

HO₂-R24: HO₂ + CH₃(CH₂)₇CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₄CH₃

TS24: HO₂ + CH₃(CH₂)₇CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₄CH₃

C	-2.45045100	4.50093900	1.34852900
H	-1.83635600	4.61724100	2.24690500
H	-1.96968700	5.06498300	0.54256200
H	-3.41924100	4.96693400	1.54745700
C	-2.61051200	3.02425200	0.97802000
H	-3.25666600	2.93511700	0.09626400
H	-3.11878400	2.49330500	1.78894900
C	-1.27172000	2.33283300	0.69192600
H	-0.75684400	2.86435100	-0.12611600
H	-0.61280500	2.42682900	1.56457700
C	-1.38771800	0.87574800	0.30910700
H	-2.20536000	0.66151900	-0.38730200
H	-1.88312000	0.28887300	1.42241900
C	-0.10960500	0.13108000	-0.00166500
H	0.58148000	0.22219000	0.84704900
H	0.39298700	0.64374800	-0.83843200
C	-0.30398100	-1.34648600	-0.36427100
H	-0.97386000	-1.41819900	-1.23043300
H	-0.81795600	-1.85592100	0.45925800
C	1.00846700	-2.07272600	-0.67787900
H	1.67981100	-2.00013500	0.18814600
H	1.52146300	-1.55855500	-1.50131500
C	0.82037900	-3.54879600	-1.04592100
H	0.15199800	-3.62159900	-1.91247900

H	0.30766700	-4.06286200	-0.22390600
C	2.13643400	-4.26777500	-1.35582300
H	2.81309600	-4.24396200	-0.49564100
H	1.96719100	-5.31645200	-1.61521800
H	2.65581000	-3.79757600	-2.19690400
O	-2.27157300	-0.19639800	2.43959700
O	-1.32724500	0.19641300	3.42073200
H	-0.77976500	-0.59684900	3.51673900

HO₂-R25: HO₂ + CH₃(CH₂)₇CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₃CH₃

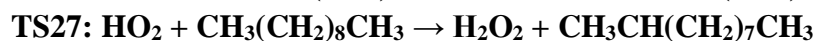
TS25: HO₂ + CH₃(CH₂)₇CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₃CH₃

C	-2.28978000	4.57437700	1.19920800
H	-1.40105000	4.90730100	1.74443900
H	-2.21927400	4.97037200	0.18125300
H	-3.16178300	5.03259900	1.67382500
C	-2.39497500	3.04663900	1.19208500
H	-3.31122900	2.74608500	0.66924100
H	-2.50092200	2.68325500	2.22172300
C	-1.19051200	2.36215600	0.53633500
H	-1.08395500	2.72667900	-0.49330600
H	-0.27282800	2.65670600	1.05893600
C	-1.29424600	0.83213300	0.51834900
H	-2.21295600	0.54047600	-0.01704600
H	-1.42477700	0.45186900	1.54038300
C	-0.12480000	0.13164200	-0.13447500
H	0.94467300	0.41303000	0.64398400
H	0.20419400	0.59869800	-1.06874500
C	-0.14800700	-1.37879600	-0.17663200
H	-1.07079500	-1.69456500	-0.69166600
H	-0.23290700	-1.76839200	0.84574800
C	1.06200000	-2.01272300	-0.87315000
H	1.97645500	-1.69640200	-0.35968400
H	1.13280800	-1.62585700	-1.89808600
C	1.00242000	-3.54362000	-0.91362600
H	0.08307500	-3.85837200	-1.42320700
H	0.92946700	-3.92703500	0.11118900
C	2.21226400	-4.17462500	-1.60865500
H	3.14330200	-3.90739600	-1.09941200
H	2.14150800	-5.26582400	-1.62127400
H	2.29424600	-3.83513000	-2.64614000
O	1.86376800	0.61425300	1.37646500
O	1.60295600	-0.17722800	2.52291400
H	1.25592700	0.47139600	3.15306900

2.2.10 C10 (*n*-C₁₀H₂₂)



C	4.66221300	-1.07601800	-0.35731300
H	4.73362900	-0.79808600	-1.41028300
H	4.94996100	0.13469300	0.23531800
H	5.50243800	-1.68094200	-0.01652900
C	3.29982400	-1.48817600	0.13148700
H	3.09875500	-2.50857000	-0.23657200
H	3.30956500	-1.57095400	1.22505000
C	2.16171300	-0.56076100	-0.31339000
H	2.35919600	0.45120100	0.05608400
H	2.16212100	-0.49316400	-1.40879300
C	0.78263200	-1.02513500	0.16678400
H	0.59484000	-2.04416100	-0.19659200
H	0.78408700	-1.08864800	1.26262500
C	-0.36121900	-0.10974100	-0.28396200
H	-0.17508500	0.90775800	0.08229000
H	-0.36004100	-0.04266400	-1.37967800
C	-1.74225100	-0.57509700	0.19153800
H	-1.92607500	-1.59377000	-0.17415400
H	-1.74378400	-0.64148800	1.28726900
C	-2.88799500	0.33749300	-0.26047100
H	-2.70721200	1.35505500	0.10927600
H	-2.88340300	0.40789700	-1.35603500
C	-4.26946900	-0.13254000	0.20865200
H	-4.27538000	-0.20315000	1.30429300
H	-4.45041600	-1.15035400	-0.16120600
C	-5.41703700	0.77795700	-0.24304600
H	-5.23923900	1.79402100	0.12973200
H	-5.40961600	0.85091100	-1.33751100
C	-6.79327000	0.29639500	0.22584500
H	-7.58869100	0.96591500	-0.11342300
H	-7.01432300	-0.70401600	-0.15968500
H	-6.84426800	0.24732600	1.31824600
O	5.19824200	1.14112900	0.76412400
O	4.89465900	2.15311500	-0.18032900
H	5.76889000	2.38497100	-0.52682300



C	-5.68173100	4.08286700	0.06616200
H	-5.40614600	4.65147700	0.96582700

H	-5.33117600	4.65802900	-0.79628000
H	-6.77324200	4.03654200	0.03315300
C	-5.06245200	2.70772200	0.09869600
H	-5.51081200	2.03524800	0.83611100
H	-5.49000900	2.10865200	-1.03515400
C	-3.55605700	2.62164900	0.02322000
H	-3.20922900	3.13767400	-0.88112100
H	-3.13673100	3.19343100	0.86835600
C	-2.99962900	1.19291900	0.05410000
H	-3.34869500	0.68988100	0.96506000
H	-3.41514800	0.62974000	-0.78868400
C	-1.46923700	1.13939500	0.00093500
H	-1.12225300	1.64321700	-0.91030200
H	-1.05525600	1.71191000	0.84155600
C	-0.90669300	-0.28625600	0.03491700
H	-1.25573500	-0.79149400	0.94490000
H	-1.31969800	-0.85725300	-0.80634800
C	0.62399300	-0.34325200	-0.01815600
H	0.97280600	0.16081100	-0.92879200
H	1.03664400	0.22973800	0.82255800
C	1.18742300	-1.76841200	0.01743900
H	0.77583500	-2.34188100	-0.82339800
H	0.83865600	-2.27362600	0.92771200
C	2.71814000	-1.82726000	-0.03518100
H	3.06692100	-1.32243600	-0.94434400
H	3.12988900	-1.25593500	0.80582800
C	3.27112900	-3.25515500	-0.00074700
H	4.36407700	-3.26247600	-0.03905700
H	2.96755800	-3.77501600	0.91359100
H	2.90538700	-3.84155100	-0.84969700
O	-5.86152900	1.62341700	-2.05648300
O	-5.52060700	2.56220200	-3.06117000
H	-6.36327900	3.01087400	-3.22536900

HO₂-R28: HO₂ + CH₃(CH₂)₈CH₃ → H₂O₂ + CH₃CH₂CH(CH₂)₆CH₃

TS28: HO₂ + CH₃(CH₂)₈CH₃ → H₂O₂ + CH₃CH₂CH(CH₂)₆CH₃

C	-5.62778700	4.27060800	0.32641300
H	-5.33941000	4.64758600	1.31263900
H	-5.21211700	4.94451900	-0.42627200
H	-6.71756800	4.31787300	0.25771600
C	-5.12640200	2.83883800	0.11440500
H	-5.58909400	2.17299200	0.86073200
H	-5.45989100	2.46595600	-0.86123500

C	-3.62604900	2.68786500	0.21822200
H	-3.15711500	3.42832600	-0.81247200
H	-3.18117900	3.23856000	1.05398600
C	-3.04561800	1.30714700	0.01678000
H	-3.49956200	0.63062000	0.75973200
H	-3.36355100	0.91637900	-0.95903400
C	-1.51883500	1.23336900	0.14064900
H	-1.06324200	1.91276000	-0.58930800
H	-1.22108800	1.60666100	1.12856600
C	-0.96067800	-0.18069200	-0.05571300
H	-1.42069800	-0.85728100	0.67623700
H	-1.26030200	-0.55518800	-1.04330900
C	0.56453500	-0.25997600	0.07240500
H	1.02453700	0.41591900	-0.66002900
H	0.86400200	0.11469600	1.05969500
C	1.12461000	-1.67353200	-0.12254900
H	0.82383100	-2.04991900	-1.10912800
H	0.66668300	-2.34942500	0.61156400
C	2.65014400	-1.75430200	0.00235500
H	3.10809300	-1.08001900	-0.73156800
H	2.95143100	-1.37934800	0.98802100
C	3.19923700	-3.17051300	-0.19438700
H	4.28855200	-3.19408400	-0.10136200
H	2.78763900	-3.86123200	0.54845800
H	2.94209100	-3.56000900	-1.18458500
O	-2.79170600	4.05490800	-1.75787400
O	-3.40351900	3.43134400	-2.87410500
H	-2.68334700	2.89516000	-3.23756200

HO₂-R29: HO₂ + CH₃(CH₂)₈CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₅CH₃

TS29: HO₂ + CH₃(CH₂)₈CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₅CH₃

C	-5.76642700	4.05918100	0.17492000
H	-5.34101300	4.70026700	0.95354200
H	-5.56153300	4.53340200	-0.79027300
H	-6.85083000	4.04516000	0.31293500
C	-5.17948700	2.64637900	0.23592400
H	-5.42954100	2.18755500	1.19979400
H	-5.64669400	2.01755900	-0.52962900
C	-3.65708600	2.62073700	0.05022800
H	-3.38770500	3.09359200	-0.90382600
H	-3.19140200	3.25139200	0.82573400
C	-3.03609700	1.24498700	0.12553800
H	-3.42287800	0.63019400	0.94516600

H	-3.54147700	0.56113000	-0.92576100
C	-1.54112800	1.14203800	-0.06941900
H	-1.27559200	1.54848000	-1.05353800
H	-1.05181300	1.80308100	0.66539000
C	-0.97800500	-0.27722700	0.07471900
H	-1.24189600	-0.67045600	1.06490100
H	-1.46376700	-0.93127000	-0.65748000
C	0.54193500	-0.34310000	-0.10794900
H	0.80251800	0.04494800	-1.10087900
H	1.02534500	0.32541300	0.61684400
C	1.11600300	-1.75576700	0.04850600
H	0.63336000	-2.42464200	-0.67561000
H	0.85537100	-2.14507100	1.04144700
C	2.63603800	-1.82540100	-0.13587500
H	2.89612600	-1.44073800	-1.12948300
H	3.11813100	-1.15398100	0.58534700
C	3.20146700	-3.23944300	0.02788800
H	4.28627500	-3.25543800	-0.10983700
H	2.98739400	-3.63759600	1.02486400
H	2.76380600	-3.92728500	-0.70252900
O	-3.94235800	-0.00557600	-1.89519000
O	-3.32700700	0.65302000	-2.98895700
H	-4.03449000	1.22949000	-3.31364100

HO₂-R30: HO₂ + CH₃(CH₂)₈CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₄CH₃

TS30: HO₂ + CH₃(CH₂)₈CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₄CH₃

C	-5.93819800	4.08913100	0.56520100
H	-5.54732600	4.71274400	1.37555600
H	-5.68054400	4.57637400	-0.38038500
H	-7.02845000	4.08257600	0.64852900
C	-5.36391000	2.67105800	0.63095200
H	-5.66795600	2.19667100	1.57214200
H	-5.80043700	2.06333500	-0.17081700
C	-3.83613400	2.63287500	0.51544000
H	-3.53109200	3.10211600	-0.42683700
H	-3.39767100	3.23835300	1.31944600
C	-3.25771700	1.21381600	0.58063800
H	-3.57423900	0.73985500	1.52461300
H	-3.69448500	0.59737000	-0.21551000
C	-1.74946200	1.14272900	0.50285200
H	-1.43423800	1.63726800	-0.71704100
H	-1.23864000	1.88103200	1.13084600
C	-1.11391800	-0.22844000	0.53350500

H	-1.42083600	-0.72723000	1.46823400
H	-1.53129400	-0.84091200	-0.27580400
C	0.41741100	-0.22534300	0.44562300
H	0.72504700	0.27451800	-0.47863500
H	0.82319900	0.37581200	1.26941500
C	1.02483000	-1.63114200	0.49717000
H	0.62129100	-2.23001900	-0.32970800
H	0.70610100	-2.13406400	1.42007800
C	2.55584200	-1.63934300	0.42244700
H	2.87315600	-1.13480300	-0.49788600
H	2.96012600	-1.04359300	1.25002600
C	3.15634800	-3.04736800	0.46687900
H	4.24816800	-3.01815200	0.41183400
H	2.88448000	-3.56527200	1.39230800
H	2.79836900	-3.65654400	-0.36919200
O	-1.20597700	2.03647100	-1.81653900
O	0.04195600	2.70117500	-1.73481800
H	-0.21708900	3.63272400	-1.67802900

2.2.11 C11 (*n*-C₁₁H₂₄)

HO₂-R31: HO₂ + CH₃(CH₂)₉CH₃ → H₂O₂ + CH₂(CH₂)₉CH₃

TS31: HO₂ + CH₃(CH₂)₉CH₃ → H₂O₂ + CH₂(CH₂)₉CH₃

C	-5.30946800	-0.95251700	0.38403200
H	-5.36654600	-0.65338500	1.43204100
H	-5.53745100	0.26091400	-0.22892300
H	-6.17814500	-1.52166300	0.05321900
C	-3.96855600	-1.43696600	-0.09842300
H	-3.81593200	-2.46039600	0.28403100
H	-3.98313800	-1.53462700	-1.19073300
C	-2.78788000	-0.55761400	0.33293200
H	-2.94422600	0.45972900	-0.04165400
H	-2.77786100	-0.48335300	1.42786700
C	-1.43328300	-1.08251800	-0.15427200
H	-1.44499800	-1.14919500	-1.24985800
H	-1.28600000	-2.10746400	0.21120200
C	-0.24894500	-0.21450600	0.28551500
H	-0.23454400	-0.15128300	1.38135400
H	-0.39988800	0.81080200	-0.07525100
C	1.10727500	-0.73058700	-0.20845400
H	1.09336400	-0.79059300	-1.30446800
H	1.25618500	-1.75770600	0.14952700
C	2.29233500	0.13493400	0.23457900
H	2.30706500	0.19399000	1.33068000

H	2.14262300	1.16218500	-0.12205800
C	3.64868000	-0.37916300	-0.26139700
H	3.63402900	-0.43719400	-1.35756100
H	3.79794500	-1.40696600	0.09438800
C	4.83410100	0.48524700	0.18215100
H	4.85047000	0.54294400	1.27847500
H	4.68555700	1.51353400	-0.17269100
C	6.19081900	-0.02711600	-0.31472500
H	6.17518600	-0.08407100	-1.41002700
H	6.34022600	-1.05424700	0.04014800
C	7.36871700	0.84306200	0.13345000
H	7.43330000	0.88952700	1.22525200
H	8.31986900	0.45185500	-0.23851000
H	7.26519000	1.86888900	-0.23432400
O	-5.74150200	1.26904900	-0.77246400
O	-5.41047000	2.28023200	0.16364800
H	-6.27926900	2.54999300	0.49608500

HO₂-R32: HO₂ + CH₃(CH₂)₉CH₃ → H₂O₂ + CH₃CH(CH₂)₈CH₃

TS32: HO₂ + CH₃(CH₂)₉CH₃ → H₂O₂ + CH₃CH(CH₂)₈CH₃

C	-5.47136500	3.26514600	-0.02785900
H	-5.20484800	3.85067500	0.86363700
H	-5.11865200	3.82744400	-0.89786900
H	-6.56236500	3.21178200	-0.06692500
C	-4.84431200	1.89444600	0.03229100
H	-5.29312900	1.23244800	0.77885600
H	-5.26163000	1.27303400	-1.09345200
C	-3.33700600	1.81600600	-0.03301200
H	-2.98803600	2.31585100	-0.94556200
H	-2.92583900	2.40709100	0.80279500
C	-2.77227600	0.39161500	0.03003000
H	-3.18240300	-0.19227900	-0.80122800
H	-3.12049500	-0.09344200	0.95099500
C	-1.24141200	0.34612000	-0.01843400
H	-0.83280200	0.94287100	0.80784000
H	-0.89542100	0.82803200	-0.94178200
C	-0.67024500	-1.07461600	0.05448900
H	-1.07862700	-1.67062600	-0.77155400
H	-1.01754500	-1.55710000	0.97738700
C	0.86087300	-1.12360200	0.00514000
H	1.26874100	-0.52273200	0.82850700
H	1.20798600	-0.64548400	-0.91995600
C	1.43294000	-2.54372600	0.08553400

H	1.02532300	-3.14483100	-0.73757400
H	1.08525500	-3.02162100	1.01068300
C	2.96390700	-2.59366700	0.03692300
H	3.37235300	-1.99003400	0.85814700
H	3.31266600	-2.11943500	-0.88979700
C	3.53710600	-4.01306200	0.12287500
H	3.13054400	-4.61627900	-0.69805500
H	3.18831200	-4.48676700	1.04867600
C	5.06732000	-4.05276600	0.07523200
H	5.50341700	-3.48700300	0.90477200
H	5.44349400	-5.07770300	0.13867200
H	5.44535800	-3.61728300	-0.85520700
O	-5.62351200	0.76784400	-2.10831700
O	-5.27922700	1.68998100	-3.12722700
H	-6.12258400	2.13199300	-3.30536000

HO₂-R33: HO₂ + CH₃(CH₂)₉CH₃ → H₂O₂ + H₂+CH₃CH₂CH(CH₂)₇CH₃

TS33: HO₂ + CH₃(CH₂)₉CH₃ → H₂O₂ + H₂+CH₃CH₂CH(CH₂)₇CH₃

C	-5.47266800	3.37699100	0.07576400
H	-5.13634800	3.88988000	0.98228000
H	-5.11946000	3.94907800	-0.78590700
H	-6.56540800	3.39842700	0.06834300
C	-4.94989900	1.93759600	0.03070700
H	-5.36151700	1.37427000	0.88346600
H	-5.32766300	1.42889000	-0.86430200
C	-3.44314700	1.82055300	0.07755700
H	-3.00597800	2.43724500	-1.04563000
H	-2.97370200	2.46659500	0.82788000
C	-2.84759200	0.43280200	0.00818800
H	-3.20935400	-0.07397900	-0.89543800
H	-3.24557800	-0.15296400	0.85392100
C	-1.31493800	0.39376400	0.04749000
H	-0.96678700	0.89225100	0.96124800
H	-0.91762800	0.97705500	-0.78948500
C	-0.74742900	-1.02909100	-0.00156700
H	-1.09130100	-1.52355100	-0.91924500
H	-1.15755000	-1.61535900	0.83153000
C	0.78346100	-1.07686500	0.05297100
H	1.12773900	-0.58787000	0.97353800
H	1.19186700	-0.48466000	-0.77570200
C	1.35617200	-2.49754200	-0.00961000
H	1.01200400	-2.98551100	-0.93073900
H	0.94657300	-3.09040200	0.81876000

C	2.88700500	-2.54556100	0.04440500
H	3.23254100	-2.06015900	0.96660000
H	3.29699300	-1.95096500	-0.78243100
C	3.46187500	-3.96522800	-0.02335900
H	3.11636700	-4.44997400	-0.94463200
H	3.05365900	-4.55951000	0.80336100
C	4.99200000	-4.00246700	0.02916900
H	5.36675200	-3.55518400	0.95536100
H	5.36973700	-5.02758100	-0.02086300
H	5.42962500	-3.44609700	-0.80583300
O	-2.67296500	2.95515700	-2.06565200
O	-1.41548300	3.55167600	-1.80270400
H	-1.64766100	4.48089500	-1.65868200

HO₂-R34: HO₂ + CH₃(CH₂)₉CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₆CH₃

TS34: HO₂ + CH₃(CH₂)₉CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₆CH₃

C	-5.51389100	3.15036400	0.15354300
H	-5.15458200	3.73535300	1.00615400
H	-5.22140600	3.68252600	-0.75737400
H	-6.60630400	3.14083900	0.19481300
C	-4.94367500	1.72951700	0.17410200
H	-5.27919600	1.21337900	1.08133800
H	-5.34660800	1.15621800	-0.66772200
C	-3.41117000	1.69766200	0.11885300
H	-3.05723700	2.22834200	-0.77525900
H	-3.01052300	2.27108700	0.97129600
C	-2.80769500	0.31258600	0.15631100
H	-3.22652300	-0.29669800	-0.97594100
H	-3.26648900	-0.34922900	0.89854000
C	-1.30235000	0.20426500	0.08109400
H	-0.87257300	0.80812200	0.89781700
H	-0.95174600	0.67295500	-0.84718300
C	-0.76305000	-1.22841900	0.17466500
H	-1.19289500	-1.82645500	-0.63613200
H	-1.10882100	-1.68283600	1.11205600
C	0.76607600	-1.30160600	0.11041500
H	1.19427100	-0.68656200	0.91306600
H	1.10881200	-0.85458100	-0.83143900
C	1.31502300	-2.72871900	0.22148200
H	0.88609400	-3.34394000	-0.57970300
H	0.97222500	-3.17552500	1.16386300
C	2.84410100	-2.80494500	0.15433500
H	3.27351800	-2.18274000	0.95069600

H	3.18746900	-2.36597800	-0.79150700
C	3.39557300	-4.23021000	0.27765700
H	2.96689000	-4.85256900	-0.51725000
H	3.05321300	-4.66799100	1.22336900
C	4.92399900	-4.29705400	0.20910000
H	5.38186400	-3.71085900	1.01232900
H	5.28411400	-5.32549100	0.30226400
H	5.29515800	-3.90027800	-0.74118300
O	-3.54911300	-0.79637100	-2.00945000
O	-2.82765600	-0.08884200	-3.00312400
H	-3.49325300	0.52174900	-3.35304600

HO₂-R35: HO₂ + CH₃(CH₂)₉CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₅CH₃

TS35: HO₂ + CH₃(CH₂)₉CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₅CH₃

C	-5.44351400	3.30950200	0.18825100
H	-5.12239100	3.79246400	1.11670100
H	-5.06537700	3.91054700	-0.64467700
H	-6.53580600	3.34748100	0.15546600
C	-4.93095800	1.86856500	0.10797700
H	-5.35674300	1.28294000	0.93205100
H	-5.29466100	1.40275900	-0.81579300
C	-3.40240700	1.76890800	0.15342500
H	-2.97561600	2.34988300	-0.67220700
H	-3.03780900	2.23236100	1.07940800
C	-2.88491400	0.32725100	0.07402700
H	-3.24493100	-0.14707200	-0.84794400
H	-3.32746300	-0.25932900	0.89630500
C	-1.38169900	0.19087300	0.15738500
H	-0.92277200	0.81675500	0.93076700
H	-0.90544700	0.81973100	-0.94226800
C	-0.80173300	-1.20337400	0.07787800
H	-1.14904600	-1.69032500	-0.84217500
H	-1.22584900	-1.79829500	0.90424600
C	0.72899600	-1.26179900	0.15064500
H	1.06228600	-0.78802600	1.08287900
H	1.15160400	-0.66470600	-0.66390100
C	1.28140500	-2.68985900	0.08131600
H	0.95267600	-3.15883700	-0.85511800
H	0.84604900	-3.29039300	0.89116100
C	2.80980600	-2.75725000	0.16850200
H	3.13979100	-2.29628600	1.10872800
H	3.24430700	-2.14958000	-0.63555500
C	3.36884400	-4.18225400	0.08249300

H	3.04107200	-4.64109500	-0.85829400
H	2.93287300	-4.79039900	0.88469800
C	4.89655000	-4.23974600	0.17237100
H	5.25306900	-3.81985400	1.11836900
H	5.26305400	-5.26804400	0.10662400
H	5.36161900	-3.66882100	-0.63751200
O	-0.53956600	1.36104400	-1.93900700
O	0.71184000	1.94412700	-1.62402200
H	0.47968200	2.87040700	-1.46216400

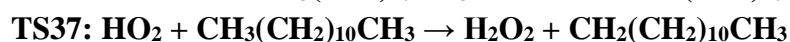
HO₂-R36: HO₂ + CH₃(CH₂)₉CH₃ → H₂O₂ + CH₃(CH₂)₄CH(CH₂)₄CH₃

TS36: HO₂ + CH₃(CH₂)₉CH₃ → H₂O₂ + CH₃(CH₂)₄CH(CH₂)₄CH₃

C	-5.50183200	3.17234000	0.11174700
H	-5.15227400	3.74853300	0.97437000
H	-5.18668600	3.70608600	-0.79056600
H	-6.59509000	3.17413500	0.13296600
C	-4.94388300	1.74630300	0.13520400
H	-5.30463500	1.22742300	1.03155300
H	-5.33943100	1.18470300	-0.71974700
C	-3.41230400	1.69497900	0.10642000
H	-3.05147600	2.21597300	-0.79032200
H	-3.01676400	2.25781700	0.96215700
C	-2.84559100	0.27113100	0.12880800
H	-3.23688000	-0.29347000	-0.72550400
H	-3.20492300	-0.24824700	1.02613800
C	-1.31280800	0.22727600	0.10515700
H	-0.92435700	0.78990500	0.97017000
H	-0.93498700	0.76115800	-0.77707800
C	-0.72239400	-1.16360700	0.14406100
H	-1.11565300	-1.75624800	-1.00612800
H	-1.20705800	-1.82973200	0.86566700
C	0.78353700	-1.28402200	0.10979400
H	1.19488300	-0.69473400	0.94640000
H	1.16402300	-0.80603600	-0.80182700
C	1.30827500	-2.72239400	0.19884000
H	0.89488800	-3.30609200	-0.63073500
H	0.93408700	-3.18591700	1.12076900
C	2.83768500	-2.80868900	0.17358300
H	3.25104200	-2.21123100	0.99725300
H	3.20998400	-2.35012600	-0.75154400
C	3.37172500	-4.24217100	0.27480500
H	2.95900400	-4.83854100	-0.54762600
H	2.99961900	-4.70089800	1.19914800

C	4.90072800	-4.32189000	0.24622200
H	5.34185800	-3.76138000	1.07673600
H	5.24846100	-5.35593700	0.32215200
H	5.30128600	-3.90458100	-0.68304100
O	-1.41322900	-2.24432000	-2.05259500
O	-0.65220400	-1.54027000	-3.01871700
H	-1.29759300	-0.91640200	-3.38277400

2.2.12 C12 (*n*-C₁₂H₂₆)



C	5.93935900	-0.93323700	-0.34549800
H	6.00514300	-0.64137100	-1.39504700
H	6.15133000	0.28659200	0.26044100
H	6.80882300	-1.49319900	-0.00135400
C	4.59713100	-1.42433300	0.12651000
H	4.45598700	-2.45154000	-0.25017700
H	4.60108000	-1.51409800	1.21959300
C	3.41472700	-0.55664200	-0.32333200
H	3.56040800	0.46455900	0.04500500
H	3.41516700	-0.49075000	-1.41883300
C	2.05883400	-1.08697300	0.15425900
H	1.92177800	-2.11550700	-0.20508600
H	2.05997900	-1.14550000	1.25036700
C	0.87355200	-0.22979700	-0.30386700
H	1.01442600	0.79900700	0.05100200
H	0.87004000	-0.17449000	-1.40021800
C	-0.48452300	-0.75074100	0.17975700
H	-0.48161100	-0.80313300	1.27623800
H	-0.62366600	-1.78116100	-0.17264600
C	-1.66993000	0.10469400	-0.28157500
H	-1.67313400	0.15664200	-1.37813500
H	-1.53007200	1.13510300	0.06997800
C	-3.02854200	-0.41422800	0.20292600
H	-3.02548400	-0.46563200	1.29947900
H	-3.16819700	-1.44494600	-0.14823600
C	-4.21387800	0.44107800	-0.25895300
H	-4.21676900	0.49276000	-1.35555500
H	-4.07434700	1.47169100	0.09240700
C	-5.57260900	-0.07752100	0.22496800
H	-5.57094600	-0.12915400	1.32168000
H	-5.71318100	-1.10828100	-0.12621800
C	-6.75877900	0.77682100	-0.23659200

H	-6.76060300	0.82876700	-1.33226600
H	-6.62016600	1.80633000	0.11546800
C	-8.11170900	0.24941900	0.25034200
H	-8.15431100	0.21913600	1.34378000
H	-8.93544400	0.87980700	-0.09626500
H	-8.29466300	-0.76626400	-0.11477100
O	6.33846000	1.30064300	0.79904700
O	6.01521300	2.30164200	-0.15066000
H	6.88725300	2.57509700	-0.47139500

HO₂-R38: HO₂ + CH₃(CH₂)₁₀CH₃ → H₂O₂ + CH₃CH(CH₂)₉CH₃

TS38: HO₂ + CH₃(CH₂)₁₀CH₃ → H₂O₂ + CH₃CH(CH₂)₉CH₃

C	-6.18426800	3.27763300	-0.20620700
H	-5.72038200	3.92553400	0.54338500
H	-6.08787200	3.78439500	-1.17701800
H	-7.25065300	3.20266100	0.01949500
C	-5.52190000	1.92227700	-0.25167000
H	-5.74518600	1.38604300	0.96884200
H	-6.05374600	1.18779300	-0.86470600
C	-4.02080700	1.88731300	-0.42412100
H	-3.77282200	2.40673600	-1.36542900
H	-3.55080900	2.48130700	0.37015300
C	-3.41426800	0.47922900	-0.45086000
H	-3.66605200	-0.03978000	0.47993100
H	-3.88160900	-0.09746800	-1.25942300
C	-1.89386100	0.48183600	-0.64396600
H	-1.64422000	1.01619500	-1.57033200
H	-1.42788700	1.05158300	0.17037200
C	-1.28206400	-0.92251100	-0.69117500
H	-1.74469100	-1.49116900	-1.50835300
H	-1.53661000	-1.45766000	0.23247100
C	0.23999700	-0.92322600	-0.87413200
H	0.70230900	-0.35651700	-0.05550500
H	0.49415000	-0.38496100	-1.79671500
C	0.85216400	-2.32742100	-0.92466100
H	0.38941700	-2.89444600	-1.74290500
H	0.59833700	-2.86536100	-0.00206700
C	2.37428400	-2.32881500	-1.10780400
H	2.83718100	-1.76205100	-0.28947400
H	2.62798100	-1.79049900	-2.03043700
C	2.98650700	-3.73279500	-1.15878600
H	2.52292700	-4.30091300	-1.97601200
H	2.73524300	-4.27125100	-0.23549600

C	4.50826000	-3.73563100	-1.34489000
H	4.97226200	-3.16870700	-0.52852100
H	4.75943800	-3.19855200	-2.26783000
C	5.11070100	-5.14266600	-1.39476900
H	4.69147600	-5.72345200	-2.22259000
H	6.19551900	-5.10893600	-1.52941000
H	4.90805300	-5.69295000	-0.47040500
O	-5.95260500	0.97641900	2.06734000
O	-6.05581600	-0.43047400	1.94261300
H	-7.01381900	-0.57308400	1.94109400

HO₂-R39: HO₂ + CH₃(CH₂)₁₀CH₃ → H₂O₂ + H₂+CH₃CH₂CH(CH₂)₈CH₃

TS39: HO₂ + CH₃(CH₂)₁₀CH₃ → H₂O₂ + H₂+CH₃CH₂CH(CH₂)₈CH₃

C	-6.36580400	3.11379600	-0.57155400
H	-5.78740300	3.82749200	0.02117200
H	-6.30009000	3.42423800	-1.61861700
H	-7.41286300	3.19080400	-0.26733600
C	-5.84023500	1.68653900	-0.38691300
H	-5.96757900	1.36658300	0.65493300
H	-6.45733100	0.99248000	-0.97950500
C	-4.39731400	1.49913000	-0.79540500
H	-4.14055300	1.98396300	-1.74333600
H	-3.68225400	2.27381100	0.05227200
C	-3.79278600	0.12496200	-0.62181300
H	-3.88133100	-0.17948800	0.42879300
H	-4.40405500	-0.59504900	-1.19141200
C	-2.33115500	0.01405000	-1.07142400
H	-2.25514400	0.30733500	-2.12646600
H	-1.72860900	0.73329300	-0.50635300
C	-1.75033100	-1.39308300	-0.89275100
H	-2.35925500	-2.11358800	-1.45484700
H	-1.83061000	-1.68445400	0.16234900
C	-0.28885100	-1.51119000	-1.33812900
H	0.31820700	-0.79018000	-0.77605000
H	-0.20718700	-1.21917100	-2.39327100
C	0.29673000	-2.91638600	-1.15609900
H	-0.30937000	-3.63742700	-1.72008800
H	0.21231600	-3.20889500	-0.10141600
C	1.76004500	-3.03353400	-1.59626600
H	2.36526800	-2.31168500	-1.03270000
H	1.84493000	-2.74168100	-2.65119300
C	2.34756300	-4.43742700	-1.41200000
H	1.74488100	-5.16009900	-1.97779300

H	2.26070400	-4.73091400	-0.35756900
C	3.81247900	-4.55435600	-1.84715100
H	4.41491400	-3.83320300	-1.28139600
H	3.90026700	-4.26203700	-2.90079400
C	4.39035700	-5.96020700	-1.65852000
H	3.82929400	-6.69972600	-2.23884700
H	5.43476700	-6.01026100	-1.97909800
H	4.35061500	-6.26659100	-0.60835000
O	-3.06408300	2.91100700	0.84780300
O	-3.22272600	2.22282400	2.07648600
H	-3.90056600	2.74809900	2.52690900

HO₂-R40: HO₂ + CH₃(CH₂)₁₀CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₇CH₃

TS40: HO₂ + CH₃(CH₂)₁₀CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₇CH₃

C	-7.19976400	2.61065400	-0.14348100
H	-6.65815800	3.18798100	0.61220300
H	-7.13905100	3.16100600	-1.08804900
H	-8.25094100	2.57869500	0.15533300
C	-6.61872300	1.20100800	-0.28167100
H	-6.71347600	0.66767100	0.66925700
H	-7.20386800	0.63337800	-1.01535100
C	-5.14509600	1.20270100	-0.70752800
H	-5.04597200	1.73657300	-1.66754900
H	-4.55230200	1.78038100	0.01314200
C	-4.53722600	-0.17175200	-0.86672400
H	-4.56563000	-0.68251000	0.38516700
H	-5.18931100	-0.89181800	-1.37247600
C	-3.09081200	-0.25049700	-1.29798400
H	-2.99028200	0.27104100	-2.26416300
H	-2.46912700	0.32246200	-0.59703500
C	-2.54459500	-1.67629000	-1.44137000
H	-3.16434100	-2.22689100	-2.16025600
H	-2.65073500	-2.20203000	-0.48529500
C	-1.08096300	-1.72267600	-1.89438100
H	-0.46125400	-1.17022100	-1.17588200
H	-0.97988200	-1.19277400	-2.85045500
C	-0.53106600	-3.14529800	-2.04562400
H	-1.14944400	-3.69723900	-2.76519000
H	-0.63280400	-3.67549100	-1.08995600
C	0.93333300	-3.19230900	-2.49707300
H	1.55114500	-2.63811500	-1.77844500
H	1.03431500	-2.66394600	-3.45399600
C	1.48537700	-4.61427400	-2.64539700

H	0.86971300	-5.16899500	-3.36554900
H	1.38336500	-5.14372700	-1.68907000
C	2.95071800	-4.66243900	-3.09373700
H	3.56589000	-4.10777700	-2.37464000
H	3.05272000	-4.13518400	-4.05011800
C	3.49387000	-6.08721400	-3.23666100
H	2.92260400	-6.65596100	-3.97723300
H	4.54034100	-6.08664500	-3.55416400
H	3.43482900	-6.62940100	-2.28758000
O	-4.55589200	-1.07625100	1.51061900
O	-3.78588800	-0.12653500	2.22738400
H	-2.92711900	-0.56748100	2.30707900

HO₂-R41: HO₂ + CH₃(CH₂)₁₀CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₆CH₃

TS41: HO₂ + CH₃(CH₂)₁₀CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₆CH₃

C	-7.03519100	2.77320900	-0.49797200
H	-6.40363700	3.54674700	-0.04994200
H	-7.18774800	3.04003200	-1.54845600
H	-8.00866300	2.81018100	-0.00139800
C	-6.39298300	1.38937800	-0.36664500
H	-6.28777900	1.13537800	0.69539400
H	-7.06326700	0.63338100	-0.79376900
C	-5.02266000	1.29335700	-1.04709400
H	-5.12776300	1.54976800	-2.10900500
H	-4.34824600	2.04436900	-0.61914600
C	-4.37718300	-0.09243900	-0.92816300
H	-4.28791200	-0.37649300	0.12896600
H	-5.05153900	-0.84307100	-1.37254600
C	-3.02772700	-0.21260400	-1.59898300
H	-2.98473200	0.25230200	-2.58968800
H	-2.21364000	0.62992300	-0.92417800
C	-2.31616100	-1.54279900	-1.51394500
H	-2.97707400	-2.31472800	-1.94276900
H	-2.18655800	-1.81820200	-0.45965200
C	-0.96098400	-1.58212500	-2.23095800
H	-0.30528400	-0.81976600	-1.79683400
H	-1.10271600	-1.30502100	-3.28362300
C	-0.27559300	-2.95050400	-2.15648800
H	-0.93540600	-3.71360800	-2.59028300
H	-0.13917300	-3.22883700	-1.10359800
C	1.08121700	-2.99091200	-2.86877600
H	1.73992700	-2.22972600	-2.43164900
H	0.94599200	-2.70676200	-3.92064500

C	1.77235700	-4.35699200	-2.80084400
H	1.11460300	-5.11904700	-3.23941600
H	1.90787200	-4.64268400	-1.74943400
C	3.13025600	-4.39481200	-3.51140400
H	3.78700900	-3.63353500	-3.07308600
H	2.99515700	-4.10976700	-4.56204900
C	3.81568600	-5.76235800	-3.43901900
H	3.19784200	-6.53958900	-3.90014200
H	4.77936400	-5.75472800	-3.95610500
H	3.99844800	-6.05906900	-2.40129600
O	-1.49310500	1.33010600	-0.28149000
O	-1.31855700	0.65084100	0.95015300
H	-1.92485800	1.12291600	1.53985300

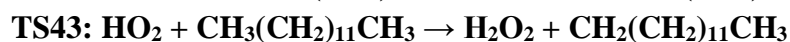
HO₂-R42: HO₂ + CH₃(CH₂)₁₀CH₃ → H₂O₂ + CH₃(CH₂)₄CH(CH₂)₅CH₃

TS42: HO₂ + CH₃(CH₂)₁₀CH₃ → H₂O₂ + CH₃(CH₂)₄CH(CH₂)₅CH₃

C	-7.25634100	2.57366900	-0.24160500
H	-6.66933900	3.27496600	0.35982900
H	-7.35721100	3.00244700	-1.24369000
H	-8.25651500	2.51736800	0.19694900
C	-6.58939000	1.19603200	-0.29293100
H	-6.53529300	0.77853000	0.71980300
H	-7.21741400	0.50790100	-0.87206300
C	-5.18217000	1.22565800	-0.89994500
H	-5.23556600	1.64336600	-1.91397500
H	-4.55426300	1.91474000	-0.32034800
C	-4.50905500	-0.15008900	-0.95018300
H	-4.44992800	-0.56381900	0.06286000
H	-5.13634700	-0.83936900	-1.53026500
C	-3.10213000	-0.11898200	-1.55994400
H	-3.16043800	0.29609200	-2.57975600
H	-2.46719700	0.57772500	-0.99767400
C	-2.42497700	-1.46869900	-1.63874700
H	-3.08155000	-2.27171600	-1.99181300
H	-2.26965400	-1.86013800	-0.35288500
C	-1.03009300	-1.52306700	-2.22013000
H	-0.37334300	-0.84963800	-1.65490300
H	-1.06733900	-1.10980700	-3.24196000
C	-0.41936700	-2.92913200	-2.26637400
H	-1.07415100	-3.58448900	-2.85510000
H	-0.39938900	-3.34633100	-1.25445000
C	0.99256300	-2.95715400	-2.86185600
H	1.64872500	-2.30983300	-2.26574600

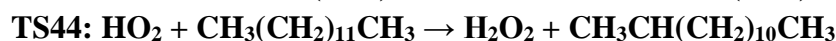
H	0.97298100	-2.52401500	-3.87077400
C	1.59682400	-4.36396000	-2.92776900
H	0.94348100	-5.01087200	-3.52798000
H	1.61026800	-4.79859800	-1.92014300
C	3.01392300	-4.39970000	-3.51161800
H	3.66763800	-3.75646000	-2.90996900
H	3.00095200	-3.96286700	-4.51775700
C	3.60656300	-5.81041300	-3.57592300
H	2.99419300	-6.46864900	-4.20054500
H	4.61692600	-5.80152100	-3.99442400
H	3.66359700	-6.26073800	-2.57990100
O	-2.10935000	-2.13710100	0.79584100
O	-2.18466300	-3.54954100	0.86845800
H	-3.09092700	-3.69844500	1.17612700

2.2.13 C13 (*n*-C₁₃H₂₈)



C	-6.57881300	-0.82710500	0.36816500
H	-6.63416400	-0.52047000	1.41409400
H	-6.75185600	0.39118900	-0.25277000
H	-7.46592400	-1.36337000	0.03145800
C	-5.25320200	-1.36554000	-0.09919200
H	-5.14371800	-2.39261800	0.28831500
H	-5.26117400	-1.46682200	-1.19126000
C	-4.04389700	-0.53020300	0.34021000
H	-4.16096700	0.49226300	-0.03484900
H	-4.03810500	-0.45661800	1.43521200
C	-2.70607000	-1.10297300	-0.13910900
H	-2.71349200	-1.16823600	-1.23480700
H	-2.59727600	-2.13283500	0.22615400
C	-1.49465600	-0.27745600	0.30872100
H	-1.48333200	-0.21762600	1.40478000
H	-1.60908300	0.75341200	-0.04977900
C	-0.15435900	-0.83753400	-0.18052100
H	-0.16554500	-0.89478800	-1.27670900
H	-0.04084400	-1.86976700	0.17583100
C	1.05652700	-0.01218900	0.26934000
H	1.06952500	0.04264100	1.36568700
H	0.94058600	1.02059200	-0.08405500
C	2.39746400	-0.56707500	-0.22425500
H	2.38430200	-0.62123900	-1.32061200
H	2.51377400	-1.60013600	0.12864100

C	3.60771000	0.25921800	0.22565400
H	3.62238400	0.31149400	1.32210000
H	3.48975200	1.29272600	-0.12511900
C	4.94881600	-0.29237600	-0.27131000
H	4.93383200	-0.34462500	-1.36776500
H	5.06733900	-1.32589200	0.07951800
C	6.15867100	0.53457000	0.17773600
H	6.17596300	0.58566200	1.27437200
H	6.04016300	1.56877100	-0.17138100
C	7.50030800	-0.01393100	-0.32128400
H	7.48361300	-0.06493100	-1.41685800
H	7.62023800	-1.04668100	0.02844800
C	8.70238200	0.81995300	0.13172800
H	8.76769100	0.85895900	1.22378300
H	9.64217500	0.40366700	-0.24187600
H	8.62826600	1.85020900	-0.23080700
O	-6.90849200	1.40362700	-0.80426900
O	-6.55855100	2.40655600	0.13382900
H	-7.42305500	2.70944700	0.44847100



C	-4.26466400	0.85007800	-2.65225800
H	-3.80949600	1.65840100	-2.07331800
H	-3.87609400	0.91862000	-3.67857000
H	-5.34183300	1.02764300	-2.69621100
C	-3.94807200	-0.49883400	-2.05641900
H	-4.58799800	-0.48294800	-0.86712700
H	-4.47034800	-1.32999700	-2.54055300
C	-2.50549800	-0.80147600	-1.72325300
H	-1.92219500	-0.76262300	-2.65857700
H	-2.10163500	0.00034200	-1.09230400
C	-2.28089600	-2.16056200	-1.04792100
H	-2.70106900	-2.95147200	-1.68243500
H	-2.84205600	-2.19206700	-0.10713400
C	-0.80410700	-2.46395400	-0.77261800
H	-0.38099500	-1.66583400	-0.14916800
H	-0.24611500	-2.43933800	-1.71780100
C	-0.57632700	-3.81517500	-0.08556000
H	-1.00993800	-4.61272200	-0.70291700
H	-1.12602600	-3.83401500	0.86409900
C	0.90083200	-4.12847800	0.17850900
H	1.33681400	-3.32731200	0.78929900

H	1.44857400	-4.11663400	-0.77275400
C	1.12774000	-5.47482000	0.87552700
H	0.68524100	-6.27549000	0.26860700
H	0.58566800	-5.48342900	1.82993600
C	2.60532200	-5.79346200	1.13094500
H	3.04928000	-4.99078200	1.73402400
H	3.14620900	-5.78910700	0.17572700
C	2.83189600	-7.13695900	1.83359900
H	2.38421900	-7.93934500	1.23274500
H	2.29444300	-7.13950300	2.79073600
C	4.30951300	-7.45874000	2.08371600
H	4.75884500	-6.65592500	2.68297000
H	4.84720000	-7.45894400	1.12651100
C	4.53704600	-8.80060500	2.78927800
H	4.08778000	-9.60301800	2.19135100
H	4.00143300	-8.79956300	3.74643300
C	6.01626100	-9.11390600	3.03306800
H	6.48510400	-8.34721100	3.65813400
H	6.14416900	-10.07617700	3.53676300
H	6.57193300	-9.15585200	2.09086400
O	-5.15180400	-0.43816200	0.18100400
O	-6.46442800	-0.00013400	-0.12131500
H	-6.97095600	-0.82561000	-0.10435200

HO₂-R45: HO₂ + CH₃(CH₂)₁₁CH₃ → H₂O₂ + H₂+CH₃CH₂CH(CH₂)₉CH₃

TS45: HO₂ + CH₃(CH₂)₁₁CH₃ → H₂O₂ + H₂+CH₃CH₂CH(CH₂)₉CH₃

C	-4.20483900	0.82706400	-2.83661600
H	-3.80822300	1.65357500	-2.24237900
H	-3.67632000	0.81680900	-3.79497400
H	-5.25893000	1.03226400	-3.03998500
C	-4.03766600	-0.50505500	-2.09952800
H	-4.60824800	-0.48923500	-1.16342000
H	-4.47749000	-1.31650600	-2.70162000
C	-2.60124200	-0.86884800	-1.80012800
H	-1.91278000	-0.68069000	-2.63090000
H	-2.19641200	0.10032800	-0.94795200
C	-2.34344600	-2.16989200	-1.07591200
H	-2.77968100	-2.98872100	-1.67166200
H	-2.89876900	-2.17750900	-0.12850300
C	-0.86156500	-2.47207600	-0.82007100
H	-0.42031400	-1.65365600	-0.23912500
H	-0.32836700	-2.48425400	-1.77896500
C	-0.62803300	-3.80144400	-0.09400800

H	-1.07796500	-4.61660300	-0.67562900
H	-1.15769400	-3.78828900	0.86755600
C	0.85307500	-4.11288700	0.14930700
H	1.30350100	-3.29755900	0.73003500
H	1.38139500	-4.12663600	-0.81267600
C	1.09058400	-5.44197900	0.87514800
H	0.63798800	-6.25681500	0.29521800
H	0.56468100	-5.42753300	1.83861400
C	2.57233900	-5.75458300	1.11337800
H	3.02532100	-4.93893500	1.69180900
H	3.09757900	-5.77019300	0.14965500
C	2.81152500	-7.08266000	1.84063400
H	2.35770700	-7.89830700	1.26272200
H	2.28735000	-7.06666500	2.80502200
C	4.29331400	-7.39562900	2.07693900
H	4.74810100	-6.58035500	2.65484500
H	4.81814600	-7.41232300	1.11279900
C	4.53435800	-8.72328700	2.80448600
H	4.08080900	-9.53824800	2.22714500
H	4.01057700	-8.70637500	3.76804000
C	6.01762300	-9.02677000	3.03572200
H	6.49123900	-8.24699400	3.64066800
H	6.15521600	-9.97906900	3.55550300
H	6.56183700	-9.08427400	2.08769100
O	-1.89552000	0.93919200	-0.15636300
O	-2.80925600	0.77989900	0.91516700
H	-2.28424800	0.29728000	1.57067500

HO₂-R46: HO₂ + CH₃(CH₂)₁₁CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₈CH₃

TS46: HO₂ + CH₃(CH₂)₁₁CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₈CH₃

C	-4.47894400	0.45607700	-2.95778900
H	-4.08224700	1.33511600	-2.44015100
H	-4.01442500	0.41765400	-3.94855800
H	-5.55152500	0.61281800	-3.10004400
C	-4.20608700	-0.82356800	-2.16304000
H	-4.70337900	-0.76932100	-1.19011100
H	-4.64672300	-1.68108100	-2.68547100
C	-2.70949000	-1.08336500	-1.94816200
H	-2.20979800	-1.14553800	-2.92964800
H	-2.25292400	-0.22325100	-1.44165200
C	-2.39461900	-2.34588000	-1.17840600
H	-2.98446200	-3.21356300	-1.49406700
H	-2.95214500	-2.15042500	0.03976800

C	-0.93929500	-2.65999000	-0.91541000
H	-0.46812300	-1.81279800	-0.40071000
H	-0.42418500	-2.73393800	-1.88760900
C	-0.69736900	-3.95056100	-0.12293300
H	-1.16718300	-4.79014500	-0.65138600
H	-1.20041200	-3.87510700	0.84782000
C	0.78802000	-4.25845700	0.09589700
H	1.25554000	-3.42049500	0.62872100
H	1.29309500	-4.31934900	-0.87695400
C	1.03596500	-5.55447900	0.87580300
H	0.57001900	-6.39274800	0.34153500
H	0.52907800	-5.49460400	1.84752800
C	2.52112100	-5.86165800	1.09930200
H	2.98577900	-5.02538600	1.63750300
H	3.02903400	-5.91619700	0.12766300
C	2.77032800	-7.16120300	1.87315300
H	2.30675900	-7.99765400	1.33400200
H	2.26134200	-7.10750200	2.84428100
C	4.25526800	-7.46736500	2.09830700
H	4.71922200	-6.63228600	2.63941400
H	4.76549900	-7.51957400	1.12757500
C	4.50618300	-8.76809800	2.86972700
H	4.04371200	-9.60286000	2.32891200
H	3.99660300	-8.71592800	3.83963400
C	5.99240000	-9.06500100	3.09026100
H	6.47564000	-8.26398500	3.65874100
H	6.13650500	-9.99745800	3.64319000
H	6.52266200	-9.15883000	2.13723000
O	-3.44051000	-1.98172500	1.11318700
O	-4.71406400	-2.59850500	1.05549400
H	-4.55936800	-3.44520200	1.49965400

HO₂-R47: HO₂ + CH₃(CH₂)₁₁CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₇CH₃

TS47: HO₂ + CH₃(CH₂)₁₁CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₇CH₃

C	-4.31055300	0.60007900	-3.11421200
H	-3.86833700	1.45427400	-2.59232200
H	-3.83814100	0.53470600	-4.09962300
H	-5.37111700	0.81741300	-3.26867400
C	-4.11484200	-0.69378200	-2.31894700
H	-4.62540900	-0.60828100	-1.35222900
H	-4.59937500	-1.52448700	-2.84725100
C	-2.64046700	-1.03615400	-2.07838100
H	-2.12780100	-1.12679100	-3.04488000

H	-2.15519700	-0.20977200	-1.54786800
C	-2.44353000	-2.32906600	-1.27802600
H	-2.93284900	-3.16319700	-1.80856300
H	-2.96055200	-2.24963200	-0.31339100
C	-0.99932700	-2.70523400	-1.03993500
H	-0.52436200	-1.69385900	-0.27768000
H	-0.35635400	-2.58282200	-1.91796500
C	-0.72529700	-3.96728900	-0.25476400
H	-1.19168300	-4.81238600	-0.78770600
H	-1.24326600	-3.91699400	0.71231400
C	0.76227700	-4.27239500	-0.03826500
H	1.23070700	-3.43144000	0.48608700
H	1.25994700	-4.33688600	-1.01407500
C	1.00960600	-5.56733000	0.74326100
H	0.53675400	-6.40595900	0.21566800
H	0.51005400	-5.50386300	1.71888500
C	2.49534200	-5.87851300	0.95687000
H	2.96777600	-5.04040200	1.48522100
H	2.99475700	-5.94118500	-0.01854100
C	2.74566300	-7.17397100	1.73715900
H	2.27398500	-8.01206800	1.20774800
H	2.24542300	-7.11183600	2.71240200
C	4.23128500	-7.48457800	1.95144300
H	4.70357100	-6.64721000	2.48166900
H	4.73248200	-7.54652500	0.97663800
C	4.48361400	-8.78021400	2.73090900
H	4.01297500	-9.61730300	2.20086600
H	3.98288000	-8.71829000	3.70487600
C	5.97050700	-9.08146900	2.94067100
H	6.46207200	-8.27792200	3.49832700
H	6.11561700	-10.01002900	3.49982400
H	6.49186600	-9.18520400	1.98379000
O	-0.15250500	-0.80922700	0.42964800
O	-1.11224500	-0.73782000	1.47017400
H	-0.67014900	-1.19981700	2.19771700

HO₂-R48: HO₂ + CH₃(CH₂)₁₁CH₃ → H₂O₂ + CH₃(CH₂)₄CH(CH₂)₆CH₃

TS48: HO₂ + CH₃(CH₂)₁₁CH₃ → H₂O₂ + CH₃(CH₂)₄CH(CH₂)₆CH₃

C	-4.23812300	0.78663900	-2.90137000
H	-3.87466200	1.61293000	-2.28215000
H	-3.70882700	0.83400200	-3.85846100
H	-5.29899900	0.96300600	-3.09983200
C	-4.01410000	-0.56191000	-2.21093400

H	-4.58128800	-0.59208700	-1.27311000
H	-4.42077200	-1.36512500	-2.83758600
C	-2.53844000	-0.85246700	-1.91451400
H	-1.96920600	-0.82268100	-2.85324900
H	-2.13263000	-0.04757600	-1.28780300
C	-2.30789700	-2.19855200	-1.21954800
H	-2.71152400	-3.00441900	-1.84603100
H	-2.87120700	-2.22923200	-0.28139800
C	-0.82815200	-2.48094000	-0.93023500
H	-0.40884900	-1.67319700	-0.31705700
H	-0.26340100	-2.45544200	-1.87728400
C	-0.56013800	-3.80938500	-0.25982400
H	-1.12273000	-4.64418000	-0.69242900
H	-1.18538500	-3.71995700	0.93731800
C	0.87633600	-4.14664900	0.07008300
H	1.30800700	-3.34661900	0.68510400
H	1.45417500	-4.13739600	-0.86900200
C	1.07287200	-5.49990700	0.76466700
H	0.64496800	-6.29211300	0.13675500
H	0.50523700	-5.50729100	1.70191300
C	2.54265200	-5.82290400	1.05539400
H	2.96934000	-5.02904100	1.68181000
H	3.11081900	-5.80699400	0.11614900
C	2.74700600	-7.17565700	1.74663500
H	2.32034900	-7.97016200	1.12050200
H	2.17869600	-7.19089600	2.68550500
C	4.21614200	-7.49905000	2.04065000
H	4.64332000	-6.70496100	2.66697200
H	4.78564600	-7.48377800	1.10215000
C	4.42222400	-8.85126800	2.73278900
H	3.99770800	-9.64538300	2.10637100
H	3.85217800	-8.86664000	3.66972000
C	5.89253500	-9.16415700	3.02568100
H	6.33568000	-8.40567100	3.67881800
H	6.00476800	-10.13341400	3.51952300
H	6.48264800	-9.19089600	2.10409800
O	-1.67915500	-3.61464900	2.01695900
O	-3.03343800	-3.99957100	1.86223900
H	-3.03263100	-4.91329700	2.18354600

HO₂-R49: $\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_5\text{CH}_3$

TS49: $\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{11}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_5\text{CH}_3$

C	-3.86454600	0.19925300	-3.62886200
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H	-3.39534200	1.05418900	-3.13178600
H	-3.42574600	0.11791000	-4.62850900
H	-4.92692100	0.42849200	-3.75084500
C	-3.65753100	-1.08880300	-2.82673900
H	-4.13671000	-0.98868900	-1.84522400
H	-4.16835400	-1.91868200	-3.33051800
C	-2.18085600	-1.45069100	-2.63038100
H	-1.70129100	-1.55269700	-3.61281600
H	-1.66907100	-0.61971500	-2.12817400
C	-1.96579300	-2.73638200	-1.82456400
H	-2.47892400	-3.56777500	-2.32604400
H	-2.44481800	-2.63113700	-0.84269000
C	-0.48901000	-3.09497800	-1.62666000
H	0.02472200	-2.26894600	-1.12341400
H	-0.00822700	-3.20735000	-2.60697400
C	-0.28524800	-4.37942000	-0.81403000
H	-0.80335700	-5.21347400	-1.31658300
H	-0.77001700	-4.27875800	0.16523200
C	1.16013100	-4.77388500	-0.61662000
H	1.67358900	-3.76029000	0.11720900
H	1.77633900	-4.67289300	-1.51629400
C	1.44068500	-6.02908700	0.17741300
H	0.94134100	-6.87382300	-0.32531100
H	0.95851100	-5.95533300	1.16139000
C	2.92978600	-6.35620800	0.34539400
H	3.43208000	-5.51197100	0.83173400
H	3.38890000	-6.45234200	-0.64658600
C	3.18429900	-7.63678300	1.14800400
H	2.67290400	-8.47803600	0.66214400
H	2.72799200	-7.53898000	2.14185600
C	4.67104300	-7.97379800	1.30697600
H	5.18406900	-7.13138700	1.78892200
H	5.12669500	-8.07686100	0.31354800
C	4.92974700	-9.25041400	2.11513100
H	4.41597800	-10.09192000	1.63445800
H	4.47671800	-9.14624900	3.10868700
C	6.41760400	-9.58068400	2.26578000
H	6.95290200	-8.77223300	2.77381600
H	6.56743100	-10.49449400	2.84743900
H	6.89097800	-9.72698700	1.28973900
O	2.07674200	-2.87147900	0.80216000
O	1.15111300	-2.77797900	1.87155000
H	1.61098000	-3.23686500	2.59000200

2.2.14 C14 (*n*-C₁₄H₃₀)



C	-7.18823900	-0.93570000	0.34504100
H	-7.18492800	-1.26516100	1.38506000
H	-7.38107600	0.41970500	0.50276200
H	-8.09569300	-1.21805700	-0.18897100
C	-5.89517000	-1.08047600	-0.41023000
H	-5.78884500	-2.13601100	-0.71265900
H	-5.95230100	-0.51324900	-1.34735200
C	-4.65323200	-0.65361400	0.38196600
H	-4.76312200	0.39552100	0.67751000
H	-4.60443900	-1.23358000	1.31259300
C	-3.34681600	-0.83257000	-0.39827200
H	-3.39854500	-0.25008700	-1.32700400
H	-3.24506300	-1.88274800	-0.70251700
C	-2.10171500	-0.41307800	0.39130500
H	-2.05156800	-0.99323000	1.32194400
H	-2.20337700	0.63695200	0.69358400
C	-0.79299400	-0.59180900	-0.38638500
H	-0.84288300	-0.01103000	-1.31654700
H	-0.69296400	-1.64215100	-0.68983100
C	0.45297100	-0.17400300	0.40291600
H	0.50127500	-0.75290400	1.33443500
H	0.35418400	0.87685700	0.70428000
C	1.76227800	-0.35621500	-0.37310000
H	1.71450500	0.22291600	-1.30446500
H	1.86034800	-1.40721800	-0.67475400
C	3.00846100	0.06025300	0.41659400
H	3.05401900	-0.51652600	1.34956000
H	2.91218500	1.11213800	0.71543500
C	4.31847600	-0.12726800	-0.35699000
H	4.27401800	0.45009000	-1.28962300
H	4.41388100	-1.17914200	-0.65636400
C	5.56457500	0.28700400	0.43405100
H	5.60624200	-0.28747200	1.36863400
H	5.47135400	1.34005200	0.72991200
C	6.87557300	0.09311600	-0.33586700
H	6.83599900	0.66785400	-1.27054600
H	6.96940000	-0.95995300	-0.63210200
C	8.12198900	0.50574900	0.45560100
H	8.16062100	-0.06656300	1.39055200
H	8.03055000	1.55888800	0.74834900

C	9.42719500	0.30367900	-0.31964900
H	9.43294000	0.88929200	-1.24454400
H	10.29534500	0.60897300	0.27127200
H	9.56553700	-0.74692500	-0.59430100
O	-7.52787800	1.57094500	0.58931400
O	-7.27249200	2.07446300	-0.71093900
H	-8.16476000	2.20909300	-1.06318400

HO₂-R51: HO₂ + CH₃(CH₂)₁₂CH₃ → H₂O₂ + CH₃CH(CH₂)₁₁CH₃

TS51: HO₂ + CH₃(CH₂)₁₂CH₃ → H₂O₂ + CH₃CH(CH₂)₁₁CH₃

C	-6.83626600	3.49867800	-0.30465100
H	-6.36799100	4.19350800	0.39791000
H	-6.76462200	3.94372200	-1.30754200
H	-7.89695700	3.42371800	-0.05349200
C	-6.16202700	2.14994500	-0.27572200
H	-6.43747100	1.67900000	0.95974400
H	-6.66429800	1.39093000	-0.88364500
C	-4.65501600	2.11245800	-0.38244400
H	-4.36900800	2.54426200	-1.35624100
H	-4.22010600	2.77881100	0.37311500
C	-4.04336600	0.71111700	-0.25575100
H	-4.49338600	0.05243300	-1.00960100
H	-4.31099300	0.28847900	0.71931900
C	-2.51931100	0.69822700	-0.41647100
H	-2.07186500	1.37170900	0.32576900
H	-2.25382300	1.10950000	-1.39916600
C	-1.90190300	-0.69686700	-0.26728400
H	-2.35565600	-1.37422600	-1.00244100
H	-2.16173300	-1.10186600	0.71906500
C	-0.37844500	-0.71567500	-0.43624900
H	0.07440500	-0.02853900	0.29022700
H	-0.11938000	-0.32238200	-1.42784500
C	0.24051500	-2.10785500	-0.26670800
H	-0.21704100	-2.79755100	-0.98790800
H	-0.01366600	-2.49698100	0.72768300
C	1.76308900	-2.12972700	-0.44339400
H	2.22023800	-1.43376200	0.27196300
H	2.01680700	-1.74864600	-1.44111200
C	2.38275900	-3.51993500	-0.26063400
H	1.92238800	-4.21746100	-0.97243400
H	2.13247900	-3.89827000	0.73893800
C	3.90466800	-3.54404100	-0.44292000
H	4.36492100	-2.84281300	0.26532800

H	4.15472000	-3.17070500	-1.44450400
C	4.52463700	-4.93285200	-0.25225500
H	4.06335800	-5.63568900	-0.95849000
H	4.27720600	-5.30534700	0.75039900
C	6.04618000	-4.95949600	-0.43742800
H	6.50745600	-4.25690500	0.26739600
H	6.29355200	-4.58946800	-1.43991900
C	6.65603200	-6.35080800	-0.24226000
H	6.23971500	-7.06882700	-0.95603100
H	7.74068000	-6.33570000	-0.38133800
H	6.45563100	-6.73247700	0.76390900
O	-6.68176700	1.29243800	2.05925000
O	-8.07775000	1.47442500	2.21627200
H	-8.42423300	0.58201100	2.06861300

HO₂-R52: HO₂ + CH₃(CH₂)₁₂CH₃ → H₂O₂ + H₂+CH₃CH₂CH(CH₂)₁₀CH₃

TS52: HO₂ + CH₃(CH₂)₁₂CH₃ → H₂O₂ + H₂+CH₃CH₂CH(CH₂)₁₀CH₃

C	-6.70004400	3.93276800	-0.70096800
H	-6.26202600	4.57512400	0.06659000
H	-6.42685300	4.34139800	-1.67884200
H	-7.78764000	3.98920800	-0.60860700
C	-6.21044500	2.48912100	-0.55033100
H	-6.52725900	2.08480500	0.41827400
H	-6.69625100	1.85533300	-1.30975800
C	-4.71431600	2.32705300	-0.69229300
H	-4.28156300	2.90457400	-1.51621400
H	-4.21449900	3.02076900	0.35614300
C	-4.14391400	0.93425900	-0.55540200
H	-4.62498600	0.28848900	-1.30854400
H	-4.43925500	0.51279300	0.41468900
C	-2.62196400	0.85087200	-0.72399500
H	-2.13992500	1.50651500	0.01076700
H	-2.34828000	1.24856700	-1.70930500
C	-2.07097900	-0.57251200	-0.58093700
H	-2.55747300	-1.22602400	-1.31672500
H	-2.34563200	-0.97039700	0.40475700
C	-0.55082600	-0.65998900	-0.75468800
H	-0.06491800	-0.00333900	-0.02144400
H	-0.27680700	-0.26596800	-1.74178200
C	0.00418100	-2.08149700	-0.60578600
H	-0.48008700	-2.73811900	-1.34023000
H	-0.27131600	-2.47568700	0.38101900
C	1.52483800	-2.16725100	-0.77656900

H	2.00807700	-1.50662800	-0.04503800
H	1.80026100	-1.77724100	-1.76496100
C	2.08262800	-3.58684400	-0.61997300
H	1.60180200	-4.24767800	-1.35293100
H	1.80507000	-3.97727900	0.36771800
C	3.60398400	-3.67050700	-0.78606400
H	4.08400500	-3.00731600	-0.05468900
H	3.88165000	-3.28248300	-1.77467000
C	4.16382500	-5.08850600	-0.62469000
H	3.68634200	-5.75256700	-1.35719100
H	3.88515400	-5.47778200	0.36331800
C	5.68568400	-5.17211100	-0.78694400
H	6.16299100	-4.50885500	-0.05524000
H	5.96464000	-4.78486400	-1.77446600
C	6.23535000	-6.59223700	-0.62192000
H	5.80367000	-7.27222900	-1.36329800
H	7.32206700	-6.61765800	-0.74178900
H	6.00116800	-6.99381200	0.36913700
O	-3.81186700	3.59498200	1.31974700
O	-4.34435600	2.88345500	2.42372300
H	-3.59146900	2.34644700	2.71194300

HO₂-R53: HO₂ + CH₃(CH₂)₁₂CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₉CH₃

TS53: HO₂ + CH₃(CH₂)₁₂CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₉CH₃

C	-6.66470800	4.02746400	-0.27101300
H	-6.30590400	4.56265700	0.61379600
H	-6.35031700	4.59657100	-1.15209500
H	-7.75755000	4.03727500	-0.24217800
C	-6.12333600	2.59582000	-0.30811000
H	-6.47681100	2.04340500	0.56755500
H	-6.52654900	2.07352100	-1.18404400
C	-4.59126400	2.54023700	-0.35421900
H	-4.23698600	3.09486400	-1.23956600
H	-4.17499400	3.07247500	0.51064600
C	-4.01343400	1.14429700	-0.41160100
H	-4.53643100	0.47858500	-1.10718400
H	-4.38321900	0.57329400	0.75811400
C	-2.50815500	1.01219300	-0.45585100
H	-2.06964100	1.53055900	0.40651800
H	-2.14258500	1.55808400	-1.34145900
C	-1.99467100	-0.43228800	-0.51145400
H	-2.43030300	-0.93512400	-1.38454800
H	-2.35448400	-0.97499100	0.37003200

C	-0.46709600	-0.52987900	-0.58102300
H	-0.03373000	-0.02912600	0.29423600
H	-0.10697100	0.02469900	-1.45747200
C	0.05230700	-1.97083600	-0.64669100
H	-0.37722400	-2.47062800	-1.52470900
H	-0.31171500	-2.52639200	0.22719800
C	1.58052700	-2.06941800	-0.70684000
H	2.00897400	-1.57283000	0.17335900
H	1.94491500	-1.50943300	-1.57795400
C	2.10238000	-3.50929900	-0.77807100
H	1.67697600	-4.00501900	-1.66035300
H	1.73559200	-4.07056900	0.09114500
C	3.63100900	-3.60593700	-0.83275900
H	4.05581200	-3.11268300	0.05115700
H	3.99782700	-3.04158200	-1.70005300
C	4.15522000	-5.04448300	-0.90860700
H	3.73214100	-5.53838600	-1.79322500
H	3.78877900	-5.61029000	-0.04194700
C	5.68398400	-5.14075700	-0.96228100
H	6.10730800	-4.65027500	-0.07726500
H	6.05037100	-4.57433500	-1.82721300
C	6.19830600	-6.58127300	-1.04168900
H	5.82013300	-7.08742700	-1.93565400
H	7.29077300	-6.61500900	-1.07876600
H	5.87764100	-7.16452000	-0.17254500
O	-4.65539100	0.09698100	1.81606900
O	-5.92988800	-0.49933100	1.65393800
H	-5.71193800	-1.43478300	1.52935500

HO₂-R54: HO₂ + CH₃(CH₂)₁₂CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₈CH₃

TS54: HO₂ + CH₃(CH₂)₁₂CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₈CH₃

C	-6.15136900	5.30590000	0.20488100
H	-5.69664900	5.56041000	1.16720100
H	-5.74172800	5.99007800	-0.54513100
H	-7.22448900	5.50171700	0.28178600
C	-5.87410600	3.84635500	-0.16673700
H	-6.32603800	3.18714400	0.58411200
H	-6.36933200	3.61076800	-1.11704600
C	-4.37945200	3.52748800	-0.27970100
H	-3.92446500	4.18547600	-1.03154300
H	-3.88459800	3.75566700	0.67058000
C	-4.09825100	2.06682300	-0.65149100
H	-4.58994500	1.83454900	-1.61100500

H	-4.56245300	1.40040000	0.08655200
C	-2.63142900	1.72562200	-0.77769200
H	-2.15597700	1.88544900	0.47822000
H	-2.03883500	2.48814800	-1.29418700
C	-2.27299700	0.30893000	-1.16395800
H	-2.73938600	0.08903900	-2.13847800
H	-2.73981000	-0.39130200	-0.45825100
C	-0.76662000	0.03551800	-1.25682600
H	-0.29709100	0.26833200	-0.29401100
H	-0.32166000	0.72453500	-1.98580900
C	-0.43411600	-1.40678700	-1.65468400
H	-0.90997800	-1.63723800	-2.61676600
H	-0.87914400	-2.09582500	-0.92478400
C	1.07026900	-1.68237200	-1.75653800
H	1.54651500	-1.44893100	-0.79556100
H	1.51448300	-0.99593900	-2.48892200
C	1.40501400	-3.12580600	-2.14940500
H	0.92818100	-3.35908600	-3.11026200
H	0.96114400	-3.81218900	-1.41653100
C	2.90941000	-3.40134500	-2.25243900
H	3.38641000	-3.16748300	-1.29180700
H	3.35308900	-2.71534700	-2.98571500
C	3.24488100	-4.84460300	-2.64461200
H	2.76739800	-5.07957100	-3.60494300
H	2.80302800	-5.53162900	-1.91090900
C	4.74902700	-5.12064700	-2.75031300
H	5.22648900	-4.88884100	-1.79046600
H	5.19075900	-4.43351700	-3.48236400
C	5.07385100	-6.56409400	-3.14614500
H	4.63818000	-6.81465500	-4.11862800
H	6.15304400	-6.72734200	-3.21416100
H	4.67621100	-7.27425100	-2.41407900
O	-1.78829500	1.98584300	1.60805500
O	-2.65012600	1.14322600	2.35360700
H	-2.10960900	0.35013700	2.48427300

HO₂-R55: HO₂ + CH₃(CH₂)₁₂CH₃ → H₂O₂ + CH₃(CH₂)₄CH(CH₂)₇CH₃

TS55: HO₂ + CH₃(CH₂)₁₂CH₃ → H₂O₂ + CH₃(CH₂)₄CH(CH₂)₇CH₃

C	-6.31635200	5.07984400	-0.81937300
H	-5.87724600	5.45072100	0.11225800
H	-5.91063700	5.68291200	-1.63806600
H	-7.39341200	5.26375400	-0.77410200
C	-6.01027300	3.59306100	-1.02220400

H	-6.45547000	3.01290600	-0.20521900
H	-6.49428400	3.24263600	-1.94205500
C	-4.50992800	3.28804800	-1.09575100
H	-4.06368400	3.86835300	-1.91454100
H	-4.02587400	3.63995500	-0.17537400
C	-4.19741500	1.80111800	-1.29424300
H	-4.68466400	1.44690600	-2.21169600
H	-4.63245200	1.22180800	-0.47325700
C	-2.69445300	1.50747500	-1.37909200
H	-2.19272100	1.87360200	-0.47431300
H	-2.25924900	2.08591200	-2.21134500
C	-2.34927900	0.05060400	-1.58947100
H	-2.97635700	-0.44895500	-2.33628700
H	-2.80666500	-0.56874500	-0.47642400
C	-0.88484700	-0.31329600	-1.68076100
H	-0.36065100	0.04975900	-0.78745600
H	-0.44597700	0.24502900	-2.52438900
C	-0.60770400	-1.80936900	-1.87451000
H	-1.13661800	-2.16022000	-2.77009300
H	-1.02898000	-2.36425200	-1.02851700
C	0.88360600	-2.13655700	-2.00709200
H	1.41160100	-1.78138500	-1.11280900
H	1.30508900	-1.57560100	-2.85150000
C	1.16803900	-3.63023700	-2.20119400
H	0.63910900	-3.98652200	-3.09479600
H	0.74769800	-4.19043400	-1.35603300
C	2.65950000	-3.95839500	-2.33327000
H	3.18811700	-3.60089400	-1.44009900
H	3.07975000	-3.39819300	-3.17870800
C	2.94609600	-5.45178100	-2.52547300
H	2.41866500	-5.81041300	-3.41918100
H	2.52597800	-6.01286500	-1.68043300
C	4.43759300	-5.78062700	-2.65608600
H	4.96464800	-5.42289500	-1.76317700
H	4.85761400	-5.22083500	-3.50071100
C	4.71418000	-7.27484500	-2.84699600
H	4.22959400	-7.65443800	-3.75225300
H	5.78553200	-7.47565600	-2.93537900
H	4.33567500	-7.85805400	-2.00147500
O	-3.15940700	-1.09814600	0.53104000
O	-4.48520800	-1.53469200	0.29216300
H	-4.36603400	-2.47399900	0.08811200

HO₂-R56: HO₂ + CH₃(CH₂)₁₂CH₃ → H₂O₂ + CH₃(CH₂)₅CH(CH₂)₆CH₃

TS56: HO₂ + CH₃(CH₂)₁₂CH₃ → H₂O₂ + CH₃(CH₂)₅CH(CH₂)₆CH₃

C	-6.15640300	5.32190900	-0.78083900
H	-5.62306300	5.73185700	0.08270900
H	-5.81219500	5.86322900	-1.66792400
H	-7.21952600	5.54218700	-0.64936700
C	-5.90838400	3.81704100	-0.92053600
H	-6.29276600	3.29986800	-0.03295300
H	-6.48362300	3.42953400	-1.77041600
C	-4.42925900	3.46158000	-1.10894000
H	-4.04411900	3.97987500	-1.99699100
H	-3.85386600	3.84918200	-0.25844300
C	-4.17172400	1.95729000	-1.24905600
H	-4.74753500	1.56952000	-2.09995700
H	-4.55690000	1.44110100	-0.36035900
C	-2.69181700	1.60479200	-1.43324500
H	-2.11682800	1.98192100	-0.58069500
H	-2.30341600	2.11991500	-2.32127200
C	-2.44457800	0.09814500	-1.57637300
H	-3.01775500	-0.28431300	-2.43751600
H	-2.84428300	-0.42751000	-0.69988400
C	-0.99483800	-0.28307900	-1.76827300
H	-0.41395900	0.07245000	-0.60049100
H	-0.44684500	0.37489400	-2.45102500
C	-0.67535100	-1.74962700	-1.94600800
H	-1.22599600	-2.11791800	-2.82736800
H	-1.08047500	-2.31690900	-1.09730700
C	0.81604400	-2.06091900	-2.12262900
H	1.36942900	-1.68271200	-1.25521900
H	1.19724200	-1.50828200	-2.99056600
C	1.10653300	-3.55459100	-2.30590700
H	0.54610900	-3.93032500	-3.17190700
H	0.72558800	-4.10682800	-1.43676400
C	2.59473600	-3.87093700	-2.49214300
H	3.15564800	-3.49170300	-1.62818900
H	2.97458700	-3.32268100	-3.36393500
C	2.88724700	-5.36507400	-2.66874100
H	2.32670700	-5.74496900	-3.53298500
H	2.50775300	-5.91403700	-1.79686600
C	4.37509700	-5.68338900	-2.85526900
H	4.93560300	-5.30401100	-1.99218800
H	4.75416300	-5.13636200	-3.72712600
C	4.65731400	-7.17856700	-3.02948500

H	4.13919900	-7.57950900	-3.90650700
H	5.72588200	-7.37172500	-3.15868900
H	4.31979700	-7.74881200	-2.15815600
O	0.04633800	0.35299300	0.46367900
O	-0.76783700	-0.32073600	1.40796200
H	-0.23264200	-1.09573700	1.63425400

2.2.15 C15 (*n*-C₁₅H₃₂)

HO₂-R57: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + CH₂(CH₂)₁₃CH₃

TS57: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + CH₂(CH₂)₁₃CH₃

C	-6.12298800	3.08140600	-1.10927500
H	-5.75721200	3.70918400	-0.29489900
H	-6.06907400	3.56929600	-2.08245200
H	-7.47914700	3.12493500	-0.86712500
C	-5.72349600	1.63094400	-1.06352200
H	-6.28186700	1.07082500	-1.82326600
H	-4.66480900	1.55657900	-1.36459200
C	-5.90359900	0.97157800	0.30987400
H	-5.32375000	1.53109300	1.05502800
H	-6.95292100	1.05659300	0.61223100
C	-5.47868700	-0.50049700	0.33457500
H	-6.05967500	-1.05655900	-0.41251200
H	-4.42807400	-0.58304200	0.02595900
C	-5.65628100	-1.16247900	1.70539000
H	-5.07497300	-0.60739800	2.45309300
H	-6.70616900	-1.07654800	2.01301500
C	-5.23919500	-2.63736900	1.73402300
H	-5.81863800	-3.19137000	0.98409600
H	-4.18803500	-2.72291400	1.42888700
C	-5.42279000	-3.30025600	3.10369000
H	-6.47407600	-3.21460100	3.40770700
H	-4.84445400	-2.74575100	3.85418500
C	-5.00675200	-4.77547000	3.13447100
H	-5.58335100	-5.32949000	2.38231600
H	-3.95453700	-4.86129200	2.83322400
C	-5.19552400	-5.43807900	4.50359800
H	-6.24782400	-5.35175100	4.80414000
H	-4.61942900	-4.88369000	5.25590300
C	-4.78066200	-6.91357500	4.53668100
H	-5.35555800	-7.46786600	3.78340800
H	-3.72770900	-7.00036600	4.23836500
C	-4.97362300	-7.57472900	5.90596800
H	-6.02651800	-7.48674800	6.20396600

H	-4.39857900	-7.02038400	6.65909300
C	-4.56087700	-9.05074200	5.94163400
H	-5.13522200	-9.60520200	5.18802700
H	-3.50751000	-9.13934000	5.64527300
C	-4.75690600	-9.71018100	7.31115600
H	-5.81007100	-9.62082200	7.60842600
H	-4.18176700	-9.15689100	8.06522700
C	-4.34707400	-11.18689200	7.34961500
H	-4.92215400	-11.74027300	6.59710700
H	-3.29470700	-11.27712600	7.05344000
C	-4.54716700	-11.83566600	8.72236500
H	-5.59671800	-11.79363700	9.03050600
H	-4.24512100	-12.88676400	8.71618200
H	-3.95748600	-11.32530600	9.49057100
O	-8.63006000	3.15437200	-0.69732600
O	-8.80601800	3.38747600	0.68946400
H	-9.01125700	4.33360400	0.71832700

HO₂-R58: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + CH₃CH(CH₂)₁₂CH₃

TS58: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + CH₃CH(CH₂)₁₂CH₃

C	-5.16444800	3.10192500	-2.33243500
H	-4.18529700	3.60210900	-2.33228600
H	-5.59298800	3.21887500	-3.33069700
H	-5.80516600	3.63226900	-1.62256300
C	-5.01424900	1.64844300	-1.95854400
H	-6.25555800	1.14282900	-2.12540100
H	-4.46506900	1.05604600	-2.69699100
C	-4.65273100	1.32294500	-0.52757000
H	-3.68305600	1.79734300	-0.30155700
H	-5.37580500	1.79942900	0.14660900
C	-4.56227500	-0.17730500	-0.22143900
H	-5.52406300	-0.65027900	-0.45061300
H	-3.82613900	-0.63746600	-0.89309500
C	-4.18033800	-0.47814600	1.23194500
H	-3.22043400	0.00215400	1.46290000
H	-4.91887100	-0.01848200	1.90125300
C	-4.08323600	-1.97642700	1.54027200
H	-5.04104900	-2.45639900	1.30201700
H	-3.34022500	-2.43538900	0.87505200
C	-3.71401900	-2.28142400	2.99648700
H	-4.45824200	-1.82349800	3.66090600
H	-2.75693500	-1.79994300	3.23594900
C	-3.61649600	-3.77987800	3.30430100

H	-4.57244400	-4.26151600	3.06111100
H	-2.86982300	-4.23733600	2.64214900
C	-3.25354100	-4.08623000	4.76184900
H	-4.00110100	-3.62991200	5.42370200
H	-2.29822500	-3.60353300	5.00582200
C	-3.15481400	-5.58478100	5.06888200
H	-4.10968500	-6.06762500	4.82365800
H	-2.40639800	-6.04079400	4.40770700
C	-2.79374300	-5.89177700	6.52677500
H	-3.54294800	-5.43719100	7.18797200
H	-1.83958400	-5.40770000	6.77247800
C	-2.69276600	-7.39039400	6.83290300
H	-3.64707700	-7.87454700	6.58792900
H	-1.94401000	-7.84488600	6.17103700
C	-2.33028400	-7.69795900	8.29010600
H	-3.07943100	-7.24548700	8.95311200
H	-1.37637800	-7.21322500	8.53621200
C	-2.22640200	-9.19632700	8.59655300
H	-3.17997700	-9.68096100	8.35389700
H	-1.47902700	-9.64878000	7.93327300
C	-1.85997300	-9.49292600	10.05381600
H	-2.60770200	-9.08391500	10.74082700
H	-1.79265500	-10.56866000	10.23898100
H	-0.89407100	-9.04966400	10.31632100
O	-7.36220000	0.72646300	-2.26270200
O	-7.78750000	1.20938800	-3.52467000
H	-7.66940000	0.43654200	-4.09649000

HO₂-R59: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + H₂+CH₃CH₂CH(CH₂)₁₁CH₃

TS59: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + H₂+CH₃CH₂CH(CH₂)₁₁CH₃

C	-5.17116900	2.91897200	-2.46574500
H	-4.13819100	3.27485900	-2.40271500
H	-5.52446100	3.10144500	-3.48382900
H	-5.77717500	3.52134100	-1.78492700
C	-5.26529300	1.43185800	-2.11116400
H	-6.29901600	1.08431300	-2.22445200
H	-4.67403700	0.84408600	-2.83184100
C	-4.77773400	1.09676700	-0.72001900
H	-3.85234200	1.61017800	-0.43772600
H	-5.64923500	1.74216300	0.08873900
C	-4.82958900	-0.35055100	-0.28896900
H	-5.85504400	-0.72786500	-0.39920000
H	-4.22699900	-0.94277900	-0.99745500

C	-4.32418600	-0.60957500	1.13575000
H	-3.29264800	-0.24551300	1.22192500
H	-4.91418400	-0.01473000	1.84295100
C	-4.37438400	-2.08709900	1.54035900
H	-5.40527600	-2.45380600	1.44922200
H	-3.77993400	-2.67776200	0.83118000
C	-3.86966700	-2.34858400	2.96376200
H	-4.46751200	-1.76158200	3.67296100
H	-2.84082600	-1.97720900	3.05587300
C	-3.91103000	-3.82626900	3.36968700
H	-4.93900400	-4.19945200	3.27341600
H	-3.30873100	-4.41227900	2.66332900
C	-3.41187900	-4.08495200	4.79562500
H	-4.01607200	-3.50038400	5.50155400
H	-2.38502400	-3.70912500	4.89275300
C	-3.44910500	-5.56247200	5.20261200
H	-4.47518300	-5.93961700	5.10185800
H	-2.84138200	-6.14659100	4.49930000
C	-2.95541100	-5.81881800	6.63087700
H	-3.56497600	-5.23637300	7.33395100
H	-1.93038800	-5.43912200	6.73252600
C	-2.98886300	-7.29638300	7.03815800
H	-4.01340000	-7.67693100	6.93430200
H	-2.37705300	-7.87859400	6.33677000
C	-2.49876600	-7.55143400	8.46767300
H	-3.11094600	-6.97022800	9.16978000
H	-1.47430000	-7.17065100	8.57288300
C	-2.53064700	-9.02861700	8.87658700
H	-3.55397200	-9.40938800	8.77194200
H	-1.91787800	-9.60969500	8.17655300
C	-2.04030700	-9.27213300	10.30679700
H	-2.65675300	-8.73323500	11.03339600
H	-2.07378900	-10.33396400	10.56643000
H	-1.00770000	-8.93159700	10.43421600
O	-6.46750900	2.27894300	0.76889400
O	-7.69725100	1.66681500	0.41995500
H	-7.83608800	1.04210000	1.14709300

HO₂-R60: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₁₀CH₃

TS60: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₁₀CH₃

C	-5.34325400	2.80417300	-2.51379200
H	-4.37934400	3.30485600	-2.37512600
H	-5.63032300	2.92232200	-3.56209000

H	-6.08273600	3.33577000	-1.90670400
C	-5.26720900	1.32597100	-2.12310000
H	-6.23337200	0.84515300	-2.30330000
H	-4.54401100	0.81298800	-2.76848500
C	-4.86663300	1.11654000	-0.65736800
H	-3.88798300	1.59355200	-0.47906300
H	-5.57241100	1.64195700	-0.00132600
C	-4.76947700	-0.33129900	-0.23369800
H	-6.02928700	-0.80882600	-0.36119000
H	-4.26218300	-0.97143600	-0.96404000
C	-4.38507500	-0.61861000	1.20025000
H	-3.40187600	-0.15723700	1.39069500
H	-5.08248100	-0.10686500	1.87584900
C	-4.31687200	-2.10944100	1.55397400
H	-5.29268000	-2.56828300	1.35817500
H	-3.60145600	-2.60510800	0.88502600
C	-3.91518000	-2.37183700	3.00948400
H	-4.63076000	-1.87366100	3.67614900
H	-2.94053600	-1.90703700	3.20795900
C	-3.84747200	-3.86134700	3.36472400
H	-4.82028500	-4.32577900	3.15787600
H	-3.12680100	-4.35897900	2.70271300
C	-3.46153200	-4.12927200	4.82384800
H	-4.18236900	-3.63109600	5.48504500
H	-2.48851300	-3.66559100	5.03208000
C	-3.39773700	-5.61930400	5.17795700
H	-4.36961800	-6.08308500	4.96479500
H	-2.67382100	-6.11692500	4.51953200
C	-3.02008800	-5.88941300	6.63889400
H	-3.74421200	-5.39195100	7.29710200
H	-2.04820300	-5.42593100	6.85277800
C	-2.95757600	-7.37978400	6.99198700
H	-3.92944800	-7.84310600	6.77760600
H	-2.23325500	-7.87721300	6.33383900
C	-2.58092400	-7.65116000	8.45273800
H	-3.30496100	-7.15443900	9.11192700
H	-1.60877000	-7.18853700	8.66813500
C	-2.51819000	-9.14135000	8.80669200
H	-3.49001000	-9.60353900	8.59449900
H	-1.79582800	-9.63832300	8.14760600
C	-2.13808500	-9.40162600	10.26734900
H	-2.86191400	-8.94707200	10.95132300
H	-2.10118500	-10.47230100	10.48709800

H	-1.15492800	-8.98057100	10.50074800
O	-7.15078000	-1.20889100	-0.40961200
O	-7.33573300	-1.68123500	-1.73210100
H	-7.22405300	-2.63823000	-1.63307300

HO₂-R61: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₉CH₃

TS61: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₉CH₃

C	-5.07678300	2.77174200	-2.49110500
H	-4.04031700	3.11466300	-2.41110700
H	-5.40728400	2.95114500	-3.51797200
H	-5.68406500	3.39936900	-1.83162700
C	-5.20130400	1.29277900	-2.11386800
H	-6.24222000	0.97104300	-2.23845500
H	-4.60920600	0.68680600	-2.81111800
C	-4.75352700	0.99854000	-0.67802100
H	-3.71296200	1.32401500	-0.54987300
H	-5.35164100	1.59455500	0.01995300
C	-4.86794700	-0.48234100	-0.29723300
H	-5.90159700	-0.82319700	-0.43676800
H	-4.26054300	-1.08505700	-0.99304300
C	-4.42418600	-0.79688400	1.11290700
H	-3.51714700	-0.26687900	1.42244400
H	-5.33166000	-0.15522500	1.88277600
C	-4.46727800	-2.24023800	1.55929900
H	-5.48046500	-2.63890600	1.41540800
H	-3.82696300	-2.82920900	0.88195800
C	-4.01108200	-2.46974900	3.00542600
H	-4.64326000	-1.88206100	3.68127700
H	-2.99334400	-2.07729300	3.12527100
C	-4.03660600	-3.94252000	3.42932200
H	-5.05383300	-4.33823300	3.31023600
H	-3.40316500	-4.52702200	2.74938000
C	-3.57204300	-4.16785600	4.87238600
H	-4.20958100	-3.58775300	5.55201400
H	-2.55812400	-3.76429100	4.99127000
C	-3.58216700	-5.63914300	5.30288600
H	-4.59538800	-6.04493100	5.18450800
H	-2.94240000	-6.21883200	4.62482800
C	-3.11627000	-5.85636600	6.74681400
H	-3.75893400	-5.27944000	7.42444700
H	-2.10544400	-5.44476000	6.86523300
C	-3.11592000	-7.32641200	7.18171200
H	-4.12627900	-7.73942900	7.06367100

H	-2.47184000	-7.90338600	6.50536100
C	-2.64971500	-7.53821500	8.62614200
H	-3.29517500	-6.96338000	9.30320100
H	-1.64042000	-7.12250600	8.74528000
C	-2.64326300	-9.00721600	9.06455900
H	-3.65137100	-9.42327400	8.94678700
H	-1.99733400	-9.58201200	8.38959900
C	-2.17601200	-9.20588700	10.50931200
H	-2.82458700	-8.67264900	11.21168500
H	-2.18133400	-10.26281300	10.79014800
H	-1.15766600	-8.82987500	10.65088500
O	-6.18343700	0.38030900	2.52322500
O	-7.40262000	-0.15321600	2.03599700
H	-7.62847600	-0.81304700	2.70819400

HO₂-R62: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + CH₃(CH₂)₄CH(CH₂)₈CH₃

TS62: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + CH₃(CH₂)₄CH(CH₂)₈CH₃

C	-5.22405700	2.54727700	-2.66966100
H	-4.21478900	2.96727500	-2.60952400
H	-5.56089300	2.64158800	-3.70582800
H	-5.87775400	3.16993300	-2.05058100
C	-5.24666000	1.08841400	-2.20438100
H	-6.26138700	0.68652100	-2.31017200
H	-4.61112700	0.48507500	-2.86416000
C	-4.78335000	0.90676200	-0.75477900
H	-3.76559700	1.30594600	-0.64862700
H	-5.41780700	1.51350700	-0.09556900
C	-4.81338600	-0.55092600	-0.28312400
H	-5.82948900	-0.94715700	-0.38073900
H	-4.18256400	-1.15885200	-0.94441000
C	-4.33962800	-0.72995500	1.16446900
H	-3.31104300	-0.34308000	1.25979500
H	-4.94913800	-0.11130400	1.83531000
C	-4.35218800	-2.16103600	1.65173700
H	-5.65744800	-2.51628300	1.62187200
H	-3.95699200	-2.87796500	0.92348300
C	-3.90570000	-2.42711300	3.07156800
H	-4.50161800	-1.81885900	3.76404000
H	-2.87009400	-2.06440200	3.17971000
C	-3.96737300	-3.90230600	3.48779800
H	-4.99692300	-4.26125600	3.37734800
H	-3.35651200	-4.49585800	2.79526800
C	-3.49392000	-4.15473400	4.92323300

H	-4.10438200	-3.56022700	5.61501100
H	-2.46405100	-3.79196100	5.03738000
C	-3.55986000	-5.63077100	5.33189400
H	-4.58898900	-5.99214800	5.20883900
H	-2.94574600	-6.22422000	4.64196600
C	-3.10213900	-5.89637900	6.77042100
H	-3.71559300	-5.30281400	7.46056300
H	-2.07199700	-5.53839800	6.89556700
C	-3.17671900	-7.37412800	7.17161500
H	-4.20647200	-7.73139900	7.04102600
H	-2.56097600	-7.96697900	6.48264600
C	-2.72785500	-7.64716800	8.61139500
H	-3.34254000	-7.05432200	9.30142500
H	-1.69706200	-7.29315700	8.74378300
C	-2.80755200	-9.12535500	9.01009200
H	-3.83741800	-9.47864000	8.87757600
H	-2.19279600	-9.71797700	8.32155300
C	-2.35908500	-9.39023200	10.45029400
H	-2.97876700	-8.83952600	11.16516500
H	-2.42702100	-10.45233100	10.70196900
H	-1.32128800	-9.07814400	10.60498600
O	-6.81474300	-2.80039400	1.65837700
O	-7.12570100	-3.32180400	0.37872000
H	-7.10111300	-4.27854900	0.52760200

HO₂-R63: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + CH₃(CH₂)₅CH(CH₂)₇CH₃

TS63: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + CH₃(CH₂)₅CH(CH₂)₇CH₃

C	-5.06065800	0.81366900	-3.32116200
H	-3.97475600	0.90892700	-3.42171500
H	-5.48914100	0.82353400	-4.32732400
H	-5.42247600	1.70414000	-2.79748600
C	-5.43658700	-0.46367100	-2.56466800
H	-6.52885000	-0.54688700	-2.50910700
H	-5.09406700	-1.33791300	-3.13197600
C	-4.85488000	-0.52226500	-1.14737300
H	-3.76150000	-0.43876700	-1.20294500
H	-5.19729000	0.35289400	-0.58035500
C	-5.22763300	-1.79619000	-0.38164200
H	-6.32075100	-1.87844700	-0.32802800
H	-4.88359300	-2.67217000	-0.94750800
C	-4.64960300	-1.84643100	1.03705400
H	-3.55609300	-1.76561700	0.98650800
H	-4.99800300	-0.97716300	1.60506900

C	-5.02583100	-3.12295800	1.79856100
H	-6.11784800	-3.22261400	1.83996200
H	-4.66922300	-4.00132200	1.23499600
C	-4.46445800	-3.20122100	3.19990100
H	-5.07580500	-2.18389600	3.84687100
H	-3.42333800	-2.87163700	3.28213300
C	-4.78007700	-4.43459300	4.01394200
H	-5.86920600	-4.56223400	4.07571600
H	-4.41831400	-5.31619400	3.45945900
C	-4.16822300	-4.44218700	5.42075300
H	-4.50389500	-3.55207700	5.96569700
H	-3.07771900	-4.35333000	5.33765800
C	-4.51404500	-5.69861500	6.22691200
H	-5.60500700	-5.78148600	6.31866100
H	-4.18935800	-6.58770600	5.67072800
C	-3.88628000	-5.72172300	7.62546200
H	-4.20378200	-4.82892700	8.17953000
H	-2.79505700	-5.64808000	7.53272900
C	-4.24131200	-6.97284100	8.43645500
H	-5.33256900	-7.04314100	8.53348300
H	-3.92863000	-7.86564500	7.87938200
C	-3.60749300	-7.00172900	9.83194400
H	-3.91731900	-6.10811000	10.38953500
H	-2.51588600	-6.93473700	9.73558900
C	-3.96504300	-8.25091500	10.64499600
H	-5.05545700	-8.31698300	10.74364400
H	-3.65625700	-9.14407600	10.08812400
C	-3.32469800	-8.27159000	12.03613000
H	-3.64249700	-7.40942800	12.63114200
H	-3.59741000	-9.17469900	12.58929200
H	-2.23253200	-8.24075000	11.96883800
O	-5.67956400	-1.31431800	4.39687600
O	-7.04608400	-1.64781900	4.22484400
H	-7.27761600	-2.03956000	5.07994300

HO₂-R64: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + CH₃(CH₂)₆CH(CH₂)₆CH₃

TS64: HO₂ + CH₃(CH₂)₁₃CH₃ → H₂O₂ + CH₃(CH₂)₆CH(CH₂)₆CH₃

C	-4.30091600	0.24318400	-3.85127100
H	-3.22718500	0.17507200	-4.05349500
H	-4.82048400	0.23816600	-4.81362100
H	-4.48651000	1.21327000	-3.37922700
C	-4.76963400	-0.90712600	-2.95551800
H	-5.85250900	-0.82999100	-2.79918400

H	-4.60508200	-1.86136700	-3.47094900
C	-4.06546400	-0.94203200	-1.59427500
H	-2.98144000	-1.01924600	-1.75142800
H	-4.22940100	0.01392800	-1.07975700
C	-4.52909500	-2.08916200	-0.68998300
H	-5.61208200	-2.01069300	-0.53105300
H	-4.36682500	-3.04461200	-1.20583200
C	-3.82161000	-2.12329700	0.66949100
H	-2.73784500	-2.20304200	0.51114400
H	-3.98370200	-1.16747300	1.18436200
C	-4.28991300	-3.26857700	1.57334000
H	-5.36837200	-3.18608900	1.74324600
H	-4.13308500	-4.22494000	1.05802900
C	-3.56586100	-3.30293500	2.92530700
H	-3.70529400	-2.34704900	3.44598700
H	-2.47989300	-3.38797500	2.75150800
C	-3.98471700	-4.43519900	3.83489600
H	-5.29105700	-4.19720800	4.09557500
H	-4.07807300	-5.40028700	3.32458500
C	-3.32205400	-4.52358200	5.19126400
H	-3.45768500	-3.57541100	5.72713600
H	-2.23453500	-4.61864200	5.03568900
C	-3.80660500	-5.68833100	6.06328500
H	-4.88699800	-5.59290300	6.22030000
H	-3.65398800	-6.63071000	5.52143900
C	-3.09948300	-5.76520500	7.42109100
H	-3.25277300	-4.82223000	7.96138200
H	-2.01653500	-5.85225200	7.26292300
C	-3.57821600	-6.93054100	8.29385700
H	-4.66149000	-6.84435200	8.44858800
H	-3.42262900	-7.87412800	7.75468500
C	-2.87871300	-7.00647000	9.65571800
H	-3.03517200	-6.06368700	10.19605500
H	-1.79480400	-7.09147200	9.50258900
C	-3.35668000	-8.17195800	10.52899700
H	-4.43979500	-8.08823700	10.68049400
H	-3.19753900	-9.11459600	9.99116200
C	-2.65565900	-8.23645900	11.88919500
H	-2.82584100	-7.32128800	12.46517200
H	-3.01854000	-9.07699900	12.48730000
H	-1.57381700	-8.35536800	11.77157400
O	-6.42201200	-3.94648400	4.37668400
O	-7.21309800	-4.53828100	3.36166200

H	-7.51340800	-5.35946600	3.77832400
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2.2.16 C16 (n-C₁₆H₃₄)

HO₂-R65: $\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_2(\text{CH}_2)_{14}\text{CH}_3$

TS65: $\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_2(\text{CH}_2)_{14}\text{CH}_3$

C	-4.72437400	6.69231600	0.47154600
H	-5.69072300	5.91100600	1.06714900
H	-3.99466800	6.75418600	1.28070900
H	-5.27398300	7.62127400	0.31978000
C	-4.28240900	5.96593700	-0.77030200
H	-5.14249600	5.81138700	-1.43301700
H	-3.59866200	6.62752600	-1.32883900
C	-3.58058000	4.62829600	-0.50317800
H	-2.71690900	4.80166500	0.15141000
H	-4.25925300	3.97278700	0.05302800
C	-3.11607800	3.92367500	-1.78215000
H	-3.98209200	3.74788600	-2.43324100
H	-2.44509500	4.58896600	-2.34167600
C	-2.40343800	2.59215500	-1.52034800
H	-1.54099700	2.76735700	-0.86417000
H	-3.07615800	1.92616200	-0.96522300
C	-1.93114500	1.88698100	-2.79688900
H	-2.79298300	1.71137700	-3.45368100
H	-1.25873100	2.55482700	-3.35118200
C	-1.21671600	0.55636000	-2.53489700
H	-0.36103500	0.73113700	-1.86972600
H	-1.89213100	-0.11519300	-1.98921800
C	-0.72971600	-0.14213600	-3.80965800
H	-1.58436700	-0.31733500	-4.47595700
H	-0.05412300	0.53046700	-4.35414800
C	-0.01340700	-1.47160600	-3.54690500
H	-0.69197400	-2.14844100	-3.01163400
H	0.83465100	-1.29708500	-2.87194800
C	0.48953300	-2.16217500	-4.81981200
H	-0.35755400	-2.33800800	-5.49557500
H	1.16757400	-1.48409900	-5.35432900
C	1.20906700	-3.48967500	-4.55595100
H	0.52858400	-4.17162700	-4.02965100
H	2.05018100	-3.31430300	-3.87256600
C	1.72647500	-4.17301900	-5.82695100
H	0.88612200	-4.35033100	-6.51070500
H	2.40589400	-3.48979900	-6.35304800
C	2.44987900	-5.49817400	-5.56179400

H	1.76886800	-6.18428000	-5.04156300
H	3.28593800	-5.32105600	-4.87264300
C	2.97793800	-6.17647800	-6.83084600
H	2.14278800	-6.35676800	-7.52047000
H	3.65794200	-5.48996900	-7.35223200
C	3.70555100	-7.49930600	-6.56562200
H	3.02605200	-8.18728900	-6.04785700
H	4.53892000	-7.31970500	-5.87529100
C	4.23418300	-8.16683700	-7.83861000
H	4.75018500	-9.10463100	-7.61411100
H	3.42002300	-8.39470300	-8.53404300
H	4.94180100	-7.51577000	-8.36182400
O	-6.53191300	5.26618200	1.54815700
O	-5.88651200	4.45570500	2.51498700
H	-6.08609500	4.91767900	3.34254600

HO₂-R66: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + CH₃CH(CH₂)₁₃CH₃

TS66: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + CH₃CH(CH₂)₁₃CH₃

C	-4.49888000	7.22611200	0.25443400
H	-4.91798200	6.62898300	1.06904100
H	-3.64022500	7.78120300	0.65860500
H	-5.24944500	7.95866400	-0.05167000
C	-4.06794500	6.35615900	-0.89993000
H	-5.22711900	5.84510100	-1.36786800
H	-3.73918000	6.91874700	-1.77931500
C	-3.20585000	5.15417000	-0.59118600
H	-2.27411500	5.51209600	-0.12152200
H	-3.69998300	4.53840000	0.17096400
C	-2.85298700	4.29298600	-1.81065400
H	-3.77606600	3.91777700	-2.26725700
H	-2.36986500	4.92360100	-2.56802100
C	-1.93327500	3.11431500	-1.47347100
H	-1.01002700	3.49418700	-1.01656200
H	-2.41355200	2.48673800	-0.71182300
C	-1.57717000	2.25078500	-2.68881500
H	-2.49936100	1.85597600	-3.13400800
H	-1.11540700	2.88330700	-3.45819800
C	-0.63353700	1.08789200	-2.36157900
H	0.29095200	1.48588700	-1.92325900
H	-1.08961000	0.45756700	-1.58721300
C	-0.28390500	0.22208900	-3.57731800
H	-1.20645900	-0.19523900	-4.00117400
H	0.14852400	0.85827600	-4.36065100

C	0.69031800	-0.91872400	-3.26238600
H	0.26459200	-1.55243900	-2.47353500
H	1.61554400	-0.49833600	-2.84718500
C	1.03172700	-1.78663300	-4.47899300
H	0.10897900	-2.22529300	-4.88040300
H	1.43469100	-1.14781700	-5.27580800
C	2.03456800	-2.90577900	-4.17670100
H	1.63716100	-3.54268800	-3.37567800
H	2.95926300	-2.46467400	-3.78237600
C	2.36936000	-3.77499400	-5.39422200
H	1.44686900	-4.22903000	-5.77878400
H	2.75048000	-3.13474700	-6.20056300
C	3.39230400	-4.87837400	-5.10154300
H	3.01439500	-5.51782300	-4.29308100
H	4.31574700	-4.42287700	-4.72085300
C	3.72382700	-5.74786400	-6.31949800
H	2.80207700	-6.21031600	-6.69624400
H	4.09455700	-5.10778000	-7.13101000
C	4.75626500	-6.84392600	-6.03268200
H	4.38660700	-7.48516500	-5.22304400
H	5.67732200	-6.38188700	-5.65678800
C	5.08125500	-7.70572800	-7.25630800
H	5.81738800	-8.47847800	-7.01757300
H	4.18520600	-8.20687800	-7.63616900
H	5.48950000	-7.09878400	-8.07075800
O	-6.26229900	5.39697300	-1.74936200
O	-7.13121300	6.51014400	-1.85921000
H	-7.11883900	6.69394400	-2.81016300

HO₂-R67: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + H₂+CH₃CH₂CH(CH₂)₁₂CH₃

TS67: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + H₂+CH₃CH₂CH(CH₂)₁₂CH₃

C	-4.62795800	7.12684400	-0.03958900
H	-5.05424700	6.57983000	0.80457400
H	-3.70863800	7.61214900	0.30268100
H	-5.33295000	7.91195200	-0.32443700
C	-4.35054300	6.18593000	-1.21589200
H	-5.28860500	5.74182700	-1.56938500
H	-3.95798600	6.76657800	-2.06631600
C	-3.36361000	5.08374300	-0.90477900
H	-2.48847200	5.41802400	-0.33740100
H	-3.98797200	4.35447400	0.04796000
C	-3.04077200	4.10003800	-2.00478000
H	-3.96903400	3.62910800	-2.35546500

H	-2.65894100	4.66303700	-2.87243400
C	-2.01827100	3.02383400	-1.61677800
H	-1.08143700	3.51051900	-1.31765900
H	-2.37685600	2.48676700	-0.73078200
C	-1.73356600	2.02331700	-2.74163000
H	-2.66997000	1.52743100	-3.02949200
H	-1.39276800	2.56537300	-3.63338600
C	-0.69297000	0.96061400	-2.36874400
H	0.25059400	1.45535800	-2.10471200
H	-1.02196800	0.43380000	-1.46369200
C	-0.43485700	-0.06064600	-3.48165600
H	-1.37748400	-0.56335100	-3.73463600
H	-0.11967400	0.46675300	-4.39141100
C	0.61828800	-1.11473200	-3.11947800
H	0.31349700	-1.62962000	-2.19911100
H	1.56684700	-0.61384100	-2.88642400
C	0.85152500	-2.15118200	-4.22386800
H	-0.09610100	-2.65827500	-4.44751300
H	1.14406100	-1.63555000	-5.14785900
C	1.91464900	-3.19918100	-3.87355500
H	1.62942400	-3.70750600	-2.94329000
H	2.86609000	-2.69369000	-3.66310700
C	2.12989400	-4.24363500	-4.97414100
H	1.17927300	-4.75349300	-5.17775800
H	2.40576700	-3.73425200	-5.90667700
C	3.20028300	-5.28772100	-4.63466400
H	2.92893300	-5.79341000	-3.69878300
H	4.15316100	-4.77900100	-4.43879100
C	3.40439300	-6.33575600	-5.73381500
H	2.45247900	-6.84777300	-5.92651800
H	3.67104100	-5.83017100	-6.67127700
C	4.47853700	-7.37825000	-5.40173700
H	4.21358700	-7.88295400	-4.46455300
H	5.43052800	-6.86739900	-5.21210500
C	4.67165300	-8.42199400	-6.50557000
H	5.44286400	-9.14961800	-6.23765100
H	3.74535900	-8.97394400	-6.69408700
H	4.97218100	-7.95100000	-7.44694500
O	-4.59185200	3.69657600	0.83807800
O	-5.76716300	3.28991200	0.15859400
H	-5.55954400	2.37880000	-0.09648000

HO₂-R68: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₁₁CH₃

TS68: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₁₁CH₃

C	-4.82093400	7.01526800	-0.00650000
H	-5.36395700	6.45808500	0.76329700
H	-3.95309800	7.48112800	0.47184300
H	-5.47609600	7.81670000	-0.35826600
C	-4.39931700	6.09818800	-1.15739600
H	-5.28619800	5.66947600	-1.63342300
H	-3.89119900	6.68816400	-1.92966600
C	-3.47185500	4.96241800	-0.70575800
H	-2.56754500	5.39521400	-0.24577200
H	-3.95625300	4.38241900	0.09017400
C	-3.03817600	4.02978600	-1.81357500
H	-4.18246300	3.42979800	-2.21618900
H	-2.77189800	4.54329100	-2.74423700
C	-2.09884300	2.90083800	-1.45302000
H	-1.17119400	3.34307000	-1.05312600
H	-2.52462600	2.31818100	-0.62622200
C	-1.74714700	1.96893800	-2.61901100
H	-2.66698400	1.50930700	-2.99782200
H	-1.33626400	2.56476700	-3.44434700
C	-0.74589900	0.87138100	-2.24093800
H	0.18273400	1.33367600	-1.88147700
H	-1.14429700	0.29361000	-1.39703800
C	-0.42357400	-0.08229000	-3.39633500
H	-1.35238100	-0.55453300	-3.74146200
H	-0.04270000	0.49597100	-4.24830200
C	0.59204900	-1.17175400	-3.03222300
H	0.22481500	-1.73268200	-2.16302800
H	1.53106800	-0.70034500	-2.71428300
C	0.87781600	-2.14847900	-4.17807100
H	-0.06107700	-2.62826000	-4.48363800
H	1.22966200	-1.58714600	-5.05348900
C	1.90614700	-3.22997100	-3.82616200
H	1.56625000	-3.77700000	-2.93714400
H	2.85302100	-2.75157700	-3.54393700
C	2.16103200	-4.22500300	-4.96360300
H	1.21469500	-4.71020000	-5.23582700
H	2.48821500	-3.67738000	-5.85706700
C	3.19984300	-5.29993600	-4.62276100
H	2.88068400	-5.83860800	-3.72098600
H	4.15103600	-4.81589000	-4.36572100
C	3.43474800	-6.30607200	-5.75456500

H	2.48440800	-6.79465200	-6.00670000
H	3.74739800	-5.76781900	-6.65905700
C	4.47899000	-7.37799800	-5.42122000
H	4.16954600	-7.91327500	-4.51516500
H	5.43039300	-6.89065300	-5.17519600
C	4.69956500	-8.38242800	-6.55599700
H	5.44863500	-9.13233800	-6.28670400
H	3.77313100	-8.91145300	-6.80114900
H	5.04374400	-7.88137500	-7.46641900
O	-5.18258600	2.86013200	-2.52658100
O	-5.79405000	3.66652300	-3.51755700
H	-5.53775000	3.22316000	-4.33966700

HO₂-R69: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₁₀CH₃

TS69: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₁₀CH₃

C	-4.69167300	7.04399900	0.03776800
H	-5.04956900	6.52109200	0.93001800
H	-3.77287900	7.57265900	0.31102000
H	-5.43985500	7.79524900	-0.22999500
C	-4.44555300	6.06509600	-1.11371300
H	-5.38930700	5.57671700	-1.38463500
H	-4.12357700	6.62090700	-2.00330900
C	-3.40301700	4.99247600	-0.77941600
H	-2.45728800	5.47878000	-0.50686600
H	-3.72754200	4.43120300	0.10363100
C	-3.15174400	4.01179400	-1.93072400
H	-4.09475200	3.53149300	-2.22093000
H	-2.81868500	4.57239500	-2.82027800
C	-2.12143000	2.94780700	-1.62899500
H	-1.24022000	3.31909700	-1.09521700
H	-2.69332900	2.22258300	-0.64167800
C	-1.79986600	1.95321000	-2.71988300
H	-2.72532200	1.46292600	-3.05083200
H	-1.43935600	2.51056900	-3.60026000
C	-0.75532900	0.89803300	-2.33289200
H	0.17439400	1.40326400	-2.04229700
H	-1.09896500	0.35925300	-1.44214800
C	-0.45943800	-0.10300400	-3.45438300
H	-1.39117400	-0.60671800	-3.74381800
H	-0.11982200	0.43931900	-4.34644200
C	0.58676200	-1.15788400	-3.07506100
H	0.25418700	-1.68844100	-2.17351800
H	1.52452700	-0.65673200	-2.80254800

C	0.86114000	-2.17570100	-4.18724800
H	-0.07865200	-2.67405100	-4.45877800
H	1.19429400	-1.64608900	-5.08926200
C	1.90292200	-3.23578200	-3.81005400
H	1.57566500	-3.75630600	-2.90063700
H	2.84784500	-2.74030300	-3.55195500
C	2.15711400	-4.26503400	-4.91658500
H	1.21057800	-4.75803200	-5.17385700
H	2.48447400	-3.74509700	-5.82632600
C	3.19507700	-5.33002500	-4.54280000
H	2.87132200	-5.84523800	-3.62906200
H	4.14476800	-4.83911900	-4.29335300
C	3.43635700	-6.36481400	-5.64691300
H	2.48624700	-6.85519300	-5.89651800
H	3.76065700	-5.85054800	-6.56116600
C	4.47197000	-7.43318300	-5.27650600
H	4.14932500	-7.94577900	-4.36201200
H	5.42260700	-6.94431500	-5.03050800
C	4.70143400	-8.46448900	-6.38502200
H	5.44385200	-9.21112000	-6.08950800
H	3.77561500	-8.99508300	-6.62908400
H	5.05877600	-7.98600000	-7.30246500
O	-3.25859200	1.57752100	0.18764000
O	-4.50808200	1.24367700	-0.39168400
H	-4.36847200	0.33104500	-0.68471400

HO₂-R70: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + CH₃(CH₂)₄CH(CH₂)₉CH₃

TS70: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + CH₃(CH₂)₄CH(CH₂)₉CH₃

C	-4.87527500	6.98150100	-0.04161000
H	-5.41255400	6.41984100	0.72913300
H	-4.01190900	7.45509100	0.43676900
H	-5.53732100	7.77754400	-0.39373500
C	-4.44038500	6.06637500	-1.18985700
H	-5.32706600	5.63493400	-1.66939200
H	-3.93730100	6.66186200	-1.96149500
C	-3.50985000	4.93271700	-0.74300800
H	-2.61636400	5.36389400	-0.27172900
H	-4.00974700	4.34290600	0.03624100
C	-3.08830400	4.00344500	-1.88564900
H	-3.97791500	3.55651100	-2.34151200
H	-2.60303100	4.59348900	-2.67377600
C	-2.13571200	2.88724600	-1.43792600
H	-1.22087600	3.33716900	-1.01732200

H	-2.58812100	2.32000300	-0.61456400
C	-1.73118000	1.93379100	-2.53920200
H	-2.88055700	1.30315700	-2.87300800
H	-1.51698900	2.42642600	-3.49424400
C	-0.75463900	0.83240200	-2.19244100
H	0.18930400	1.30225800	-1.86958400
H	-1.11982600	0.27871200	-1.31817100
C	-0.46254700	-0.14201500	-3.34016800
H	-1.39676600	-0.63137400	-3.63761800
H	-0.11877200	0.42523200	-4.21490200
C	0.58215500	-1.20664900	-2.98649600
H	0.25527200	-1.75130200	-2.09136000
H	1.52597900	-0.71554900	-2.71579400
C	0.83718500	-2.20674500	-4.11926600
H	-0.10531100	-2.70866600	-4.37329100
H	1.14310100	-1.66159000	-5.02180300
C	1.89775100	-3.26224800	-3.78480000
H	1.60528400	-3.79183800	-2.86881800
H	2.84761400	-2.76192000	-3.55570000
C	2.12028200	-4.28155400	-4.90742900
H	1.17188400	-4.78971600	-5.12490100
H	2.39755800	-3.75131900	-5.82787600
C	3.19278400	-5.32928900	-4.58700400
H	2.92385700	-5.85064500	-3.65907800
H	4.14524900	-4.82236000	-4.38460400
C	3.39608500	-6.35921000	-5.70342200
H	2.44516900	-6.87158400	-5.89992700
H	3.65692300	-5.83823300	-6.63407800
C	4.47526800	-7.40272700	-5.39202000
H	4.21765900	-7.92079200	-4.46010000
H	5.42692200	-6.89159400	-5.20150500
C	4.66438300	-8.43112400	-6.51089700
H	5.43961000	-9.15974100	-6.25770300
H	3.73859300	-8.98353400	-6.70051600
H	4.95716100	-7.94688000	-7.44798700
O	-3.88511200	0.70933200	-3.12010600
O	-4.55972900	1.48148900	-4.09723300
H	-4.33497700	1.02464400	-4.92121500

HO₂-R71: $\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_8\text{CH}_3$

TS71: $\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_8\text{CH}_3$

C	-4.73688600	7.01317000	-0.31482800
H	-4.98548500	6.55735000	0.64880300

H	-3.80891600	7.57853200	-0.18239600
H	-5.52864100	7.72715800	-0.55843900
C	-4.58585300	5.94990700	-1.40658000
H	-5.54006200	5.42565600	-1.53966700
H	-4.37177100	6.43861700	-2.36511700
C	-3.48624800	4.92502000	-1.10534400
H	-2.53165000	5.45001200	-0.96859800
H	-3.70259200	4.43550800	-0.14706200
C	-3.32415000	3.85587200	-2.19108700
H	-4.28057800	3.33642500	-2.33207400
H	-3.09747800	4.34308800	-3.14876900
C	-2.23492000	2.82660900	-1.86976300
H	-1.27847300	3.34443000	-1.72155900
H	-2.46936700	2.33333000	-0.92026500
C	-2.06374300	1.75857000	-2.95641400
H	-3.02140600	1.25326300	-3.13481800
H	-1.80307100	2.24579200	-3.91079200
C	-1.00466900	0.72657000	-2.64295700
H	-0.10135800	1.14180300	-2.18352800
H	-1.51379900	0.06997200	-1.57685400
C	-0.72415500	-0.34070700	-3.67544500
H	-1.66143900	-0.84518900	-3.94562800
H	-0.38450500	0.15356200	-4.60059900
C	0.32479300	-1.37311200	-3.24205500
H	-0.00801200	-1.85497300	-2.31541100
H	1.25784800	-0.85172200	-2.99348400
C	0.61239300	-2.44417500	-4.29970300
H	-0.32242100	-2.95714500	-4.56141100
H	0.96234300	-1.96261800	-5.22203300
C	1.64628000	-3.47947800	-3.84216200
H	1.29157800	-3.95691100	-2.91959200
H	2.57865600	-2.96483400	-3.57607100
C	1.94885700	-4.56180500	-4.88456600
H	1.01558300	-5.06899100	-5.16201400
H	2.32157900	-4.08865100	-5.80225400
C	2.96531100	-5.60264700	-4.40134300
H	2.58856300	-6.07420700	-3.48439400
H	3.89637400	-5.09410000	-4.11899400
C	3.27925500	-6.69051300	-5.43437100
H	2.34834700	-7.19567800	-5.72380700
H	3.66683200	-6.22247900	-6.34877100
C	4.28512100	-7.73530500	-4.93783100
H	3.89650700	-8.20326400	-4.02509500

H	5.21483000	-7.23084300	-4.64736800
C	4.59650400	-8.81973200	-5.97346500
H	5.31490900	-9.54791500	-5.58657000
H	3.69176000	-9.36585100	-6.25904100
H	5.02141700	-8.38660300	-6.88459700
O	-2.02428800	-0.51259300	-0.66866300
O	-3.31618600	-0.86388100	-1.13280200
H	-3.20793700	-1.79518800	-1.37614800

HO₂-R72: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + CH₃(CH₂)₆CH(CH₂)₇CH₃

TS72: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + CH₃(CH₂)₆CH(CH₂)₇CH₃

C	-5.14760400	6.73170300	-0.09129100
H	-5.70327000	6.19863000	0.68670200
H	-4.28551600	7.20777000	0.38682900
H	-5.79406900	7.52593200	-0.47521800
C	-4.70660400	5.77992400	-1.20710800
H	-5.59196800	5.34857600	-1.68989100
H	-4.18348900	6.34827600	-1.98594900
C	-3.79919200	4.64590500	-0.71622000
H	-2.91261400	5.07730200	-0.23290500
H	-4.32266000	4.07719800	0.06340400
C	-3.35619800	3.68932200	-1.82858400
H	-4.24345900	3.25851300	-2.30976000
H	-2.83512000	4.25924600	-2.60889700
C	-2.44815800	2.55417000	-1.34169100
H	-1.55408800	2.98248400	-0.86929300
H	-2.96590100	1.98889400	-0.55611300
C	-2.02636900	1.59369100	-2.45852500
H	-2.91676400	1.15470600	-2.92016900
H	-1.51812500	2.15926400	-3.25015900
C	-1.10179600	0.46872700	-1.97569900
H	-0.19256300	0.91034900	-1.53451100
H	-1.58367900	-0.08622700	-1.16086100
C	-0.67896900	-0.49700000	-3.05930900
H	-1.82846600	-1.09968900	-3.44062400
H	-0.40607400	-0.01019900	-4.00218600
C	0.24243200	-1.63242700	-2.67252700
H	-0.21294300	-2.21472200	-1.86122700
H	1.16069500	-1.19927000	-2.24252800
C	0.62111800	-2.56106100	-3.83262600
H	-0.29300400	-2.98433300	-4.26412500
H	1.09298100	-1.96816600	-4.62680300
C	1.56375500	-3.69832000	-3.42279800

H	1.08830800	-4.29458300	-2.63354200
H	2.47419800	-3.27549300	-2.97820300
C	1.94943400	-4.61663400	-4.58760600
H	1.03766000	-5.03167100	-5.03615000
H	2.43013900	-4.02025200	-5.37398800
C	2.88153400	-5.76556100	-4.18507800
H	2.39926100	-6.36455800	-3.40182600
H	3.79257400	-5.35201700	-3.73322400
C	3.26741600	-6.67859400	-5.35385400
H	2.35627500	-7.08995300	-5.80774900
H	3.75198600	-6.08014700	-6.13648300
C	4.19595800	-7.83191300	-4.95557000
H	3.71176100	-8.43092600	-4.17476500
H	5.10657600	-7.42142900	-4.50236800
C	4.57515100	-8.73696200	-6.13132400
H	5.23900600	-9.54661900	-5.81560200
H	3.68749100	-9.19205300	-6.58220700
H	5.08988100	-8.17194100	-6.91501900
O	-2.83062800	-1.68455600	-3.71797900
O	-3.49698400	-0.88284100	-4.67655500
H	-3.26194100	-1.31183800	-5.51252200

4. Cartesian coordinates for all optimized geometries at the M06-2X/6-311++G(d,p) level

3.1 Hydrogen abstraction reaction of n -C_nH_{2n+2} (n = 1-16) by OH radical

3.1.1 C1 (CH₄)



OH

O	0.00000000	0.00000000	0.10800100
H	0.00000000	0.00000000	-0.86401200

H₂O

O	0.00000000	0.00000000	0.11657000
H	0.00000000	0.76160200	-0.46627900
H	0.00000000	-0.76160200	-0.46627900

CH₄

C	0.00000000	0.00000000	0.00000000
H	0.62889200	0.62889200	0.62889200
H	-0.62889200	-0.62889200	0.62889200
H	-0.62889200	0.62889200	-0.62889200
H	0.62889200	-0.62889200	-0.62889200

CH₃

C	0.00000000	0.00000000	0.00006500
H	0.00000000	1.07889700	-0.00013000
H	-0.93435200	-0.53944800	-0.00013000
H	0.93435200	-0.53944800	-0.00013000



C	1.21668300	0.00903500	0.00048400
H	1.61595300	-0.93574300	-0.36159600
H	1.43845900	0.83359000	-0.67238600
H	0.03428100	-0.15106300	0.00406500
H	1.50593400	0.21749300	1.02741800
O	-1.30868800	-0.10901900	0.00005100
H	-1.42522200	0.85365700	-0.00081000

3.1.2 C2 (C₂H₆)



CH₃CH₃

C	0.00000000	0.00000000	0.76355700
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H	0.50661500	0.88267500	1.15886400
H	0.51111200	-0.88007900	1.15886400
H	-1.01772700	-0.00259700	1.15886400
C	0.00000000	0.00000000	-0.76355700
H	1.01772700	-0.00259700	-1.15886400
H	-0.51111200	-0.88007900	-1.15886400
H	-0.50661500	0.88267500	-1.15886400

CH₂CH₃

C	0.69394200	0.00000000	-0.00052900
H	1.08534200	-0.00001100	1.02692500
H	1.10430600	0.88506600	-0.49171800
H	1.10430700	-0.88505500	-0.49173600
C	-0.79383800	0.00000000	-0.02428000
H	-1.34729000	0.92566200	0.05269000
H	-1.34728900	-0.92566300	0.05268900

TS2: OH + CH₃CH₃ → H₂O + CH₂CH₃

C	1.44476100	-0.47270600	0.02498200
H	1.21376400	-1.12854100	0.86572300
H	2.47842200	-0.13291600	0.13728500
H	1.38398600	-1.06333900	-0.89013900
C	0.49615700	0.70831300	-0.02347200
H	0.49347300	1.29938300	0.89329100
H	0.64828500	1.35882500	-0.88572200
H	-0.58565400	0.29533100	-0.15983400
O	-1.88805800	-0.27517600	-0.08767100
H	-2.17332500	0.15902200	0.73170000

3.1.3 C3 (C₃H₈)

OH-R3: OH + CH₃CH₂CH₃ → H₂O + CH₂CH₂CH₃

C₃H₈

C	1.26630200	-0.26115500	0.00000100
H	1.29782400	-0.90642500	-0.88222200
H	1.29820000	-0.90584900	0.88263100
H	2.16899000	0.35336200	-0.00039500
C	0.00000000	0.59262300	0.00000100
H	0.00000100	1.24800500	0.87618800
H	-0.00000100	1.24793600	-0.87623400
C	-1.26630200	-0.26115500	0.00000200
H	-1.29806000	-0.90605800	0.88248300
H	-2.16899000	0.35336200	-0.00010500
H	-1.29796500	-0.90621600	-0.88237000

CH₂CH₂CH₃

C	-1.21854500	-0.24535400	-0.03866400
H	-1.27015700	-0.98436000	0.76485800
H	-1.27357400	-0.78035300	-0.98921400
H	-2.09471600	0.40081500	0.04076500
C	0.07853700	0.56002600	0.05292500
H	0.10510100	1.31949700	-0.73579800
H	0.08212400	1.12354100	0.99898400
C	1.29434600	-0.29585300	-0.03262900
H	2.25404800	0.12175000	-0.30604400
H	1.27114800	-1.31380900	0.33666200

TS3: OH + CH₃CH₂CH₃ → H₂O + CH₂CH₂CH₃

C	-1.38807700	-0.90939700	0.17737000
H	-1.71666000	-0.77575800	1.21137200
H	-0.53238100	-1.58826800	0.18134500
H	-2.20158400	-1.38239900	-0.37561600
C	-0.99483500	0.42958100	-0.44174800
H	-0.70780600	0.28420600	-1.48751800
H	-1.85667400	1.10702700	-0.44910300
C	0.14496400	1.08846200	0.31034000
H	1.04941100	0.35023800	0.31375700
H	0.49786800	2.01835800	-0.13766600
H	-0.06919500	1.23849800	1.37113700
O	2.07149500	-0.59383000	-0.01121600
H	2.39275300	-0.15313800	-0.81374600

OH-R4: OH + CH₃CH₂CH₃ → H₂O + CH₃CHCH₃

C	1.28955300	-0.20046500	0.00399700
H	1.30120100	-1.02183500	-0.72132100
H	1.45214100	-0.65876500	0.99127700
H	2.14435000	0.44591400	-0.19992500
C	0.00000000	0.54352300	-0.05033500
H	-0.00000100	1.61381000	0.11399100
C	-1.28955300	-0.20046500	0.00399600
H	-1.45215600	-0.65874100	0.99128600
H	-2.14434800	0.44590800	-0.19995300
H	-1.30118800	-1.02185200	-0.72130200

TS4: OH + CH₃CH₂CH₃ → H₂O + CH₃CHCH₃

C	0.96002200	1.27759100	-0.13807200
H	0.86986500	1.29894500	-1.22656600

H	0.46625800	2.16490500	0.26108900
H	2.02414600	1.33981400	0.11174200
C	0.35997700	0.00039000	0.42342600
H	-0.74974300	-0.00871200	0.12337000
H	0.36997900	0.00155700	1.51700600
C	0.97623400	-1.27048100	-0.13493900
H	0.49257000	-2.16272600	0.26544300
H	0.88775100	-1.29494500	-1.22352300
H	2.04075900	-1.31909100	0.11628800
O	-2.20654500	-0.01303900	-0.19579200
H	-2.52662400	0.03955800	0.71900200

3.1.4 C4 (*n*-C₄H₁₀)



n-C₄H₁₀

C	-1.94913700	0.11990400	0.00006500
H	-2.08746800	0.75066200	-0.88229600
H	-2.08755700	0.75008100	0.88282500
H	-2.73888400	-0.63424800	-0.00022600
C	-0.56178600	-0.51694100	-0.00007100
H	-0.45277700	-1.16550700	0.87655500
H	-0.45287800	-1.16535900	-0.87681800
C	0.56178600	0.51694100	-0.00007100
H	0.45277500	1.16550800	0.87655400
H	0.45288000	1.16535800	-0.87681900
C	1.94913700	-0.11990400	0.00006500
H	2.08749400	-0.75060400	-0.88233400
H	2.73888400	0.63424800	-0.00015100
H	2.08753100	-0.75014000	0.88278800

CH₂(CH₂)₂CH₃

C	1.87880700	-0.13045500	0.01867600
H	2.01272100	-0.86326100	-0.78142200
H	2.00271800	-0.65258100	0.97116400
H	2.67905900	0.60721000	-0.06593600
C	0.50319000	0.52392000	-0.06829600
H	0.39184700	1.26416500	0.73117000
H	0.40658900	1.06927600	-1.01218600
C	-0.63601800	-0.49340800	0.03605000
H	-0.51283800	-1.05668400	0.97616200
H	-0.53735700	-1.23817100	-0.76242800
C	-1.98621100	0.13170200	-0.01279700
H	-2.85760100	-0.43764600	-0.30695900

H	-2.14374400	1.11713500	0.40863700
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TS5: OH + CH₃(CH₂)₂CH₃ → H₂O + CH₂(CH₂)₂CH₃

C	0.98022200	0.86912500	0.00289100
H	1.02531900	1.40872900	0.95090900
H	0.94915100	1.57676300	-0.82849900
H	2.01522900	0.34112500	-0.12126500
C	-0.13102400	-0.16011100	-0.05141800
H	-0.05984000	-0.72761600	-0.98476000
H	-0.01241600	-0.88357300	0.76304100
C	-1.51919900	0.47832000	0.04951900
H	-1.63939500	1.20470500	-0.76098800
H	-1.58769100	1.04369800	0.98495100
C	-2.63857400	-0.55757300	-0.01283100
H	-2.54508500	-1.28103900	0.80128200
H	-3.62142800	-0.08916100	0.06630400
H	-2.60432600	-1.11113600	-0.95455800
O	3.12979400	-0.53408700	-0.07439200
H	2.89358000	-0.98836900	0.74975900

OH-R6: OH + CH₃(CH₂)₂CH₃ → H₂O + CH₃CHCH₂CH₃

CH₃CHCH₂CH₃

C	-1.92830400	0.16594000	-0.06554900
H	-2.00242700	0.68707600	-1.02266100
H	-2.07778400	0.90201300	0.72827400
H	-2.74155700	-0.55974200	-0.00866600
C	-0.56506500	-0.50893300	0.07603100
H	-0.53475900	-1.07201600	1.02340900
H	-0.43719600	-1.26584300	-0.70893200
C	0.57413500	0.45204800	0.02382600
H	0.39065300	1.48465100	0.30222900
C	1.97660600	-0.04412100	-0.05242000
H	2.08716000	-0.79573900	-0.84167500
H	2.68556200	0.76169200	-0.24772300
H	2.28611400	-0.53169400	0.88441600

TS6: OH + CH₃(CH₂)₂CH₃ → H₂O + CH₃CHCH₂CH₃

C	-1.81301800	-0.96272200	-0.04103300
H	-1.82942800	-2.02319300	0.23068200
H	-1.95240600	-0.89198100	-1.12217000
H	-2.66063400	-0.47618600	0.44381600
C	-0.49528100	-0.33268000	0.37344400
H	-0.54244600	0.77707800	0.06801100

H	-0.37638700	-0.32870600	1.46223400
C	0.73187800	-0.92240100	-0.30157000
H	0.59690900	-0.87891700	-1.38712700
H	0.79685700	-1.98566400	-0.03839500
C	2.02121500	-0.20762400	0.09214300
H	2.17192800	-0.24475300	1.17471700
H	2.89241300	-0.66278400	-0.38217000
H	1.98090400	0.84155600	-0.21047200
O	-0.45901800	2.24141500	-0.20350300
H	-0.07432800	2.49478900	0.65099000

3.1.5 C5 (*n*-C₅H₁₂)



n-C₅H₁₂

C	2.54053900	-0.32850200	-0.00000500
H	2.57219600	-0.97317400	-0.88251100
H	2.57222500	-0.97314000	0.88252300
H	3.44376400	0.28516500	-0.00003300
C	1.27623300	0.52766200	0.00000000
H	1.27462900	1.18434100	0.87696700
H	1.27461600	1.18432900	-0.87697500
C	0.00000000	-0.31090800	0.00001200
H	0.00000100	-0.96974400	0.87746400
H	-0.00000100	-0.96976800	-0.87742200
C	-1.27623300	0.52766200	0.00000100
H	-1.27461600	1.18433200	-0.87697300
H	-1.27462900	1.18433800	0.87697000
C	-2.54053900	-0.32850200	-0.00000600
H	-2.57221700	-0.97315500	0.88251300
H	-3.44376400	0.28516500	-0.00001400
H	-2.57220400	-0.97316000	-0.88252100

CH₂(CH₂)₃CH₃

C	-2.58001500	-0.34646500	-0.02517600
H	-2.58112200	-1.34047800	0.40498300
H	-3.52683900	0.06754500	-0.34465900
C	-1.34956000	0.49014800	0.02506700
H	-1.35785400	1.21617200	-0.79636900
H	-1.33844000	1.09455500	0.94711800
C	-0.06060700	-0.33269100	-0.02973700
H	-0.05254200	-0.92631200	-0.95087600
H	-0.05730000	-1.04931600	0.80040100
C	1.20035800	0.52503500	0.03590700

H	1.18684300	1.11643100	0.95796600
H	1.18959200	1.24292000	-0.79146700
C	2.47763500	-0.30894000	-0.02391300
H	2.51796100	-0.89047800	-0.94866300
H	3.37026600	0.31836500	0.01670900
H	2.52256300	-1.01192400	0.81196600

TS7: OH + CH₃(CH₂)₃CH₃ → H₂O + CH₂(CH₂)₃CH₃

C	-1.62508700	0.85783700	-0.01069700
H	-1.58982000	1.56301600	-0.84403000
H	-1.65283100	1.40110700	0.93587100
H	-2.66901800	0.34605700	-0.12448900
C	-0.53053900	-0.18896400	-0.07163600
H	-0.65973700	-0.91395200	0.73954900
H	-0.61317800	-0.75036300	-1.00756500
C	0.86646200	0.42867900	0.02917600
H	0.95365200	0.97816100	0.97426900
H	0.99438200	1.16807100	-0.77038500
C	1.98321800	-0.60924700	-0.05918200
H	1.89684000	-1.14796400	-1.00882200
H	1.84640900	-1.35426300	0.73210500
C	3.37141300	0.01535800	0.05498200
H	3.49097100	0.52619100	1.01397000
H	4.15760900	-0.73797400	-0.02398600
H	3.53237900	0.75241200	-0.73603700
O	-3.81121800	-0.49192500	-0.04223200
H	-3.59072100	-0.91707500	0.80154500

OH-R8: OH + CH₃(CH₂)₃CH₃ → H₂O + CH₃CH(CH₂)₂CH₃
CH₃CH(CH₂)₂CH₃

C	2.59741700	-0.22868900	-0.08508400
H	2.57519700	-0.94230600	-0.91600200
H	2.85538700	-0.80856000	0.81382800
H	3.41182700	0.47520600	-0.26215100
C	1.28585900	0.46249900	0.06185500
H	1.26633300	1.49774000	0.38646400
C	0.01790400	-0.31923700	0.12203400
H	-0.06905700	-0.82778800	1.09818800
H	0.05178500	-1.12853500	-0.62037400
C	-1.23532500	0.52798900	-0.10139800
H	-1.16573800	1.01090300	-1.08117600
H	-1.25769800	1.33334500	0.64053200
C	-2.51959900	-0.29120600	-0.01265300

H	-2.61951700	-0.75469800	0.97247900
H	-3.40250200	0.32799600	-0.18275100
H	-2.52354700	-1.09143600	-0.75756400

TS8: OH + CH₃(CH₂)₃CH₃ → H₂O + CH₃CH(CH₂)₂CH₃

C	2.09777000	-1.32533900	-0.13487500
H	2.14530100	-1.28215100	-1.22530600
H	1.90148000	-2.36356500	0.15158500
H	3.07528900	-1.04411800	0.25954900
C	1.00107700	-0.41620100	0.39121700
H	0.98935300	-0.39359200	1.48604800
H	1.27334700	0.65459700	0.06730600
C	-0.38384000	-0.70695200	-0.16034800
H	-0.66659600	-1.73183400	0.11714900
H	-0.34806500	-0.68161300	-1.25568800
C	-1.44851400	0.26714700	0.33804600
H	-1.16414500	1.28051900	0.03631000
H	-1.46186800	0.25456700	1.43385200
C	-2.83981200	-0.05996200	-0.19728000
H	-3.15111200	-1.06166000	0.11053100
H	-3.58574100	0.64934900	0.16638500
H	-2.85202100	-0.02878900	-1.28969700
O	1.50997700	2.09284100	-0.25854100
H	1.20487300	2.45340100	0.58974200

**OH-R9: OH + CH₃(CH₂)₃CH₃ → H₂O + CH₃CH₂CHCH₂CH₃
CH₃CH₂CHCH₂CH₃**

C	-2.50695500	-0.40190700	0.06557100
H	-2.44724400	-1.03762600	0.95186000
H	-2.54933200	-1.05307200	-0.81102300
H	-3.44109100	0.16061100	0.11240400
C	-1.29733400	0.52798700	-0.01394600
H	-1.40705200	1.19397300	-0.88552500
H	-1.28156200	1.19752000	0.85605000
C	0.00000000	-0.20230300	-0.09870000
H	0.00000000	-1.22195200	-0.47483400
C	1.29733400	0.52798700	-0.01394600
H	1.28156200	1.19752100	0.85605000
H	1.40705200	1.19397300	-0.88552600
C	2.50695500	-0.40190700	0.06557100
H	2.54933200	-1.05307200	-0.81102200
H	3.44109100	0.16061100	0.11240300
H	2.44724400	-1.03762600	0.95186000

TS9: OH + CH₃(CH₂)₃CH₃ → H₂O + CH₃CH₂CHCH₂CH₃

C	2.53202900	-0.25604500	-0.30884200
H	2.50797900	0.83517100	-0.35740800
H	2.59120300	-0.63473900	-1.33230300
H	3.44171400	-0.55718600	0.21374200
C	1.28385500	-0.78565300	0.39235800
H	1.31192800	-1.88134300	0.43407700
H	1.26612000	-0.44254000	1.43350600
C	0.00003300	-0.35551600	-0.29611800
H	0.00005200	-0.64501000	-1.35408700
H	-0.00034000	0.79981100	-0.34609900
C	-1.28359400	-0.78593700	0.39250500
H	-1.26582000	-0.44265500	1.43357400
H	-1.31144500	-1.88164000	0.43422000
C	-2.53186300	-0.25645200	-0.30859300
H	-2.59110900	-0.63513000	-1.33206400
H	-3.44146300	-0.55771300	0.21407500
H	-2.50782700	0.83476000	-0.35694500
O	-0.00146700	2.22514900	0.08154300
H	0.00798200	2.04463800	1.03551300

3.1.6 C6 (*n*-C₆H₁₄)**OH-R10: OH + CH₃(CH₂)₄CH₃ → H₂O + CH₂(CH₂)₄CH₃*****n*-C₆H₁₄**

C	-3.20106000	0.20961500	0.00000200
H	-3.27882500	0.85046900	-0.88247200
H	-3.27882700	0.85045200	0.88248700
H	-4.05823200	-0.46680300	-0.00000600
C	-1.87880500	-0.55378100	-0.00000300
H	-1.83095200	-1.20892400	0.87685300
H	-1.83095300	-1.20891600	-0.87686400
C	-0.66565300	0.37359100	0.00000100
H	-0.71269900	1.03056800	0.87748000
H	-0.71269600	1.03057100	-0.87747600
C	0.66565300	-0.37359100	0.00000100
H	0.71269600	-1.03057200	-0.87747500
H	0.71269800	-1.03056700	0.87748000
C	1.87880500	0.55378100	-0.00000300
H	1.83095200	1.20892400	0.87685300
H	1.83095300	1.20891600	-0.87686400
C	3.20106000	-0.20961500	0.00000200
H	3.27882700	-0.85046500	-0.88247500
H	4.05823200	0.46680300	-0.00000100

H	3.27882600	-0.85045600	0.88248500
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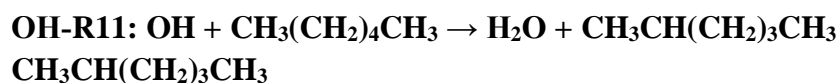
CH₂(CH₂)₄CH₃

C	-3.12755500	-0.22409400	0.01820800
H	-3.19638000	-0.80856300	0.93952500
H	-3.20354500	-0.91959800	-0.82176300
H	-3.99035600	0.44373000	-0.02018700
C	-1.81292000	0.55012600	-0.03546200
H	-1.77395300	1.14928100	-0.95164500
H	-1.76713900	1.25869500	0.79863800
C	-0.59151500	-0.36482400	0.01758300
H	-0.63601500	-1.07501700	-0.81732000
H	-0.62931400	-0.96607000	0.93445300
C	0.73059000	0.39518800	-0.03516100
H	0.77817300	1.10346000	0.80058000
H	0.77395100	0.99402900	-0.95182100
C	1.95185600	-0.52498300	0.02043400
H	1.91060700	-1.24174600	-0.80820300
H	1.88727800	-1.13589200	0.93612700
C	3.24426700	0.21359400	-0.01091700
H	3.31641100	1.20509400	0.41903400
H	4.16194300	-0.27744300	-0.30552900

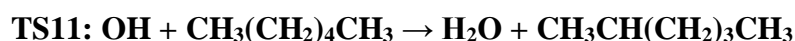
TS10: OH + CH₃(CH₂)₄CH₃ → H₂O + CH₂(CH₂)₄CH₃

C	-2.58633500	-0.86513300	0.25924300
H	-2.91147000	0.20485100	-0.07886800
H	-2.64194800	-0.87440900	1.35005200
H	-3.35193100	-1.51951000	-0.16002800
C	-1.18947600	-1.13044600	-0.26516000
H	-0.89820200	-2.15491700	0.00093600
H	-1.19165300	-1.08300000	-1.35871500
C	-0.15413900	-0.15203800	0.28503000
H	-0.16971900	-0.18782900	1.38183700
H	-0.44351600	0.86548400	-0.00222400
C	1.26122200	-0.43624700	-0.20947700
H	1.27446200	-0.40714700	-1.30577000
H	1.54959900	-1.45580800	0.07501700
C	2.29465300	0.54888000	0.33219200
H	2.27779600	0.52125000	1.42725700
H	2.00589000	1.56559400	0.04445700
C	3.70575500	0.25297600	-0.16885300
H	3.74856000	0.30092700	-1.26012400
H	4.43098600	0.96694600	0.22650100

H	4.02331000	-0.74900100	0.13168500
O	-3.10848900	1.59835400	-0.30481100
H	-2.82433300	1.91178300	0.56862300

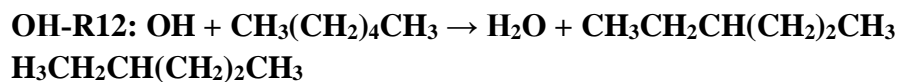


C	3.15954900	0.23408700	0.08122600
H	3.20159000	0.77404500	1.03077500
H	3.25882300	0.96904800	-0.72196200
H	4.02416600	-0.43100000	0.03571600
C	1.84863600	-0.53724700	-0.04640100
H	1.83749400	-1.09473600	-0.98937800
H	1.77960300	-1.28292100	0.75323700
C	0.62488400	0.37343200	0.01217500
H	0.68367200	1.11253500	-0.79590600
H	0.63414200	0.93983500	0.95042200
C	-0.69499400	-0.38886700	-0.09916400
H	-0.76004200	-1.13199000	0.70786400
H	-0.68691200	-0.97932500	-1.03187300
C	-1.89941800	0.48897300	-0.06128500
H	-1.80599800	1.50784500	-0.42212800
C	-3.25661100	-0.09962700	0.11466700
H	-3.28053700	-0.78618200	0.96804600
H	-4.01739400	0.66627200	0.27206200
H	-3.56088200	-0.68793000	-0.76418400

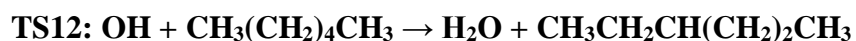


C	-2.81072400	-1.02688000	-0.08312500
H	-2.76558100	-2.11549100	0.01892400
H	-2.91703000	-0.80438900	-1.14884300
H	-3.70832200	-0.67844200	0.43068100
C	-1.55587000	-0.38802800	0.48511600
H	-1.65981900	0.76005500	0.41931200
H	-1.46801400	-0.56508400	1.56223300
C	-0.27326700	-0.75701300	-0.23936000
H	-0.38052500	-0.51881600	-1.30508800
H	-0.13096200	-1.84476800	-0.18070500
C	0.95583300	-0.04593700	0.31987600
H	1.06832200	-0.29764600	1.38159700
H	0.79094600	1.03645200	0.27208900
C	2.24192000	-0.40268500	-0.42140000
H	2.12816900	-0.14736900	-1.48065300
H	2.39523300	-1.48680200	-0.38002300

C	3.46320800	0.31227600	0.15077000
H	3.61341500	0.04657300	1.20046700
H	4.37297300	0.05299300	-0.39428800
H	3.33696600	1.39672600	0.09854000
O	-1.81572900	2.14085600	-0.10545900
H	-2.27654200	1.88875800	-0.92183200



C	-3.18153300	-0.13785400	0.11479900
H	-3.22554800	-0.71156900	1.04433900
H	-3.34492100	-0.83401100	-0.71216500
H	-4.00889300	0.57422700	0.12165900
C	-1.83535500	0.56670800	-0.02466300
H	-1.82001900	1.15900200	-0.94556500
H	-1.69568900	1.27235300	0.80045900
C	-0.66179000	-0.41198200	-0.04399300
H	-0.80474200	-1.12435700	-0.87487500
H	-0.68542800	-1.03042900	0.86500800
C	0.66949600	0.24859100	-0.15952900
H	0.71757900	1.26091600	-0.55235300
C	1.93024200	-0.54423400	-0.08498500
H	2.07399600	-1.10742500	-1.02166100
H	1.83248500	-1.30678900	0.69767800
C	3.16639800	0.31656900	0.17471200
H	3.07609500	0.84207600	1.12789600
H	4.07489600	-0.28801400	0.20218200
H	3.28543600	1.06723100	-0.61065000



C	3.05546700	-0.46890300	0.21832900
H	3.12912800	-0.82701100	1.24832700
H	3.14974100	0.61941500	0.23488500
H	3.89859600	-0.87909600	-0.34047600
C	1.72218700	-0.87785100	-0.40206300
H	1.68248900	-0.55451400	-1.44886200
H	1.63311000	-1.97098500	-0.41723900
C	0.53112500	-0.30076600	0.34345900
H	0.65793200	0.84882700	0.36358300
H	0.56096800	-0.56795000	1.40676200
C	-0.82648400	-0.60683200	-0.26362400
H	-0.97388400	-1.69508100	-0.27896200
H	-0.83718900	-0.28594500	-1.31368300

C	-1.98359000	0.05484500	0.48207300
H	-1.81264100	1.13561800	0.51128500
H	-1.98055200	-0.28785600	1.52229700
C	-3.33664100	-0.24601800	-0.15668200
H	-3.53303300	-1.32138300	-0.16973000
H	-4.15147200	0.23705500	0.38581100
H	-3.36660400	0.10937000	-1.19017600
O	0.78991800	2.25602500	-0.10010700
H	0.65167700	2.06449100	-1.04191500

3.1.7 C7 (*n*-C₇H₁₆)



n-C₇H₁₆

C	3.81416600	-0.35993000	-0.00002900
H	3.84532500	-1.00456900	-0.88246000
H	3.84537500	-1.00454500	0.88241700
H	4.71775200	0.25298000	-0.00006300
C	2.55088300	0.49759000	-0.00000600
H	2.54978500	1.15411600	0.87693800
H	2.54974500	1.15410200	-0.87696000
C	1.27413700	-0.34028600	0.00002900
H	1.27432400	-0.99864000	-0.87745000
H	1.27434400	-0.99860100	0.87753700
C	0.00000000	0.50075400	0.00002200
H	0.00000000	1.15863900	-0.87765400
H	0.00000000	1.15865900	0.87768400
C	-1.27413700	-0.34028600	0.00003000
H	-1.27434600	-0.99859500	0.87754200
H	-1.27432200	-0.99864500	-0.87744500
C	-2.55088300	0.49759000	-0.00001300
H	-2.54974600	1.15409100	-0.87697500
H	-2.54978400	1.15412700	0.87692200
C	-3.81416600	-0.35993000	-0.00002500
H	-3.84537600	-1.00453100	0.88243200
H	-4.71775200	0.25298000	-0.00006900
H	-3.84532400	-1.00458300	-0.88244500

CH₂(CH₂)₅CH₃

C	-3.74620600	-0.34130000	-0.02064100
H	-3.78838000	-1.02372900	0.83230600
H	-3.77866800	-0.94617200	-0.93072700
H	-4.64403500	0.27955400	0.00153100
C	-2.47531700	0.50358400	0.02276200

H	-2.46565900	1.19941200	-0.82319600
H	-2.47089400	1.11932000	0.92877300
C	-1.20627700	-0.34519400	-0.01325200
H	-1.21358000	-1.04238400	0.83356000
H	-1.21077600	-0.96307200	-0.91955400
C	0.07481600	0.48410700	0.02596900
H	0.08325500	1.09667200	0.93583300
H	0.07759000	1.18543200	-0.81736300
C	1.34009000	-0.36787400	-0.02324300
H	1.33598600	-0.97929600	-0.93251700
H	1.34247500	-1.06757100	0.82098000
C	2.62414000	0.46391500	0.01422100
H	2.61125400	1.08464400	0.92529500
H	2.62634100	1.17506100	-0.82012400
C	3.85950600	-0.36608300	-0.02358400
H	4.80360700	0.04825900	-0.35069100
H	3.86697000	-1.35306700	0.42251200

TS13: OH + CH₃(CH₂)₅CH₃ → H₂O + CH₂(CH₂)₅CH₃

C	-2.96829800	0.84391600	-0.00058500
H	-2.97830900	1.53110000	-0.84942900
H	-3.03244100	1.40409200	0.93430300
H	-3.97643300	0.26380900	-0.10276700
C	-1.80625400	-0.12885100	-0.03977300
H	-1.87371200	-0.82655600	0.80241300
H	-1.86362900	-0.73227200	-0.95116900
C	-0.45327300	0.58553700	0.01178700
H	-0.38319300	1.28577200	-0.82889500
H	-0.39728200	1.19127600	0.92414600
C	0.72929300	-0.37928200	-0.03203400
H	0.67146900	-0.98158000	-0.94668000
H	0.65492300	-1.08325300	0.80568000
C	2.08060100	0.32878000	0.02204700
H	2.14103000	0.92635200	0.93999500
H	2.15282900	1.03819200	-0.81141900
C	3.26543600	-0.63297900	-0.03201700
H	3.20687800	-1.22388600	-0.95256600
H	3.18865800	-1.34516900	0.79679100
C	4.60930900	0.08823300	0.03183500
H	4.70094000	0.65760300	0.96053800
H	5.44485100	-0.61283300	-0.01507400
H	4.71360600	0.79072400	-0.79918300
O	-5.04327800	-0.67320900	-0.05376500

H	-4.76485200	-1.12982500	0.75587700
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OH-R14: OH + CH₃(CH₂)₅CH₃ → H₂O + CH₃CH(CH₂)₄CH₃
CH₃CH(CH₂)₄CH₃

C	3.77579800	-0.33570000	-0.00530900
H	3.80510000	-1.05136500	-0.83111000
H	3.82416100	-0.90378500	0.92748100
H	4.67249300	0.28419800	-0.06669000
C	2.50372200	0.50658100	-0.06125800
H	2.50926000	1.23766700	0.75451500
H	2.48243200	1.08344500	-0.99218100
C	1.23591100	-0.33918600	0.03377200
H	1.22898700	-1.07250200	-0.78213400
H	1.25644200	-0.91725000	0.96591700
C	-0.04456800	0.48910000	-0.02013700
H	-0.07275100	1.06128100	-0.95437800
H	-0.03663300	1.22401800	0.79362000
C	-1.31164100	-0.35900500	0.08514400
H	-1.26987900	-0.94710900	1.01837000
H	-1.32329800	-1.10568400	-0.72145500
C	-2.57105500	0.43758300	0.04060700
H	-2.53855000	1.47334700	0.36208300
C	-3.89001400	-0.24242900	-0.09075900
H	-4.15383300	-0.79766100	0.82198700
H	-4.69721800	0.46562400	-0.28407900
H	-3.87563700	-0.97589100	-0.90431000

TS14: OH + CH₃(CH₂)₅CH₃ → H₂O + CH₃CH(CH₂)₄CH₃

C	3.38803600	-1.03624000	-0.18567500
H	3.42868000	-0.82098200	-1.25741200
H	3.34858500	-2.12402900	-0.07334900
H	4.31553100	-0.68465500	0.26956500
C	2.17062500	-0.39169100	0.45325800
H	2.14216700	-0.57046500	1.53326400
H	2.27823900	0.75604000	0.38402900
C	0.84749700	-0.75093800	-0.19965300
H	0.89464400	-0.50410200	-1.26782600
H	0.70432800	-1.83857700	-0.14219800
C	-0.34508100	-0.03991400	0.43451600
H	-0.17159400	1.04140100	0.39783900
H	-0.40476900	-0.31110100	1.49560400
C	-1.66950600	-0.37151600	-0.24748600
H	-1.83226600	-1.45633600	-0.22560600

H	-1.61252200	-0.09054900	-1.30644300
C	-2.86515500	0.32926800	0.39370900
H	-2.69679600	1.41131600	0.37792800
H	-2.92588000	0.04222900	1.44917500
C	-4.18178600	0.00159800	-0.30584300
H	-4.37843400	-1.07354400	-0.28148200
H	-5.02562400	0.50723400	0.16777900
H	-4.15180900	0.30931400	-1.35449600
O	2.40419900	2.13553800	-0.15205900
H	2.78614400	1.87910700	-1.00685100

OH-R15: OH + CH₃(CH₂)₅CH₃ → H₂O + CH₃CH₂CH(CH₂)₃CH₃
CH₃CH₂CH(CH₂)₃CH₃

C	-3.76703800	-0.42864700	0.06357600
H	-3.75250200	-1.06724800	0.95071400
H	-3.80190200	-1.08031800	-0.81347100
H	-4.68980700	0.15444200	0.08515300
C	-2.53400900	0.47048900	0.02136400
H	-2.58283200	1.12408500	-0.85654100
H	-2.52696800	1.12925700	0.89661600
C	-1.23164500	-0.32468800	-0.01881100
H	-1.17546900	-0.97977500	0.85819300
H	-1.23578900	-0.98205800	-0.89652800
C	0.01268600	0.56155500	-0.06352400
H	0.02489400	1.22322600	0.81399300
H	-0.06361700	1.23900000	-0.93158700
C	1.28967700	-0.20482200	-0.12797500
H	1.27209200	-1.21111200	-0.53809700
C	2.60502900	0.48025600	0.02674800
H	2.58418200	1.10874400	0.92687100
H	2.76017300	1.18292500	-0.80827300
C	3.78306100	-0.48998600	0.09526700
H	3.83479500	-1.09608000	-0.81263600
H	4.73190100	0.03875200	0.20156900
H	3.67428500	-1.16878000	0.94415300

TS15: OH + CH₃(CH₂)₅CH₃ → H₂O + CH₃CH₂CH(CH₂)₃CH₃

C	3.62231700	-0.31796400	0.28526000
H	3.66579100	-0.40009600	1.37468300
H	3.66222700	0.74258000	0.02557400
H	4.50983700	-0.80426300	-0.12337600
C	2.34085800	-0.94626200	-0.25573300
H	2.33257500	-0.89596800	-1.34926300

H	2.30207800	-2.01068400	0.00759600
C	1.09161500	-0.26599500	0.27895700
H	1.09290600	-0.24716500	1.37541400
H	1.16677000	0.83588200	-0.04406600
C	-0.22571300	-0.79753100	-0.25804900
H	-0.32819300	-1.85130500	0.03447700
H	-0.20183900	-0.77997300	-1.35356700
C	-1.43516600	-0.00961300	0.23861600
H	-1.32742500	1.03663300	-0.07129100
H	-1.44567100	-0.01313000	1.33593400
C	-2.76366500	-0.55659400	-0.27828000
H	-2.86783500	-1.60255100	0.03033900
H	-2.74893200	-0.55714000	-1.37337500
C	-3.96051800	0.24907900	0.22020800
H	-3.88708700	1.29161500	-0.10019900
H	-4.90210200	-0.15254700	-0.15942100
H	-4.00809900	0.23974300	1.31237800
O	1.25029800	2.30311200	-0.35359400
H	0.96424700	2.61276200	0.52103100

**OH-R16: OH + CH₃(CH₂)₅CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₂CH₃
CH₃(CH₂)₂CH(CH₂)₂CH₃**

C	3.81767600	-0.23506000	0.16192600
H	4.00574000	-0.78761100	-0.76247400
H	3.79959800	-0.95705900	0.98262500
H	4.66080800	0.43839000	0.32730000
C	2.49889200	0.52839000	0.08175600
H	2.33889500	1.09611500	1.00377200
H	2.54351600	1.26108100	-0.73096900
C	1.30006900	-0.39356800	-0.14548300
H	1.47332800	-0.97716000	-1.06641200
H	1.25127300	-1.13815400	0.66093000
C	0.00000000	0.33080900	-0.23160900
H	0.00000000	1.34680000	-0.61828400
C	-1.30006900	-0.39356800	-0.14548300
H	-1.25127300	-1.13815300	0.66093100
H	-1.47332800	-0.97716100	-1.06641100
C	-2.49889200	0.52838900	0.08175600
H	-2.54351600	1.26108100	-0.73097000
H	-2.33889500	1.09611600	1.00377200
C	-3.81767600	-0.23506000	0.16192600
H	-3.79959900	-0.95705900	0.98262600
H	-4.66080800	0.43839000	0.32729900

H	-4.00574000	-0.78761100	-0.76247400
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TS16: OH + CH₃(CH₂)₅CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₂CH₃

C	-3.82862200	-0.60140700	-0.20205900
H	-3.90600300	-1.65964800	0.06171200
H	-3.85019800	-0.52839500	-1.29246400
H	-4.71457100	-0.09415000	0.18449500
C	-2.54550900	0.00816700	0.35610500
H	-2.48976300	1.06983200	0.09476500
H	-2.55628000	-0.04532400	1.45044800
C	-1.29224000	-0.69044300	-0.16623800
H	-1.32176000	-1.75377600	0.10853000
H	-1.28245300	-0.65396900	-1.26177200
C	-0.00593400	-0.08058100	0.36373600
H	-0.00750000	-0.04712100	1.45979100
H	-0.00997300	1.01861700	0.02477800
C	1.27633100	-0.70053700	-0.16318300
H	1.25824100	-0.69042600	-1.25903700
H	1.30980100	-1.75663900	0.13744300
C	2.53417300	0.01010400	0.33126400
H	2.54056500	0.00900200	1.42709000
H	2.48991800	1.05808000	0.01678000
C	3.81473300	-0.63477100	-0.19187400
H	3.83444100	-0.62585400	-1.28460600
H	4.70296600	-0.10862900	0.16301900
H	3.88881600	-1.67577600	0.13363700
O	0.01398300	2.47782400	-0.33408700
H	0.28428300	2.79839200	0.54157600

3.1.8 C8 (*n*-C₈H₁₈)

OH-R17: OH + CH₃(CH₂)₆CH₃ → H₂O + CH₂(CH₂)₆CH₃

***n*-C₈H₁₈**

C	4.46560400	0.25915700	-0.00018000
H	4.52300000	0.90198200	0.88228000
H	4.52274800	0.90216000	-0.88252600
H	5.34364500	-0.38977000	-0.00037200
C	3.16840100	-0.54605800	-0.00007600
H	3.14079900	-1.20200900	-0.87703500
H	3.14100700	-1.20213300	0.87679700
C	1.92693900	0.34316100	0.00012600
H	1.95349800	1.00107100	-0.87731200
H	1.95365500	1.00091300	0.87767700
C	0.61989100	-0.44559300	0.00016400

H	0.59386000	-1.10307800	0.87775700
H	0.59383100	-1.10310000	-0.87741100
C	-0.61989100	0.44559400	0.00016000
H	-0.59382500	1.10310200	-0.87741400
H	-0.59386700	1.10307600	0.87775400
C	-1.92693900	-0.34316100	0.00010800
H	-1.95365500	-1.00092400	0.87765100
H	-1.95349700	-1.00105900	-0.87733800
C	-3.16840100	0.54605800	-0.00007900
H	-3.14080800	1.20201300	-0.87703600
H	-3.14099900	1.20212900	0.87679700
C	-4.46560400	-0.25915700	-0.00017100
H	-4.52298600	-0.90199100	0.88228300
H	-5.34364600	0.38976900	-0.00034300
H	-4.52276200	-0.90215200	-0.88252200

CH₂(CH₂)₆CH₃

C	-4.39118300	-0.27418200	0.01334300
H	-4.44223900	-0.88073000	0.92148200
H	-4.44717500	-0.95292200	-0.84179500
H	-5.27312100	0.36897300	-0.01034600
C	-3.09920200	0.53842200	-0.02293200
H	-3.07693300	1.15729200	-0.92656000
H	-3.07444300	1.23065000	0.82566700
C	-1.85208600	-0.34219400	0.01268000
H	-1.87538000	-1.03573500	-0.83689200
H	-1.87388700	-0.96338800	0.91657300
C	-0.55032300	0.45453000	-0.02153300
H	-0.52836900	1.14949500	0.82668300
H	-0.52795800	1.07328400	-0.92681900
C	0.69460800	-0.42848200	0.01757900
H	0.66953100	-1.12686800	-0.82780300
H	0.67493700	-1.04363700	0.92552700
C	1.99560000	0.36813000	-0.02542000
H	2.02508300	1.06559700	0.82014400
H	2.02142300	0.98064700	-0.93361400
C	3.24159500	-0.51932900	0.01575000
H	3.21648600	-1.22784500	-0.82049300
H	3.19714800	-1.14135800	0.92505600
C	4.51306600	0.25473400	-0.01306900
H	4.56177900	1.24042000	0.43329600
H	5.44066900	-0.20365200	-0.32849200

TS17: OH + CH₃(CH₂)₆CH₃ → H₂O + CH₂(CH₂)₆CH₃

C	-3.64525900	0.77966300	0.00795700
H	-3.68252500	1.46560600	-0.84110100
H	-3.74115400	1.33524300	0.94278700
H	-4.62565800	0.15450300	-0.09852500
C	-2.43798600	-0.13695000	-0.02459000
H	-2.46969000	-0.82743300	0.82573900
H	-2.46783600	-0.75204000	-0.92951800
C	-1.12078800	0.64228300	0.01512900
H	-1.09591800	1.26818100	0.91507400
H	-1.08302700	1.32784100	-0.83958000
C	0.10724900	-0.26486900	-0.00777000
H	0.07427400	-0.89725200	-0.90306300
H	0.07247700	-0.94497900	0.85188100
C	1.42222700	0.51084100	0.01444300
H	1.45317800	1.14636600	0.90782900
H	1.45662700	1.18889700	-0.84689100
C	2.65247400	-0.39275800	-0.00563200
H	2.62001600	-1.03168900	-0.89670100
H	2.62172200	-1.06835300	0.85802600
C	3.96807400	0.38257700	0.00897700
H	3.99841600	1.02126600	0.89849200
H	3.99743500	1.05543800	-0.85494800
C	5.18901400	-0.53363200	-0.00995200
H	5.18902700	-1.16255700	-0.90414800
H	6.12003800	0.03645900	-0.00112500
H	5.19205000	-1.19495100	0.86050100
O	-5.64257700	-0.83745200	-0.07656700
H	-5.29887000	-1.34386800	0.67643400

**OH-R18: OH + CH₃(CH₂)₆CH₃ → H₂O + CH₃CH(CH₂)₅CH₃
CH₃CH(CH₂)₅CH₃**

C	-4.41658700	0.27483500	0.06703500
H	-4.49004100	0.98207300	-0.76333400
H	-4.45265800	0.85023900	0.99586900
H	-5.29754500	-0.36947400	0.03774200
C	-3.12413700	-0.53284700	-0.01989300
H	-3.08225200	-1.25217600	0.80523500
H	-3.11735800	-1.12229100	-0.94319600
C	-1.87758600	0.34840300	0.02135400
H	-1.88586500	0.94331800	0.94286700
H	-1.91491100	1.06611600	-0.80740500
C	-0.57637900	-0.44595700	-0.05543600

H	-0.56815500	-1.04049100	-0.97719200
H	-0.54141000	-1.16354700	0.77344000
C	0.66845500	0.43594100	-0.01109300
H	0.66371100	1.03178100	0.90863800
H	0.63879700	1.14961600	-0.84297400
C	1.97004600	-0.36198600	-0.08244100
H	1.96188400	-0.97541700	-1.00008900
H	2.00342500	-1.08619900	0.74367800
C	3.19552600	0.48617100	-0.04655800
H	3.12659400	1.50858400	-0.40282200
C	4.53811100	-0.13501000	0.12896100
H	4.83231600	-0.72227500	-0.75397800
H	5.31547100	0.61211700	0.29557900
H	4.54330600	-0.82926700	0.97637100

TS18: OH + CH₃(CH₂)₆CH₃ → H₂O + CH₃CH(CH₂)₅CH₃

C	4.03643800	-0.91536800	-0.10743800
H	4.09428700	-0.72075800	-1.18229300
H	4.04871300	-2.00115200	0.02778000
H	4.93294300	-0.50808200	0.36309000
C	2.77148900	-0.32095100	0.48625700
H	2.72599500	-0.47429300	1.56962400
H	2.81895500	0.82892300	0.38928100
C	1.48605000	-0.76657800	-0.18809600
H	1.39981300	-1.85869100	-0.10549900
H	1.54719600	-0.54396000	-1.26078500
C	0.24160100	-0.10513700	0.39812800
H	0.35738200	0.98276000	0.33529200
H	0.16966100	-0.35107100	1.46455600
C	-1.04521400	-0.52647500	-0.30633500
H	-1.15023100	-1.61741100	-0.25571800
H	-0.97383100	-0.27311600	-1.37121900
C	-2.29182800	0.12808100	0.28332300
H	-2.18174700	1.21857500	0.24230600
H	-2.37121600	-0.13244400	1.34598100
C	-3.57898400	-0.27577900	-0.43181400
H	-3.68664300	-1.36533300	-0.39157100
H	-3.49800200	-0.01317400	-1.49232600
C	-4.81669600	0.38622100	0.16847000
H	-4.73745700	1.47539600	0.11770700
H	-5.72645000	0.09148100	-0.35837500
H	-4.93369200	0.11151700	1.22008000
O	2.87707800	2.19757500	-0.18358400

H	3.33056900	1.94615100	-1.00421300
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OH-R19: OH + CH₃(CH₂)₆CH₃ → H₂O + CH₃CH₂CH(CH₂)₄CH₃
CH₃CH₂CH(CH₂)₄CH₃

C	4.43167500	-0.19180800	0.09259100
H	4.53843400	-0.86820100	-0.75961600
H	4.47436500	-0.79655400	1.00236400
H	5.29157600	0.48085200	0.09649300
C	3.11482000	0.57641000	0.01420700
H	3.03823200	1.26541400	0.86239200
H	3.10168100	1.19664900	-0.88865100
C	1.89787700	-0.34584500	0.00606800
H	1.91218900	-0.97089500	0.90748400
H	1.97144500	-1.03382700	-0.84536400
C	0.57325300	0.40808400	-0.06548400
H	0.55965000	1.03467700	-0.96517900
H	0.49316000	1.09051200	0.78841000
C	-0.64315800	-0.51691200	-0.08150100
H	-0.62779100	-1.16018100	0.80974100
H	-0.55337700	-1.21048700	-0.93529800
C	-1.94416500	0.20796600	-0.14846100
H	-1.95710100	1.21842100	-0.54863700
C	-3.23838900	-0.52069000	-0.01614900
H	-3.17324000	-1.22758000	0.82082600
H	-3.40867000	-1.14578500	-0.90819200
C	-4.43401400	0.41089100	0.17893100
H	-4.52247300	1.10458600	-0.66085500
H	-5.36851700	-0.14826400	0.25297800
H	-4.31695700	1.00208700	1.08989400

TS19: OH + CH₃(CH₂)₆CH₃ → H₂O + CH₃CH₂CH(CH₂)₄CH₃

C	-4.20575700	-0.37626300	0.26633700
H	-4.25731700	0.71483300	0.24722500
H	-4.26844000	-0.69618900	1.30959800
H	-5.07717800	-0.77142400	-0.25879200
C	-2.90410100	-0.85780300	-0.36905400
H	-2.85856500	-1.95356000	-0.35100200
H	-2.87503600	-0.56872100	-1.42618900
C	-1.67518900	-0.30575200	0.33260100
H	-1.68867300	-0.54372600	1.40308800
H	-1.76109500	0.84822200	0.32434600
C	-0.34402000	-0.67501100	-0.29781300
H	-0.34550000	-0.37358300	-1.35362200

H	-0.23843400	-1.76806000	-0.29598000
C	0.85182300	-0.04324100	0.41106400
H	0.87107200	-0.37980900	1.45456200
H	0.71495100	1.04388500	0.43911700
C	2.18477500	-0.37667400	-0.25325300
H	2.16545800	-0.03758700	-1.29651200
H	2.31584700	-1.46545300	-0.28674000
C	3.38149300	0.25286700	0.45613900
H	3.40439900	-0.09080500	1.49597500
H	3.24480100	1.33890900	0.49358200
C	4.70715700	-0.07718600	-0.22495100
H	4.71174300	0.27832700	-1.25873200
H	5.55069900	0.38496700	0.29159700
H	4.87653800	-1.15699100	-0.24492700
O	-1.84434700	2.24202700	-0.18655400
H	-1.70758700	2.01492600	-1.12058600

**OH-R20: OH + CH₃(CH₂)₆CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₃CH₃
CH₃(CH₂)₂CH(CH₂)₃CH₃**

C	-4.42493000	0.37776300	0.12374100
H	-4.49241600	1.04049700	-0.74305800
H	-4.40394000	1.00456000	1.01913800
H	-5.33508300	-0.22435900	0.15711600
C	-3.17524300	-0.49519000	0.04208600
H	-3.13461700	-1.16357300	0.90912500
H	-3.23145800	-1.13975700	-0.84203200
C	-1.89051600	0.32682000	-0.01936300
H	-1.82710700	0.97393700	0.86307000
H	-1.92811600	0.99305300	-0.88961800
C	-0.62991400	-0.53327900	-0.10251700
H	-0.71510600	-1.20593200	-0.97356500
H	-0.58175200	-1.20084100	0.76917700
C	0.62918700	0.25964200	-0.19370300
H	0.58106400	1.26297800	-0.60879600
C	1.96200800	-0.39590600	-0.06918500
H	2.13967300	-1.06081600	-0.93232400
H	1.96431000	-1.05999000	0.80663900
C	3.12374200	0.59231200	0.03723400
H	2.95952300	1.24040300	0.90395300
H	3.11814600	1.24340500	-0.84328400
C	4.47571900	-0.10502700	0.15582100
H	4.66895800	-0.73325300	-0.71786700
H	5.29238300	0.61474800	0.23801600

H	4.50522500	-0.74787100	1.03962200
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TS20: OH + CH₃(CH₂)₆CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₃CH₃

C	-4.40362900	-0.55328800	-0.13830100
H	-4.49224000	-1.61156700	0.12177000
H	-4.45087100	-0.47377300	-1.22748500
H	-5.27115900	-0.03362100	0.27282500
C	-3.09727600	0.03182400	0.39136500
H	-3.02943600	1.09363700	0.13366300
H	-3.08273700	-0.02632500	1.48539000
C	-1.86895300	-0.68583500	-0.16350000
H	-1.88555700	-0.64665300	-1.25888900
H	-1.90876500	-1.74928800	0.10959300
C	-0.56072300	-0.09739800	0.33611800
H	-0.53543100	-0.06557400	1.43188700
H	-0.55885700	1.00279400	0.00008400
C	0.69899200	-0.73599400	-0.22248000
H	0.65293900	-0.72616500	-1.31741300
H	0.72465200	-1.79193800	0.07888200
C	1.97731400	-0.04208100	0.24039100
H	2.01260100	-0.03842200	1.33722800
H	1.94475200	1.00705500	-0.07700300
C	3.24703800	-0.69425100	-0.30127900
H	3.20789800	-0.69930700	-1.39577800
H	3.27563400	-1.74360700	0.01214400
C	4.51395300	0.01778100	0.16545700
H	4.58578700	0.00919500	1.25633500
H	5.41266800	-0.45680400	-0.23305700
H	4.51403100	1.06169500	-0.15913300
O	-0.50605200	2.46041200	-0.36118400
H	-0.10778100	2.76082100	0.47180600

3.1.9 C9 (n-C₉H₂₀)

OH-R21: OH + CH₃(CH₂)₇CH₃ → H₂O + CH₂(CH₂)₇CH₃

n-C₉H₂₀

C	-5.08834600	-0.37898600	-0.00009600
H	-5.11906800	-1.02367900	0.88229400
H	-5.11900300	-1.02358000	-0.88256100
H	-5.99237600	0.23325600	-0.00009600
C	-3.82574400	0.47947700	-0.00000200
H	-3.82511300	1.13602000	-0.87691400
H	-3.82518700	1.13593800	0.87697000
C	-2.54830400	-0.35739500	0.00001300

H	-2.54798800	-1.01568500	-0.87749800
H	-2.54803100	-1.01572000	0.87749800
C	-1.27497100	0.48479700	0.00005800
H	-1.27558700	1.14266700	0.87770600
H	-1.27553700	1.14267500	-0.87758300
C	0.00000000	-0.35531600	0.00009000
H	-0.00000600	-1.01334300	-0.87741300
H	0.00000600	-1.01326300	0.87765200
C	1.27497100	0.48479700	0.00003800
H	1.27557100	1.14271900	0.87764700
H	1.27555400	1.14262300	-0.87764300
C	2.54830400	-0.35739500	0.00007000
H	2.54796800	-1.01579700	-0.87735800
H	2.54805200	-1.01560800	0.87763800
C	3.82574400	0.47947700	-0.00008500
H	3.82519700	1.13607500	0.87678500
H	3.82510300	1.13588300	-0.87709900
C	5.08834600	-0.37898600	-0.00006200
H	5.11897000	-1.02375000	-0.88240400
H	5.99237600	0.23325600	-0.00021300
H	5.11910100	-1.02350900	0.88245100

CH₂(CH₂)₇CH₃

C	5.13670000	-0.37637700	-0.02452400
H	5.14881400	-1.35675000	0.43592500
H	6.07855800	0.03605800	-0.36045700
C	3.89909600	0.45055800	0.00641100
H	3.88573600	1.08039400	0.91121000
H	3.89813600	1.15306000	-0.83515600
C	2.61723000	-0.38508800	-0.02068000
H	2.62278400	-1.07630100	0.83049200
H	2.61342200	-1.00553000	-0.92382900
C	1.34989600	0.46413000	0.02198500
H	1.34966300	1.15707700	-0.82822300
H	1.35816300	1.08563800	0.92574800
C	0.07071900	-0.36888700	-0.00702900
H	0.06720200	-1.05725300	0.84678900
H	0.06719900	-0.99545200	-0.90716100
C	-1.19928000	0.47819600	0.02236800
H	-1.19521000	1.16626000	-0.83176700
H	-1.19694500	1.10507600	0.92239500
C	-2.47747300	-0.35595200	-0.00880000
H	-2.48404600	-1.04241800	0.84677600

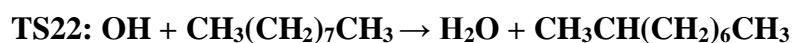
H	-2.47813300	-0.98540200	-0.90721000
C	-3.74973900	0.48842600	0.01414900
H	-3.74092400	1.17419700	-0.84001000
H	-3.74932100	1.11495500	0.91275600
C	-5.01756900	-0.36146500	-0.02144800
H	-5.05797800	-1.03474400	0.83885500
H	-5.91773000	0.25626000	-0.00681800
H	-5.04686800	-0.97636400	-0.92491400

TS21: OH + CH₃(CH₂)₇CH₃ → H₂O + CH₂(CH₂)₇CH₃

C	4.27681900	0.80761600	0.00772900
H	4.36137700	1.36657900	0.94165500
H	4.30526700	1.49236400	-0.84263200
H	5.26744000	0.19801100	-0.09493800
C	3.08443400	-0.12818700	-0.02611000
H	3.12491900	-0.74243400	-0.93121000
H	3.12630900	-0.81840800	0.82400700
C	1.75500500	0.62995400	0.01279100
H	1.70763900	1.31635800	-0.84077100
H	1.71916300	1.25391400	0.91374100
C	0.54139300	-0.29623700	-0.01323600
H	0.58673300	-0.97858000	0.84417600
H	0.58421100	-0.92511600	-0.91060500
C	-0.78531000	0.45901200	0.01155800
H	-0.82990600	1.13995900	-0.84700400
H	-0.82597900	1.09051600	0.90740200
C	-2.00198700	-0.46298000	-0.01216000
H	-1.95922300	-1.14259700	0.84767100
H	-1.96060900	-1.09595700	-0.90695600
C	-3.32751700	0.29399800	0.00890900
H	-3.37091800	0.97344700	-0.85120000
H	-3.36881000	0.92812400	0.90312400
C	-4.54718700	-0.62446000	-0.01360100
H	-4.50220600	-1.30317800	0.84507600
H	-4.50610000	-1.25560100	-0.90805600
C	-5.86310100	0.14919500	0.01041000
H	-5.93790300	0.81483400	-0.85356200
H	-6.72518700	-0.52042400	-0.00634000
H	-5.93414500	0.76564300	0.91050500
O	6.29794800	-0.77946300	-0.06830600
H	5.95905400	-1.28921500	0.68461100

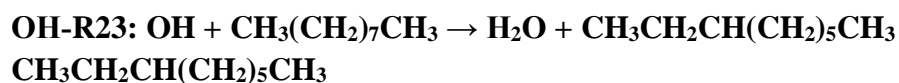


C	5.17309800	-0.25076300	-0.10399600
H	5.15834000	-0.97723100	-0.92378800
H	5.44143700	-0.81306200	0.80308700
H	5.97759600	0.46134900	-0.29370200
C	3.85255700	0.42409000	0.03741900
H	3.81769000	1.45698800	0.36758500
C	2.59567300	-0.37673600	0.07640900
H	2.56291300	-0.98276500	0.99841000
H	2.60311100	-1.10792200	-0.74435600
C	1.32556300	0.46952100	-0.00326200
H	1.34651400	1.06178100	-0.92509000
H	1.32016000	1.18665200	0.82615300
C	0.04787500	-0.36403300	0.03984300
H	0.03578000	-0.96291000	0.95872300
H	0.05273800	-1.07822500	-0.79260000
C	-1.22213500	0.48061000	-0.02815600
H	-1.20970000	1.08184000	-0.94535600
H	-1.22823200	1.19257300	0.80615700
C	-2.50027400	-0.35323400	0.01179100
H	-2.50970900	-0.95946600	0.92598900
H	-2.49810900	-1.06145000	-0.82590600
C	-3.77237700	0.48967800	-0.04552800
H	-3.76303700	1.09346500	-0.95950600
H	-3.77226600	1.19677700	0.79109900
C	-5.04050600	-0.35929600	-0.00113000
H	-5.07742800	-0.95330000	0.91593100
H	-5.94041700	0.25794700	-0.03709200
H	-5.07422300	-1.05205800	-0.84607600



C	4.63422900	-0.92192500	-0.19169700
H	4.65673700	-0.72714400	-1.26786800
H	4.64853100	-2.00778400	-0.05728900
H	5.54676200	-0.51686600	0.24908300
C	3.39077600	-0.32499100	0.44343500
H	3.38017200	-0.47897300	1.52756500
H	3.43756800	0.82490800	0.34558900
C	2.08302200	-0.76707500	-0.18903900
H	1.99697700	-1.85907300	-0.10469400
H	2.10954600	-0.54338700	-1.26290300
C	0.86007800	-0.10323200	0.43831500

H	0.97782700	0.98445300	0.37515000
H	0.82104500	-0.35242800	1.50572700
C	-0.44985000	-0.51732000	-0.22662800
H	-0.55660200	-1.60818400	-0.17865400
H	-0.41201500	-0.25817300	-1.29183000
C	-1.67478400	0.13785400	0.40677400
H	-1.55925900	1.22788500	0.37234100
H	-1.72230700	-0.13269100	1.46871900
C	-2.98421600	-0.25279700	-0.27328900
H	-3.09942300	-1.34343100	-0.24321700
H	-2.93782800	0.02159600	-1.33450100
C	-4.21022100	0.40014100	0.36111500
H	-4.09023700	1.48868000	0.33574300
H	-4.25925000	0.12041200	1.41919900
C	-5.51075700	0.00911400	-0.33595000
H	-5.66140000	-1.07310900	-0.29991400
H	-6.37625900	0.48360800	0.13074900
H	-5.49206800	0.30593300	-1.38804900
O	3.48090600	2.19300500	-0.22978500
H	3.91456800	1.94111500	-1.06087000



C	-5.05895600	-0.54544500	0.11616700
H	-4.92498900	-1.25693200	0.93412700
H	-5.12237200	-1.11463800	-0.81456100
H	-6.01150000	-0.03332200	0.26287700
C	-3.89390200	0.44112700	0.06435200
H	-4.07034200	1.17165600	-0.74198400
H	-3.86618100	1.03721700	0.98618100
C	-2.57285600	-0.22109200	-0.13489100
H	-2.54974300	-1.21783900	-0.56763400
C	-1.30555200	0.56183500	-0.08047700
H	-1.31824800	1.22096300	0.79876700
H	-1.24566500	1.24193300	-0.94771400
C	-0.04940700	-0.30876400	-0.04961900
H	-0.04578100	-0.96352900	-0.92911400
H	-0.09008800	-0.96631900	0.82614300
C	1.24204100	0.50398400	-0.01923300
H	1.23715800	1.16138300	0.85877400
H	1.27679600	1.16192700	-0.89626900
C	2.49635100	-0.36568100	0.00889100
H	2.49894000	-1.02687900	-0.86639300

H	2.46525800	-1.02056700	0.88832500
C	3.79087500	0.44421600	0.03053400
H	3.78739900	1.10406800	0.90494800
H	3.82017100	1.09715100	-0.84861000
C	5.03511700	-0.44011200	0.05748700
H	5.06748100	-1.09093800	-0.82030700
H	5.95128300	0.15366700	0.06888100
H	5.03814700	-1.07941300	0.94430000

TS23: OH + CH₃(CH₂)₇CH₃ → H₂O + CH₃CH₂CH(CH₂)₅CH₃

C	-4.79380400	-0.27355200	0.36124000
H	-4.81682600	0.81695400	0.30027200
H	-4.83028600	-0.55083600	1.41794500
H	-5.69223500	-0.66447300	-0.11960000
C	-3.52716900	-0.81526700	-0.29598000
H	-3.51383200	-1.91080200	-0.24329900
H	-3.52165000	-0.56058300	-1.36218300
C	-2.26122000	-0.28000900	0.35073200
H	-2.24639600	-0.48853100	1.42727300
H	-2.31565300	0.87548500	0.31249000
C	-0.96263700	-0.70498700	-0.31172000
H	-0.98457500	-0.41911800	-1.37173500
H	-0.89590300	-1.80097700	-0.29675900
C	0.27574900	-0.10765500	0.35261000
H	0.32198300	-0.44359800	1.39542700
H	0.17335300	0.98327100	0.38311200
C	1.57324400	-0.48206200	-0.35884100
H	1.53369800	-0.12405200	-1.39503600
H	1.65822100	-1.57445400	-0.41419000
C	2.81543200	0.08606400	0.32242300
H	2.86966600	-0.29056200	1.35118700
H	2.72078000	1.17619100	0.39933000
C	4.11156300	-0.25689900	-0.40839000
H	4.05901500	0.13028800	-1.43181900
H	4.19893100	-1.34566200	-0.49479800
C	5.34641100	0.30460700	0.29156200
H	5.43598400	-0.09734900	1.30420400
H	6.26238400	0.05786300	-0.24889500
H	5.28658400	1.39328600	0.37145400
O	-2.36897400	2.25268100	-0.24251200
H	-2.21687400	1.99477700	-1.16610700

OH-R24: OH + CH₃(CH₂)₇CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₄CH₃

CH₃(CH₂)₂CH(CH₂)₄CH₃

C	-5.10763300	-0.18947200	0.22501700
H	-5.09402400	-0.85801100	1.08984200
H	-5.31128900	-0.79720100	-0.66059700
H	-5.93935500	0.50592400	0.35274200
C	-3.77787600	0.54610100	0.08606300
H	-3.81810100	1.22641100	-0.77106800
H	-3.60054500	1.16863700	0.96859200
C	-2.59636500	-0.40804600	-0.09259500
H	-2.78811200	-1.04838800	-0.97101800
H	-2.55132300	-1.09977500	0.76001100
C	-1.28544000	0.28585500	-0.24061800
H	-1.27608700	1.29122600	-0.65351200
C	-0.00133400	-0.46928200	-0.18365100
H	0.10670600	-1.10046600	-1.08254300
H	-0.02759400	-1.17363400	0.65899200
C	1.23043100	0.42834500	-0.06251300
H	1.13917200	1.04057900	0.84175000
H	1.25048900	1.12587800	-0.90821400
C	2.53974600	-0.35431000	-0.02045900
H	2.62748000	-0.96603000	-0.92681000
H	2.51724000	-1.05596800	0.82243000
C	3.77098100	0.54053500	0.10343300
H	3.68242300	1.14976800	1.00936400
H	3.79194300	1.24112100	-0.73833400
C	5.07307600	-0.25553000	0.14339800
H	5.19268600	-0.85084500	-0.76560900
H	5.94251700	0.39873100	0.23234100
H	5.08226200	-0.94312200	0.99317800

TS24: OH + CH₃(CH₂)₇CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₄CH₃

C	-4.94294600	-0.60787800	-0.25237300
H	-4.99974200	-1.69738200	-0.18016600
H	-4.95928500	-0.34446800	-1.31343600
H	-5.84211200	-0.19413600	0.20777400
C	-3.67746400	-0.08055500	0.41818800
H	-3.64644300	1.01193400	0.35775800
H	-3.68991100	-0.33314000	1.48391500
C	-2.40586900	-0.64394100	-0.21258300
H	-2.39570700	-0.40896400	-1.28491600
H	-2.41466100	-1.74003200	-0.14245100
C	-1.13423800	-0.11857700	0.42985400
H	-1.12986000	-0.30024500	1.51118200

H	-1.16043100	1.03638200	0.36209200
C	0.15845800	-0.58898700	-0.21362100
H	0.14212700	-0.34348800	-1.28358600
H	0.20725600	-1.68457200	-0.15577700
C	1.40571100	0.01427600	0.42815600
H	1.43462500	-0.26194500	1.48909500
H	1.33031900	1.10725300	0.39457900
C	2.69911500	-0.43317000	-0.24714300
H	2.67022600	-0.15429700	-1.30794000
H	2.76731300	-1.52787700	-0.21944300
C	3.94894700	0.16538700	0.39422500
H	3.98193300	-0.11976600	1.45142300
H	3.87479800	1.25793200	0.37205800
C	5.23391200	-0.27855700	-0.29982900
H	5.23066100	0.02055700	-1.35146500
H	6.11690600	0.15915800	0.16981500
H	5.33973400	-1.36615700	-0.26508300
O	-1.18153300	2.40053900	-0.22667000
H	-1.11924700	2.11095600	-1.15131900

**OH-R25: OH + CH₃(CH₂)₇CH₃ → H₂O + CH₃(CH₂)₃CH(CH₂)₃CH₃
CH₃(CH₂)₃CH(CH₂)₃CH₃**

C	-5.01868600	-0.56513000	0.16547100
H	-4.90510100	-1.31713900	0.95077700
H	-5.10585400	-1.09268500	-0.78804500
H	-5.95657700	-0.03486800	0.34188300
C	-3.82629000	0.38784700	0.15137100
H	-3.96690800	1.14518800	-0.62766500
H	-3.77524100	0.92961100	1.10220900
C	-2.50271800	-0.33520900	-0.08396900
H	-2.54780200	-0.87476400	-1.03766500
H	-2.35682700	-1.09376400	0.69360300
C	-1.29874700	0.60668700	-0.09583100
H	-1.25440900	1.15821000	0.85327500
H	-1.45926700	1.37769700	-0.86919600
C	0.00000000	-0.08791300	-0.32688400
H	0.00000300	-0.99781000	-0.92176500
C	1.29874600	0.60668500	-0.09581600
H	1.25440200	1.15820100	0.85329400
H	1.45927100	1.37770200	-0.86917400
C	2.50271700	-0.33521100	-0.08395300
H	2.54780400	-0.87475900	-1.03765300
H	2.35682300	-1.09377100	0.69361300

C	3.82628800	0.38784400	0.15139500
H	3.77524900	0.92957500	1.10225200
H	3.96689100	1.14521200	-0.62761600
C	5.01869000	-0.56512600	0.16544500
H	5.10584200	-1.09265300	-0.78808700
H	5.95658100	-0.03486300	0.34185200
H	4.90512600	-1.31715800	0.95073200

TS25: OH + CH₃(CH₂)₇CH₃ → H₂O + CH₃(CH₂)₃CH(CH₂)₃CH₃

C	-5.07814800	0.01561200	0.32453200
H	-5.06555100	1.10847900	0.32850600
H	-5.13945300	-0.31881400	1.36346100
H	-5.98723700	-0.30818400	-0.18601300
C	-3.82625200	-0.53822700	-0.35078400
H	-3.86510500	-1.63309900	-0.36044400
H	-3.80233900	-0.22128100	-1.39935700
C	-2.54149300	-0.08471200	0.33813100
H	-2.56533700	-0.39392700	1.39017600
H	-2.49046900	1.01026900	0.33864000
C	-1.28187600	-0.64131400	-0.32073900
H	-1.27073000	-0.36367800	-1.38297800
H	-1.30737100	-1.73888900	-0.29572000
C	0.00071400	-0.16340800	0.33729700
H	-0.00013100	-0.37671200	1.41284000
H	0.00354600	0.99347900	0.30304200
C	1.28280200	-0.64358000	-0.31982300
H	1.27032800	-0.37028600	-1.38298700
H	1.30942200	-1.74104200	-0.28899700
C	2.54197700	-0.08156700	0.33516100
H	2.56440000	-0.38012900	1.39036700
H	2.49122100	1.01327800	0.32362200
C	3.82722800	-0.54312100	-0.34741300
H	3.80397300	-0.23876400	-1.39971300
H	3.86642700	-1.63803500	-0.34375800
C	5.07847300	0.01920400	0.32213000
H	5.13778900	-0.30072100	1.36576700
H	5.98822100	-0.31224900	-0.18230500
H	5.06651000	1.11202200	0.31086400
O	0.00352000	2.37045800	-0.25389300
H	-0.05682400	2.10131000	-1.18482200

3.1.10 C₁₀ (*n*-C₁₀H₂₂)

OH-R26: OH + CH₃(CH₂)₈CH₃ → H₂O + CH₂(CH₂)₈CH₃

n-C₁₀H₂₂

C	5.73542100	-0.29095000	-0.00038600
H	6.62285900	0.34508700	-0.00081200
H	5.78299900	-0.93488000	-0.88260000
H	5.78344100	-0.93432100	0.88221200
C	4.45022800	0.53328000	-0.00032700
H	4.43206200	1.18932500	-0.87743100
H	4.43243600	1.18979300	0.87643400
C	3.19580900	-0.33769400	0.00016000
H	3.21279400	-0.99602100	-0.87716800
H	3.21314600	-0.99557000	0.87781900
C	1.90035000	0.46998600	0.00020500
H	1.88358300	1.12761800	-0.87747700
H	1.88374800	1.12780700	0.87774800
C	0.64803400	-0.40352200	0.00039600
H	0.66504500	-1.06119000	0.87801900
H	0.66491900	-1.06135500	-0.87710600
C	-0.64803400	0.40352200	0.00040200
H	-0.66492500	1.06135900	-0.87709600
H	-0.66503900	1.06118700	0.87802800
C	-1.90034900	-0.46998600	0.00021500
H	-1.88374500	-1.12780700	0.87775800
H	-1.88358500	-1.12761700	-0.87746700
C	-3.19580900	0.33769400	0.00017400
H	-3.21279000	0.99603000	-0.87714800
H	-3.21315000	0.99556100	0.87784000
C	-4.45022800	-0.53328000	-0.00032700
H	-4.43244400	-1.18979700	0.87643100
H	-4.43205400	-1.18932100	-0.87743400
C	-5.73542100	0.29094900	-0.00039600
H	-5.78298800	0.93488800	-0.88260500
H	-6.62285900	-0.34508700	-0.00084000
H	-5.78345300	0.93431200	0.88220700

CH₂(CH₂)₈CH₃

C	5.78500600	0.28015100	-0.01535600
H	6.71539400	-0.15974200	-0.34841700
H	5.82499100	1.25839700	0.44803100
C	4.52352800	-0.51015000	0.01035200
H	4.48870500	-1.13958100	0.91493500
H	4.50519800	-1.21211300	-0.83145200
C	3.26651300	0.36230400	-0.02098100
H	3.28930300	1.05337700	0.83002000
H	3.28301000	0.98223600	-0.92433500

C	1.97536300	-0.45038700	0.01822200
H	1.96409900	-1.07182700	0.92201600
H	1.95780400	-1.14323300	-0.83190200
C	0.71997800	0.41796500	-0.01383600
H	0.73494800	1.04376200	-0.91439200
H	0.73382000	1.10666000	0.83962300
C	-0.57240700	-0.39449200	0.01413900
H	-0.58660500	-1.02211800	0.91353100
H	-0.58632500	-1.08170300	-0.84055800
C	-1.82865100	0.47278900	-0.01596200
H	-1.81394100	1.10161100	-0.91452900
H	-1.81596000	1.15882000	0.83972300
C	-3.12022100	-0.34068700	0.00925400
H	-3.13467000	-0.97080000	0.90710500
H	-3.13405800	-1.02627700	-0.84696100
C	-4.37869600	0.52395500	-0.01868900
H	-4.36437600	1.15105500	-0.91679200
H	-4.36293500	1.20887900	0.83604600
C	-5.66005500	-0.30565900	0.01022500
H	-5.70322100	-0.92077400	0.91300100
H	-6.55030200	0.32617300	-0.00804000
H	-5.70703100	-0.97753700	-0.85086300

TS26: OH + CH₃(CH₂)₈CH₃ → H₂O + CH₂(CH₂)₈CH₃

C	-4.93835500	0.73569800	0.00274400
H	-5.90863800	0.09526200	-0.10392800
H	-4.98393100	1.41785500	-0.84898300
H	-5.04518900	1.29335400	0.93513800
C	-3.71681400	-0.16210100	-0.02323100
H	-3.73582800	-0.78247900	-0.92482300
H	-3.73879900	-0.84827700	0.83085300
C	-2.41215300	0.63815800	0.01369200
H	-2.38443300	1.31958600	-0.84468700
H	-2.39801700	1.26915300	0.91028300
C	-1.16969100	-0.24934900	-0.00331700
H	-1.19201200	-0.88709900	-0.89511200
H	-1.19417800	-0.92507100	0.86013900
C	0.13253500	0.54764900	0.01534100
H	0.15298900	1.18813400	0.90544100
H	0.15626600	1.22167400	-0.84948100
C	1.37739200	-0.33621300	0.00013300
H	1.35442500	-0.97987500	-0.88760900
H	1.35665200	-1.00726100	0.86742100

C	2.67926100	0.46150900	0.01058400
H	2.70201500	1.10608400	0.89776100
H	2.69977600	1.13190000	-0.85725700
C	3.92480600	-0.42097800	-0.00439900
H	3.90198800	-1.06694400	-0.89071700
H	3.90624100	-1.09071500	0.86418100
C	5.22755900	0.37587900	0.00305400
H	5.24911100	1.02025300	0.88871300
H	5.24450300	1.04396100	-0.86492200
C	6.46332700	-0.52044200	-0.01266500
H	6.47224800	-1.15385200	-0.90366100
H	7.38517500	0.06450800	-0.00782200
H	6.47773100	-1.17726800	0.86109900
O	-6.91454400	-0.90837100	-0.07915800
H	-6.56894600	-1.40477200	0.67961600

OH-R27: OH + CH₃(CH₂)₈CH₃ → H₂O + CH₃CH(CH₂)₇CH₃
CH₃CH(CH₂)₇CH₃

C	-5.81704200	-0.15806800	0.14069000
H	-6.60184600	0.58050200	0.31062100
H	-5.81307600	-0.85421800	0.98654700
H	-6.10705700	-0.74637200	-0.74293400
C	-4.48151700	0.47772300	-0.03630900
H	-4.42408000	1.50084500	-0.39255200
C	-3.24661700	-0.35669600	-0.07143800
H	-3.26659300	-1.07325500	0.76182400
H	-3.23698700	-0.97886600	-0.98313100
C	-1.95403800	0.45693500	-0.01573300
H	-1.95196200	1.06376600	0.89681900
H	-1.93676500	1.16081600	-0.85625800
C	-0.69910500	-0.41065900	-0.05552700
H	-0.70657500	-1.01939700	-0.96796000
H	-0.71933100	-1.11557600	0.78457900
C	0.59290800	0.40083100	-0.00079100
H	0.59862600	1.01186000	0.90996700
H	0.61536600	1.10359000	-0.84255600
C	1.84885000	-0.46676200	-0.03421600
H	1.84408400	-1.07714700	-0.94551900
H	1.82516300	-1.17026100	0.80696600
C	3.14100300	0.34397600	0.02360000
H	3.14555400	0.95521000	0.93448700
H	3.16656600	1.04734700	-0.81780300
C	4.39818900	-0.52246800	-0.00686600

H	4.39478400	-1.12899900	-0.91908100
H	4.36907000	-1.22675000	0.83165700
C	5.68079700	0.30289600	0.05904100
H	5.71318400	0.89649800	0.97652900
H	6.56975300	-0.33069500	0.03820200
H	5.74155700	0.99484500	-0.78511300

TS27: OH + CH₃(CH₂)₈CH₃ → H₂O + CH₃CH(CH₂)₇CH₃

C	-5.27885600	-0.92158200	-0.07973800
H	-6.17915500	-0.42866100	0.28991200
H	-5.28930400	-1.95747900	0.27416900
H	-5.32426200	-0.94030400	-1.17091400
C	-4.02097600	-0.21483600	0.39390400
H	-4.00272400	-0.11675400	1.48442700
H	-4.07661700	0.86388900	-0.00549000
C	-2.72395500	-0.81702600	-0.11852000
H	-2.64531500	-1.84846400	0.25135900
H	-2.76403000	-0.88201300	-1.21193600
C	-1.48531900	-0.02981500	0.30131000
H	-1.46928300	0.06622800	1.39440900
H	-1.55863200	0.98608900	-0.10419400
C	-0.18051500	-0.66869700	-0.16688800
H	-0.20110300	-0.77431400	-1.25823100
H	-0.10599200	-1.68460100	0.23983200
C	1.05577700	0.12950600	0.23979700
H	1.07383000	0.23963000	1.33105600
H	0.98149600	1.14389800	-0.17064100
C	2.36276100	-0.50807300	-0.22443000
H	2.34263400	-0.62249500	-1.31507000
H	2.43998500	-1.52094800	0.18945200
C	3.59763100	0.29547300	0.17554300
H	3.61914000	0.41002200	1.26638700
H	3.51992300	1.30874700	-0.23758800
C	4.90653200	-0.33814900	-0.28970900
H	4.88355100	-0.45167100	-1.37902300
H	4.98384300	-1.34963100	0.12384600
C	6.13039800	0.47880500	0.11721200
H	6.18831900	0.57679400	1.20456700
H	7.05710500	0.01577300	-0.22753600
H	6.08176100	1.48654200	-0.30381500
O	-4.02066100	2.30340900	-0.39514300
H	-3.57075900	2.61881600	0.40527100

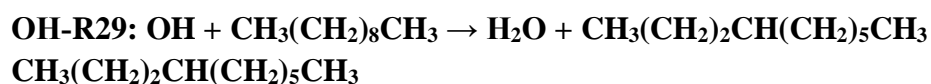
OH-R28: OH + CH₃(CH₂)₈CH₃ → H₂O + CH₃CH₂CH(CH₂)₆CH₃
CH₃CH₂CH(CH₂)₆CH₃

C	5.71245100	0.46986700	0.13586400
H	6.65375900	-0.06628800	0.26850800
H	5.59347900	1.16167000	0.97278900
H	5.78816100	1.06238100	-0.77927700
C	4.52639900	-0.48978800	0.05762900
H	4.48363900	-1.10731400	0.96462700
H	4.68931300	-1.20397800	-0.76603200
C	3.22076000	0.20608700	-0.12827000
H	3.22078200	1.21020200	-0.54412900
C	1.93575500	-0.54827600	-0.08589100
H	1.93032900	-1.21544700	0.78738900
H	1.86431200	-1.21922300	-0.95938000
C	0.69933800	0.34985500	-0.05177200
H	0.71237900	1.01099800	-0.92638500
H	0.75202300	0.99984200	0.82902100
C	-0.60952000	-0.43470100	-0.03081100
H	-0.62138400	-1.09782200	0.84278800
H	-0.65537100	-1.08614200	-0.91218500
C	-1.84550700	0.46107200	-0.00095600
H	-1.83145300	1.12681300	-0.87251300
H	-1.80280900	1.10977500	0.88242000
C	-3.15484200	-0.32378900	0.01237600
H	-3.17049000	-0.98900000	0.88449200
H	-3.19649600	-0.97394900	-0.87025100
C	-4.39349100	0.56896200	0.03833400
H	-4.37553800	1.23379300	-0.83210600
H	-4.35265600	1.21582400	0.92150100
C	-5.69285000	-0.23265000	0.04706900
H	-5.74082100	-0.88416900	0.92365500
H	-6.56888900	0.41870700	0.06455500
H	-5.76323600	-0.86650700	-0.84092100

TS28: OH + CH₃(CH₂)₈CH₃ → H₂O + CH₃CH₂CH(CH₂)₆CH₃

C	5.39946100	-0.27926700	0.28892800
H	6.28621400	-0.66912700	-0.21396400
H	5.46091700	-0.55895300	1.34379200
H	5.42125000	0.81137800	0.22994000
C	4.11749900	-0.81933800	-0.33938900
H	4.10378700	-1.91483300	-0.28610300
H	4.08834000	-0.56507500	-1.40534600

C	2.86739000	-0.28174800	0.33554400
H	2.87804200	-0.48707500	1.41274900
H	2.92125400	0.87359700	0.29278700
C	1.55302200	-0.70787400	-0.29424900
H	1.48351700	-1.80353500	-0.26925100
H	1.55164800	-0.42995400	-1.35656800
C	0.33229900	-0.10119200	0.39376800
H	0.43706600	0.98982600	0.40853900
H	0.31206800	-0.42434700	1.44149400
C	-0.98344400	-0.48177200	-0.27974300
H	-1.07505000	-1.57444100	-0.31346000
H	-0.96742300	-0.14241400	-1.32282600
C	-2.20578100	0.10561600	0.42132200
H	-2.10355000	1.19639300	0.47263900
H	-2.23415800	-0.24942000	1.45863900
C	-3.52087000	-0.24621300	-0.26913200
H	-3.62289300	-1.33715900	-0.32505300
H	-3.49356700	0.11293100	-1.30532400
C	-4.74435900	0.33840100	0.43293100
H	-4.63666400	1.42686900	0.49406400
H	-4.77518200	-0.02652800	1.46531000
C	-6.05047500	-0.01079600	-0.27592900
H	-6.19156000	-1.09398300	-0.32048300
H	-6.91385200	0.41889000	0.23588100
H	-6.04772000	0.36547500	-1.30229900
O	2.96546800	2.24971200	-0.26645000
H	2.80530500	1.98887300	-1.18786700



C	-5.75697900	-0.06676800	0.22071900
H	-6.56416100	0.66191700	0.31713000
H	-5.77185000	-0.70290800	1.10973500
H	-5.97735400	-0.69919300	-0.64345400
C	-4.40144600	0.61608900	0.06468800
H	-4.20983700	1.26861200	0.92237600
H	-4.41023900	1.26085400	-0.82048000
C	-3.25184100	-0.38420200	-0.06210900
H	-3.23885700	-1.04133000	0.81868900
H	-3.45699900	-1.05344200	-0.91569100
C	-1.91717800	0.25922600	-0.22374400
H	-1.87058900	1.25253000	-0.66273800
C	-0.66000500	-0.53685800	-0.13362100

H	-0.58878900	-1.22800500	-0.99123700
H	-0.69781300	-1.18531400	0.75279100
C	0.60380900	0.32176900	-0.08646900
H	0.55141700	0.98938800	0.78106900
H	0.63104300	0.96697400	-0.97263400
C	1.88699100	-0.50175400	-0.02135900
H	1.93329700	-1.16958600	-0.89036500
H	1.85962800	-1.14948500	0.86341700
C	3.14778500	0.35788800	0.02175600
H	3.10694700	1.02004200	0.89535000
H	3.17026400	1.01219400	-0.85843700
C	4.43536600	-0.46166200	0.07146000
H	4.47414700	-1.12170100	-0.80199200
H	4.41276800	-1.11466000	0.95074500
C	5.68572000	0.41347300	0.11194400
H	5.68102800	1.05737800	0.99540700
H	6.59721300	-0.18696600	0.13933100
H	5.73541300	1.05950200	-0.76860400

TS29: OH + CH₃(CH₂)₈CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₅CH₃

C	5.54985800	-0.60227100	-0.15974700
H	6.43165400	-0.08229400	0.21940800
H	5.57857600	-0.55722800	-1.25149500
H	5.62882400	-1.65312500	0.13172900
C	4.26131100	0.01754500	0.37394800
H	4.20417300	1.07206300	0.08549700
H	4.26463400	-0.00757300	1.46924700
C	3.01368700	-0.69814000	-0.13888500
H	3.01597300	-0.69726000	-1.23505700
H	3.03958400	-1.75206100	0.17043800
C	1.72216300	-0.07010100	0.35606800
H	1.73436500	1.01689400	-0.02045900
H	1.71298900	0.00378300	1.45004000
C	0.44496200	-0.70932500	-0.16031400
H	0.39640700	-1.74534900	0.20106100
H	0.48489200	-0.76325600	-1.25419800
C	-0.81504900	0.03963400	0.26689000
H	-0.76685000	1.06233000	-0.12528200
H	-0.83532000	0.12211800	1.36095400
C	-2.10180000	-0.62724100	-0.21192400
H	-2.15222900	-1.64851300	0.18496600
H	-2.07487600	-0.72207400	-1.30417400
C	-3.35905100	0.13575800	0.19718800

H	-3.30924500	1.15588600	-0.20293500
H	-3.38510900	0.23512400	1.28948800
C	-4.64882800	-0.52866400	-0.27839100
H	-4.69972900	-1.54586500	0.12499000
H	-4.61939400	-0.63062100	-1.36867200
C	-5.89560300	0.25074500	0.13234700
H	-5.87499300	1.26227700	-0.28167800
H	-6.80838400	-0.23588800	-0.21689800
H	-5.95780500	0.33940700	1.22029000
O	1.70820400	2.46671200	-0.41423100
H	1.29633300	2.78987900	0.40350300

**OH-R30: OH + CH₃(CH₂)₈CH₃ → H₂O + CH₃(CH₂)₃CH(CH₂)₄CH₃
CH₃(CH₂)₃CH(CH₂)₄CH₃**

C	5.67665500	0.50502600	0.20223900
H	6.59933000	-0.04116200	0.40710200
H	5.56384000	1.27430300	0.97064300
H	5.79332100	1.01177700	-0.75922600
C	4.46440400	-0.42264400	0.18333100
H	4.39106300	-0.95343900	1.13874300
H	4.59737800	-1.19037800	-0.58671300
C	3.15957800	0.32694400	-0.07209500
H	3.01975600	1.08998800	0.70213400
H	3.22847300	0.86300000	-1.02623200
C	1.93593500	-0.58837600	-0.09765800
H	1.88142800	-1.15528800	0.84241300
H	2.07752400	-1.35037800	-0.88320700
C	0.65185500	0.13799200	-0.31315300
H	0.67852400	1.10632300	-0.80650000
C	-0.66060400	-0.55530800	-0.17560800
H	-0.64831300	-1.18869700	0.72195100
H	-0.81011500	-1.25376900	-1.01709800
C	-1.85303200	0.39927200	-0.11076500
H	-1.86237300	1.02474500	-1.01123200
H	-1.71991500	1.08046600	0.73728600
C	-3.19069000	-0.32321600	0.01845100
H	-3.17969800	-0.95058200	0.91820500
H	-3.31889400	-1.00664800	-0.83009400
C	-4.38359700	0.62765300	0.08427500
H	-4.39467500	1.25299700	-0.81496100
H	-4.25341900	1.30937300	0.93173000
C	-5.71395600	-0.10924600	0.21647800
H	-5.72954500	-0.72278000	1.12116900

H	-6.55531700	0.58456300	0.26748300
H	-5.87766000	-0.77300300	-0.63655900

TS30: OH + CH₃(CH₂)₈CH₃ → H₂O + CH₃(CH₂)₃CH(CH₂)₄CH₃

C	-5.65829500	-0.05192400	0.25437600
H	-6.55166100	-0.41804800	-0.25529400
H	-5.67028900	1.04015100	0.21181400
H	-5.72859100	-0.34315100	1.30569500
C	-4.38342900	-0.60478400	-0.37748300
H	-4.34711400	-0.32767300	-1.43693100
H	-4.39984100	-1.69979700	-0.34549000
C	-3.12114900	-0.09825500	0.31600800
H	-3.09396200	0.99682800	0.27829300
H	-3.15655500	-0.37111100	1.37778700
C	-1.83777200	-0.64789700	-0.30147100
H	-1.80972100	-0.39848300	-1.37017200
H	-1.84181600	-1.74469500	-0.24588500
C	-0.57981800	-0.12513700	0.36981100
H	-0.59707200	-0.31355100	1.44984800
H	-0.60606600	1.03021900	0.30873800
C	0.72642800	-0.58993700	-0.24980500
H	0.73033000	-0.34168900	-1.31923400
H	0.77744600	-1.68553100	-0.19347600
C	1.95869000	0.01558700	0.41818400
H	1.96384700	-0.25774900	1.48027300
H	1.88340800	1.10843700	0.38003900
C	3.26735800	-0.43302500	-0.22621800
H	3.26136900	-0.16005500	-1.28892500
H	3.33681200	-1.52745700	-0.19093100
C	4.50155100	0.17143600	0.43941100
H	4.50999000	-0.10539100	1.49933300
H	4.42726500	1.26373400	0.40702800
C	5.80269900	-0.27683800	-0.22087500
H	5.82330600	0.01293900	-1.27492300
H	6.67403600	0.16641000	0.26510300
H	5.90900300	-1.36395600	-0.17402800
O	-0.62432300	2.39672500	-0.27499700
H	-0.55711600	2.11046200	-1.20031500

3.1.11 C11 (*n*-C₁₁H₂₄)

OH-R31: OH + CH₃(CH₂)₉CH₃ → H₂O + CH₂(CH₂)₉CH₃

***n*-C₁₁H₂₄**

C	-6.36257300	-0.39256700	-0.00038000
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H	-6.39293700	-1.03732800	0.88197400
H	-6.39268600	-1.03713200	-0.88288500
H	-7.26703900	0.21903600	-0.00044100
C	-5.10059100	0.46680400	-0.00010600
H	-5.10034200	1.12340100	-0.87697800
H	-5.10059600	1.12322000	0.87690100
C	-3.82254300	-0.36913400	-0.00000900
H	-3.82168400	-1.02740100	-0.87753800
H	-3.82187200	-1.02748900	0.87745500
C	-2.54983100	0.47398400	0.00016200
H	-2.55101100	1.13183400	0.87782300
H	-2.55082700	1.13189400	-0.87745500
C	-1.27419500	-0.36510800	0.00026300
H	-1.27366700	-1.02315200	-0.87723700
H	-1.27372300	-1.02303800	0.87784900
C	0.00000000	0.47610400	0.00023800
H	-0.00002000	1.13405300	0.87780800
H	0.00002100	1.13391100	-0.87743800
C	1.27419500	-0.36510900	0.00032900
H	1.27363700	-1.02327200	-0.87708200
H	1.27375200	-1.02292000	0.87800400
C	2.54983100	0.47398200	0.00006500
H	2.55098900	1.13204700	0.87756600
H	2.55084900	1.13167900	-0.87771200
C	3.82254300	-0.36913500	0.00013400
H	3.82164300	-1.02771700	-0.87715900
H	3.82191400	-1.02717400	0.87783400
C	5.10059100	0.46680300	-0.00032900
H	5.10061300	1.12358400	0.87640600
H	5.10032200	1.12303600	-0.87747400
C	6.36257300	-0.39256500	-0.00027600
H	6.39263400	-1.03754400	-0.88248100
H	7.26703800	0.21903800	-0.00067800
H	6.39299100	-1.03691300	0.88237800

CH₂(CH₂)₉CH₃

C	-6.41286700	-0.38297200	-0.02559600
H	-6.42769000	-1.35811800	0.44578000
H	-7.35326000	0.02742300	-0.36807500
C	-5.17412100	0.44242500	0.00001500
H	-5.17167600	1.13889700	-0.84652200
H	-5.16026700	1.07853800	0.90041800
C	-3.89337400	-0.39522200	-0.02039100

H	-3.88951800	-1.02138800	-0.91958500
H	-3.90075300	-1.08097300	0.83518300
C	-2.62494300	0.45255500	0.01823600
H	-2.63325200	1.07950900	0.91823700
H	-2.62301500	1.14034500	-0.83615500
C	-1.34677200	-0.38221000	-0.00444500
H	-1.34283800	-1.01375200	-0.90110300
H	-1.34525000	-1.06579100	0.85323300
C	-0.07591600	0.46361400	0.02199100
H	-0.07912300	1.09585100	0.91824900
H	-0.07780600	1.14655100	-0.83624500
C	1.20158700	-0.37217700	-0.00185600
H	1.20232800	-1.00688600	-0.89637400
H	1.20526500	-1.05293900	0.85808800
C	2.47353000	0.47225600	0.01793400
H	2.47415300	1.10629700	0.91295400
H	2.46929100	1.15355800	-0.84162300
C	3.75001900	-0.36466000	-0.00877600
H	3.74889900	-0.99979000	-0.90319700
H	3.75568300	-1.04571700	0.85114100
C	5.02409300	0.47714800	0.00819300
H	5.02542100	1.10915800	0.90296100
H	5.01627500	1.15769700	-0.85016000
C	6.29014700	-0.37559400	-0.02270600
H	6.31809300	-0.99569900	-0.92266000
H	7.19163000	0.24029600	-0.01157500
H	6.32911700	-1.04404800	0.84143900

TS31: OH + CH₃(CH₂)₉CH₃ → H₂O + CH₂(CH₂)₉CH₃

C	5.56994400	0.77066200	0.00469000
H	5.66732000	1.32956300	0.93738900
H	5.60760600	1.45349700	-0.84686900
H	6.54933300	0.14382000	-0.10021400
C	4.36099500	-0.14392300	-0.02369200
H	4.38921800	-0.76254900	-0.92625800
H	4.39169300	-0.83111500	0.82932700
C	3.04548600	0.63829100	0.01351100
H	3.00930800	1.32106300	-0.84349700
H	3.02216400	1.26730800	0.91131800
C	1.81508500	-0.26574600	-0.00628000
H	1.84805300	-0.94311600	0.85560900
H	1.84620700	-0.90107800	-0.89954700
C	0.50257200	0.51410400	0.01356600

H	0.47048700	1.18964600	-0.84981500
H	0.47379200	1.15250700	0.90495200
C	-0.73113000	-0.38518200	-0.00371000
H	-0.70226300	-1.05780000	0.86214400
H	-0.70041200	-1.02658200	-0.89287400
C	-2.04221300	0.39715000	0.00854400
H	-2.07069500	1.06879900	-0.85808100
H	-2.07174500	1.04004600	0.89673200
C	-3.27828300	-0.49889300	-0.00713200
H	-3.25098700	-1.16999900	0.85999800
H	-3.24917600	-1.14218500	-0.89505100
C	-4.58755900	0.28611800	0.00397200
H	-4.61531500	0.95733600	-0.86323700
H	-4.61654200	0.93025500	0.89147900
C	-5.82684000	-0.60600600	-0.01079600
H	-5.79776400	-1.27623500	0.85519900
H	-5.79802300	-1.24736900	-0.89842100
C	-7.12568700	0.19635400	0.00276700
H	-7.18486600	0.85350100	-0.86890900
H	-8.00228600	-0.45437500	-0.00736500
H	-7.18392100	0.82456600	0.89562700
O	7.56646100	-0.84815500	-0.07524200
H	7.22290200	-1.35184300	0.67965300

OH-R32: OH + CH₃(CH₂)₉CH₃ → H₂O + CH₃CH(CH₂)₈CH₃

CH₃CH(CH₂)₈CH₃

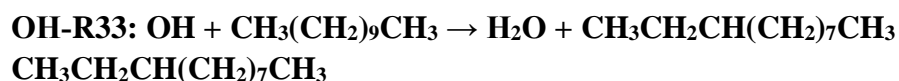
C	-6.45289100	-0.25534300	-0.11652300
H	-6.72501400	-0.82758500	0.78318400
H	-6.43683400	-0.97232100	-0.94459800
H	-7.25555900	0.46033000	-0.30051200
C	-5.13170100	0.41561900	0.03674900
H	-5.09612500	1.44522600	0.37687100
C	-3.87619200	-0.38755600	0.07126700
H	-3.88174800	-1.10948900	-0.75764500
H	-3.84756800	-1.00387900	0.98653700
C	-2.60462400	0.45772100	0.00534400
H	-2.60076700	1.16523100	0.84297600
H	-2.62197400	1.06061400	-0.90965100
C	-1.32814100	-0.37796300	0.04252100
H	-1.33212000	-1.08326500	-0.79747300
H	-1.31881000	-0.98653400	0.95505300
C	-0.05704300	0.46584800	-0.01401200
H	-0.05131800	1.16838100	0.82822900

H	-0.06752600	1.07733700	-0.92441900
C	1.22020900	-0.37003700	0.01808800
H	1.21703400	-1.06896200	-0.82715900
H	1.22752100	-0.98561700	0.92585700
C	2.49220900	0.47313000	-0.02948700
H	2.49495800	1.17204100	0.81581400
H	2.48593300	1.08867300	-0.93728700
C	3.76873500	-0.36344400	0.00448700
H	3.76869600	-1.06065600	-0.84239600
H	3.77343100	-0.98159400	0.91071500
C	5.04265300	0.47772300	-0.03672300
H	5.03997400	1.17471300	0.80834700
H	5.03856300	1.09245100	-0.94343300
C	6.30900400	-0.37415500	0.00315800
H	6.34430900	-1.05782200	-0.84912100
H	7.21025900	0.24162700	-0.02295900
H	6.34136800	-0.97815900	0.91384500

TS32: OH + CH₃(CH₂)₉CH₃ → H₂O + CH₃CH(CH₂)₈CH₃

C	5.88381500	-0.95494000	-0.12265600
H	5.91319300	-0.98021200	-1.21423600
H	5.88941100	-1.98887300	0.23701600
H	6.79408400	-0.46866700	0.23109300
C	4.63984900	-0.23325200	0.36502000
H	4.63830000	-0.12898500	1.45509800
H	4.70064100	0.84268600	-0.04109200
C	3.32977600	-0.82534900	-0.12541200
H	3.24632000	-1.85389000	0.25141000
H	3.35353700	-0.89683500	-1.21887200
C	2.10498100	-0.02376600	0.30760600
H	2.18218200	0.98910600	-0.10477700
H	2.10559000	0.07862600	1.40022800
C	0.78755100	-0.65273400	-0.13814100
H	0.70919000	-1.66551900	0.27560500
H	0.79163600	-0.76495000	-1.22898800
C	-0.43533500	0.15944000	0.28118200
H	-0.35777000	1.17049200	-0.13688000
H	-0.43661300	0.27667700	1.37183200
C	-1.75443800	-0.46937800	-0.16005300
H	-1.83506000	-1.47851100	0.26222200
H	-1.75049800	-0.59191500	-1.24994000
C	-2.97664100	0.34826900	0.25091200
H	-2.89573400	1.35687700	-0.17258600

H	-2.98044300	0.47226000	1.34075800
C	-4.29608600	-0.27963200	-0.18998900
H	-4.38042800	-1.28684600	0.23657100
H	-4.29116000	-0.40772900	-1.27943200
C	-5.51883700	0.54121700	0.21403500
H	-5.43294400	1.54641200	-0.21300700
H	-5.52307100	0.66826000	1.30210500
C	-6.82981000	-0.09895900	-0.23480400
H	-6.94830600	-1.09269900	0.20539900
H	-7.69301700	0.50209600	0.05804200
H	-6.85413400	-0.21361300	-1.32172700
O	4.65412200	2.28082200	-0.43716200
H	4.21317100	2.60367500	0.36525200



C	6.33529500	-0.58235200	0.13300300
H	6.40448600	-1.13369300	-0.80799500
H	6.19010900	-1.30882700	0.93577100
H	7.28909500	-0.07825900	0.29827900
C	5.17619200	0.41149600	0.08980200
H	5.14406200	0.99062500	1.02230500
H	5.36321100	1.15587500	-0.70132400
C	3.85291500	-0.23883800	-0.13249800
H	3.82737700	-1.23082900	-0.57594200
C	2.59087400	0.55285800	-0.08404300
H	2.54070500	1.23506600	-0.95023200
H	2.60305100	1.20996800	0.79666200
C	1.32832300	-0.30881100	-0.06241600
H	1.35946300	-0.96860600	0.81203400
H	1.32496100	-0.96153000	-0.94345400
C	0.04279100	0.51338400	-0.03719700
H	0.01740500	1.17338000	-0.91296900
H	0.04798100	1.16889800	0.84220800
C	-1.21821000	-0.34712700	-0.01737100
H	-1.19480800	-1.00488000	0.85994500
H	-1.22125800	-1.00494700	-0.89500800
C	-2.50566100	0.47350700	0.00175000
H	-2.52819600	1.13191800	-0.87522700
H	-2.50374500	1.13072200	0.87987500
C	-3.76623700	-0.38742000	0.01866800
H	-3.74585500	-1.04455700	0.89680100
H	-3.76717400	-1.04669200	-0.85809300

C	-5.05545100	0.43106700	0.03322300
H	-5.07429500	1.08646700	-0.84436100
H	-5.05374200	1.08862900	0.90937400
C	-6.30574800	-0.44501200	0.04909400
H	-6.31835500	-1.08752500	0.93350700
H	-7.21809200	0.15470900	0.05702600
H	-6.33688700	-1.09243400	-0.83127100

TS33: OH + CH₃(CH₂)₉CH₃ → H₂O + CH₃CH₂CH(CH₂)₇CH₃

C	-6.00118600	-0.19624800	0.36033600
H	-6.00689200	0.89138400	0.25807300
H	-6.04559800	-0.43285800	1.42652200
H	-6.90393900	-0.59110400	-0.10906800
C	-4.74082000	-0.78178000	-0.27097600
H	-4.74542300	-1.87475900	-0.17847300
H	-4.72691100	-0.56578300	-1.34550400
C	-3.46907300	-0.24377100	0.36197400
H	-3.46297300	-0.41223600	1.44556800
H	-3.50396100	0.90983000	0.28058900
C	-2.17480400	-0.71573800	-0.27673600
H	-2.18672500	-0.47088400	-1.34708300
H	-2.12724200	-1.81134500	-0.21906900
C	-0.92926100	-0.11472300	0.37070600
H	-0.89647700	-0.40676400	1.42723700
H	-1.01026900	0.97834200	0.35447200
C	0.36497200	-0.54410900	-0.31495200
H	0.33976100	-0.22851000	-1.36536400
H	0.42780000	-1.63925000	-0.32478500
C	1.61435800	0.02626100	0.35163800
H	1.65696900	-0.31455500	1.39323600
H	1.53781800	1.11965500	0.38895500
C	2.90582400	-0.36521100	-0.36211900
H	2.86798800	-0.00794800	-1.39852400
H	2.97427400	-1.45870300	-0.41646100
C	4.15832200	0.18509500	0.31490300
H	4.20927500	-0.18932500	1.34469900
H	4.08146500	1.27695600	0.38895200
C	5.44749300	-0.17938500	-0.41786900
H	5.39741700	0.20392500	-1.44287000
H	5.51895300	-1.26960500	-0.49978000
C	6.69242200	0.36742200	0.27585900
H	6.77984000	-0.03181800	1.28977200
H	7.60310000	0.10597300	-0.26668900

H	6.64811600	1.45714100	0.35169200
O	-3.53355300	2.26939800	-0.32009100
H	-3.36742900	1.98017800	-1.23193700

OH-R34: OH + CH₃(CH₂)₉CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₆CH₃
CH₃(CH₂)₂CH(CH₂)₆CH₃

C	6.39318400	-0.15406200	0.25168100
H	6.61420100	-0.72488600	-0.65415700
H	6.38594700	-0.85393100	1.09146100
H	7.21085700	0.55147900	0.41094100
C	5.05136900	0.56221900	0.13021000
H	4.85728000	1.14985300	1.03300800
H	5.08434100	1.27279600	-0.70240300
C	3.88774900	-0.40554600	-0.08947400
H	3.84658800	-1.12462700	0.74037000
H	4.09878900	-1.01360000	-0.98633200
C	2.56730300	0.27203300	-0.22707800
H	2.54329900	1.28140800	-0.62956200
C	1.29335400	-0.49988000	-0.16653600
H	1.31053700	-1.16816900	0.70575100
H	1.21658900	-1.17086500	-1.03954700
C	0.04609700	0.38194900	-0.11085300
H	0.03266400	1.03932300	-0.98830300
H	0.10866400	1.03657500	0.76591500
C	-1.25180100	-0.41911300	-0.05885300
H	-1.23828900	-1.07622300	0.81925400
H	-1.30675500	-1.07722300	-0.93474400
C	-2.49820000	0.46133100	-0.01047200
H	-2.51061700	1.11929500	-0.88794100
H	-2.44490600	1.11856500	0.86602000
C	-3.79711100	-0.33925900	0.03784000
H	-3.78779700	-0.99426300	0.91774100
H	-3.84808800	-1.00028000	-0.83619400
C	-5.04587500	0.53881500	0.07774100
H	-5.05355400	1.19204600	-0.80158500
H	-4.99478000	1.19800700	0.95121900
C	-6.33496800	-0.27786600	0.12426800
H	-6.35816400	-0.91612400	1.01156100
H	-7.21825400	0.36343800	0.14891900
H	-6.41515500	-0.92633000	-0.75225500

TS34: OH + CH₃(CH₂)₉CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₆CH₃

C	-6.12414000	-0.62444400	-0.23522900
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H	-6.17750200	-1.71078300	-0.12346900
H	-6.14499000	-0.39938100	-1.30489600
H	-7.02281600	-0.19691500	0.21316500
C	-4.85773500	-0.06989600	0.41129900
H	-4.82900700	1.01955100	0.30974600
H	-4.86638300	-0.28308200	1.48560000
C	-3.58688400	-0.65344600	-0.20233700
H	-3.57857100	-0.45421400	-1.28166600
H	-3.59417600	-1.74649900	-0.09436900
C	-2.31523600	-0.10480000	0.42020900
H	-2.30966500	-0.24923000	1.50715300
H	-2.34513400	1.04645900	0.31275300
C	-1.02260800	-0.59757500	-0.20667600
H	-1.03847100	-0.39032900	-1.28473700
H	-0.97500900	-1.69052300	-0.11057700
C	0.22560600	0.02520000	0.41436600
H	0.24755500	-0.20561900	1.48615400
H	0.15821000	1.11645800	0.33504800
C	1.51904800	-0.46030600	-0.23447000
H	1.49648600	-0.22922800	-1.30664000
H	1.57782400	-1.55304300	-0.15707000
C	2.76972600	0.15718100	0.38634200
H	2.79378700	-0.07376500	1.45828000
H	2.71086600	1.24959500	0.30877100
C	4.06318200	-0.32702300	-0.26352500
H	4.03925700	-0.09713300	-1.33595000
H	4.12231300	-1.41976600	-0.18537300
C	5.31598200	0.28975700	0.35449700
H	5.33882000	0.05970500	1.42528400
H	5.25589000	1.38072200	0.27506000
C	6.60016500	-0.20469600	-0.30621000
H	6.60744900	0.03878100	-1.37202400
H	7.48552400	0.24610400	0.14639300
H	6.69196700	-1.29025300	-0.21391100
O	-2.36984200	2.39551300	-0.31283100
H	-2.20812500	2.08857100	-1.21967700

OH-R35: OH + CH₃(CH₂)₉CH₃ → H₂O + CH₃(CH₂)₃CH(CH₂)₅CH₃

C	-6.28950400	-0.65182600	0.21006700
H	-6.15913500	-1.39707300	0.99904000
H	-7.23757200	-0.13984200	0.38584200
H	-6.36783000	-1.18603000	-0.74043500
C	-5.11732000	0.32594500	0.18813500

H	-5.07165700	0.86879100	1.13849600
H	-5.27940700	1.07969400	-0.59008200
C	-3.78034000	-0.36876400	-0.05692500
H	-3.61234200	-1.12408000	0.71923500
H	-3.82149500	-0.90883900	-1.01038400
C	-2.59615400	0.59766500	-0.07884000
H	-2.78156500	1.36866100	-0.84654800
H	-2.55125400	1.14605500	0.87210400
C	-1.28679500	-0.06941200	-0.32973800
H	-1.27740900	-0.98983800	-0.90759900
C	-0.00026900	0.65682400	-0.13023000
H	-0.02715600	1.19217800	0.82884900
H	0.11274300	1.44421300	-0.89528800
C	1.22804800	-0.25226000	-0.17471400
H	1.25170100	-0.77646100	-1.13739500
H	1.12938900	-1.02476200	0.59621400
C	2.53929400	0.50324200	0.02305800
H	2.51257800	1.03058200	0.98441500
H	2.63319500	1.27644500	-0.74922800
C	3.76623000	-0.40408000	-0.01978900
H	3.79438900	-0.93161200	-0.98109200
H	3.67284800	-1.17778700	0.75204800
C	5.07964000	0.34923400	0.17920200
H	5.04984600	0.87560400	1.13936700
H	5.17170400	1.12107400	-0.59259300
C	6.29669300	-0.57137400	0.13451700
H	6.35829900	-1.08776200	-0.82701500
H	7.22642000	-0.01718700	0.27740500
H	6.23658200	-1.33318400	0.91618800

TS35: OH + CH₃(CH₂)₉CH₃ → H₂O + CH₃(CH₂)₃CH(CH₂)₅CH₃

C	6.23791600	0.06353500	0.25200700
H	6.29802400	-0.00798000	1.34133000
H	6.22361900	1.12470100	-0.01018800
H	7.14864500	-0.37253600	-0.16316600
C	4.98779100	-0.63965600	-0.27024600
H	4.96348700	-0.58486500	-1.36392300
H	5.02842300	-1.70443500	-0.01493300
C	3.70177700	-0.03517000	0.28809500
H	3.64721800	1.02584200	0.01794300
H	3.72826000	-0.07684900	1.38413900
C	2.44269300	-0.73749000	-0.21341200
H	2.46273700	-1.79347800	0.08872800

H	2.42940800	-0.72888600	-1.30938200
C	1.16343400	-0.10090200	0.30271700
H	1.17705900	0.98547900	-0.07506100
H	1.17279600	-0.02600300	1.39659100
C	-0.12643600	-0.73165500	-0.19196600
H	-0.17913800	-1.76510700	0.17612200
H	-0.10263400	-0.79213800	-1.28596100
C	-1.37339100	0.03127700	0.24878600
H	-1.32295000	1.05020100	-0.15284100
H	-1.37540400	0.12331800	1.34226800
C	-2.67321500	-0.62872300	-0.20342800
H	-2.72706100	-1.64517500	0.20524500
H	-2.66371600	-0.73557100	-1.29483300
C	-3.91701500	0.15046000	0.21626300
H	-3.86455300	1.16518600	-0.19709600
H	-3.92461500	0.26343100	1.30749800
C	-5.22016800	-0.50795900	-0.23024400
H	-5.27421600	-1.51924300	0.18740000
H	-5.20891900	-0.62461800	-1.31935800
C	-6.45306500	0.28859100	0.18951200
H	-6.43005100	1.29405200	-0.23897300
H	-7.37570000	-0.19449700	-0.13811600
H	-6.49675300	0.39302400	1.27691600
O	1.16019700	2.43327200	-0.47886300
H	0.76253300	2.76611300	0.34205800

**OH-R36: OH + CH₃(CH₂)₉CH₃ → H₂O + CH₃(CH₂)₄CH(CH₂)₄CH₃
CH₃(CH₂)₄CH(CH₂)₄CH₃**

C	6.37247500	-0.22168500	0.08784100
H	6.46410500	-0.84707300	-0.80422200
H	6.41561600	-0.87985400	0.95966700
H	7.23991800	0.44028900	0.12369600
C	5.06367900	0.56412600	0.06609500
H	5.00222800	1.20413700	0.95301100
H	5.05004600	1.23472200	-0.79995900
C	3.83687500	-0.34356400	0.01535900
H	3.84566900	-1.01208500	0.88505200
H	3.90218100	-0.98955800	-0.86904900
C	2.51942400	0.42566600	-0.01895200
H	2.51195200	1.09366100	-0.88838800
H	2.44544900	1.06761900	0.86631700
C	1.29575700	-0.48748400	-0.08063300
H	1.29471800	-1.16014200	0.78906300

H	1.39152800	-1.15377400	-0.95530100
C	0.00000000	0.24682600	-0.14503300
H	0.00000000	1.27846100	-0.48609600
C	-1.29575700	-0.48748400	-0.08063300
H	-1.29471800	-1.16014300	0.78906300
H	-1.39152800	-1.15377400	-0.95530100
C	-2.51942400	0.42566600	-0.01895100
H	-2.51195200	1.09366100	-0.88838700
H	-2.44544900	1.06761800	0.86631700
C	-3.83687500	-0.34356500	0.01535900
H	-3.84566900	-1.01208500	0.88505200
H	-3.90218100	-0.98955900	-0.86904800
C	-5.06367900	0.56412500	0.06609500
H	-5.05004500	1.23472200	-0.79995900
H	-5.00222800	1.20413700	0.95301100
C	-6.37247500	-0.22168500	0.08784000
H	-6.41561700	-0.87985400	0.95966700
H	-7.23991800	0.44029000	0.12369500
H	-6.46410500	-0.84707300	-0.80422300

TS36: OH + CH₃(CH₂)₉CH₃ → H₂O + CH₃(CH₂)₄CH(CH₂)₄CH₃

C	-6.36498300	-0.40418600	-0.27480200
H	-6.43683600	-1.49093900	-0.17890700
H	-6.37885000	-0.16414400	-1.34133400
H	-7.25753500	0.03186000	0.17803400
C	-5.08896100	0.11608100	0.38182800
H	-5.04851200	1.20752300	0.29939700
H	-5.10502800	-0.11162600	1.45320100
C	-3.82649100	-0.47918600	-0.23752700
H	-3.81051000	-0.25208100	-1.31076300
H	-3.86486900	-1.57267300	-0.15576200
C	-2.54214500	0.03457500	0.40725200
H	-2.55783600	-0.19298400	1.47993300
H	-2.49617000	1.12632800	0.32227400
C	-1.28261100	-0.56425800	-0.21415200
H	-1.27085600	-0.35446500	-1.29150300
H	-1.30837800	-1.65799100	-0.11811200
C	-0.00056000	-0.04552700	0.41315200
H	-0.00035900	-0.19492400	1.49941800
H	-0.00242800	1.10668900	0.31107400
C	1.28201600	-0.56345400	-0.21393800
H	1.27097500	-0.35322000	-1.29134300
H	1.30747600	-1.65728500	-0.11936100

C	2.54177500	0.03370000	0.40875700
H	2.55737000	-0.19645900	1.48085100
H	2.49647400	1.12581300	0.32722100
C	3.82595200	-0.47883100	-0.23736800
H	3.80972600	-0.24992300	-1.31024100
H	3.86420100	-1.57245100	-0.15760300
C	5.08870200	0.11517700	0.38261300
H	5.10496900	-0.11420100	1.45361800
H	5.04856000	1.20676900	0.30193400
C	6.36439900	-0.40442200	-0.27516800
H	6.37795500	-0.16298200	-1.34139200
H	7.25716500	0.03088300	0.17793800
H	6.43610800	-1.49130600	-0.18073300
O	-0.00248300	2.45669400	-0.31270100
H	0.04449200	2.14221200	-1.23012900

3.1.12 C12 (*n*-C₁₂H₂₆)



n-C₁₂H₂₆

C	7.00721800	0.31339100	-0.00030200
H	7.04990500	0.95751700	0.88201500
H	7.04974800	0.95726500	-0.88281200
H	7.89975600	-0.31548600	-0.00029200
C	5.72875900	-0.52125800	-0.00007000
H	5.71594800	-1.17776700	-0.87691700
H	5.71611100	-1.17752700	0.87696000
C	4.46730700	0.33952000	-0.00007000
H	4.47915800	0.99762800	-0.87764200
H	4.47929200	0.99782700	0.87735000
C	3.17839100	-0.47856900	0.00011700
H	3.16696700	-1.13630000	0.87780400
H	3.16683000	-1.13647700	-0.87743600
C	1.91916800	0.38496500	0.00012700
H	1.93099400	1.04278600	-0.87746200
H	1.93106300	1.04287000	0.87765200
C	0.62937400	-0.43208100	0.00021100
H	0.61742300	-1.08988200	0.87782200
H	0.61736100	-1.08994800	-0.87735000
C	-0.62937400	0.43208100	0.00021900
H	-0.61737500	1.08994400	-0.87734400
H	-0.61740900	1.08988600	0.87782700
C	-1.91916800	-0.38496500	0.00016000
H	-1.93105600	-1.04285800	0.87769400

H	-1.93100200	-1.04279800	-0.87742000
C	-3.17839100	0.47856900	0.00014700
H	-3.16682800	1.13647400	-0.87740800
H	-3.16696900	1.13630200	0.87783200
C	-4.46730700	-0.33952000	-0.00004200
H	-4.47930500	-0.99781100	0.87739000
H	-4.47914500	-0.99764400	-0.87760200
C	-5.72875900	0.52125800	-0.00007800
H	-5.71592800	1.17775700	-0.87693200
H	-5.71613000	1.17753600	0.87694500
C	-7.00721800	-0.31339100	-0.00033200
H	-7.04992900	-0.95750300	0.88199500
H	-7.89975600	0.31548600	-0.00035600
H	-7.04972400	-0.95728000	-0.88283200

CH₂(CH₂)₁₀CH₃

C	-7.05825800	0.29716400	-0.01673200
H	-7.09366600	1.27004500	0.45824200
H	-7.99018000	-0.13227700	-0.35902900
C	-5.80217300	-0.50178100	0.00518500
H	-5.77245400	-1.13719800	0.90573600
H	-5.78749400	-1.19820200	-0.84121100
C	-4.53937400	0.36263500	-0.01897400
H	-4.55892800	1.04873000	0.83612100
H	-4.55056300	0.98804800	-0.91861400
C	-3.25358000	-0.45866200	0.01721400
H	-3.23970300	-1.14715500	-0.83650200
H	-3.24712300	-1.08482600	0.91777900
C	-1.99262900	0.40178700	-0.00927400
H	-2.00287600	1.08626200	0.84762200
H	-2.00291000	1.03217000	-0.90668400
C	-0.70537200	-0.41887600	0.01562800
H	-0.69536000	-1.10223200	-0.84221500
H	-0.69541300	-1.05064600	0.91217000
C	0.55610400	0.44086500	-0.01012700
H	0.54779500	1.12240300	0.84916900
H	0.54483300	1.07450900	-0.90532600
C	1.84292300	-0.38060200	0.01010000
H	1.85124500	-1.06160800	-0.84962700
H	1.85361400	-1.01495600	0.90481500
C	3.10531000	0.47790600	-0.01465300
H	3.09705300	1.15921600	0.84485800
H	3.09541000	1.11184300	-0.90969000

C	4.39111200	-0.34477700	0.00666400
H	4.40036500	-1.02611000	-0.85300600
H	4.40089000	-0.97950100	0.90131900
C	5.65573700	0.51100500	-0.01649600
H	5.64436200	1.19195100	0.84148700
H	5.64631700	1.14243700	-0.91161800
C	6.93115200	-0.32785500	0.00914200
H	6.97366200	-0.99606000	-0.85503200
H	7.82587700	0.29771700	-0.00589500
H	6.96954200	-0.94741700	0.90908400

TS37: OH + CH₃(CH₂)₁₀CH₃ → H₂O + CH₂(CH₂)₁₀CH₃

C	6.21187800	0.64017300	-0.02939200
H	6.30839600	1.19586400	0.90579200
H	6.28789500	1.32309100	-0.87809500
H	7.14972100	-0.04730600	-0.11515800
C	4.97487600	-0.23549000	-0.07106700
H	4.97928400	-0.83542100	-0.98628500
H	4.99556000	-0.94074700	0.76563800
C	3.68517600	0.58796300	-0.01120300
H	3.66410800	1.28934100	-0.85367200
H	3.68488700	1.19818500	0.89986400
C	2.42820500	-0.27876100	-0.04165800
H	2.44760700	-0.97455800	0.80566200
H	2.43576700	-0.89619400	-0.94780600
C	1.13876500	0.53766600	0.00329400
H	1.11869800	1.22980200	-0.84723100
H	1.13423200	1.15978500	0.90657200
C	-0.11945700	-0.32697800	-0.02043500
H	-0.10210100	-1.01564900	0.83296900
H	-0.11217600	-0.95297500	-0.92096700
C	-1.40926600	0.48922500	0.01598200
H	-1.42673300	1.17674900	-0.83840900
H	-1.41619800	1.11654000	0.91569000
C	-2.66766800	-0.37505800	-0.00662700
H	-2.65196200	-1.06060400	0.84936700
H	-2.65887900	-1.00454500	-0.90476500
C	-3.95787100	0.44083000	0.02434400
H	-3.97322800	1.12641600	-0.83168000
H	-3.96736200	1.07025500	0.92257800
C	-5.21589500	-0.42364900	0.00028800
H	-5.20264300	-1.10825800	0.85729100
H	-5.20571500	-1.05484800	-0.89684600

C	-6.50761600	0.39052400	0.02715100
H	-6.51898400	1.07389000	-0.82892500
H	-6.51726500	1.01951700	0.92400800
C	-7.75545900	-0.48874000	0.00046400
H	-7.77632600	-1.15955400	0.86337900
H	-8.66951900	0.10816300	0.01728000
H	-7.77490800	-1.10739700	-0.90069300
O	8.28402400	-0.89847600	0.01598400
H	8.66165200	-0.48795100	0.80972300

OH-R38: OH + CH₃(CH₂)₁₀CH₃ → H₂O + CH₃CH(CH₂)₉CH₃

CH₃CH(CH₂)₉CH₃

C	7.09477600	-0.17337400	0.14998800
H	7.38303500	-0.76405000	-0.73262600
H	7.08576300	-0.86865300	0.99652000
H	7.88325900	0.56116200	0.32041100
C	5.76300800	0.46948800	-0.02968700
H	5.71163100	1.49211400	-0.38826300
C	4.52324900	-0.35777600	-0.06325800
H	4.53668600	-1.06969900	0.77411700
H	4.51225200	-0.98501800	-0.97143900
C	3.23556600	0.46409800	-0.01555800
H	3.22455600	1.16260400	-0.86065700
H	3.23527700	1.07680000	0.89306900
C	1.97520900	-0.39573000	-0.05256700
H	1.98815400	-1.09417600	0.79305400
H	1.98157400	-1.01152100	-0.96026600
C	0.68837200	0.42464700	-0.00842600
H	0.67311600	1.12026900	-0.85626400
H	0.68406500	1.04344500	0.89709500
C	-0.57316500	-0.43486300	-0.03827900
H	-0.55811000	-1.12944600	0.81043800
H	-0.56837900	-1.05488900	-0.94304000
C	-1.86020700	0.38532000	0.00462100
H	-1.87636700	1.07879000	-0.84497100
H	-1.86388600	1.00659200	0.90851400
C	-3.12193800	-0.47410500	-0.02177700
H	-3.10470200	-1.16874000	0.82688700
H	-3.11958900	-1.09413500	-0.92656300
C	-4.40862500	0.34607600	0.02475200
H	-4.42708800	1.04118500	-0.82367100
H	-4.41114800	0.96633400	0.92954200
C	-5.67191900	-0.51163200	-0.00034600

H	-5.65032400	-1.20739800	0.84547700
H	-5.67034700	-1.12749100	-0.90629900
C	-6.94868700	0.32371900	0.05327000
H	-7.00170400	1.00733000	-0.79816900
H	-7.84220100	-0.30355400	0.03616600
H	-6.97935400	0.92693700	0.96453600

TS38: OH + CH₃(CH₂)₁₀CH₃ → H₂O + CH₃CH(CH₂)₉CH₃

C	6.52314300	-0.85655700	-0.08608600
H	6.55586300	-0.90638100	-1.17675900
H	6.55961300	-1.88110900	0.29772300
H	7.41740900	-0.33453800	0.25753200
C	5.25690200	-0.16161700	0.38263500
H	5.24619600	-0.03966700	1.47082800
H	5.29015300	0.90897700	-0.04071500
C	3.96619000	-0.79677700	-0.10520900
H	3.90848500	-1.82166500	0.28609600
H	3.99764800	-0.88346900	-1.19739900
C	2.71804800	-0.02218300	0.30988700
H	2.77299100	0.98793500	-0.11269400
H	2.70768300	0.09180500	1.40130900
C	1.42027500	-0.68861800	-0.13897400
H	1.36464800	-1.69941900	0.28319700
H	1.43473100	-0.81019400	-1.22873000
C	0.17452000	0.09619100	0.26487600
H	0.23109400	1.10614900	-0.15914300
H	0.16149500	0.22040900	1.35468000
C	-1.12549000	-0.56689200	-0.18274300
H	-1.18460300	-1.57571600	0.24379900
H	-1.11072000	-0.69432600	-1.27198800
C	-2.36989600	0.22290600	0.21575700
H	-2.30943300	1.23177500	-0.21044400
H	-2.38501900	0.35034500	1.30509100
C	-3.67109000	-0.43715300	-0.23306500
H	-3.73344000	-1.44535500	0.19455900
H	-3.65518300	-0.56610000	-1.32217800
C	-4.91413700	0.35585900	0.16263300
H	-4.85102600	1.36493000	-0.26316800
H	-4.93193100	0.48368800	1.25203100
C	-6.21714100	-0.29987000	-0.28826600
H	-6.27945300	-1.30725400	0.13765400
H	-6.19824100	-0.42625500	-1.37623900
C	-7.44945200	0.50610700	0.11508600

H	-7.41703800	1.50862600	-0.31975600
H	-8.37189400	0.02591800	-0.21741500
H	-7.50199300	0.61815000	1.20133600
O	5.20646700	2.34029200	-0.45418000
H	4.75899400	2.66204300	0.34504800

**OH-R39: OH + CH₃(CH₂)₁₀CH₃ → H₂O + CH₃CH₂CH(CH₂)₈CH₃
CH₃CH₂CH(CH₂)₈CH₃**

C	-6.98510900	0.51003100	0.14955500
H	-7.06815000	1.06848600	-0.78609500
H	-6.84893900	1.23160500	0.95829100
H	-7.92913900	-0.01218400	0.31453800
C	-5.80879500	-0.46275100	0.09226600
H	-5.76306800	-1.05035400	1.01891000
H	-5.98560400	-1.20250000	-0.70550300
C	-4.49815200	0.21342300	-0.12804800
H	-4.49211900	1.20986900	-0.56203400
C	-3.22202500	-0.55602100	-0.09088000
H	-3.16242800	-1.22893300	-0.96373400
H	-3.22035800	-1.22166600	0.78346500
C	-1.97465800	0.32730500	-0.06409900
H	-2.01561800	0.97934500	0.81576400
H	-1.98365900	0.98706900	-0.93981800
C	-0.67544100	-0.47326600	-0.04730000
H	-0.64064700	-1.12591900	-0.92826700
H	-0.66872200	-1.13576200	0.82685000
C	0.57162300	0.40716000	-0.02224300
H	0.53888000	1.05812500	0.85985100
H	0.56381000	1.07118400	-0.89516600
C	1.87119900	-0.39415200	-0.01000400
H	1.90219700	-1.04625200	-0.89142700
H	1.87955200	-1.05741500	0.86349800
C	3.11992400	0.48413800	0.01162100
H	3.09102700	1.13480700	0.89416100
H	3.11070700	1.14867100	-0.86093800
C	4.41807200	-0.31918900	0.01962100
H	4.44615000	-0.97120100	-0.86215500
H	4.42858700	-0.98326600	0.89269200
C	5.66964200	0.55563400	0.03811300
H	5.64194800	1.20484000	0.92005800
H	5.65739100	1.21880300	-0.83369700
C	6.95728000	-0.26476100	0.04288700
H	7.01424300	-0.90180700	-0.84377800

H	7.84277800	0.37385600	0.05468700
H	6.99983100	-0.91470600	0.92092600

TS39: OH + CH₃(CH₂)₁₀CH₃ → H₂O + CH₃CH₂CH(CH₂)₈CH₃

C	-6.61543000	-0.20418000	0.25786800
H	-6.61911500	0.84497900	-0.04735600
H	-6.67986300	-0.23761700	1.34877100
H	-7.50993900	-0.68171300	-0.14586700
C	-5.34419100	-0.89218700	-0.23200700
H	-5.33860700	-1.94352600	0.08184700
H	-5.31818900	-0.89431000	-1.32638800
C	-4.08489200	-0.22012500	0.28954700
H	-4.10521100	-0.14153300	1.38317600
H	-4.12574700	0.86429700	-0.09207500
C	-2.77489800	-0.81760200	-0.19268300
H	-2.78552900	-0.87629700	-1.28697300
H	-2.70054900	-1.85021800	0.17412700
C	-1.55218400	-0.02505800	0.26354900
H	-1.56471200	0.06364200	1.35723000
H	-1.62353800	0.99362100	-0.13566800
C	-0.23141400	-0.65160600	-0.17533500
H	-0.22370100	-0.75123200	-1.26741000
H	-0.15959300	-1.66926900	0.22752500
C	0.98821600	0.15336900	0.26661200
H	0.97734700	0.25921200	1.35836300
H	0.91711800	1.16890400	-0.14162500
C	2.31131700	-0.47282000	-0.16638100
H	2.31703300	-0.58937200	-1.25692500
H	2.38862200	-1.48419800	0.25108300
C	3.52933600	0.34338800	0.25954300
H	3.52254900	0.46355000	1.34980800
H	3.45218800	1.35347400	-0.16112100
C	4.85330900	-0.28233600	-0.17076200
H	4.85788000	-0.40909600	-1.26036500
H	4.93536400	-1.28994600	0.25528600
C	6.07137000	0.53979100	0.24464400
H	6.06585500	0.66615700	1.33279100
H	5.98788500	1.54514600	-0.18249800
C	7.38714800	-0.09826000	-0.19301800
H	7.42079200	-0.21297800	-1.27970700
H	8.24686400	0.50430100	0.10692000
H	7.50366400	-1.09174900	0.24827000
O	-4.16005700	2.31287200	-0.49186100

H	-3.78453300	2.65854900	0.33421400
OH-R40: OH + CH₃(CH₂)₁₀CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₇CH₃			
CH₃(CH₂)₂CH(CH₂)₇CH₃			
C	-7.03426800	0.02685300	0.27352600
H	-7.27436500	0.66437300	-0.58158500
H	-7.04104400	0.65523700	1.16814500
H	-7.83280300	-0.71043500	0.37652700
C	-5.67497500	-0.64155600	0.08989900
H	-5.46319600	-1.29920300	0.93885800
H	-5.69183600	-1.27905000	-0.80042400
C	-4.53689900	0.37073100	-0.04698300
H	-4.51500600	1.01986000	0.83948600
H	-4.76279100	1.04542200	-0.89095800
C	-3.19980300	-0.25962400	-0.23699300
H	-3.15240800	-1.24496600	-0.69367300
C	-1.94594800	0.54182000	-0.14839800
H	-1.97888100	1.17914300	0.74618000
H	-1.88479700	1.24346200	-0.99820400
C	-0.67837800	-0.31233700	-0.12260300
H	-0.65572300	-0.94562300	-1.01747400
H	-0.72208000	-0.99168700	0.73625400
C	0.60266000	0.51429100	-0.05598300
H	0.57989400	1.15024100	0.83740400
H	0.64115600	1.19348900	-0.91646800
C	1.86575100	-0.34315200	-0.03313500
H	1.88343000	-0.98397900	-0.92312200
H	1.83035100	-1.01798000	0.83072100
C	3.15128500	0.47873200	0.02121900
H	3.13632100	1.11840500	0.91208600
H	3.18548500	1.15445000	-0.84211400
C	4.41236700	-0.38150000	0.03848900
H	4.42382400	-1.02565800	-0.84938500
H	4.38203400	-1.05376100	0.90481500
C	5.70095700	0.43682500	0.08197200
H	5.68970000	1.07892900	0.96946400
H	5.72925300	1.10757300	-0.78367100
C	6.95120900	-0.43937300	0.09571800
H	6.99011100	-1.07321600	-0.79419700
H	7.86341100	0.16010400	0.12075600
H	6.95621100	-1.09538900	0.97021300

TS40: OH + CH₃(CH₂)₁₀CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₇CH₃

C	-6.74243700	-0.58886400	-0.17659100
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H	-6.83687900	-1.61862900	0.17838800
H	-6.75361100	-0.61147400	-1.26933600
H	-7.62473100	-0.03794000	0.15491800
C	-5.45636500	0.05152500	0.33831000
H	-5.38969600	1.08884600	-0.00481400
H	-5.47207400	0.08460200	1.43332500
C	-4.20710100	-0.69648300	-0.12211800
H	-4.19356900	-0.74571000	-1.21713300
H	-4.24629100	-1.73484100	0.23456600
C	-2.91791200	-0.05626900	0.36321500
H	-2.91760500	0.05187200	1.45435500
H	-2.92314100	1.01865700	-0.04716800
C	-1.63790500	-0.71355900	-0.12268300
H	-1.66627300	-0.79445400	-1.21527700
H	-1.59731200	-1.74051600	0.26455500
C	-0.37973400	0.04135300	0.29944300
H	-0.36558300	0.14130400	1.39213400
H	-0.42523800	1.05776800	-0.10912500
C	0.90931200	-0.63327900	-0.16187700
H	0.89082700	-0.73896200	-1.25327100
H	0.95466700	-1.65063300	0.24551300
C	2.16469300	0.13200200	0.24942300
H	2.18602200	0.23480200	1.34131500
H	2.11443200	1.15048600	-0.15446200
C	3.45588700	-0.53298000	-0.22051700
H	3.43095300	-0.64099500	-1.31172900
H	3.51102200	-1.54956900	0.18769700
C	4.70936900	0.24055500	0.18063800
H	4.73753000	0.34644600	1.27221500
H	4.65193900	1.25833700	-0.22463000
C	6.00251900	-0.41745600	-0.29467600
H	5.97289800	-0.52182400	-1.38476200
H	6.05958600	-1.43359500	0.11059200
C	7.24524200	0.36976100	0.11362000
H	7.30916500	0.45836300	1.20145900
H	8.16048500	-0.11064700	-0.23787000
H	7.21704700	1.38142100	-0.29974500
O	-2.89452500	2.45959800	-0.47089500
H	-2.50177600	2.80226500	0.34833800

OH-R41: $\text{OH} + \text{CH}_3(\text{CH}_2)_{10}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_6\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_6\text{CH}_3$

C	-6.92713800	0.61602700	0.29170500
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H	-7.04418900	1.11315700	-0.67489900
H	-6.78170900	1.39188100	1.04802000
H	-7.86160300	0.09859000	0.51752800
C	-5.74280400	-0.34664000	0.26677200
H	-5.65923100	-0.85481700	1.23375800
H	-5.91820500	-1.12958500	-0.47919400
C	-4.42355600	0.35529900	-0.04504700
H	-4.24136800	1.13927600	0.69897400
H	-4.50190500	0.86090900	-1.01507500
C	-3.22980000	-0.59886600	-0.07020700
H	-3.43011000	-1.39842100	-0.80451700
H	-3.14997500	-1.11300700	0.89757800
C	-1.93473800	0.06969700	-0.38397600
H	-1.95147400	0.96943200	-0.99386200
C	-0.63704600	-0.64316900	-0.20986400
H	-0.51787900	-1.41214100	-0.99260100
H	-0.64936900	-1.19840800	0.73781900
C	0.57907900	0.28313700	-0.24372500
H	0.47465400	1.03812500	0.54372500
H	0.59003600	0.82793400	-1.19524000
C	1.90014100	-0.46030700	-0.06847700
H	2.00250000	-1.21291700	-0.85989200
H	1.88192000	-1.01224200	0.87926100
C	3.11606200	0.46274000	-0.08963400
H	3.00967400	1.21902700	0.69758100
H	3.14003600	1.01002900	-1.03985900
C	4.43618400	-0.27999100	0.09918300
H	4.54449100	-1.03634600	-0.68799300
H	4.41119300	-0.82816500	1.04907500
C	5.65408200	0.64109400	0.08233800
H	5.54245900	1.39778700	0.86657100
H	5.68064500	1.18468900	-0.86836100
C	6.96459100	-0.11647100	0.27929000
H	7.10587900	-0.86033800	-0.50934200
H	7.82523800	0.55515400	0.26449000
H	6.96796100	-0.64491200	1.23629900

TS41: OH + CH₃(CH₂)₁₀CH₃ → H₂O + CH₃(CH₂)₃CH(CH₂)₆CH₃

C	-6.83287100	-0.04760900	0.28261900
H	-6.85269300	1.03996600	0.17571800
H	-6.88565400	-0.27648000	1.35025700
H	-7.73118200	-0.44855500	-0.19081100
C	-5.56366500	-0.62959700	-0.33443600

H	-5.57611200	-1.72148600	-0.24456700
H	-5.54053900	-0.40841700	-1.40721400
C	-4.29510900	-0.08440300	0.31707200
H	-4.31608200	-0.30554700	1.39115100
H	-4.27293800	1.00755900	0.22537800
C	-3.01707700	-0.65830500	-0.28923000
H	-2.99723300	-0.44922400	-1.36646000
H	-3.02076800	-1.75216800	-0.19087700
C	-1.75416300	-0.11088100	0.35232200
H	-1.76187600	-0.26212300	1.43830600
H	-1.78477300	1.04102900	0.25184900
C	-0.45269100	-0.59734700	-0.26093600
H	-0.45466500	-0.38327000	-1.33777800
H	-0.40433600	-1.69081600	-0.17099500
C	0.78578500	0.02367700	0.38091200
H	0.79160300	-0.21084200	1.45212900
H	0.71903700	1.11517700	0.30433600
C	2.08933200	-0.45911900	-0.24947500
H	2.08315400	-0.22499200	-1.32121000
H	2.14770700	-1.55203700	-0.17422600
C	3.32959900	0.15754300	0.39265100
H	3.33611400	-0.07511500	1.46448700
H	3.27177500	1.25007900	0.31593500
C	4.63380000	-0.32531100	-0.23640800
H	4.62770300	-0.09366200	-1.30870500
H	4.69193700	-1.41817500	-0.15904500
C	5.87578700	0.29084400	0.40365600
H	5.88049700	0.05923800	1.47436400
H	5.81670300	1.38191200	0.32483000
C	7.17120300	-0.20223000	-0.23584000
H	7.19597800	0.04194500	-1.30122500
H	8.04848200	0.24912000	0.23172300
H	7.26234200	-1.28777100	-0.14267800
O	-1.80636600	2.39275600	-0.36828000
H	-1.64282600	2.08903000	-1.27587000

**OH-R42: OH + CH₃(CH₂)₁₀CH₃ → H₂O + CH₃(CH₂)₄CH(CH₂)₅CH₃
CH₃(CH₂)₄CH(CH₂)₅CH₃**

C	-6.97660000	0.01315500	0.38214300
H	-7.17773900	0.77782000	-0.37284500
H	-6.95920800	0.50710500	1.35726500
H	-7.81129800	-0.69050000	0.37757100
C	-5.64797700	-0.68569400	0.10430200

H	-5.47586800	-1.46432700	0.85535800
H	-5.69463900	-1.19617000	-0.86386600
C	-4.46687000	0.28188300	0.10474100
H	-4.41943400	0.79331200	1.07418200
H	-4.63938100	1.06304500	-0.64599400
C	-3.12955000	-0.39886800	-0.17250900
H	-3.17275900	-0.90449600	-1.14457600
H	-2.95311100	-1.17998600	0.57564500
C	-1.95181200	0.57578800	-0.16521800
H	-1.90623800	1.08968700	0.80475500
H	-2.14683700	1.37272400	-0.90371300
C	-0.63759900	-0.06982100	-0.44547000
H	-0.62085300	-0.95730200	-1.07299500
C	0.64308800	0.65614900	-0.20956400
H	0.59351400	1.17838700	0.75566900
H	0.77252200	1.45313500	-0.96199200
C	1.87449300	-0.24978200	-0.23766300
H	1.92687400	-0.75667000	-1.20858200
H	1.75625400	-1.03604800	0.51645900
C	3.17661000	0.50608800	0.01201700
H	3.11652500	1.01922600	0.97970900
H	3.29372000	1.29082700	-0.74535900
C	4.40705800	-0.39731200	-0.00262700
H	4.47630800	-0.90290300	-0.97370700
H	4.28456200	-1.18827400	0.74737300
C	5.70857500	0.35440900	0.26775400
H	5.63638300	0.85816000	1.23789200
H	5.83069500	1.14412100	-0.48154500
C	6.92893500	-0.56281000	0.25328700
H	7.03900800	-1.04837900	-0.71998600
H	7.84926700	-0.01274800	0.45932500
H	6.83162600	-1.34885900	1.00679400

TS42: OH + CH₃(CH₂)₁₀CH₃ → H₂O + CH₃(CH₂)₄CH(CH₂)₅CH₃

C	-6.95475200	-0.37546300	-0.20194300
H	-7.03186400	-1.46111700	-0.09807900
H	-6.98530800	-0.14176600	-1.26950500
H	-7.83655600	0.06917500	0.26342700
C	-5.66444700	0.14054500	0.42970600
H	-5.61889700	1.23128100	0.34063200
H	-5.66344200	-0.08130000	1.50242500
C	-4.41642100	-0.46576800	-0.20793300
H	-4.41687700	-0.24376900	-1.28236000

H	-4.46040400	-1.55859600	-0.12038000
C	-3.11820200	0.04234200	0.41314400
H	-3.11750800	-0.18085500	1.48682300
H	-3.06697900	1.13358600	0.32366100
C	-1.87291300	-0.56727400	-0.22635000
H	-1.87721000	-0.36253500	-1.30482900
H	-1.90476100	-1.66039900	-0.12551900
C	-0.57717700	-0.05543600	0.37820700
H	-0.56260900	-0.19821000	1.46528100
H	-0.56836900	1.09603200	0.26905500
C	0.69171200	-0.58813700	-0.26403600
H	0.66680800	-0.38480700	-1.34241100
H	0.70989100	-1.68143300	-0.16157300
C	1.96428800	0.00391100	0.33683800
H	1.98922400	-0.21265700	1.41157400
H	1.92882700	1.09511000	0.24110900
C	3.23644300	-0.53059800	-0.31579000
H	3.21113000	-0.31532300	-1.39112800
H	3.26318700	-1.62326000	-0.22142300
C	4.51008300	0.05852600	0.28501100
H	4.53401200	-0.15120000	1.36141900
H	4.48655200	1.15054800	0.18575500
C	5.78502700	-0.47951700	-0.36047600
H	5.75936800	-0.27112600	-1.43567100
H	5.80698700	-1.57003600	-0.25817000
C	7.04926500	0.12029700	0.24983200
H	7.10335900	-0.09461300	1.32031700
H	7.95126700	-0.27908000	-0.21796500
H	7.06128800	1.20670100	0.12920400
O	-0.56766400	2.44310600	-0.36146200
H	-0.61723500	2.12423200	-1.27722800

3.1.13 C13 (*n*-C₁₃H₂₈)



n-C₁₃H₂₈

C	-7.63686300	-0.40343800	-0.00035400
H	-7.66682700	-1.04791200	0.88222500
H	-7.66651700	-1.04833000	-0.88263900
H	-8.54174800	0.20754800	-0.00065800
C	-6.37546600	0.45679100	-0.00033800
H	-6.37565800	1.11311400	-0.87741700
H	-6.37593200	1.11348900	0.87646100
C	-5.09682400	-0.37823500	0.00003500

H	-5.09546900	-1.03673900	-0.87731900
H	-5.09572300	-1.03635400	0.87767800
C	-3.82473100	0.46582800	0.00003100
H	-3.82640600	1.12386400	0.87755600
H	-3.82622800	1.12357500	-0.87771100
C	-2.54844000	-0.37227200	0.00028900
H	-2.54736800	-1.03042300	-0.87713400
H	-2.54750700	-1.03011300	0.87794400
C	-1.27489000	0.46992200	0.00023500
H	-1.27542500	1.12789800	0.87778600
H	-1.27538500	1.12771300	-0.87745500
C	0.00000100	-0.37024000	0.00034200
H	0.00000300	-1.02833000	-0.87713600
H	0.00000100	-1.02812600	0.87797400
C	1.27488900	0.46992600	0.00024000
H	1.27544700	1.12785500	0.87782700
H	1.27535700	1.12776500	-0.87741400
C	2.54844100	-0.37226500	0.00020900
H	2.54738000	-1.03031100	-0.87729200
H	2.54749800	-1.03021100	0.87778500
C	3.82473200	0.46583500	0.00007200
H	3.82641000	1.12373500	0.87769900
H	3.82622700	1.12371800	-0.87756700
C	5.09682300	-0.37823100	-0.00005800
H	5.09549300	-1.03655200	-0.87754900
H	5.09569100	-1.03653300	0.87744800
C	6.37546900	0.45679000	-0.00021300
H	6.37591500	1.11329100	0.87673300
H	6.37568700	1.11331000	-0.87714500
C	7.63686100	-0.40344500	-0.00038700
H	7.66655100	-1.04811900	-0.88283000
H	8.54174900	0.20753600	-0.00050000
H	7.66678400	-1.04813700	0.88203400

CH₂(CH₂)₁₁CH₃

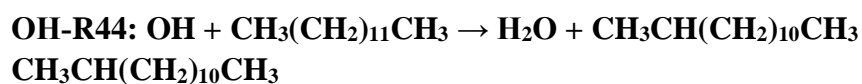
C	7.68853600	-0.38745300	-0.02650300
H	7.70554400	-1.35792300	0.45437800
H	8.62775500	0.02071900	-0.37480200
C	6.44900200	0.43691100	-0.00537900
H	6.43458000	1.07778200	0.89163700
H	6.44576500	1.12869100	-0.85569900
C	5.16901400	-0.40208100	-0.02100300
H	5.17752900	-1.08375500	0.83780900

H	5.16519800	-1.03247500	-0.91723000
C	3.89990500	0.44483700	0.01444700
H	3.89696200	1.12877500	-0.84302500
H	3.90825900	1.07583700	0.91161200
C	2.62231600	-0.39094400	-0.00364300
H	2.62207500	-1.07107000	0.85677300
H	2.61793900	-1.02605700	-0.89776700
C	1.35096900	0.45421400	0.02067300
H	1.35161600	1.13376200	-0.84024400
H	1.35473200	1.08996400	0.91443700
C	0.07385100	-0.38229000	0.00150800
H	0.07165100	-1.05994200	0.86391800
H	0.07223600	-1.02018200	-0.89074300
C	-1.19832400	0.46175000	0.02001100
H	-1.19564200	1.13972700	-0.84215400
H	-1.19774200	1.09921800	0.91256900
C	-2.47472600	-0.37580100	-0.00135800
H	-2.47814200	-1.05293900	0.86145400
H	-2.47397900	-1.01430500	-0.89317600
C	-3.74785900	0.46693800	0.01402400
H	-3.74397700	1.14480300	-0.84824800
H	-3.74992600	1.10456100	0.90649100
C	-5.02320600	-0.37180700	-0.01005600
H	-5.02811700	-1.04983400	0.85225800
H	-5.02107100	-1.01007000	-0.90224200
C	-6.29842500	0.46832700	0.00376200
H	-6.29158300	1.14566700	-0.85713100
H	-6.30055200	1.10366000	0.89616700
C	-7.56333200	-0.38623900	-0.02377600
H	-7.60111800	-1.05162000	0.84279300
H	-8.46564600	0.22845800	-0.01458400
H	-7.59066200	-1.00961300	-0.92148200

TS43: OH + CH₃(CH₂)₁₁CH₃ → H₂O + CH₂(CH₂)₁₁CH₃

C	6.85602300	0.73941500	-0.00153400
H	6.96274800	1.29784900	0.93043000
H	6.89869000	1.42159700	-0.85341000
H	7.82696400	0.10058300	-0.11039800
C	5.63689300	-0.16166100	-0.02549900
H	5.65665100	-0.78236400	-0.92681700
H	5.66205400	-0.84761900	0.82860400
C	4.33013400	0.63507400	0.01259200
H	4.29985000	1.31654400	-0.84568200

H	4.31495800	1.26598300	0.90924400
C	3.08998600	-0.25572300	-0.00359500
H	3.11660600	-0.93123800	0.85995300
H	3.11348800	-0.89355800	-0.89529400
C	1.78594800	0.53823700	0.01550600
H	1.76045600	1.21212300	-0.84938100
H	1.76458900	1.17889200	0.90547600
C	0.54254600	-0.34771700	0.00103200
H	0.56470900	-1.01871100	0.86833300
H	0.56584000	-0.99127600	-0.88678000
C	-0.75993900	0.44887600	0.01231800
H	-0.78113300	1.11951600	-0.85530700
H	-0.78245600	1.09331900	0.89958800
C	-2.00574600	-0.43359300	-0.00217200
H	-1.98627100	-1.10312400	0.86635800
H	-1.98309500	-1.07895600	-0.88874100
C	-3.30637800	0.36605900	0.00638500
H	-3.32523200	1.03542200	-0.86229200
H	-3.32814100	1.01200800	0.89258000
C	-4.55448700	-0.51324500	-0.00757800
H	-4.53634800	-1.18260600	0.86114200
H	-4.53374000	-1.15895800	-0.89397200
C	-5.85311700	0.28931500	0.00141600
H	-5.87178100	0.95881200	-0.86737000
H	-5.87364000	0.93583000	0.88742300
C	-7.10438600	-0.58601900	-0.01142500
H	-7.08436000	-1.25450000	0.85617400
H	-7.08402100	-1.22978900	-0.89753500
C	-8.39231400	0.23384300	0.00009100
H	-8.44256100	0.88955200	-0.87323000
H	-9.27762900	-0.40505200	-0.00847200
H	-8.44204000	0.86499100	0.89139300
O	8.83913000	-0.89710000	-0.07944900
H	8.52083900	-1.36562900	0.70835400



C	-7.73109200	-0.25828200	-0.12592400
H	-8.00551900	-0.83773600	0.76844500
H	-7.71427300	-0.96827300	-0.95997900
H	-8.53260500	0.45981700	-0.30543200
C	-6.40949000	0.40996300	0.03546500
H	-6.37344000	1.43702900	0.38307600

C	-5.15486400	-0.39475900	0.06618900
H	-5.15881200	-1.10916800	-0.76921700
H	-5.12929400	-1.01930100	0.97594100
C	-3.88239300	0.44996300	0.01118300
H	-3.87979500	1.14954900	0.85543800
H	-3.89722500	1.06145900	-0.89814500
C	-2.60664400	-0.38707000	0.04312500
H	-2.61003300	-1.08529500	-0.80275600
H	-2.59897300	-1.00324600	0.95056100
C	-1.33488100	0.45629100	-0.00480100
H	-1.32976900	1.15199300	0.84308900
H	-1.34387500	1.07510500	-0.91026800
C	-0.05812900	-0.38054900	0.02194300
H	-0.06156900	-1.07371400	-0.82804500
H	-0.05130900	-1.00223200	0.92555700
C	1.21420900	0.46235300	-0.01989600
H	1.21741600	1.15535900	0.83023200
H	1.20795400	1.08418100	-0.92338800
C	2.49054800	-0.37508900	0.00775900
H	2.48878800	-1.06644800	-0.84370200
H	2.49493400	-0.99877900	0.90999800
C	3.76362400	0.46703100	-0.02908200
H	3.76436900	1.15943900	0.82156400
H	3.76091400	1.08952800	-0.93215800
C	5.03915600	-0.37115900	0.00254900
H	5.04043600	-1.06279300	-0.84890000
H	5.04098000	-0.99524400	0.90471300
C	6.31411600	0.46881900	-0.03005500
H	6.31016400	1.16035300	0.81948500
H	6.31287600	1.08935700	-0.93281200
C	7.57941300	-0.38475200	0.00731600
H	7.61549800	-1.06342900	-0.84892200
H	8.48144200	0.23009300	-0.01348900
H	7.60929400	-0.99416700	0.91447800

TS44: OH + CH₃(CH₂)₁₁CH₃ → H₂O + CH₃CH(CH₂)₁₀CH₃

C	7.13854600	-0.87829300	-0.13009600
H	7.15765400	-0.93210900	-1.22088900
H	7.17536100	-1.90162300	0.25692700
H	8.03916000	-0.35888500	0.20064800
C	5.88118100	-0.17614500	0.35158300
H	5.88433600	-0.05008500	1.43934300
H	5.91407300	0.89277600	-0.07610700

C	4.58178500	-0.80722300	-0.11812300
H	4.52403300	-1.83036500	0.27772200
H	4.59965100	-0.89818200	-1.21025000
C	3.34240900	-0.02511500	0.30899000
H	3.39768600	0.98344700	-0.11729700
H	3.34503000	0.09220100	1.40008300
C	2.03610000	-0.68584200	-0.12325900
H	1.97894400	-1.69454600	0.30370200
H	2.03839000	-0.81198800	-1.21257500
C	0.79939900	0.10818900	0.29030100
H	0.85738500	1.11580600	-0.13908000
H	0.79882300	0.23758500	1.37956900
C	-0.50931100	-0.54912500	-0.14016300
H	-0.57015600	-1.55545900	0.29198700
H	-0.50674100	-0.68198300	-1.22884200
C	-1.74452600	0.25047200	0.26728600
H	-1.68161400	1.25706700	-0.16397000
H	-1.74804900	0.38277300	1.35613000
C	-3.05436700	-0.40279200	-0.16596000
H	-3.12029700	-1.40805000	0.26795900
H	-3.04898900	-0.53805000	-1.25437200
C	-4.28818500	0.40193100	0.23583000
H	-4.21992800	1.40784100	-0.19630100
H	-4.29527700	0.53555800	1.32449800
C	-5.59867200	-0.24685200	-0.20148400
H	-5.67049200	-1.25167600	0.23293200
H	-5.59076700	-0.38351400	-1.28988100
C	-6.83242900	0.56137600	0.19452000
H	-6.75798000	1.56470900	-0.23906000
H	-6.84041200	0.69574000	1.28168100
C	-8.13460900	-0.09768000	-0.25253200
H	-8.24212900	-1.08982500	0.19401400
H	-9.00555900	0.49492400	0.03463900
H	-8.15537200	-0.21983000	-1.33870900
O	5.83111300	2.32244000	-0.49522000
H	5.39040700	2.64882500	0.30589600

**OH-R45: OH + CH₃(CH₂)₁₁CH₃ → H₂O + CH₃CH₂CH(CH₂)₉CH₃
CH₃CH₂CH(CH₂)₉CH₃**

C	7.61107100	-0.60952000	0.14752100
H	7.68264900	-1.15581200	-0.79624200
H	7.45942800	-1.33994100	0.94551300
H	8.56599000	-0.10996300	0.32003500

C	6.45608000	0.38906800	0.10450900
H	6.42168600	0.96284400	1.04024600
H	6.64979900	1.13730300	-0.68136300
C	5.13124400	-0.25449900	-0.12800200
H	5.10365100	-1.24449600	-0.57579700
C	3.87240300	0.54242800	-0.08226900
H	3.82828900	1.22699700	-0.94691600
H	3.88411900	1.19720700	0.80015100
C	2.60606600	-0.31384900	-0.06753300
H	2.63139400	-0.97621600	0.80515300
H	2.60291500	-0.96408100	-0.95041300
C	1.32409500	0.51394600	-0.04427300
H	1.30426700	1.17620900	-0.91847000
H	1.32951200	1.16727700	0.83676100
C	0.05915100	-0.34087300	-0.03039100
H	0.07722500	-1.00112400	0.84517800
H	0.05557000	-0.99625800	-0.90986100
C	-1.22448500	0.48566800	-0.01248900
H	-1.24166000	1.14653700	-0.88771200
H	-1.22185200	1.14050000	0.86739800
C	-2.48923700	-0.36954800	-0.00129300
H	-2.47321300	-1.02916600	0.87486400
H	-2.49031900	-1.02576200	-0.88016000
C	-3.77355700	0.45607200	0.01267200
H	-3.78902900	1.11627600	-0.86310500
H	-3.77362200	1.11161900	0.89206000
C	-5.03760200	-0.39991100	0.02139600
H	-5.02379600	-1.05939200	0.89790700
H	-5.03701400	-1.05694800	-0.85705500
C	-6.32373800	0.42345300	0.03214400
H	-6.33608700	1.08132100	-0.84370000
H	-6.32360900	1.07860600	0.91010600
C	-7.57740200	-0.44793500	0.03975800
H	-7.59611600	-1.09328200	0.92200100
H	-8.48755700	0.15513300	0.04576300
H	-7.60716100	-1.09238100	-0.84284600

TS45: OH + CH₃(CH₂)₁₁CH₃ → H₂O + CH₃CH₂CH(CH₂)₉CH₃

C	-7.22704800	-0.09683800	0.28867700
H	-7.20767700	0.94377900	-0.04386200
H	-7.28519400	-0.10032900	1.38040900
H	-8.13533500	-0.56309500	-0.09712300
C	-5.97574300	-0.82777600	-0.19038000

H	-5.99437400	-1.87090200	0.14910200
H	-5.95579500	-0.85714700	-1.28449500
C	-4.69758200	-0.17459700	0.30865200
H	-4.70769600	-0.07402100	1.40061100
H	-4.71631000	0.90279400	-0.09413400
C	-3.40515100	-0.81068600	-0.17154900
H	-3.42415700	-0.88614900	-1.26472000
H	-3.35254300	-1.83895800	0.21084400
C	-2.16141400	-0.03983200	0.26459300
H	-2.16146000	0.06107400	1.35725200
H	-2.21507600	0.97574800	-0.14516900
C	-0.85843100	-0.69846400	-0.18027200
H	-0.86435200	-0.81133000	-1.27106400
H	-0.80268000	-1.71247200	0.23416800
C	0.38168900	0.08713600	0.23908800
H	0.38376300	0.20685200	1.32947200
H	0.32707700	1.09873600	-0.18121200
C	1.68752400	-0.57134900	-0.19822600
H	1.68308400	-0.69623100	-1.28785900
H	1.74541800	-1.58102800	0.22644200
C	2.92604500	0.22086400	0.21355800
H	2.93022800	0.34691400	1.30314400
H	2.86727200	1.23016000	-0.21187000
C	4.23323700	-0.43533200	-0.22335900
H	4.22769200	-0.56408300	-1.31259000
H	4.29459900	-1.44344900	0.20460100
C	5.47025200	0.36127600	0.18386900
H	5.47761400	0.48921200	1.27336700
H	5.40815900	1.37014900	-0.24255500
C	6.77930500	-0.29064300	-0.25487200
H	6.77081300	-0.41720600	-1.34294400
H	6.84065500	-1.29779700	0.17173300
C	8.00547600	0.51896800	0.15975900
H	8.04766400	0.63128200	1.24641300
H	8.93232500	0.04141100	-0.16417000
H	7.97418900	1.52134900	-0.27548300
O	-4.71333700	2.34268200	-0.52493300
H	-4.33015100	2.69690200	0.29393500

**OH-R46: OH + CH₃(CH₂)₁₁CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₈CH₃
CH₃(CH₂)₂CH(CH₂)₈CH₃**

C	7.66973400	-0.10026800	0.31236800
H	7.91156700	-0.71200700	-0.56089500

H	7.65856800	-0.75806700	1.18551000
H	8.47615700	0.62288200	0.44851000
C	6.32133300	0.59172700	0.13619700
H	6.10634300	1.22070900	1.00582100
H	6.35765000	1.26078000	-0.73002200
C	5.17248000	-0.40012800	-0.05204800
H	5.12977200	-1.07996000	0.81021800
H	5.40201700	-1.04687300	-0.91665200
C	3.84647100	0.25476100	-0.23725100
H	3.81798100	1.25047500	-0.67245200
C	2.57987200	-0.52908100	-0.17625200
H	2.59684500	-1.18655900	0.70401300
H	2.51463400	-1.21050800	-1.04205300
C	1.32500300	0.34325000	-0.13981900
H	1.31453800	0.99252100	-1.02334800
H	1.37522100	1.00643700	0.73124800
C	0.03214100	-0.46612900	-0.09174000
H	0.04343400	-1.11724000	0.79086500
H	-0.01268400	-1.13025000	-0.96363000
C	-1.21935100	0.40776300	-0.05781500
H	-1.22887300	1.06021500	-0.93941900
H	-1.17532400	1.07074600	0.81480800
C	-2.51501600	-0.39860700	-0.01343200
H	-2.50731100	-1.04930100	0.86947200
H	-2.55747200	-1.06333400	-0.88488500
C	-3.76620800	0.47600500	0.01532900
H	-3.77261100	1.12776100	-0.86684700
H	-3.72518100	1.13973700	0.88761900
C	-5.06190900	-0.33017900	0.05592900
H	-5.05789700	-0.98020600	0.93956200
H	-5.10176500	-0.99629900	-0.81477600
C	-6.31497200	0.54242500	0.07920600
H	-6.31754200	1.19066500	-0.80384800
H	-6.27475400	1.20672700	0.94935400
C	-7.60076600	-0.27983700	0.11861500
H	-7.62866100	-0.91381300	1.00884400
H	-8.48713300	0.35753600	0.13256100
H	-7.67039500	-0.93299000	-0.75531000

TS46: OH + CH₃(CH₂)₁₁CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₈CH₃

C	-7.34121100	-0.62271900	-0.23185400
H	-7.43659200	-1.64702400	0.13831800
H	-7.33562500	-0.66303300	-1.32416200

H	-8.23078500	-0.07049200	0.07725800
C	-6.06601200	0.03195000	0.29200500
H	-5.99909100	1.06406900	-0.06636300
H	-6.09826700	0.08211900	1.38606500
C	-4.80627400	-0.71666900	-0.13803400
H	-4.77520100	-0.78104400	-1.23194500
H	-4.84652300	-1.75007500	0.23254300
C	-3.52803100	-0.06340000	0.35872800
H	-3.54331100	0.05498100	1.44870500
H	-3.53475800	1.00761300	-0.06195800
C	-2.23684100	-0.71564500	-0.10376200
H	-2.24817200	-0.80246300	-1.19617800
H	-2.19568100	-1.74028800	0.28953600
C	-0.99033500	0.05012600	0.33315300
H	-0.99041900	0.15181100	1.42571300
H	-1.03979900	1.06554200	-0.07749300
C	0.31042700	-0.61277500	-0.11191600
H	0.30229000	-0.72735800	-1.20252100
H	0.36510900	-1.62617600	0.30411700
C	1.55257800	0.17201600	0.30298400
H	1.56154300	0.28777200	1.39375800
H	1.49408400	1.18508900	-0.11326400
C	2.85637500	-0.48260300	-0.14600000
H	2.84326300	-0.60498300	-1.23585400
H	2.92055600	-1.49306300	0.27585600
C	4.09615300	0.31243900	0.25668800
H	4.11161700	0.43318900	1.34680600
H	4.02855400	1.32355000	-0.16317500
C	5.40104300	-0.33563700	-0.19800400
H	5.38360000	-0.46133300	-1.28762300
H	5.47379400	-1.34489700	0.22579000
C	6.64016000	0.46561500	0.19546000
H	6.65778800	0.58922800	1.28381100
H	6.56443800	1.47331100	-0.22761600
C	7.93685900	-0.19193500	-0.26936300
H	7.94789200	-0.30354200	-1.35680900
H	8.81156600	0.39602200	0.01593900
H	8.04602800	-1.18854800	0.16666700
O	-3.50588000	2.44313000	-0.50355300
H	-3.14020700	2.80039700	0.32199800

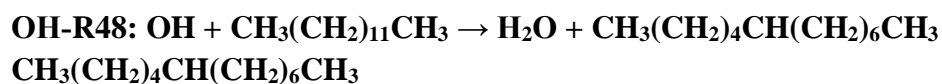
**OH-R47: OH + CH₃(CH₂)₁₁CH₃ → H₂O + CH₃(CH₂)₃CH(CH₂)₇CH₃
CH₃(CH₂)₃CH(CH₂)₇CH₃**

C	7.55310200	-0.73303400	0.26165400
H	7.63693100	-1.25199800	-0.69678800
H	8.50674900	-0.24017200	0.46040000
H	7.39848100	-1.48947300	1.03544400
C	6.39773600	0.26457500	0.23941800
H	6.34653900	0.79144400	1.19844400
H	6.58420400	1.02891200	-0.52284500
C	5.05339100	-0.40318800	-0.03804300
H	5.10022100	-0.92696100	-1.00029300
H	4.86107100	-1.16914900	0.72186400
C	3.88568200	0.58313400	-0.06052600
H	3.83451300	1.11462900	0.89963800
H	4.09608000	1.36486300	-0.81074000
C	2.56992700	-0.05760000	-0.34439400
H	2.55504100	-0.96626100	-0.94050200
C	1.29176100	0.68447500	-0.14952600
H	1.20155300	1.48767900	-0.90103000
H	1.31262900	1.20119700	0.81986100
C	0.05091300	-0.20506500	-0.22881200
H	0.12704700	-0.99315200	0.52878200
H	0.03381600	-0.71084100	-1.20144700
C	-1.25195500	0.56589000	-0.03573500
H	-1.32353900	1.35449200	-0.79468600
H	-1.23173300	1.07484200	0.93561900
C	-2.49099300	-0.32286700	-0.11317000
H	-2.41847300	-1.11216500	0.64476100
H	-2.51211900	-0.83095900	-1.08488800
C	-3.79544600	0.44614400	0.08246200
H	-3.86776300	1.23605000	-0.67499700
H	-3.77454400	0.95357800	1.05457100
C	-5.03431700	-0.44250000	0.00418800
H	-4.96261800	-1.23296100	0.76130400
H	-5.05625200	-0.95009900	-0.96796300
C	-6.33996600	0.32491100	0.20031300
H	-6.41053500	1.11337700	-0.55679500
H	-6.31667100	0.83131600	1.17133400
C	-7.56881500	-0.57748600	0.11986000
H	-7.53018900	-1.35575400	0.88653900
H	-8.49284200	-0.01341100	0.26109200
H	-7.62372400	-1.07335500	-0.85281700

TS47: OH + CH₃(CH₂)₁₁CH₃ → H₂O + CH₃(CH₂)₃CH(CH₂)₇CH₃

C	-7.42504400	0.10751100	0.22426500
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H	-7.40004200	1.15737200	-0.07940800
H	-7.49296900	0.07934000	1.31506500
H	-8.33669200	-0.33700200	-0.17978000
C	-6.17750900	-0.62588900	-0.26142300
H	-6.22822100	-1.67913700	0.03636700
H	-6.14627700	-0.61535300	-1.35619500
C	-4.89011300	-0.00921500	0.28004900
H	-4.92246300	-0.00834600	1.37673900
H	-4.82687900	1.04003200	-0.03102600
C	-3.63326000	-0.73857500	-0.18748200
H	-3.61239400	-0.76814000	-1.28296800
H	-3.66437300	-1.78312000	0.15105300
C	-2.35247800	-0.09496700	0.31572800
H	-2.36537900	0.00987100	1.40714600
H	-2.35579700	0.98037600	-0.09277600
C	-1.06378300	-0.74477400	-0.15699400
H	-1.07955900	-0.82337000	-1.25000400
H	-1.02216000	-1.77235000	0.22855100
C	0.18505500	0.01669900	0.28078500
H	0.18722700	0.11345100	1.37380100
H	0.13641400	1.03408800	-0.12483800
C	1.48317900	-0.64790100	-0.16938800
H	1.47148300	-0.76127800	-1.26010400
H	1.53715100	-1.66193000	0.24528000
C	2.72843100	0.13353400	0.24253000
H	2.73842200	0.25231900	1.33296700
H	2.67361000	1.14563200	-0.17648700
C	4.02938400	-0.52787800	-0.20490400
H	4.01558300	-0.65374900	-1.29437700
H	4.08910700	-1.53729200	0.22019600
C	5.27276500	0.26233500	0.19530700
H	5.28778600	0.38926100	1.28486800
H	5.21267000	1.27180300	-0.22994100
C	6.57579200	-0.39538100	-0.25259400
H	6.55859700	-0.52282700	-1.34046100
H	6.63626000	-1.40238900	0.17446600
C	7.80828200	0.40972800	0.15193500
H	7.85875600	0.52362900	1.23809100
H	8.73077900	-0.07221400	-0.17784000
H	7.77803000	1.41149700	-0.28477400
O	-2.33444900	2.41689900	-0.53507400
H	-2.02729700	2.78327600	0.31008400



C	7.65735500	-0.17303300	0.13523400
H	7.76843200	-0.82171500	-0.73776200
H	7.69691100	-0.80643000	1.02543300
H	8.51631400	0.50022700	0.16400600
C	6.33971000	0.59568900	0.07541900
H	6.25965400	1.25950500	0.94315500
H	6.32874300	1.24180000	-0.80912100
C	5.12448400	-0.32791400	0.03573300
H	5.13213400	-0.97355100	0.92257800
H	5.20695400	-0.99598800	-0.83066100
C	3.79840800	0.42397900	-0.03182200
H	3.79179100	1.06934200	-0.91821900
H	3.70756400	1.08770500	0.83565300
C	2.58643700	-0.50526700	-0.08151400
H	2.58669000	-1.15740400	0.80370700
H	2.69727800	-1.19086900	-0.93929600
C	1.28245700	0.21142200	-0.17249700
H	1.27295500	1.23589800	-0.53432500
C	-0.00487300	-0.53714500	-0.10469800
H	0.00123900	-1.20093700	0.77169600
H	-0.09038700	-1.21315200	-0.97296000
C	-1.23937100	0.36222100	-0.05600100
H	-1.23629000	1.02243800	-0.93138700
H	-1.17648700	1.01289500	0.82368000
C	-2.54762300	-0.42283300	-0.02005400
H	-2.55075800	-1.08391700	0.85516300
H	-2.60065300	-1.07665100	-0.89930100
C	-3.78504200	0.47055200	0.01809800
H	-3.77757500	1.13676100	-0.85318300
H	-3.73890800	1.11878800	0.90163700
C	-5.09205600	-0.31810000	0.03791700
H	-5.10181600	-0.98306500	0.91030800
H	-5.13539200	-0.96880200	-0.84425100
C	-6.33370900	0.57027000	0.06853400
H	-6.32097200	1.23551900	-0.80167700
H	-6.29243300	1.21685500	0.95187700
C	-7.63001100	-0.23626900	0.08093900
H	-7.67288400	-0.88832700	0.95738900
H	-8.50850600	0.41170300	0.10123200
H	-7.70059200	-0.87006600	-0.80709100

TS48: OH + CH₃(CH₂)₁₁CH₃ → H₂O + CH₃(CH₂)₄CH(CH₂)₆CH₃

C	-7.53508400	-0.44207400	-0.27294400
H	-7.64218900	-1.44484700	0.14917100
H	-7.53062200	-0.53969400	-1.36173200
H	-8.41798100	0.13560800	0.00793000
C	-6.25018900	0.22002700	0.21737900
H	-6.17680200	1.23315800	-0.19264500
H	-6.28317800	0.32967000	1.30698200
C	-4.99950100	-0.56598700	-0.16995100
H	-4.96666900	-0.67700300	-1.26066200
H	-5.06833100	-1.58090700	0.24074700
C	-3.70773300	0.09090000	0.30826300
H	-3.73496900	0.19267900	1.40052200
H	-3.64220100	1.10598800	-0.10073400
C	-2.45437800	-0.68157000	-0.09640100
H	-2.42084800	-0.77739200	-1.18767600
H	-2.50592200	-1.70288300	0.30432700
C	-1.17157400	-0.02736400	0.38632700
H	-1.17941000	0.10383700	1.47491100
H	-1.15626400	1.03826700	-0.04766900
C	0.11595700	-0.68856800	-0.07525200
H	0.10358900	-0.77321000	-1.16797500
H	0.15011300	-1.71450400	0.31559800
C	1.36549800	0.07172000	0.36285200
H	1.38156000	0.14369700	1.45744300
H	1.30326900	1.09818800	-0.01613900
C	2.66075600	-0.57497900	-0.12037700
H	2.63513700	-0.66143300	-1.21342000
H	2.72708300	-1.59865600	0.26829600
C	3.90676000	0.20482700	0.29265800
H	3.93446200	0.29324600	1.38569200
H	3.83622600	1.22762900	-0.09677300
C	5.20508500	-0.43212200	-0.19534100
H	5.17289400	-0.53069000	-1.28744900
H	5.28326100	-1.45148400	0.20254600
C	6.44949800	0.35955600	0.20078700
H	6.48061100	0.45900700	1.29136600
H	6.36925100	1.37628600	-0.19903400
C	7.74002600	-0.28795900	-0.29442700
H	7.73692500	-0.37677600	-1.38403100
H	8.61841100	0.29411400	-0.00830100
H	7.85460700	-1.29336400	0.11941300

O	-1.16869200	2.47076000	-0.50082600
H	-1.46321200	2.84694800	0.34446200

OH-R49: OH + CH₃(CH₂)₁₁CH₃ → H₂O + CH₃(CH₂)₅CH(CH₂)₅CH₃
CH₃(CH₂)₅CH(CH₂)₅CH₃

C	-7.56169900	-0.68458600	0.17776100
H	-7.47352600	-1.47180800	0.93108700
H	-7.62424400	-1.16817000	-0.80063200
H	-8.50198400	-0.15783100	0.35194000
C	-6.36564200	0.26218800	0.23966600
H	-6.48556100	1.05796400	-0.50346000
H	-6.33533200	0.75545700	1.21723600
C	-5.03808500	-0.45288500	-0.00199100
H	-5.06719300	-0.94768900	-0.98052800
H	-4.91656300	-1.25020300	0.74137100
C	-3.83164700	0.48069700	0.05629100
H	-3.80274700	0.97413800	1.03542100
H	-3.95447000	1.27834200	-0.68651600
C	-2.50677200	-0.23675700	-0.18708900
H	-2.53315500	-0.72646500	-1.16771400
H	-2.37929600	-1.03402400	0.55381600
C	-1.29843700	0.69781900	-0.12751600
H	-1.26644900	1.19610800	0.85122400
H	-1.44225500	1.51157400	-0.85910200
C	0.00000000	0.00959500	-0.37771400
H	0.00000000	-0.89006400	-0.98748400
C	1.29843700	0.69781800	-0.12751400
H	1.26644900	1.19610500	0.85122700
H	1.44225400	1.51157500	-0.85909800
C	2.50677200	-0.23675700	-0.18708900
H	2.53315500	-0.72646300	-1.16771600
H	2.37929600	-1.03402600	0.55381400
C	3.83164700	0.48069700	0.05629400
H	3.80274700	0.97413500	1.03542400
H	3.95447000	1.27834300	-0.68651200
C	5.03808500	-0.45288500	-0.00199000
H	5.06719300	-0.94768800	-0.98052800
H	4.91656300	-1.25020400	0.74137100
C	6.36564200	0.26218800	0.23966600
H	6.33533300	0.75545600	1.21723800
H	6.48556000	1.05796500	-0.50345800
C	7.56169900	-0.68458500	0.17775900
H	7.62424300	-1.16816800	-0.80063400

H	8.50198500	-0.15783000	0.35193700
H	7.47352800	-1.47180800	0.93108500

TS49: OH + CH₃(CH₂)₁₁CH₃ → H₂O + CH₃(CH₂)₅CH(CH₂)₅CH₃

C	-7.62682000	0.22676500	0.23891400
H	-7.61748100	1.27291900	-0.07794100
H	-7.67385800	0.21197100	1.33099000
H	-8.54192300	-0.23073900	-0.14217400
C	-6.38204900	-0.50248700	-0.26064200
H	-6.42229600	-1.55367000	0.04497500
H	-6.36744900	-0.50029200	-1.35588500
C	-5.08850400	0.12148800	0.25836800
H	-5.10332300	0.12387700	1.35524200
H	-5.04462300	1.17293500	-0.05037500
C	-3.83432900	-0.59984700	-0.22867200
H	-3.82361100	-0.60652900	-1.32523500
H	-3.87535300	-1.65006200	0.08549000
C	-2.54318200	0.03392400	0.28286300
H	-2.55621600	0.04878300	1.37963600
H	-2.49107400	1.07900900	-0.04272500
C	-1.28963800	-0.69447800	-0.19583300
H	-1.28117800	-0.72994100	-1.29122200
H	-1.31405600	-1.73712700	0.14868800
C	-0.00460000	-0.04618600	0.29065900
H	-0.00624200	0.06149100	1.38181400
H	-0.01433300	1.02812500	-0.12067200
C	1.27964800	-0.69725100	-0.19264200
H	1.25989900	-0.76678700	-1.28609200
H	1.31704900	-1.72808300	0.18438300
C	2.53405800	0.05300100	0.24854900
H	2.53720400	0.14248600	1.34211200
H	2.49437500	1.07315400	-0.15085000
C	3.82690300	-0.62020000	-0.20521000
H	3.82165900	-0.71343600	-1.29779100
H	3.86305500	-1.64217600	0.19128900
C	5.08001000	0.13471800	0.23087000
H	5.08404100	0.23185500	1.32357000
H	5.04559800	1.15572900	-0.16834200
C	6.37520400	-0.53785500	-0.21875400
H	6.36933300	-0.63502700	-1.30974700
H	6.40849200	-1.55700000	0.18139400
C	7.61870900	0.22969700	0.22308600
H	7.65591700	0.31556500	1.31225500

H	8.53496900	-0.26461300	-0.10553000
H	7.61730900	1.24210900	-0.18917700
O	0.01054700	2.46577200	-0.55638400
H	0.36726400	2.82156400	0.27365400

3.1.14 C14 (*n*-C₁₄H₃₀)



n-C₁₄H₃₀

C	-8.28000900	0.33049400	-0.00019300
H	-8.31930700	0.97459800	-0.88268400
H	-8.31937600	0.97478700	0.88215700
H	-9.17574000	-0.29383300	-0.00016100
C	-7.00584500	-0.51071000	-0.00005500
H	-6.99648200	-1.16706300	0.87695200
H	-6.99640400	-1.16723500	-0.87693300
C	-5.73997500	0.34356200	-0.00008100
H	-5.74860200	1.00189700	0.87735900
H	-5.74853200	1.00174200	-0.87763800
C	-4.45524000	-0.48110800	0.00004200
H	-4.44698800	-1.13903000	-0.87753500
H	-4.44707000	-1.13890000	0.87771700
C	-3.19171800	0.37613800	0.00003800
H	-3.20043600	1.03410500	0.87755500
H	-3.20038500	1.03402000	-0.87754300
C	-1.90584000	-0.44708100	0.00011200
H	-1.89686500	-1.10497600	-0.87746100
H	-1.89692200	-1.10491300	0.87773200
C	-0.64313000	0.41130700	0.00012200
H	-0.65223700	1.06919600	0.87770100
H	-0.65222100	1.06919100	-0.87746100
C	0.64313000	-0.41130700	0.00013300
H	0.65223500	-1.06919000	-0.87745100
H	0.65222200	-1.06919700	0.87771100
C	1.90584000	0.44708100	0.00014400
H	1.89691100	1.10491000	0.87776700
H	1.89687600	1.10498000	-0.87742600
C	3.19171800	-0.37613800	0.00008100
H	3.20038500	-1.03403000	-0.87749100
H	3.20043500	-1.03409400	0.87760600
C	4.45524000	0.48110800	0.00007400
H	4.44707500	1.13890600	0.87774500
H	4.44698300	1.13902300	-0.87750800
C	5.73997500	-0.34356200	-0.00005100

H	5.74851500	-1.00176500	-0.87759100
H	5.74862000	-1.00187400	0.87740600
C	7.00584500	0.51071000	-0.00007600
H	6.99650600	1.16708200	0.87691700
H	6.99638000	1.16721500	-0.87696800
C	8.28000900	-0.33049400	-0.00023200
H	8.31927600	-0.97462700	-0.88270300
H	9.17574000	0.29383300	-0.00025300
H	8.31940700	-0.97475800	0.88213800

CH₂(CH₂)₁₂CH₃

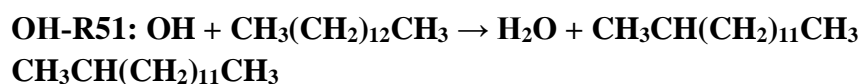
C	-8.33207500	0.30919200	-0.01747500
H	-8.36511400	1.27731900	0.46731900
H	-9.26472800	-0.11302000	-0.36669400
C	-7.07924600	-0.49491600	0.00068000
H	-7.05239000	-1.13513700	0.89790500
H	-7.06689400	-1.18675000	-0.84944800
C	-5.81301900	0.36469400	-0.01818700
H	-5.83068100	1.04682400	0.84011600
H	-5.82098800	0.99436800	-0.91487900
C	-4.53047100	-0.46179300	0.01532200
H	-4.51867400	-1.14665900	-0.84133500
H	-4.52703300	-1.09181300	0.91320800
C	-3.26622600	0.39393800	-0.00661000
H	-3.27469300	1.07513000	0.85291700
H	-3.27337300	1.02783100	-0.90157400
C	-1.98202900	-0.43156800	0.01621900
H	-1.97403100	-1.11206500	-0.84391500
H	-1.97479800	-1.06635600	0.91065100
C	-0.71748600	0.42375500	-0.00603900
H	-0.72389400	1.10258800	0.85541500
H	-0.72612200	1.06027700	-0.89922000
C	0.56651500	-0.40214400	0.01215600
H	0.57261800	-1.08079800	-0.84946200
H	0.57500400	-1.03897100	0.90514100
C	1.83166700	0.45228500	-0.01024200
H	1.82612600	1.13057700	0.85165600
H	1.82321200	1.08940200	-0.90301000
C	3.11494800	-0.37476200	0.00716200
H	3.12045400	-1.05280900	-0.85493100
H	3.12275900	-1.01230300	0.89964000
C	4.38115800	0.47819300	-0.01429800
H	4.37551100	1.15682000	0.84735800

H	4.37449900	1.11498500	-0.90733400
C	5.66323600	-0.35034700	0.00507300
H	5.66989700	-1.02897700	-0.85675700
H	5.66969400	-0.98795300	0.89770700
C	6.93176200	0.49972200	-0.01464200
H	6.92309700	1.17781300	0.84563400
H	6.92555900	1.13420200	-0.90763300
C	8.20333500	-0.34503800	0.00866500
H	8.24305600	-1.01057000	-0.85770200
H	9.10090200	0.27650000	-0.00405700
H	8.23860900	-0.96772900	0.90657100

TS50: OH + CH₃(CH₂)₁₂CH₃ → H₂O + CH₂(CH₂)₁₂CH₃

C	7.50627700	0.67418600	-0.00726800
H	7.62372100	1.23416100	0.92244100
H	7.55946300	1.35216500	-0.86191700
H	8.46668100	0.01915000	-0.11394600
C	6.27169800	-0.20582200	-0.02630300
H	6.28005900	-0.83095300	-0.92475700
H	6.28539800	-0.88789900	0.83120300
C	4.97889500	0.61356100	0.00891000
H	4.95955500	1.29104700	-0.85280700
H	4.97530600	1.24906000	0.90241100
C	3.72358400	-0.25587400	-0.00168400
H	3.73982700	-0.92775600	0.86494900
H	3.73519700	-0.89805800	-0.89048300
C	2.43321100	0.56021000	0.01541100
H	2.41798500	1.23068400	-0.85235100
H	2.42344300	1.20482000	0.90270100
C	1.17527800	-0.30509900	0.00599600
H	1.18771400	-0.97300300	0.87587100
H	1.18712000	-0.95238800	-0.87931800
C	-0.11430800	0.51228800	0.01572300
H	-0.12588700	1.18011100	-0.85424200
H	-0.12610200	1.15995300	0.90082700
C	-1.37344900	-0.35113700	0.00523500
H	-1.36328400	-1.01779200	0.87613300
H	-1.36072100	-0.99996100	-0.87899700
C	-2.66251000	0.46710800	0.01145000
H	-2.67220200	1.13387000	-0.85937400
H	-2.67545200	1.11592900	0.89570500
C	-3.92208600	-0.39568500	-0.00001100
H	-3.91299600	-1.06198000	0.87117600

H	-3.90867700	-1.04500000	-0.88388100
C	-5.21117400	0.42259500	0.00460500
H	-5.22019100	1.08900300	-0.86652400
H	-5.22495000	1.07178700	0.88859800
C	-6.47050400	-0.44023300	-0.00752400
H	-6.46236800	-1.10696100	0.86354300
H	-6.45731600	-1.08982100	-0.89140100
C	-7.76099900	0.37636100	-0.00333400
H	-7.76772600	1.04163300	-0.87361200
H	-7.77322400	1.02397700	0.88012600
C	-9.01014800	-0.50138300	-0.01636400
H	-9.03415900	-1.15521600	0.85945500
H	-9.92332300	0.09709700	-0.01347100
H	-9.02819100	-1.13745100	-0.90534100
O	9.46216400	-0.99487000	-0.08096300
H	9.11538800	-1.47771200	0.68593800



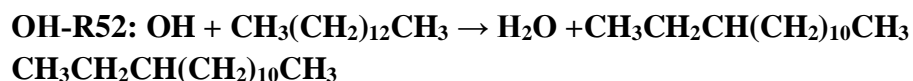
C	8.37170600	-0.18480400	0.15696100
H	8.65869200	-0.77734000	-0.72480800
H	8.35968500	-0.87912300	1.00423300
H	9.16250900	0.54726400	0.32724600
C	7.04226400	0.46240300	-0.02441800
H	6.99457200	1.48446500	-0.38508000
C	5.79949600	-0.36044400	-0.05599200
H	5.80866800	-1.06800100	0.78514000
H	5.78790700	-0.99239600	-0.96088100
C	4.51483800	0.46651400	-0.01501600
H	4.50761700	1.15998400	-0.86428300
H	4.51560100	1.08461000	0.88995800
C	3.25128600	-0.38876100	-0.04858400
H	3.26031300	-1.08204400	0.80131500
H	3.25665000	-1.01010100	-0.95250300
C	1.96751800	0.43678100	-0.01147600
H	1.95644500	1.12750100	-0.86337100
H	1.96398700	1.06082300	0.89044000
C	0.70272800	-0.41803000	-0.03864700
H	0.71340600	-1.10760600	0.81420300
H	0.70690600	-1.04338400	-0.93973400
C	-0.58122200	0.40736700	-0.00331500
H	-0.59262500	1.09606700	-0.85686400
H	-0.58459800	1.03371100	0.89707800

C	-1.84614800	-0.44732900	-0.02800400
H	-1.83445500	-1.13619300	0.82541700
H	-1.84318400	-1.07348900	-0.92853700
C	-3.12992100	0.37830700	0.00836300
H	-3.14208900	1.06680500	-0.84533400
H	-3.13220800	1.00493900	0.90856000
C	-4.39528900	-0.47586400	-0.01462500
H	-4.38224500	-1.16551000	0.83816800
H	-4.39439500	-1.10122200	-0.91573500
C	-5.67841100	0.35027200	0.02519400
H	-5.69254000	1.04035800	-0.82740000
H	-5.67945700	0.97591900	0.92627200
C	-6.94555100	-0.50182800	0.00339100
H	-6.92871900	-1.19212700	0.85378500
H	-6.94514700	-1.12356600	-0.89854000
C	-8.21855500	0.33976200	0.04909300
H	-8.26669900	1.01792700	-0.80697700
H	-9.11492500	-0.28347600	0.03437900
H	-8.24810800	0.94912800	0.95629800

TS51: OH + CH₃(CH₂)₁₂CH₃ → H₂O + CH₃CH(CH₂)₁₁CH₃

C	7.77502900	-0.79390400	-0.10009800
H	7.79715700	-0.86753200	-1.18969700
H	7.83320300	-1.80887500	0.30590000
H	8.66384200	-0.24929400	0.22205000
C	6.50231800	-0.10982100	0.36692500
H	6.49919500	0.03203800	1.45273000
H	6.51529300	0.95337100	-0.07615900
C	5.21709500	-0.77289700	-0.09778100
H	5.17796400	-1.79141100	0.31199900
H	5.24035700	-0.87864200	-1.18847800
C	3.96143600	-0.00899100	0.31438900
H	4.00032300	0.99545700	-0.12324900
H	3.95655500	0.12090100	1.40403800
C	2.66953300	-0.69836400	-0.11651500
H	2.62876000	-1.70325400	0.32116500
H	2.67936200	-0.83620100	-1.20436400
C	1.41667000	0.07756400	0.28245500
H	1.45953800	1.08203100	-0.15597700
H	1.40743500	0.21700700	1.37043600
C	0.12211300	-0.60637200	-0.14942000
H	0.07640100	-1.60982000	0.29120300
H	0.13310200	-0.74855600	-1.23686500

C	-1.12901300	0.17517600	0.24422900
H	-1.08086700	1.17914500	-0.19496000
H	-1.14103800	0.31629700	1.33190200
C	-2.42508800	-0.50388500	-0.19080900
H	-2.47561100	-1.50707300	0.24991400
H	-2.41206100	-0.64658400	-1.27821200
C	-3.67445000	0.28214200	0.19962500
H	-3.62171600	1.28601500	-0.23928300
H	-3.68862400	0.42328100	1.28725200
C	-4.97186900	-0.39239700	-0.23851200
H	-5.02621200	-1.39586200	0.20119400
H	-4.95734800	-0.53422000	-1.32604300
C	-6.21969400	0.39650900	0.15035000
H	-6.16482500	1.40075700	-0.28785500
H	-6.23586400	0.53751800	1.23812700
C	-7.51899900	-0.27407800	-0.28924400
H	-7.57301200	-1.27652600	0.14927800
H	-7.50175800	-0.41383900	-1.37560000
C	-8.75623600	0.52790700	0.10696300
H	-8.73301800	1.52456500	-0.34172400
H	-9.67595600	0.03602800	-0.21585000
H	-8.80619200	0.65448600	1.19171700
O	6.40659800	2.37673600	-0.50972600
H	5.95975700	2.70337400	0.28786800



C	-8.25844200	0.53975300	0.16339700
H	-8.34281900	1.08870400	-0.77774300
H	-8.11319200	1.26901900	0.96362800
H	-9.20504700	0.02565900	0.33888600
C	-7.08914100	-0.44162800	0.11039200
H	-7.04252500	-1.01958900	1.04305500
H	-7.27514200	-1.18861100	-0.67850200
C	-5.77490100	0.22273600	-0.12396000
H	-5.76389000	1.21557700	-0.56608600
C	-4.50433300	-0.55586700	-0.08752000
H	-4.45263200	-1.23349200	-0.95720800
H	-4.50437500	-1.21707600	0.79015900
C	-3.25042600	0.31844800	-0.06960300
H	-3.28372100	0.97519900	0.80706100
H	-3.25763300	0.97384100	-0.94861800
C	-1.95704300	-0.49153300	-0.05295100

H	-1.92935200	-1.14824400	-0.93113600
H	-1.95270100	-1.15023900	0.82407900
C	-0.70354000	0.37990200	-0.03508300
H	-0.72945500	1.03498000	0.84417600
H	-0.70879100	1.04008800	-0.91093500
C	0.59027200	-0.43067600	-0.02238500
H	0.61493200	-1.08632800	-0.90136800
H	0.59561400	-1.09062800	0.85366200
C	1.84521200	0.43879800	-0.00647500
H	1.82226200	1.09322300	0.87342700
H	1.83920000	1.09981900	-0.88170900
C	3.13776700	-0.37383700	0.00279100
H	3.15933000	-1.02901100	-0.87661600
H	3.14398700	-1.03440100	0.87837100
C	4.39445300	0.49323200	0.01637300
H	4.37461900	1.14737900	0.89658500
H	4.38794700	1.15460600	-0.85861400
C	5.68530700	-0.32180700	0.02270100
H	5.70460900	-0.97707300	-0.85688100
H	5.69277000	-0.98294400	0.89804000
C	6.94486500	0.54162400	0.03405300
H	6.92545200	1.19456600	0.91344900
H	6.93613400	1.20138300	-0.84039100
C	8.22500400	-0.29044900	0.03862400
H	8.27380600	-0.93151400	-0.84561900
H	9.11628500	0.34016200	0.04556500
H	8.26400700	-0.93723100	0.91916500

TS52: OH + CH₃(CH₂)₁₂CH₃ → H₂O + CH₃CH₂CH(CH₂)₁₀CH₃

C	-7.84597100	-0.11511100	0.24456400
H	-7.82696800	0.92454900	-0.09092900
H	-7.91499100	-0.11552600	1.33568000
H	-8.74869600	-0.58577900	-0.14883400
C	-6.58737500	-0.84299800	-0.21982900
H	-6.60575600	-1.88522100	0.12241000
H	-6.55636100	-0.87537000	-1.31361800
C	-5.31656200	-0.18386400	0.29005500
H	-5.33756300	-0.08096700	1.38165300
H	-5.33571700	0.89258400	-0.11521900
C	-4.01713000	-0.81592300	-0.17633100
H	-4.02524000	-0.89354600	-1.26947600
H	-3.96430600	-1.84326000	0.20853900
C	-2.78067300	-0.03945800	0.27040100

H	-2.79151500	0.06309400	1.36285300
H	-2.83448200	0.97529100	-0.14141600
C	-1.47084000	-0.69344200	-0.16105500
H	-1.46568000	-0.80711000	-1.25176500
H	-1.41520300	-1.70692700	0.25467600
C	-0.23801500	0.09742100	0.26973500
H	-0.24598700	0.21653800	1.36014900
H	-0.29359200	1.10901000	-0.15050100
C	1.07465300	-0.55458300	-0.15674500
H	1.07923800	-0.68022800	-1.24628800
H	1.13467800	-1.56364200	0.26910000
C	2.30567200	0.24474300	0.26368000
H	2.30159000	0.37106900	1.35323300
H	2.24391200	1.25358700	-0.16245000
C	3.61961700	-0.40375400	-0.16429100
H	3.62086800	-0.53500500	-1.25320900
H	3.68548900	-1.41044200	0.26629400
C	4.84908400	0.40254500	0.24752300
H	4.84933200	0.53284200	1.33661700
H	4.78105800	1.40961600	-0.18192800
C	6.16372000	-0.24177900	-0.18390500
H	6.16214400	-0.37612100	-1.27261600
H	6.23585000	-1.24733800	0.24874600
C	7.39311100	0.56890000	0.22056100
H	7.39473900	0.70117700	1.30800600
H	7.31844700	1.57286900	-0.21150000
C	8.69947200	-0.08589100	-0.22053900
H	8.72628800	-0.20635300	-1.30678400
H	9.56727900	0.50867500	0.07204100
H	8.80738100	-1.07840200	0.22509200
O	-5.33499000	2.33127900	-0.55022400
H	-4.95890200	2.68927400	0.27029900

OH-R53: OH + CH₃(CH₂)₁₂CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₉CH₃

C	-8.31038000	-0.01179300	0.31142500
H	-8.56396400	0.62820500	-0.53790500
H	-8.31368900	0.61172700	1.20945700
H	-9.10173200	-0.75626600	0.41819900
C	-6.94743600	-0.66785700	0.11094400
H	-6.72172300	-1.32788500	0.95441900
H	-6.96782100	-1.30100800	-0.78240600
C	-5.81908600	0.35454400	-0.03212000

H	-5.79314400	0.99891400	0.85765000
H	-6.05932500	1.03172500	-0.87009600
C	-4.47929900	-0.26444600	-0.23961100
H	-4.42938400	-1.24466400	-0.70703500
C	-3.22933900	0.54320500	-0.15230600
H	-3.26038000	1.17361200	0.74718800
H	-3.17628400	1.25132300	-0.99724900
C	-1.95765200	-0.30520000	-0.14003300
H	-1.93692400	-0.93125700	-1.04002500
H	-1.99410300	-0.99160000	0.71352700
C	-0.67959000	0.52601400	-0.07324800
H	-0.70017800	1.15461300	0.82537100
H	-0.64779700	1.21220900	-0.92841300
C	0.58643800	-0.32736500	-0.06367000
H	0.60208900	-0.96029400	-0.95934000
H	0.55665700	-1.00994000	0.79429400
C	1.86998600	0.49740900	-0.00747000
H	1.85716300	1.12932800	0.88891900
H	1.89921700	1.18055600	-0.86507900
C	3.13293000	-0.36062000	-0.00279600
H	3.14134900	-0.99632100	-0.89659800
H	3.10601700	-1.04054800	0.85742400
C	4.41949800	0.46016300	0.04340100
H	4.41374600	1.09457900	0.93812900
H	4.44549700	1.14098700	-0.81618100
C	5.68022700	-0.40079400	0.04286700
H	5.68330500	-1.03868000	-0.84959900
H	5.65735800	-1.07915500	0.90465000
C	6.96965100	0.41651000	0.08049500
H	6.96678200	1.05201400	0.97279000
H	6.99047800	1.09365400	-0.78034900
C	8.21948500	-0.46039000	0.07614800
H	8.25047100	-1.08675300	-0.81936400
H	9.13222000	0.13837800	0.09844900
H	8.23150200	-1.12373200	0.94501200

TS53: OH + CH₃(CH₂)₁₂CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₉CH₃

C	-7.95917800	-0.54118200	-0.20649900
H	-8.07045600	-1.55498800	0.18742200
H	-7.95920600	-0.60661300	-1.29763000
H	-8.83778200	0.03319000	0.09355000
C	-6.67050800	0.10293200	0.29704100
H	-6.58759300	1.12542000	-0.08479100

H	-6.69679200	0.17796700	1.38988500
C	-5.42581700	-0.67677400	-0.12166900
H	-5.39824300	-0.76132000	-1.21428700
H	-5.48525700	-1.70244500	0.26743100
C	-4.13434000	-0.03990600	0.36169400
H	-4.14357100	0.09312200	1.45006500
H	-4.12039200	1.02517600	-0.07393800
C	-2.85648800	-0.72133200	-0.09609300
H	-2.87055300	-0.81658600	-1.18779700
H	-2.83532200	-1.74347600	0.30517600
C	-1.59523200	0.02388300	0.33375700
H	-1.58825500	0.12651500	1.42619200
H	-1.63008800	1.03966700	-0.07724000
C	-0.30810700	-0.66131800	-0.11723800
H	-0.32259300	-0.77415200	-1.20797800
H	-0.26943500	-1.67613300	0.29714200
C	0.94912700	0.10125300	0.29348900
H	0.96643100	0.21221400	1.38466800
H	0.90462200	1.11689200	-0.11812400
C	2.23956600	-0.57219400	-0.16619800
H	2.21868100	-0.68784100	-1.25669500
H	2.28937900	-1.58603300	0.24941200
C	3.49404900	0.20033800	0.23449200
H	3.51862200	0.31182100	1.32542500
H	3.43909900	1.21578200	-0.17654800
C	4.78618800	-0.46342400	-0.23455800
H	4.75980800	-0.57685300	-1.32523600
H	4.84474800	-1.47793200	0.17835000
C	6.03835100	0.31523300	0.16091100
H	6.06884700	0.42454100	1.25207900
H	5.97669200	1.33167300	-0.24717500
C	7.33244800	-0.33995100	-0.31569100
H	7.30092400	-0.44662400	-1.40551700
H	7.39334700	-1.35510700	0.09149500
C	8.57373300	0.45171200	0.08845000
H	8.63984200	0.54229400	1.17599700
H	9.48968500	-0.02638500	-0.26437400
H	8.54141700	1.46264000	-0.32644000
O	-4.06945500	2.45675500	-0.52523900
H	-3.76371600	2.82391400	0.32007400

OH-R54: $\text{OH} + \text{CH}_3(\text{CH}_2)_{12}\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_8\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2)_8\text{CH}_3$

C	8.19096700	0.69812500	0.33667200
H	8.02861700	1.42761000	1.13438100
H	8.28822800	1.24987100	-0.60198800
H	9.14069900	0.19564200	0.53002100
C	7.03321000	-0.29441400	0.26532300
H	7.22732300	-1.03270500	-0.52033500
H	6.96812500	-0.85376600	1.20492500
C	5.69446900	0.38697700	-0.00613600
H	5.75460200	0.94183600	-0.95006000
H	5.49544000	1.12835700	0.77607800
C	4.52375900	-0.59385900	-0.07465000
H	4.45807600	-1.15462700	0.86768500
H	4.74158900	-1.35235200	-0.84629200
C	3.21422700	0.06085900	-0.35539300
H	3.20959200	0.97798700	-0.93859300
C	1.92923000	-0.67363300	-0.17727400
H	1.93852200	-1.19822500	0.78810100
H	1.83955900	-1.47025900	-0.93580000
C	0.69540400	0.22530700	-0.25931300
H	0.68754400	0.73604100	-1.22947200
H	0.77290100	1.00901700	0.50268800
C	-0.61408300	-0.53705400	-0.07725600
H	-0.60353300	-1.04932700	0.89250900
H	-0.68643700	-1.32264300	-0.83925500
C	-1.84635600	0.36064000	-0.15940500
H	-1.85955800	0.86969200	-1.13076900
H	-1.77147000	1.14875800	0.59954600
C	-3.15705600	-0.39916200	0.03007300
H	-3.14441400	-0.90622700	1.00249100
H	-3.23122000	-1.18893300	-0.72731400
C	-4.38945500	0.49823900	-0.05464100
H	-4.40357300	1.00330000	-1.02811100
H	-4.31392100	1.28962400	0.70094600
C	-5.70003100	-0.26034200	0.13899400
H	-5.68727700	-0.76450600	1.11310400
H	-5.77605300	-1.05289400	-0.61553100
C	-6.93352700	0.63590900	0.05287200
H	-6.94570900	1.13755900	-0.92081900
H	-6.85582900	1.42728400	0.80623100
C	-8.23538100	-0.13677000	0.25021700
H	-8.25372700	-0.62351400	1.22886700
H	-9.10646900	0.51817200	0.18531200
H	-8.34390100	-0.91571600	-0.50904500

TS54: OH + CH₃(CH₂)₁₂CH₃ → H₂O + CH₃(CH₂)₃CH(CH₂)₈CH₃

C	-8.02992700	0.08831200	0.15796700
H	-8.00267100	1.12988200	-0.17267700
H	-8.11307600	0.08844000	1.24806300
H	-8.93493400	-0.36871100	-0.24701400
C	-6.77423600	-0.65453300	-0.29110200
H	-6.82713800	-1.69986400	0.03294100
H	-6.72769200	-0.67201900	-1.38527700
C	-5.49583200	-0.02103500	0.25216200
H	-5.54135600	0.00377900	1.34813800
H	-5.43273200	1.02137000	-0.08100400
C	-4.23057400	-0.75509600	-0.18452500
H	-4.19520800	-0.80538700	-1.27892300
H	-4.26292200	-1.79307900	0.17339500
C	-2.95867900	-0.09755100	0.32325700
H	-2.98266700	0.01964300	1.41323100
H	-2.96492200	0.97322800	-0.09740700
C	-1.66116700	-0.74381500	-0.12982900
H	-1.66515400	-0.83274100	-1.22214300
H	-1.61693800	-1.76746900	0.26574900
C	-0.42192800	0.03005600	0.31350900
H	-0.42951400	0.13350700	1.40587800
H	-0.47530000	1.04454500	-0.09878000
C	0.88527100	-0.62636000	-0.12216500
H	0.88352200	-0.74539300	-1.21233000
H	0.94432300	-1.63775300	0.29821500
C	2.12036200	0.16793700	0.29574300
H	2.12230400	0.28962700	1.38589900
H	2.05830100	1.17839100	-0.12629700
C	3.43048900	-0.48158800	-0.14208800
H	3.42397500	-0.61095500	-1.23118600
H	3.49841600	-1.48898400	0.28650100
C	4.66342400	0.32325300	0.26215200
H	4.67174400	0.45196700	1.35142400
H	4.59276400	1.33092300	-0.16542700
C	5.97448000	-0.32102400	-0.18003800
H	5.96410900	-0.45491800	-1.26875600
H	6.05014500	-1.32672900	0.25166200
C	7.20702800	0.48968200	0.21467800
H	7.21742500	0.62175900	1.30211000
H	7.12872600	1.49369900	-0.21661600
C	8.50983500	-0.16483100	-0.23718300

H	8.52807900	-0.28459300	-1.32366700
H	9.37990700	0.42954300	0.04898200
H	8.62121000	-1.15762100	0.20697900
O	-2.94682200	2.40693100	-0.54806500
H	-2.64942600	2.78001900	0.29761400

OH-R55: OH + CH₃(CH₂)₁₂CH₃ → H₂O + CH₃(CH₂)₄CH(CH₂)₇CH₃
CH₃(CH₂)₄CH(CH₂)₇CH₃

C	-8.29126700	0.03148900	0.24047700
H	-8.44452500	0.77331800	-0.54780000
H	-8.32356900	0.55607800	1.19903000
H	-9.13067300	-0.66602300	0.21201400
C	-6.95612400	-0.68565000	0.05833600
H	-6.83025200	-1.43887000	0.84368500
H	-6.95570900	-1.22962000	-0.89250100
C	-5.76708300	0.27195500	0.08735600
H	-5.76754700	0.82005700	1.03760200
H	-5.89091000	1.02506300	-0.70071000
C	-4.42503600	-0.43168700	-0.09048300
H	-4.42648800	-0.98381900	-1.03778900
H	-4.29362900	-1.17737200	0.70192400
C	-3.23707400	0.52918200	-0.07456800
H	-3.23789700	1.09965800	0.86542700
H	-3.37857000	1.28567800	-0.86537200
C	-1.91909700	-0.14572800	-0.24623300
H	-1.89443600	-1.13902200	-0.68645000
C	-0.64532500	0.62198100	-0.14576900
H	-0.66990500	1.26093100	0.74816800
H	-0.56051200	1.32195200	-0.99496100
C	0.60146400	-0.26151300	-0.10930700
H	0.61258600	-0.90155800	-0.99955700
H	0.54045500	-0.93334000	0.75440700
C	1.89979100	0.53803600	-0.04584000
H	1.88775900	1.18191700	0.84206200
H	1.95374500	1.20932000	-0.91175000
C	3.14598100	-0.34332700	-0.01320100
H	3.15183400	-0.99416000	-0.89603500
H	3.09864600	-1.00764000	0.85821200
C	4.44589600	0.45633800	0.03148300
H	4.44195000	1.10651900	0.91482700
H	4.49089400	1.12149100	-0.83957800
C	5.69272000	-0.42404600	0.05828500
H	5.69321700	-1.07913500	-0.82161400

H	5.65297400	-1.08497800	0.93292500
C	6.99384900	0.37483100	0.09036500
H	6.99272800	1.02857700	0.96938100
H	7.03142400	1.03381900	-0.78395600
C	8.23089800	-0.51955000	0.11496400
H	8.26033100	-1.16508600	-0.76684900
H	9.15174600	0.06681700	0.13233600
H	8.22676500	-1.16443700	0.99772400

TS55: OH + CH₃(CH₂)₁₂CH₃ → H₂O + CH₃(CH₂)₄CH(CH₂)₇CH₃

C	-8.14252900	-0.36385100	-0.25279500
H	-8.26241800	-1.36961600	0.15872700
H	-8.14155500	-0.44973800	-1.34261600
H	-9.01702000	0.22267400	0.03608100
C	-6.84760500	0.27510500	0.24199500
H	-6.76119000	1.29190100	-0.15591200
H	-6.87650600	0.37214000	1.33287900
C	-5.60873700	-0.52318800	-0.15812100
H	-5.57928600	-0.61867300	-1.25048400
H	-5.69211100	-1.54307300	0.23767600
C	-4.30717900	0.10831700	0.32767700
H	-4.33020100	0.19209400	1.42134700
H	-4.22558700	1.12957000	-0.06158900
C	-3.06717800	-0.67734800	-0.09269800
H	-3.04561400	-0.77025600	-1.18461600
H	-3.12444000	-1.69963400	0.30508600
C	-1.77214800	-0.03738800	0.37747000
H	-1.77243800	0.10022400	1.46528600
H	-1.76255200	1.02574700	-0.06292200
C	-0.49726200	-0.71868700	-0.08868000
H	-0.51954700	-0.81524800	-1.18016000
H	-0.47188600	-1.74029500	0.31371100
C	0.76630700	0.02874400	0.33044900
H	0.78531900	0.12643100	1.42319200
H	0.72320600	1.04622400	-0.07554400
C	2.05064700	-0.64936300	-0.13877200
H	2.02434300	-0.75552500	-1.22998200
H	2.09768800	-1.66653100	0.26893300
C	3.30966200	0.11539600	0.26243100
H	3.34099700	0.21625100	1.35429500
H	3.25493000	1.13457000	-0.13907800
C	4.59700900	-0.54741000	-0.22087700
H	4.56269800	-0.65130900	-1.31226500

H	4.65635000	-1.56546300	0.18306900
C	5.85333900	0.22568000	0.17222900
H	5.89264700	0.32466900	1.26413300
H	5.78993400	1.24590300	-0.22596900
C	7.14267400	-0.42666200	-0.32092900
H	7.10175700	-0.52354500	-1.41136700
H	7.20591400	-1.44542300	0.07676600
C	8.38806000	0.36035300	0.07959600
H	8.46398800	0.44070400	1.16731600
H	9.30048300	-0.11492800	-0.28588800
H	8.35274200	1.37509600	-0.32560400
O	-1.71785700	2.45464600	-0.52470300
H	-1.41815200	2.82970400	0.31927800

**OH-R56: OH + CH₃(CH₂)₁₂CH₃ → H₂O + CH₃(CH₂)₅CH(CH₂)₆CH₃
CH₃(CH₂)₅CH(CH₂)₆CH₃**

C	-8.20377400	-0.66319800	0.24222200
H	-8.10985400	-1.44035900	1.00523100
H	-8.28000400	-1.15992100	-0.72857800
H	-9.13974100	-0.13009800	0.42027800
C	-7.00325500	0.27928100	0.27688100
H	-7.12874700	1.06521900	-0.47572800
H	-6.95936200	0.78588800	1.24707600
C	-5.68148100	-0.44455300	0.02956800
H	-5.72402600	-0.95259200	-0.94165300
H	-5.55440400	-1.23209100	0.78235900
C	-4.47089300	0.48490800	0.06102200
H	-4.42882200	0.99168300	1.03282800
H	-4.59925500	1.27274000	-0.69125500
C	-3.15151700	-0.24088500	-0.18755100
H	-3.19062700	-0.74348500	-1.16119100
H	-3.01866400	-1.02868000	0.56247000
C	-1.93935600	0.69004300	-0.15380900
H	-1.89472700	1.20102700	0.81783100
H	-2.08872300	1.49458000	-0.89443000
C	-0.64601500	-0.00580400	-0.40929100
H	-0.65505600	-0.91071700	-1.01114800
C	0.65719400	0.67963300	-0.17679600
H	0.63616400	1.18541200	0.79839900
H	0.79685800	1.48735100	-0.91582100
C	1.86183900	-0.25941200	-0.24058100
H	1.87821400	-0.75562300	-1.21815200
H	1.73815300	-1.05131800	0.50668700

C	3.19088000	0.45551600	-0.01321700
H	3.17192900	0.95490700	0.96310300
H	3.30953400	1.24830800	-0.76182400
C	4.39429500	-0.48200900	-0.07634100
H	4.41354300	-0.98129000	-1.05268600
H	4.27558900	-1.27490100	0.67198500
C	5.72449200	0.23163000	0.15146700
H	5.70659000	0.73009900	1.12841100
H	5.84336000	1.02570900	-0.59588200
C	6.92936000	-0.70442200	0.08662100
H	6.94612700	-1.20117700	-0.88950300
H	6.80946900	-1.49665900	0.83349900
C	8.25133400	0.02389100	0.31635600
H	8.26434200	0.50518000	1.29778000
H	9.10153100	-0.65922700	0.26682900
H	8.40199500	0.80231300	-0.43621700

TS56: OH + CH₃(CH₂)₁₂CH₃ → H₂O + CH₃(CH₂)₅CH(CH₂)₆CH₃

C	-8.20398000	0.25352400	0.09023200
H	-8.16838500	1.27116600	-0.30754000
H	-8.28507700	0.32577400	1.17815200
H	-9.11394400	-0.22045100	-0.28291800
C	-6.95564600	-0.52865700	-0.31048500
H	-7.01877800	-1.55032600	0.07968100
H	-6.90974600	-0.61742600	-1.40138400
C	-5.66965900	0.12267800	0.19263000
H	-5.71350700	0.21362200	1.28512100
H	-5.60635900	1.14555100	-0.19850200
C	-4.41038600	-0.64500900	-0.20144000
H	-4.37267300	-0.74222700	-1.29318900
H	-4.46751400	-1.66527100	0.19722700
C	-3.12741600	0.02157500	0.28767200
H	-3.16061800	0.11526800	1.38046100
H	-3.07080400	1.04014900	-0.11385700
C	-1.86419800	-0.73462300	-0.11672800
H	-1.82768500	-0.82771200	-1.20816400
H	-1.90355200	-1.75730800	0.28182800
C	-0.59049500	-0.06511300	0.36918900
H	-0.60419500	0.06953100	1.45729800
H	-0.58549100	0.99916700	-0.06831200
C	0.70614700	-0.71360000	-0.08477700
H	0.69801000	-0.80540000	-1.17695700
H	0.75160500	-1.73652800	0.31281900

C	1.94519700	0.06443100	0.35211200
H	1.95495800	0.14700000	1.44603700
H	1.87366000	1.08652600	-0.03689100
C	3.24986900	-0.57267300	-0.11832400
H	3.23082100	-0.67031200	-1.21055600
H	3.32548200	-1.59164300	0.28090200
C	4.48510800	0.22486900	0.29326300
H	4.50564400	0.32505500	1.38543300
H	4.40575200	1.24272800	-0.10728000
C	5.79293800	-0.40315000	-0.18067300
H	5.76868700	-0.51235200	-1.27195600
H	5.87904400	-1.41788400	0.22732100
C	7.02671400	0.40485600	0.21581100
H	7.04978400	0.51480300	1.30556100
H	6.93879200	1.41696000	-0.19403100
C	8.32680900	-0.23424800	-0.26507300
H	8.33201400	-0.33249300	-1.35385900
H	9.19763700	0.35863600	0.02194100
H	8.44816700	-1.23496800	0.15817200
O	-0.61273500	2.42937800	-0.52833200
H	-0.91585600	2.80617000	0.31366300

3.1.15 C15 (*n*-C₁₅H₃₂)



n-C₁₅H₃₂

C	8.91111800	-0.41275300	-0.00008400
H	8.94047500	-1.05745500	-0.88251700
H	8.94055700	-1.05745600	0.88234700
H	9.81639700	0.19765100	-0.00012600
C	7.65028300	0.44830100	-0.00002500
H	7.65106700	1.10480800	0.87691800
H	7.65099500	1.10482000	-0.87695800
C	6.37108300	-0.38587200	0.00002000
H	6.36939700	-1.04418100	-0.87747900
H	6.36945500	-1.04417900	0.87752000
C	5.09956900	0.45905200	0.00005900
H	5.10158600	1.11695500	-0.87756400
H	5.10162000	1.11693000	0.87770100
C	3.82269400	-0.37815300	0.00006800
H	3.82123900	-1.03614400	0.87760900
H	3.82123300	-1.03614900	-0.87746900
C	2.54975500	0.46495600	0.00006800
H	2.55075700	1.12285600	-0.87754100

H	2.55073800	1.12283300	0.87769300
C	1.27423900	-0.37425100	0.00004100
H	1.27372800	-1.03223700	0.87759700
H	1.27376800	-1.03223900	-0.87751500
C	0.00000000	0.46689000	0.00000900
H	0.00002400	1.12477700	-0.87761100
H	-0.00002100	1.12477400	0.87763200
C	-1.27424000	-0.37424700	-0.00002500
H	-1.27377300	-1.03223600	0.87753100
H	-1.27372900	-1.03223400	-0.87758100
C	-2.54975400	0.46496200	-0.00005500
H	-2.55073300	1.12284000	-0.87767900
H	-2.55075900	1.12286000	0.87755400
C	-3.82269400	-0.37814600	-0.00006200
H	-3.82123900	-1.03614000	0.87747700
H	-3.82123400	-1.03614000	-0.87760100
C	-5.09956900	0.45905800	-0.00006300
H	-5.10161600	1.11693200	-0.87770800
H	-5.10159300	1.11696500	0.87755700
C	-6.37108200	-0.38586900	-0.00002800
H	-6.36939900	-1.04417500	0.87747300
H	-6.36944700	-1.04418000	-0.87752600
C	-7.65028400	0.44829900	0.00000700
H	-7.65106900	1.10479800	-0.87694100
H	-7.65100100	1.10482500	0.87693500
C	-8.91111600	-0.41276000	0.00007100
H	-8.94047200	-1.05745600	0.88250900
H	-9.81639800	0.19764000	0.00010700
H	-8.94055200	-1.05746900	-0.88235500

CH₂(CH₂)₁₃CH₃

C	8.96388900	-0.39119600	-0.02667900
H	8.98286800	-1.35642200	0.46460300
H	9.90209500	0.01428700	-0.38081900
C	7.72394600	0.43263200	-0.01004700
H	7.70881600	1.07758100	0.88405200
H	7.72060800	1.12033500	-0.86361800
C	6.44434700	-0.40711800	-0.02203000
H	6.44051800	-1.04083900	-0.91591000
H	6.45352400	-1.08559500	0.83931500
C	5.17485500	0.43934000	0.01084300
H	5.17146900	1.12053500	-0.84881700
H	5.18311300	1.07320700	0.90599500

C	3.89760200	-0.39701300	-0.00428200
H	3.89816500	-1.07487400	0.85793200
H	3.89293200	-1.03447600	-0.89673600
C	2.62595100	0.44772400	0.01865800
H	2.62574100	1.12500500	-0.84405600
H	2.63015100	1.08584400	0.91073900
C	1.34906200	-0.38920700	0.00272000
H	1.34786800	-1.06476500	0.86678500
H	1.34678100	-1.02926100	-0.88798700
C	0.07670200	0.45456900	0.02043000
H	0.07830500	1.13034200	-0.84347900
H	0.07815500	1.09433100	0.91135500
C	-1.19963900	-0.38316100	0.00270200
H	-1.20196600	-1.05808400	0.86727400
H	-1.19986600	-1.02393200	-0.88750700
C	-2.47270200	0.45962200	0.01745600
H	-2.46998100	1.13502300	-0.84674400
H	-2.47345700	1.09979400	0.90808900
C	-3.74828600	-0.37921500	-0.00232600
H	-3.75132000	-1.05424300	0.86215500
H	-3.74663300	-1.01992400	-0.89257200
C	-5.02229200	0.46224300	0.01062800
H	-5.01895500	1.13795100	-0.85335000
H	-5.02514500	1.10210700	0.90149800
C	-6.29678500	-0.37785300	-0.01147300
H	-6.30090900	-1.05395100	0.85237100
H	-6.29409100	-1.01812200	-0.90222800
C	-7.57289600	0.46094800	0.00062300
H	-7.56695900	1.13629400	-0.86185500
H	-7.57549600	1.09835900	0.89155300
C	-8.83690500	-0.39502800	-0.02458900
H	-8.87367500	-1.05848500	0.84351100
H	-9.73988400	0.21872300	-0.01646900
H	-8.86386900	-1.02046900	-0.92087500

TS57: OH + CH₃(CH₂)₁₃CH₃ → H₂O + CH₂(CH₂)₁₃CH₃

C	-8.13838600	0.71769900	-0.00422500
H	-8.18486200	1.39625100	-0.85879400
H	-8.24834300	1.27885800	0.92570100
H	-9.10645000	0.07380900	-0.10969300
C	-6.91382300	-0.17614600	-0.02480200
H	-6.93463300	-0.85889700	0.83204600
H	-6.92952400	-0.80022200	-0.92390000

C	-5.61203900	0.62883800	0.01060400
H	-5.58590200	1.30725600	-0.85021200
H	-5.60111100	1.26314000	0.90490300
C	-4.36615900	-0.25399900	-0.00189000
H	-4.38496000	-0.89484800	-0.89153400
H	-4.38894500	-0.92681800	0.86387300
C	-3.06738700	0.54860500	0.01549600
H	-3.05072400	1.19208500	0.90351400
H	-3.04586000	1.21998500	-0.85144500
C	-1.81809900	-0.32910300	0.00441000
H	-1.83666200	-0.97542900	-0.88149500
H	-1.83631800	-0.99762600	0.87370800
C	-0.52096700	0.47621500	0.01400200
H	-0.50307600	1.12330300	0.89944100
H	-0.50385500	1.14449100	-0.85553500
C	0.73074600	-0.39793400	0.00250600
H	0.71252900	-1.04609300	-0.88211800
H	0.71553600	-1.06493100	0.87306700
C	2.02600400	0.41042000	0.00879500
H	2.04349700	1.05902900	0.89314400
H	2.04038100	1.07736900	-0.86183200
C	3.27992300	-0.46057900	-0.00274300
H	3.26302000	-1.10930800	-0.88698800
H	3.26657200	-1.12715800	0.86817800
C	4.57324700	0.35087700	0.00289500
H	4.58919700	1.00007800	0.88683200
H	4.58607900	1.01735500	-0.86811400
C	5.82937300	-0.51701900	-0.00794800
H	5.81471100	-1.16564100	-0.89233600
H	5.81697900	-1.18380600	0.86285200
C	7.12066600	0.29732300	-0.00104400
H	7.13515200	0.94664900	0.88301800
H	7.13355900	0.96433100	-0.87184900
C	8.37985900	-0.56665200	-0.01090600
H	8.36534600	-1.21341300	-0.89494500
H	8.36570200	-1.23248900	0.85884200
C	9.66033400	0.26485900	-0.00192500
H	9.70425900	0.89935300	0.88729900
H	10.55136100	-0.36610100	-0.00832000
H	9.70476300	0.91809300	-0.87741700
O	-10.11034000	-0.93189600	-0.08119300
H	-9.76444300	-1.42389100	0.68030100



C	-9.00831600	-0.25963100	-0.13353500
H	-9.28439700	-0.84582000	0.75592200
H	-8.99108400	-0.96306600	-0.97312400
H	-9.80891400	0.46060900	-0.30846600
C	-7.68635400	0.40616500	0.03482800
H	-7.64987200	1.43103900	0.38877300
C	-6.43248400	-0.39984900	0.06247000
H	-6.40871400	-1.02988000	0.96847100
H	-6.43578600	-1.10914000	-0.77727600
C	-5.15931400	0.44425000	0.01434800
H	-5.15746500	1.13885500	0.86270800
H	-5.17245200	1.06109200	-0.89139400
C	-3.88412200	-0.39374400	0.04315300
H	-3.88697200	-1.08732000	-0.80654600
H	-3.87777100	-1.01484600	0.94723200
C	-2.61188700	0.44923800	0.00113400
H	-2.60723300	1.14025200	0.85285000
H	-2.61982100	1.07303300	-0.90092300
C	-1.33548100	-0.38824400	0.02428100
H	-1.33877600	-1.07708100	-0.82922000
H	-1.32927200	-1.01447400	0.92475400
C	-0.06288200	0.45449500	-0.01281300
H	-0.05960900	1.14298100	0.84098100
H	-0.06890900	1.08109500	-0.91300800
C	1.21333300	-0.38327100	0.01038000
H	1.21118000	-1.07043300	-0.84448600
H	1.21795200	-1.01133800	0.90958600
C	2.48634800	0.45902400	-0.02288900
H	2.48787000	1.14669200	0.83157400
H	2.48272700	1.08650700	-0.92249100
C	3.76210100	-0.37938000	0.00265900
H	3.76162100	-1.06597800	-0.85265200
H	3.76429100	-1.00808800	0.90141700
C	5.03580900	0.46208500	-0.02692800
H	5.03531700	1.14982900	0.82749600
H	5.03527700	1.08948900	-0.92661000
C	6.31072600	-0.37711900	0.00257400
H	6.31286200	-1.06451900	-0.85229600
H	6.31074700	-1.00565700	0.90164300
C	7.58632300	0.46211900	-0.02392200

H	7.58167800	1.14932900	0.82912000
H	7.58675300	1.08721700	-0.92353100
C	8.85095300	-0.39256600	0.01079500
H	8.88738100	-1.06721600	-0.84861500
H	9.75346500	0.22168900	-0.00619500
H	8.87941000	-1.00629300	0.91509300

TS58: OH + CH₃(CH₂)₁₃CH₃ → H₂O + CH₃CH(CH₂)₁₂CH₃

C	8.39729600	-0.80076500	-0.14899500
H	8.40718000	-0.87668200	-1.23860800
H	8.46060300	-1.81484200	0.25847700
H	9.28936000	-0.25498800	0.16198700
C	7.12962700	-0.11624800	0.33090800
H	7.13850400	0.02767200	1.41640700
H	7.13737000	0.94612600	-0.11426600
C	5.83941200	-0.78044800	-0.11817800
H	5.85051400	-0.88818600	-1.20885400
H	5.80502500	-1.79821100	0.29386600
C	4.58851100	-0.01569000	0.30664000
H	4.62303500	0.98819600	-0.13265900
H	4.59545200	0.11560600	1.39610300
C	3.29147200	-0.70460400	-0.10939900
H	3.25435600	-1.70887100	0.33000500
H	3.28957400	-0.84378300	-1.19711300
C	2.04404700	0.07360900	0.30195400
H	2.08482200	1.07805900	-0.13674400
H	2.04567800	0.21299100	1.38997200
C	0.74358600	-0.60688100	-0.11749500
H	0.69865400	-1.60991300	0.32412500
H	0.74425500	-0.74963000	-1.20491400
C	-0.50108700	0.17943300	0.28699700
H	-0.45189800	1.18363600	-0.15157200
H	-0.50388500	0.31958800	1.37485200
C	-1.80385500	-0.49276500	-0.13860100
H	-1.85699700	-1.49564300	0.30250000
H	-1.79924300	-0.63544600	-1.22606900
C	-3.04571900	0.30082500	0.26040500
H	-2.98828400	1.30514600	-0.17694700
H	-3.05293100	0.44008400	1.34834400
C	-4.35034400	-0.36322300	-0.17216400
H	-4.41117000	-1.36641600	0.26724200
H	-4.34160200	-0.50452600	-1.25979700
C	-5.58988600	0.43640300	0.22218500

H	-5.52557000	1.44085000	-0.21397500
H	-5.60112200	0.57466500	1.31023300
C	-6.89563000	-0.22090300	-0.21653400
H	-6.96368600	-1.22440600	0.22151700
H	-6.88375200	-0.36166600	-1.30437900
C	-8.13460700	0.58268600	0.17260000
H	-8.06325300	1.58505200	-0.26376100
H	-8.14703100	0.72034800	1.25930400
C	-9.43217900	-0.08365100	-0.27702900
H	-9.53652100	-1.07517100	0.17164300
H	-10.30681100	0.50559500	0.00586300
H	-9.44883700	-0.20859900	-1.36295300
O	7.02382800	2.36880400	-0.54895500
H	6.58372800	2.69626400	0.25205100

**OH-R59: OH + CH₃(CH₂)₁₃CH₃ → H₂O + CH₃CH₂CH(CH₂)₁₁CH₃
CH₃CH₂CH(CH₂)₁₁CH₃**

C	8.88695400	-0.62986500	0.15800800
H	8.96027500	-1.17120900	-0.78847400
H	8.73167500	-1.36424100	0.95168200
H	9.84231000	-0.13303300	0.33593200
C	7.73411900	0.37125500	0.11699700
H	7.69810300	0.94000200	1.05577400
H	7.93166200	1.12338900	-0.66418100
C	6.40854600	-0.26808300	-0.12299800
H	6.38000000	-1.25689500	-0.57336300
C	5.15178000	0.53226500	-0.08018500
H	5.11161800	1.21713300	-0.94476800
H	5.16313300	1.18674000	0.80245900
C	3.88303200	-0.32051500	-0.06876800
H	3.90460100	-0.98334800	0.80366200
H	3.88006600	-0.97029800	-0.95198400
C	2.60337200	0.51091400	-0.04790100
H	2.58730300	1.17371800	-0.92175600
H	2.60875600	1.16373500	0.83351100
C	1.33591200	-0.34022900	-0.03718500
H	1.35055000	-1.00139900	0.83775100
H	1.33195400	-0.99469000	-0.91734100
C	0.05472200	0.49012500	-0.02063400
H	0.04099100	1.15194100	-0.89520100
H	0.05783200	1.14404200	0.85993200
C	-1.21269000	-0.36118400	-0.01246200
H	-1.19993800	-1.02198300	0.86286200

H	-1.21448900	-1.01619900	-0.89223500
C	-2.49432700	0.46852600	0.00073200
H	-2.50641800	1.12991100	-0.87418300
H	-2.49355000	1.12291500	0.88096200
C	-3.76128000	-0.38349900	0.00646700
H	-3.74987200	-1.04417400	0.88190900
H	-3.76096100	-1.03869800	-0.87316500
C	-5.04364500	0.44520200	0.01704000
H	-5.05479800	1.10626100	-0.85815000
H	-5.04494300	1.09991000	0.89705600
C	-6.30973700	-0.40778900	0.02096200
H	-6.29985200	-1.06853600	0.89657200
H	-6.30825400	-1.06357600	-0.85842700
C	-7.59400900	0.41851300	0.02938900
H	-7.60257200	1.07762400	-0.84556100
H	-7.59475100	1.07241700	0.90828500
C	-8.84964600	-0.45007400	0.03239600
H	-8.87191100	-1.09690200	0.91347200
H	-9.75848200	0.15499600	0.03721800
H	-8.87864800	-1.09293400	-0.85139700

TS59: OH + CH₃(CH₂)₁₃CH₃ → H₂O + CH₃CH₂CH(CH₂)₁₁CH₃

C	8.46191700	-0.03129200	0.27797300
H	8.52172300	0.00043700	1.36919300
H	8.43122300	0.99795500	-0.08723900
H	9.37437900	-0.50025700	-0.09450800
C	7.21747300	-0.78999800	-0.17534000
H	7.19468300	-0.85181400	-1.26808100
H	7.24913300	-1.82235300	0.19459100
C	5.93347100	-0.13711100	0.30876300
H	5.94357900	-0.00984700	1.39792000
H	5.94093500	0.93035200	-0.12024700
C	4.64685100	-0.79717100	-0.15437900
H	4.60683400	-1.81810600	0.24863700
H	4.66354800	-0.89449500	-1.24586400
C	3.39582900	-0.03166100	0.27012200
H	3.43893400	0.97763800	-0.15610000
H	3.39578000	0.08702700	1.36097600
C	2.09918500	-0.71057000	-0.16268800
H	2.05660900	-1.72030600	0.26359000
H	2.10303000	-0.83601500	-1.25209700
C	0.85129000	0.06527700	0.25169300
H	0.89448400	1.07385600	-0.17713200

H	0.84935200	0.19413000	1.34101600
C	-0.44805800	-0.61064700	-0.17837200
H	-0.49419200	-1.61778400	0.25370600
H	-0.44412500	-0.74337600	-1.26706800
C	-1.69437000	0.17110200	0.22984800
H	-1.64683900	1.17816400	-0.20225100
H	-1.69840400	0.30423700	1.31859000
C	-2.99515500	-0.50167300	-0.20087000
H	-3.04515500	-1.50766200	0.23347100
H	-2.98991200	-0.63716000	-1.28926100
C	-4.23986400	0.28469600	0.20346700
H	-4.18826600	1.29103800	-0.22986400
H	-4.24571200	0.41942100	1.29198400
C	-5.54192000	-0.38460000	-0.22891800
H	-5.59498900	-1.39050500	0.20531900
H	-5.53576400	-0.52012200	-1.31732900
C	-6.78523400	0.40440200	0.17392600
H	-6.73170000	1.41112400	-0.25871200
H	-6.79306100	0.53899500	1.26260600
C	-8.08909200	-0.26111100	-0.25988500
H	-8.14149700	-1.26621600	0.17269400
H	-8.08042000	-0.39405100	-1.34719500
C	-9.32183100	0.54041000	0.15097400
H	-9.30010800	1.54010200	-0.29097500
H	-10.24483300	0.05243200	-0.16838200
H	-9.36353000	0.65961100	1.23690600
O	5.92368500	2.36051600	-0.58109800
H	5.54183500	2.72909600	0.23200000

**OH-R60: OH + CH₃(CH₂)₁₃CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₁₀CH₃
CH₃(CH₂)₂CH(CH₂)₁₀CH₃**

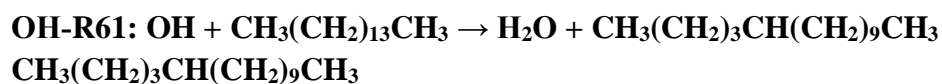
C	8.94639800	-0.05340200	0.34938100
H	9.20045700	-0.67923200	-0.51031200
H	8.93582100	-0.69441800	1.23494700
H	9.74445900	0.68050800	0.47712000
C	7.59224000	0.62105300	0.15061000
H	7.36504300	1.26485200	1.00615700
H	7.62753300	1.27318100	-0.72848900
C	6.45474900	-0.38605100	-0.02548600
H	6.69662500	-1.04757700	-0.87540000
H	6.41294400	-1.04887300	0.84999600
C	5.12383100	0.25184600	-0.23308600
H	5.08924500	1.24024100	-0.68436200

C	3.86404300	-0.54272000	-0.17007400
H	3.88099900	-1.18893100	0.71847200
H	3.80982300	-1.23528400	-1.02772300
C	2.60192900	0.31978400	-0.15248000
H	2.59261700	0.95862700	-1.04360700
H	2.64136100	0.99354400	0.71097300
C	1.31455000	-0.49824200	-0.10349900
H	1.32454900	-1.13946300	0.78633200
H	1.27942300	-1.17210600	-0.96829500
C	0.05756400	0.36829100	-0.08703900
H	0.04990900	1.01110500	-0.97572500
H	0.09265300	1.04101100	0.77849200
C	-1.23426800	-0.44413600	-0.04165900
H	-1.22827900	-1.08608800	0.84764500
H	-1.26919800	-1.11743900	-0.90682000
C	-2.48909200	0.42562100	-0.02798200
H	-2.49323500	1.06889100	-0.91637400
H	-2.45481900	1.09788900	0.83800300
C	-3.78251400	-0.38448200	0.01379300
H	-3.77972500	-1.02667100	0.90295000
H	-3.81600600	-1.05769200	-0.85149100
C	-5.03673400	0.48625000	0.02424800
H	-5.03889800	1.12888700	-0.86462500
H	-5.00397400	1.15906500	0.88989300
C	-6.33016600	-0.32360900	0.06415600
H	-6.32969900	-0.96516900	0.95397300
H	-6.36258100	-0.99811900	-0.80035500
C	-7.58603100	0.54527200	0.07134400
H	-7.58594300	1.18411100	-0.81855200
H	-7.55227700	1.21888100	0.93456300
C	-8.86952300	-0.28045900	0.11297700
H	-8.89962900	-0.90547500	1.00945900
H	-9.75786100	0.35431700	0.11649200
H	-8.93318200	-0.94265300	-0.75455700

TS60: OH + CH₃(CH₂)₁₃CH₃ → H₂O + CH₃(CH₂)₂CH(CH₂)₁₀CH₃

C	-8.56746800	-0.56700200	-0.25373000
H	-8.67760700	-1.58047600	0.14137500
H	-8.55732300	-0.63474800	-1.34467600
H	-9.45135500	0.00394400	0.03719300
C	-7.28643500	0.08420900	0.26005900
H	-7.20413000	1.10576800	-0.12439000
H	-7.32358800	0.16279100	1.35235200

C	-6.03444000	-0.69155000	-0.14393000
H	-6.09239800	-1.71564800	0.24950500
H	-5.99677300	-0.78112600	-1.23587200
C	-4.75044400	-0.04597500	0.34777000
H	-4.77091600	0.09430000	1.43507900
H	-4.73726300	1.01624200	-0.09480800
C	-3.46518600	-0.72484100	-0.09272100
H	-3.46867300	-0.82923900	-1.18365600
H	-3.44271100	-1.74350700	0.31725600
C	-2.21167700	0.03018600	0.34271000
H	-2.21640300	0.14330700	1.43412100
H	-2.24683500	1.04186200	-0.07834600
C	-0.91671800	-0.65311000	-0.08832800
H	-0.91916700	-0.77600600	-1.17805100
H	-0.87765400	-1.66388400	0.33579400
C	0.33233700	0.11946300	0.32867800
H	0.33786900	0.23982700	1.41896100
H	0.28666500	1.13135600	-0.09200800
C	1.63112600	-0.55056800	-0.11208900
H	1.62122400	-0.67697200	-1.20152000
H	1.68339100	-1.55996900	0.31392500
C	2.87678300	0.23411700	0.29257400
H	2.89051600	0.35645500	1.38251400
H	2.81869600	1.24514400	-0.12889000
C	4.17770100	-0.42505600	-0.15817900
H	4.16071700	-0.55202800	-1.24749600
H	4.24133900	-1.43391800	0.26758500
C	5.42042300	0.36916900	0.23705700
H	5.44041200	0.49288900	1.32675900
H	5.35258800	1.37931000	-0.18515900
C	6.72264900	-0.28181800	-0.22107000
H	6.70143600	-0.40905000	-1.31046000
H	6.79509200	-1.29060600	0.20390900
C	7.96441100	0.51786700	0.16724500
H	7.98595500	0.64249000	1.25540700
H	7.88876600	1.52531200	-0.25647300
C	9.25853800	-0.14203700	-0.30139300
H	9.26587100	-0.25434400	-1.38880100
H	10.13510600	0.44469600	-0.01926900
H	9.36753100	-1.13856900	0.13487800
O	-4.68981500	2.44473900	-0.55625200
H	-4.38146100	2.81815900	0.28535900



C	-8.81801300	-0.79944700	0.30997100
H	-8.64588000	-1.55697800	1.07897700
H	-8.90551600	-1.31557200	-0.64967400
H	-9.77552800	-0.31924600	0.52073800
C	-7.67537200	0.21252500	0.27972500
H	-7.87949800	0.97769100	-0.47716000
H	-7.62039600	0.73593400	1.24043400
C	-6.32596600	-0.43735400	-0.01502300
H	-6.11607100	-1.20423400	0.73927800
H	-6.37663200	-0.95742600	-0.97908700
C	-5.17068000	0.56336700	-0.04545000
H	-5.11538400	1.09076300	0.91670400
H	-5.39897900	1.34596700	-0.78948500
C	-3.85054400	-0.06012600	-0.34684700
H	-3.83120200	-0.96285300	-0.95179600
C	-2.57863900	0.69366200	-0.15592000
H	-2.59561400	1.19916800	0.81944300
H	-2.50437000	1.50622100	-0.89905400
C	-1.32919200	-0.18148200	-0.25723500
H	-1.31584300	-0.67550600	-1.23594800
H	-1.38997100	-0.97925000	0.49156900
C	-0.03274200	0.60087300	-0.06690400
H	-0.04896000	1.09753300	0.91086500
H	0.02331700	1.39949000	-0.81663300
C	1.21468700	-0.27374300	-0.16718900
H	1.23184300	-0.76924300	-1.14547400
H	1.15737100	-1.07329700	0.58125300
C	2.51295000	0.50616200	0.02613400
H	2.49609200	1.00100300	1.00477000
H	2.57011300	1.30626000	-0.72183900
C	3.75997800	-0.36898100	-0.07512900
H	3.77664900	-0.86386200	-1.05374600
H	3.70264400	-1.16914000	0.67273800
C	5.05882500	0.41002900	0.11815900
H	5.04252100	0.90471200	1.09691000
H	5.11620500	1.21030400	-0.62963600
C	6.30540100	-0.46538500	0.01637400
H	6.32213500	-0.96092200	-0.96209200
H	6.24918700	-1.26565500	0.76445000
C	7.60557400	0.31226700	0.20839900

H	7.58762900	0.80657200	1.18575000
H	7.66061700	1.11053200	-0.53967100
C	8.84217300	-0.57701700	0.10404100
H	8.89147600	-1.06050300	-0.87515100
H	9.76216900	-0.00568900	0.24239500
H	8.81923800	-1.36485700	0.86152100

TS61: OH + CH₃(CH₂)₁₃CH₃ → H₂O + CH₃(CH₂)₃CH(CH₂)₉CH₃

C	-8.63056000	0.18922700	0.16771700
H	-8.58501200	1.21698000	-0.20164500
H	-8.70856700	0.23155300	1.25741400
H	-9.54591100	-0.26525000	-0.21639400
C	-7.39104700	-0.59354000	-0.25824300
H	-7.46273000	-1.62509200	0.10390300
H	-7.34930700	-0.65170400	-1.35126800
C	-6.09881000	0.03466400	0.25759200
H	-6.01975800	1.06473700	-0.10868800
H	-6.13738800	0.09499100	1.35250300
C	-4.84877200	-0.73446200	-0.16266100
H	-4.81683100	-0.81259800	-1.25553700
H	-4.90068300	-1.76242200	0.22102300
C	-3.56335100	-0.08978200	0.32707000
H	-3.57937100	0.04550800	1.41506400
H	-3.55335600	0.97423000	-0.11092600
C	-2.27905500	-0.76460700	-0.12224200
H	-2.28813900	-0.86586700	-1.21345600
H	-2.25195100	-1.78435100	0.28476800
C	-1.02502200	-0.00773900	0.30853000
H	-1.02436700	0.10284000	1.40021100
H	-1.06488700	1.00482300	-0.10994900
C	0.26925200	-0.68697900	-0.13080000
H	0.26067900	-0.80925200	-1.22057000
H	0.31384200	-1.69788400	0.29249200
C	1.51861100	0.08886800	0.27921300
H	1.52915000	0.21032300	1.36935000
H	1.46865600	1.10022500	-0.14225400
C	2.81661900	-0.57908400	-0.16692500
H	2.80264600	-0.70558600	-1.25630400
H	2.87197400	-1.58839600	0.25893200
C	4.06286100	0.20706400	0.23309800
H	4.07973100	0.33039700	1.32288200
H	4.00289900	1.21764900	-0.18911700
C	5.36286400	-0.45196900	-0.22059300

H	5.34418100	-0.57778000	-1.31004500
H	5.42660300	-1.46134200	0.20402100
C	6.60655100	0.34069100	0.17388000
H	6.62881700	0.46318900	1.26382200
H	6.54005100	1.35175900	-0.24665300
C	7.90871200	-0.31035600	-0.28608600
H	7.88526700	-0.43088000	-1.37464900
H	7.97475600	-1.31987800	0.13415400
C	9.14121500	0.49589400	0.11617800
H	9.19915600	0.60099700	1.20286400
H	10.06312200	0.02026500	-0.22428100
H	9.10405300	1.50114800	-0.31194000
O	-3.51210600	2.40249500	-0.57519400
H	-3.21088200	2.77936200	0.26744900

**OH-R62: OH + CH₃(CH₂)₁₃CH₃ → H₂O + CH₃(CH₂)₄CH(CH₂)₈CH₃
CH₃(CH₂)₄CH(CH₂)₈CH₃**

C	8.89766600	0.00126500	0.45692500
H	9.11767900	-0.70101500	-0.35140000
H	8.87827100	-0.56514500	1.39169300
H	9.72190300	0.71485600	0.51448900
C	7.56208000	0.70157100	0.21896600
H	7.37235400	1.41890700	1.02465300
H	7.61035900	1.28409800	-0.70740700
C	6.39311700	-0.27743000	0.13477100
H	6.58205000	-0.99735800	-0.67105600
H	6.34352500	-0.86094600	1.06232500
C	5.05103100	0.40870900	-0.10344000
H	5.09752500	0.98565600	-1.03465200
H	4.85977600	1.13036300	0.69870600
C	3.88115500	-0.57286800	-0.18057300
H	3.82843400	-1.15601200	0.74884000
H	4.09063700	-1.31221700	-0.97278400
C	2.56692200	0.08539000	-0.42910000
H	2.55253100	1.01298900	-0.99534400
C	1.28580300	-0.65462900	-0.24595000
H	1.30838100	-1.19341700	0.71138800
H	1.18866300	-1.44035000	-1.01487600
C	0.04882800	0.24205900	-0.29939100
H	0.02700900	0.76625500	-1.26212800
H	0.13412900	1.01526900	0.47245100
C	-1.25610900	-0.52656800	-0.11105600
H	-1.23179300	-1.05170700	0.85155100

H	-1.33574100	-1.30218300	-0.88249900
C	-2.49202700	0.36817300	-0.16572700
H	-2.51909800	0.89001200	-1.12999100
H	-2.41006400	1.14641400	0.60263300
C	-3.79780900	-0.39848400	0.03007500
H	-3.77130100	-0.91832300	0.99544300
H	-3.87883900	-1.17845800	-0.73671100
C	-5.03413800	0.49563900	-0.02739300
H	-5.06195100	1.01368100	-0.99372000
H	-4.95203600	1.27708500	0.73779700
C	-6.33965300	-0.27016700	0.17200800
H	-6.31336300	-0.78706800	1.13914600
H	-6.42201500	-1.05300900	-0.59193700
C	-7.57719100	0.62264400	0.11254200
H	-7.60286900	1.13694900	-0.85425900
H	-7.49318000	1.40438400	0.87523000
C	-8.87389900	-0.15725000	0.31534100
H	-8.87892400	-0.65659800	1.28778000
H	-9.74795800	0.49532000	0.26923500
H	-8.98875200	-0.92674700	-0.45257900

TS62: OH + CH₃(CH₂)₁₃CH₃ → H₂O + CH₃(CH₂)₄CH(CH₂)₈CH₃

C	-8.73460700	-0.40409200	-0.29559800
H	-8.84968500	-1.40298300	0.13363500
H	-8.72842700	-0.50980700	-1.38361400
H	-9.61402400	0.18180900	-0.02089600
C	-7.44612400	0.25236800	0.19286200
H	-7.36350400	1.26123000	-0.22588500
H	-7.48162000	0.37194700	1.28133500
C	-6.20043700	-0.54694100	-0.18328300
H	-6.27858400	-1.55738400	0.23673700
H	-6.16506700	-0.66850500	-1.27278200
C	-4.90509300	0.10416500	0.29307000
H	-4.93666500	0.21955700	1.38386300
H	-4.82850900	1.11357600	-0.12797500
C	-3.65670700	-0.68446100	-0.09556400
H	-3.61850700	-0.79452800	-1.18534700
H	-3.71955300	-1.70008000	0.31789500
C	-2.37080300	-0.03546000	0.38570800
H	-2.38488900	0.11307100	1.47200300
H	-2.34162900	1.02289300	-0.06500500
C	-1.08630500	-0.71611100	-0.05579500
H	-1.09134700	-0.81814800	-1.14707700

H	-1.06465500	-1.73590000	0.35165000
C	0.16647700	0.04023100	0.37981600
H	0.17481900	0.12926200	1.47323600
H	0.11538100	1.06121100	-0.01533800
C	1.46041500	-0.62363700	-0.08318300
H	1.44278800	-0.72663300	-1.17494000
H	1.51633800	-1.64168200	0.32159100
C	2.70824100	0.15416000	0.32799600
H	2.72858400	0.25753300	1.41985100
H	2.64616800	1.17195700	-0.07572900
C	4.00682800	-0.49602600	-0.14201000
H	3.98095600	-0.60918700	-1.23269100
H	4.07698900	-1.50994300	0.27058400
C	5.25047400	0.29717800	0.25242900
H	5.27786200	0.41039200	1.34315200
H	5.17706000	1.31111300	-0.15952600
C	6.55113000	-0.34586800	-0.22109700
H	6.52138000	-0.46544600	-1.31118000
H	6.63065900	-1.35734200	0.19617700
C	7.79316200	0.45564400	0.16259800
H	7.82230200	0.57432600	1.25127700
H	7.71115900	1.46512400	-0.25500000
C	9.08595400	-0.19742000	-0.31916500
H	9.08569000	-0.30373000	-1.40720500
H	9.96270400	0.39055300	-0.04016200
H	9.20119500	-1.19596500	0.11086600
O	-2.33779100	2.44730700	-0.54347400
H	-2.63866700	2.84087700	0.29157700

**OH-R63: OH + CH₃(CH₂)₁₃CH₃ → H₂O + CH₃(CH₂)₅CH(CH₂)₇CH₃
CH₃(CH₂)₅CH(CH₂)₇CH₃**

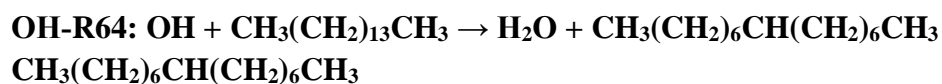
C	8.81359900	-0.81971200	0.21189900
H	8.89309200	-1.19793200	-0.81066300
H	8.68800300	-1.68011700	0.87440000
H	9.75951100	-0.33695400	0.46511100
C	7.63647600	0.14346400	0.34429400
H	7.59018000	0.53163200	1.36754600
H	7.79325000	1.00997600	-0.30721600
C	6.30119900	-0.51048300	-0.00416500
H	6.34654400	-0.90117600	-1.02812800
H	6.14245400	-1.37780300	0.64824400
C	5.11351700	0.44040800	0.12160600
H	5.27190600	1.30650900	-0.53250600

H	5.07011000	0.83198100	1.14521900
C	3.78065100	-0.21763300	-0.22421700
H	3.61748500	-1.08200900	0.42931200
H	3.82201700	-0.60704800	-1.24831000
C	2.59064800	0.73383500	-0.09889900
H	2.76722700	1.61088600	-0.74516400
H	2.54702700	1.13614800	0.92263300
C	1.28461800	0.10116400	-0.44003900
H	1.28146700	-0.73996500	-1.12838000
C	-0.00624900	0.79246000	-0.16069700
H	-0.13486000	1.64704700	-0.84718900
H	0.02457800	1.23450100	0.84446300
C	-1.22570200	-0.12211300	-0.28097800
H	-1.11617000	-0.95760300	0.41955000
H	-1.24684100	-0.56101400	-1.28551300
C	-2.54449000	0.59873800	-0.01573500
H	-2.65188900	1.43110800	-0.72187800
H	-2.51902800	1.04602600	0.98539800
C	-3.76034000	-0.31800100	-0.12735200
H	-3.65412400	-1.14812400	0.58138800
H	-3.78349700	-0.76858500	-1.12700700
C	-5.08196700	0.40110600	0.13234800
H	-5.18887900	1.23043600	-0.57736700
H	-5.05881100	0.85274100	1.13155700
C	-6.29675300	-0.51692000	0.02190600
H	-6.19127400	-1.34576700	0.73259300
H	-6.31955300	-0.97027800	-0.97668500
C	-7.62021800	0.20040500	0.27879200
H	-7.72455600	1.02729600	-0.43199900
H	-7.59628700	0.65257000	1.27621400
C	-8.82425600	-0.73137600	0.16481500
H	-8.75150600	-1.55006400	0.88553900
H	-9.76153300	-0.20332800	0.35089900
H	-8.88044000	-1.17314900	-0.83352900

TS63: OH + CH₃(CH₂)₁₃CH₃ → H₂O + CH₃(CH₂)₅CH(CH₂)₇CH₃

C	-8.79484800	0.34315200	0.11032200
H	-8.74386400	1.35640000	-0.29693500
H	-8.87035000	0.42680700	1.19783700
H	-9.71404900	-0.11905400	-0.25498800
C	-7.56108000	-0.46315700	-0.28788700
H	-7.63962800	-1.48010000	0.11181800
H	-7.52094700	-0.56256700	-1.37810200

C	-6.26270700	0.17141400	0.20465600
H	-6.18445900	1.19004900	-0.19460400
H	-6.30050100	0.27162200	1.29655300
C	-5.01732200	-0.61920300	-0.18843300
H	-4.98427200	-0.72237900	-1.27982300
H	-5.09062400	-1.63652200	0.21534500
C	-3.72257900	0.02896900	0.29425700
H	-3.74998500	0.12519900	1.38690800
H	-3.65010600	1.04603200	-0.10792000
C	-2.47322200	-0.74855200	-0.11306800
H	-2.44603500	-0.85185700	-1.20389100
H	-2.52266500	-1.76725400	0.29469500
C	-1.18697500	-0.09133600	0.35690300
H	-1.19372000	0.05723800	1.44331400
H	-1.17744700	0.96668700	-0.09558000
C	0.09785500	-0.76408500	-0.09481900
H	0.08362700	-0.86982800	-1.18562400
H	0.13062600	-1.78220400	0.31598300
C	1.35009500	0.00109100	0.32662800
H	1.36411400	0.10076800	1.41920800
H	1.29350300	1.01754800	-0.07966600
C	2.64442900	-0.66161300	-0.13695200
H	2.62263400	-0.77211700	-1.22786500
H	2.70482400	-1.67663900	0.27457500
C	3.89163100	0.12232100	0.26436200
H	3.91720400	0.23033600	1.35568100
H	3.82439600	1.13818200	-0.14348500
C	5.18991100	-0.52574800	-0.20950900
H	5.16110800	-0.63846700	-1.30017800
H	5.26245100	-1.53975500	0.20248100
C	6.43354900	0.26842500	0.18209400
H	6.46627400	0.37811000	1.27318300
H	6.35756400	1.28395600	-0.22580400
C	7.73437200	-0.36998000	-0.29891600
H	7.69977400	-0.47858200	-1.38845900
H	7.81079900	-1.38361600	0.10948600
C	8.96634400	0.43931100	0.09886900
H	9.03603900	0.53215800	1.18601200
H	9.88732700	-0.02626600	-0.25760700
H	8.91791200	1.44918000	-0.31708000
O	-1.16596500	2.39422600	-0.56442500
H	-1.16051400	2.79705700	0.31889600



C	8.88790700	-0.05296200	0.37915900
H	9.04466900	-0.81577100	-0.38801700
H	8.88682300	-0.55515300	1.35014000
H	9.74145900	0.62732800	0.35471100
C	7.57191700	0.68593900	0.14885200
H	7.44600700	1.46245700	0.91110400
H	7.60295700	1.20352800	-0.81603300
C	6.36248100	-0.24594700	0.17854300
H	6.48734400	-1.02424300	-0.58428500
H	6.33033500	-0.76533600	1.14416000
C	5.03813400	0.47824100	-0.05014900
H	5.07156800	0.99848700	-1.01509700
H	4.91333500	1.25524400	0.71370400
C	3.83036600	-0.45534200	-0.02219500
H	3.79761400	-0.97594800	0.94261300
H	3.95501400	-1.23206900	-0.78651800
C	2.50681700	0.26969500	-0.24969100
H	2.53655500	0.78680000	-1.21605200
H	2.37720300	1.04578900	0.51300800
C	1.29824900	-0.66601200	-0.22016300
H	1.26413500	-1.19258500	0.74355200
H	1.44389400	-1.45809300	-0.97482400
C	0.00000000	0.02874300	-0.45277900
H	0.00000000	0.94331000	-1.03994300
C	-1.29824900	-0.66601200	-0.22016300
H	-1.26413500	-1.19258500	0.74355100
H	-1.44389400	-1.45809300	-0.97482500
C	-2.50681700	0.26969500	-0.24969000
H	-2.53655500	0.78680100	-1.21605100
H	-2.37720300	1.04578900	0.51300900
C	-3.83036600	-0.45534200	-0.02219500
H	-3.79761400	-0.97594800	0.94261300
H	-3.95501400	-1.23206900	-0.78651800
C	-5.03813400	0.47824100	-0.05014800
H	-5.07156800	0.99848700	-1.01509600
H	-4.91333500	1.25524400	0.71370400
C	-6.36248100	-0.24594700	0.17854300
H	-6.33033500	-0.76533600	1.14416000
H	-6.48734400	-1.02424300	-0.58428500
C	-7.57191700	0.68593900	0.14885200

H	-7.60295700	1.20352800	-0.81603300
H	-7.44600700	1.46245600	0.91110400
C	-8.88790700	-0.05296200	0.37915900
H	-8.88682300	-0.55515300	1.35014000
H	-9.74145900	0.62732700	0.35471000
H	-9.04466800	-0.81577100	-0.38801700

TS64: OH + CH₃(CH₂)₁₃CH₃ → H₂O + CH₃(CH₂)₆CH(CH₂)₆CH₃

C	-8.90724500	-0.29768000	-0.31023900
H	-9.02062400	-1.29530300	0.12239500
H	-8.90417900	-0.40703400	-1.39794700
H	-9.78625400	0.28858700	-0.03489300
C	-7.61756700	0.36066800	0.17259900
H	-7.53714500	1.36877800	-0.24858800
H	-7.64991100	0.48321600	1.26076900
C	-6.37243700	-0.43891100	-0.20497400
H	-6.44939200	-1.44852000	0.21724800
H	-6.34036200	-0.56365400	-1.29435300
C	-5.07479600	0.21114000	0.26717400
H	-5.10486900	0.33165000	1.35709200
H	-5.00300900	1.22212500	-0.15213400
C	-3.82834500	-0.58139800	-0.11942100
H	-3.80243100	-0.70610600	-1.20864600
H	-3.89350300	-1.59074500	0.30497600
C	-2.53327000	0.08212000	0.34090000
H	-2.55342800	0.20012000	1.43163000
H	-2.47073800	1.09110700	-0.08349400
C	-1.28208800	-0.69557000	-0.06033900
H	-1.25685800	-0.81020600	-1.15000000
H	-1.32881000	-1.70988500	0.35839100
C	0.00304100	-0.03070700	0.40108700
H	0.00160000	0.12276000	1.48676700
H	0.01495000	1.02584700	-0.05463200
C	1.28877000	-0.69955000	-0.05443100
H	1.27023000	-0.80687500	-1.14508100
H	1.32705900	-1.71712500	0.35739700
C	2.53938200	0.07188200	0.36068600
H	2.56154300	0.16619800	1.45349000
H	2.47266000	1.09036100	-0.03854900
C	3.83332700	-0.58165000	-0.11671300
H	3.80297300	-0.68798800	-1.20789000
H	3.90325100	-1.59802000	0.29012800
C	5.07979500	0.20757100	0.27665200

H	5.11306200	0.31375300	1.36796200
H	5.00465300	1.22381900	-0.12878500
C	6.37706400	-0.43405700	-0.20789600
H	6.34089500	-0.54719800	-1.29846700
H	6.45831900	-1.44795500	0.20317600
C	7.62179600	0.36454300	0.17309100
H	7.65720000	0.47746100	1.26222500
H	7.53807000	1.37618500	-0.23879500
C	8.91137800	-0.28683200	-0.31945500
H	8.90484400	-0.38735500	-1.40802300
H	9.79005400	0.29915200	-0.04234500
H	9.02839300	-1.28768300	0.10469600
O	-0.00137900	2.44750800	-0.54114200
H	-0.31004100	2.84104800	0.29109400

3.1.16 C16 (*n*-C₁₆H₃₄)



n-C₁₆H₃₄

C	-9.55330000	-0.34393500	-0.00005100
H	-9.59047900	-0.98826600	0.88236500
H	-9.59045100	-0.98825200	-0.88247900
H	-10.45113500	0.27736900	-0.00006000
C	-8.28200800	0.50161300	-0.00002400
H	-8.27479200	1.15808700	-0.87696000
H	-8.27481900	1.15807200	0.87692400
C	-7.01321800	-0.34831600	-0.00001200
H	-7.01958500	-1.00659200	-0.87751500
H	-7.01960900	-1.00660400	0.87748100
C	-5.73130800	0.48073400	0.00001000
H	-5.72531200	1.13860300	0.87764400
H	-5.72529200	1.13861800	-0.87761200
C	-4.46489900	-0.37223100	0.00001700
H	-4.47141700	-1.03018100	-0.87753200
H	-4.47143000	-1.03018800	0.87756000
C	-3.18175800	0.45523900	0.00002900
H	-3.17493000	1.11311600	0.87763300
H	-3.17492200	1.11312700	-0.87756800
C	-1.91631900	-0.39910600	0.00002900
H	-1.92340100	-1.05702800	-0.87754500
H	-1.92340100	-1.05702900	0.87760300
C	-0.63256400	0.42740300	0.00002900
H	-0.62536500	1.08529800	0.87762100
H	-0.62536700	1.08530000	-0.87756100

C	0.63256400	-0.42740300	0.00002600
H	0.62536200	-1.08530200	-0.87756300
H	0.62537100	-1.08529600	0.87761900
C	1.91631900	0.39910600	0.00001600
H	1.92340600	1.05703300	0.87758700
H	1.92339700	1.05702500	-0.87756100
C	3.18175800	-0.45523900	0.00001300
H	3.17491900	-1.11312800	-0.87758200
H	3.17493200	-1.11311400	0.87761900
C	4.46489900	0.37223100	-0.00000300
H	4.47142900	1.03019300	0.87753600
H	4.47141900	1.03017500	-0.87755500
C	5.73130800	-0.48073400	-0.00000200
H	5.72529600	-1.13862000	-0.87762200
H	5.72530800	-1.13860000	0.87763500
C	7.01321800	0.34831600	-0.00002000
H	7.01960200	1.00661000	0.87746900
H	7.01959300	1.00658500	-0.87752700
C	8.28200800	-0.50161300	-0.00001400
H	8.27480100	-1.15809200	-0.87694700
H	8.27481000	-1.15806700	0.87693700
C	9.55330000	0.34393500	-0.00003300
H	9.59046900	0.98827300	0.88237900
H	10.45113500	-0.27736900	-0.00002700
H	9.59046200	0.98824500	-0.88246500

CH₂(CH₂)₁₄CH₃

C	-9.60656900	0.32201800	0.00959600
H	-9.63172400	1.28088500	0.51247000
H	-10.54470700	-0.09448800	-0.33105100
C	-8.35611500	-0.48593700	0.00289400
H	-8.32084600	-1.13664300	0.89225800
H	-8.35587400	-1.16807900	-0.85502800
C	-7.08726500	0.36971000	-0.01984600
H	-7.09849800	1.04884000	0.84089500
H	-7.09806200	1.00278200	-0.91401900
C	-5.80725400	-0.46103600	0.00505800
H	-5.80117000	-1.14384300	-0.85324500
H	-5.80226800	-1.09349500	0.90115800
C	-4.54011000	0.39031900	-0.01893000
H	-4.54623300	1.07322200	0.83922400
H	-4.54533800	1.02271000	-0.91488300
C	-3.25870600	-0.43950200	0.00571800

H	-3.25215400	-1.12146900	-0.85321000
H	-3.25436100	-1.07304600	0.90098000
C	-1.99122900	0.41146300	-0.01608200
H	-1.99759000	1.09300800	0.84318900
H	-1.99577600	1.04549400	-0.91098500
C	-0.70982200	-0.41835200	0.00776400
H	-0.70316800	-1.09936100	-0.85193800
H	-0.70569700	-1.05298600	0.90226600
C	0.55782100	0.43240400	-0.01288700
H	0.55151300	1.11295300	0.84718300
H	0.55340300	1.06752600	-0.90703500
C	1.83918800	-0.39750400	0.00994800
H	1.84552200	-1.07786000	-0.85027900
H	1.84354900	-1.03284800	0.90394600
C	3.10688500	0.45317700	-0.01049900
H	3.10095100	1.13307700	0.85009000
H	3.10215500	1.08900700	-0.90414800
C	4.38824300	-0.37677800	0.01117200
H	4.39414100	-1.05665100	-0.84942900
H	4.39311600	-1.01263900	0.90478800
C	5.65598300	0.47389800	-0.00949200
H	5.65042800	1.15350300	0.85135400
H	5.65088600	1.11005900	-0.90292500
C	6.93728500	-0.35581200	0.01133300
H	6.94358200	-1.03591200	-0.84928900
H	6.94360300	-0.99207400	0.90484800
C	8.20598600	0.49392500	-0.00999400
H	8.19869000	1.17210900	0.85018000
H	8.19819100	1.12867800	-0.90269300
C	9.47813400	-0.34988300	0.01052300
H	9.51656300	-1.01603300	-0.85537700
H	10.37483900	0.27271100	-0.00562000
H	9.51760500	-0.97179900	0.90866800

TS65: OH + CH₃(CH₂)₁₄CH₃ → H₂O + CH₂(CH₂)₁₄CH₃

C	8.78596600	0.65332900	-0.01129400
H	8.90539900	1.21612900	0.91646600
H	8.84105200	1.32821200	-0.86827300
H	9.74436400	-0.00494100	-0.11588200
C	7.54852300	-0.22271700	-0.02705600
H	7.55438900	-0.85046300	-0.92370400
H	7.56041000	-0.90230300	0.83245100
C	6.25851000	0.60113600	0.00644100

H	6.24129500	1.27663400	−0.85688200
H	6.25727400	1.23876400	0.89843000
C	5.00015600	−0.26392000	−0.00180000
H	5.01454900	−0.93423700	0.86607800
H	5.00902300	−0.90777000	−0.88941900
C	3.71272400	0.55681400	0.01456900
H	3.69945100	1.22588800	−0.85430600
H	3.70570500	1.20293600	0.90078200
C	2.45163200	−0.30391500	0.00727400
H	2.46214700	−0.97045700	0.87821900
H	2.46063700	−0.95265300	−0.87700900
C	1.16509700	0.51826900	0.01643600
H	1.15548300	1.18474800	−0.85458300
H	1.15621100	1.16738600	0.90051000
C	−0.09734200	−0.34037300	0.00808500
H	−0.08918600	−1.00568700	0.88003000
H	−0.08760600	−0.99060700	−0.87514600
C	−1.38318100	0.48292700	0.01379900
H	−1.39072900	1.14843200	−0.85800900
H	−1.39308600	1.13310700	0.89709500
C	−2.64628800	−0.37472600	0.00433000
H	−2.63945700	−1.03969300	0.87656200
H	−2.63594900	−1.02542800	−0.87856800
C	−3.93183600	0.44903700	0.00833100
H	−3.93842200	1.11414000	−0.86379900
H	−3.94238500	1.09964300	0.89130900
C	−5.19505900	−0.40844100	−0.00181400
H	−5.18863000	−1.07347200	0.87036700
H	−5.18434100	−1.05915100	−0.88469900
C	−6.48082900	0.41504900	0.00170100
H	−6.48730900	1.08023200	−0.87039000
H	−6.49195700	1.06555500	0.88476400
C	−7.74357300	−0.44280500	−0.00901600
H	−7.73775600	−1.10846300	0.86289200
H	−7.73309700	−1.09356900	−0.89206400
C	−9.03094200	0.37871300	−0.00550400
H	−9.03544200	1.04290400	−0.87662300
H	−9.04051200	1.02747200	0.87714700
C	−10.28338100	−0.49437300	−0.01704700
H	−10.30945300	−1.14708600	0.85955600
H	−11.19436800	0.10745300	−0.01453900
H	−10.30404800	−1.13144200	−0.90525200
O	10.73591700	−1.02283600	−0.08287300

H	10.38795100	-1.50354700	0.68484100
OH-R66: OH + CH₃(CH₂)₁₄CH₃ → H₂O + CH₃CH(CH₂)₁₃CH₃			
CH₃CH(CH₂)₁₃CH₃			
C	-9.64813900	-0.19228500	0.16313600
H	-9.63426600	-0.88408200	1.01244400
H	-9.93470000	-0.78790600	-0.71670000
H	-10.44014900	0.53885300	0.33184100
C	-8.32005500	0.45685800	-0.02108300
H	-8.27453800	1.47790900	-0.38488100
C	-7.07560300	-0.36349500	-0.05059900
H	-7.06337300	-0.99872900	-0.95318700
H	-7.08257100	-1.06796400	0.79314600
C	-5.79274700	0.46644500	-0.01367800
H	-5.79419800	1.08785500	0.88903300
H	-5.78777100	1.15681900	-0.86548900
C	-4.52722900	-0.38599200	-0.04513700
H	-4.53192400	-1.01072200	-0.94672800
H	-4.53385100	-1.07609100	0.80737900
C	-3.24542900	0.44279200	-0.01230900
H	-3.24263100	1.07028600	0.88722100
H	-3.23681700	1.13027900	-0.86685300
C	-1.97853600	-0.40895900	-0.03736800
H	-1.98218100	-1.03800400	-0.93589500
H	-1.98650800	-1.09505600	0.81832000
C	-0.69662200	0.41980700	-0.00699100
H	-0.69368700	1.04982100	0.89084700
H	-0.68804900	1.10504100	-0.86336900
C	0.57043700	-0.43176800	-0.02986600
H	0.56752300	-1.06200700	-0.92756000
H	0.56193800	-1.11677200	0.82670400
C	1.85222400	0.39720600	0.00041200
H	1.85457700	1.02798500	0.89772700
H	1.86110000	1.08175800	-0.85651400
C	3.11955500	-0.45401100	-0.02101600
H	3.11778800	-1.08440400	-0.91860400
H	3.11038500	-1.13888400	0.83565200
C	4.40095900	0.37550300	0.01057800
H	4.40213900	1.00618600	0.90795700
H	4.41040000	1.06019200	-0.84622300
C	5.66888800	-0.47493000	-0.00960600
H	5.66906800	-1.10440700	-0.90785200
H	5.65874100	-1.16068400	0.84636800
C	6.94948900	0.35534700	0.02516000

H	6.94955500	0.98501800	0.92344200
H	6.96052500	1.04165000	-0.83053600
C	8.21931500	-0.49279800	0.00576600
H	8.21965900	-1.11889000	-0.89315800
H	8.20587800	-1.17901500	0.85952700
C	9.48966600	0.35311800	0.04553800
H	9.51858700	0.96695300	0.94975500
H	10.38803000	-0.26729200	0.03244400
H	9.53428400	1.02727700	-0.81389200

TS66: OH + CH₃(CH₂)₁₄CH₃ → H₂O + CH₃CH(CH₂)₁₃CH₃

C	9.01785400	-0.82930500	-0.04696600
H	9.05667000	-0.91701700	-1.13508100
H	9.05044600	-1.84008900	0.37215100
H	9.91100400	-0.29696800	0.28349900
C	7.75007700	-0.11679400	0.39030900
H	7.73356300	0.04180400	1.47367400
H	7.78770300	0.93908100	-0.06858100
C	6.46129300	-0.76674800	-0.08258100
H	6.39921400	-1.77672200	0.34532100
H	6.49926300	-0.89343400	-1.17062700
C	5.21134000	0.02366900	0.29605100
H	5.26445000	1.01414300	-0.17100800
H	5.19947500	0.18584200	1.38132500
C	3.91625300	-0.66682500	-0.12319500
H	3.86180300	-1.65483200	0.35016100
H	3.93487300	-0.84433500	-1.20514200
C	2.66604000	0.13295500	0.23514700
H	2.70924400	1.11214000	-0.25704700
H	2.65857700	0.33036100	1.31412700
C	1.37099900	-0.57439600	-0.15590100
H	1.32473800	-1.54774800	0.34774700
H	1.38381400	-0.78574000	-1.23202900
C	0.11807100	0.22877000	0.18496300
H	0.15162300	1.19247800	-0.33758900
H	0.11589500	0.45996000	1.25722200
C	-1.17504300	-0.49822000	-0.17579100
H	-1.21094400	-1.45637400	0.35688700
H	-1.16822300	-0.74153000	-1.24531200
C	-2.43102000	0.30631800	0.15008400
H	-2.40599600	1.25602300	-0.39792500
H	-2.42917200	0.56591700	1.21587000
C	-3.72184400	-0.43701200	-0.18489500

H	-3.74825200	-1.38258300	0.37027500
H	-3.72031100	-0.70525200	-1.24853500
C	-4.98048900	0.36750300	0.13038000
H	-4.96149500	1.30726600	-0.43474700
H	-4.97643900	0.64645200	1.19128400
C	-6.26939300	-0.38676500	-0.18731400
H	-6.28898200	-1.32430600	0.38159500
H	-6.27162600	-0.67029800	-1.24702900
C	-7.52977200	0.41686100	0.12220500
H	-7.51426200	1.35229100	-0.45052100
H	-7.52630600	0.70503900	1.18081600
C	-8.81851900	-0.34126500	-0.18816600
H	-8.83299000	-1.27430700	0.38559000
H	-8.82024300	-0.62927100	-1.24522500
C	-10.07008700	0.47493800	0.12491500
H	-10.08569300	1.40043600	-0.45675000
H	-10.98134500	-0.08070600	-0.10512400
H	-10.10135400	0.74818200	1.18306400
O	7.70749800	2.35774200	-0.52230500
H	7.24673200	2.70006200	0.26062100

**OH-R67: OH + CH₃(CH₂)₁₄CH₃ → H₂O + CH₃CH₂CH(CH₂)₁₂CH₃
CH₃CH₂CH(CH₂)₁₂CH₃**

C	9.53270400	0.56146600	0.17419800
H	9.38224900	1.29599500	0.96865100
H	9.61784000	1.10380800	-0.77069800
H	10.48076300	0.05234200	0.35625900
C	8.36755200	-0.42497900	0.12492100
H	8.55904100	-1.17713900	-0.65772000
H	8.32027200	-0.99606500	1.06179300
C	7.05124800	0.23195900	-0.11866800
H	7.03733600	1.22263700	-0.56557200
C	5.78426500	-0.55251700	-0.08380200
H	5.78521800	-1.21188600	0.79523800
H	5.73777800	-1.23209700	-0.95224900
C	4.52622100	0.31596800	-0.07077700
H	4.53250500	0.96956800	-0.95113700
H	4.55440500	0.97466500	0.80459400
C	3.23661900	-0.50005500	-0.05545800
H	3.23339600	-1.15702200	0.82288500
H	3.21390200	-1.15861900	-0.93238400
C	1.97901500	0.36554600	-0.04206100
H	1.98283700	1.02365400	-0.91948200

H	2.00033000	1.02283000	0.83566700
C	0.68893500	-0.45097800	-0.02970700
H	0.68508400	-1.10886000	0.84790500
H	0.66872600	-1.10879900	-0.90717400
C	-0.56996400	0.41283400	-0.01797400
H	-0.56558500	1.07161000	-0.89491200
H	-0.55116500	1.06962200	0.86025900
C	-1.85895600	-0.40543500	-0.00842800
H	-1.86340300	-1.06393500	0.86872800
H	-1.87663700	-1.06274500	-0.88633200
C	-3.11927600	0.45633900	0.00161600
H	-3.11467000	1.11541600	-0.87509600
H	-3.10290600	1.11287700	0.88009300
C	-4.40686500	-0.36417100	0.00899500
H	-4.41139200	-1.02300100	0.88589600
H	-4.42217300	-1.02122300	-0.86913100
C	-5.66887800	0.49520500	0.01759400
H	-5.66453600	1.15438300	-0.85906300
H	-5.65481100	1.15168400	0.89617800
C	-6.95475900	-0.32765900	0.02342300
H	-6.95984100	-0.98677400	0.90030500
H	-6.96856700	-0.98507200	-0.85465000
C	-8.21954300	0.52816600	0.03052200
H	-8.21341100	1.18567300	-0.84564300
H	-8.20532500	1.18350500	0.90822500
C	-9.49466900	-0.31157200	0.03539900
H	-9.53099700	-0.95639200	0.91749400
H	-10.38969000	0.31375600	0.03963200
H	-9.53847700	-0.95508100	-0.84732000

TS67: OH + CH₃(CH₂)₁₄CH₃ → H₂O + CH₃CH₂CH(CH₂)₁₂CH₃

C	9.08464800	-0.02786900	0.22247300
H	9.15764900	0.00329300	1.31292100
H	9.04655500	1.00151600	-0.14164600
H	9.99385400	-0.49392700	-0.16141700
C	7.83697400	-0.78987500	-0.21626000
H	7.80128900	-0.85126200	-1.30870100
H	7.87597000	-1.82230200	0.15279100
C	6.55702100	-0.14076000	0.28337200
H	6.55670700	0.92709300	-0.14483100
H	6.57945500	-0.01428900	1.37244900
C	5.26667900	-0.80364000	-0.16527400
H	5.23313900	-1.82451100	0.23846400

H	5.27153800	-0.90128600	-1.25683600
C	4.01913700	-0.04009700	0.27272500
H	4.05650200	0.96941000	-0.15353100
H	4.03040800	0.07824400	1.36356200
C	2.71857200	-0.71994200	-0.14675100
H	2.68069600	-1.72968800	0.27991400
H	2.71148000	-0.84529300	-1.23615500
C	1.47498900	0.05602300	0.28012600
H	1.51579400	1.06546500	-0.14692900
H	1.48247400	0.18267400	1.36967900
C	0.17086000	-0.61663900	-0.14053600
H	0.12497500	-1.62384700	0.29137200
H	0.16655500	-0.74873200	-1.22930900
C	-1.06988500	0.16911900	0.27685100
H	-1.02030700	1.17694400	-0.15327500
H	-1.06710200	0.29992300	1.36587800
C	-2.37638900	-0.49615200	-0.14816600
H	-2.43061700	-1.50205700	0.28584000
H	-2.37673300	-0.63095400	-1.23665800
C	-3.61423300	0.29812700	0.26178500
H	-3.55612100	1.30507000	-0.16939400
H	-3.61602700	0.43044800	1.35061700
C	-4.92266300	-0.35962400	-0.16889500
H	-4.98463200	-1.36503000	0.26525200
H	-4.91891800	-0.49499400	-1.25731400
C	-6.15813200	0.44150900	0.23505300
H	-6.09292900	1.44789900	-0.19646100
H	-6.16411100	0.57445600	1.32380700
C	-7.46769200	-0.20994400	-0.20101700
H	-7.53714300	-1.21496700	0.23330400
H	-7.46056700	-0.34641600	-1.28945200
C	-8.70260500	0.59594200	0.19620200
H	-8.63000000	1.59968600	-0.23675600
H	-8.71021200	0.72962500	1.28345000
C	-10.00400400	-0.06481600	-0.25060100
H	-10.10989200	-1.05736200	0.19542800
H	-10.87569800	0.52637100	0.03727400
H	-10.02507400	-0.18637900	-1.33684500
O	6.53177800	2.35784100	-0.60338400
H	6.15715000	2.72429600	0.21404500

OH-R68: $\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_{11}\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_2\text{CH}(\text{CH}_2)_{11}\text{CH}_3$

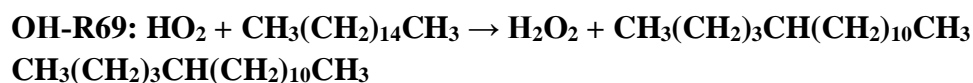
C	9.58606000	-0.04672400	0.33827500
H	9.58803200	0.57321300	1.23878200
H	9.84849900	0.59500500	-0.50703400
H	10.37214300	-0.79652900	0.44668500
C	8.22022900	-0.69343100	0.12720500
H	8.24195200	-1.32327800	-0.76844300
H	7.98540200	-1.35520600	0.96679400
C	7.09915900	0.33660500	-0.01856200
H	7.34898000	1.01585500	-0.85204600
H	7.07142900	0.97720500	0.87385000
C	5.75705800	-0.27336900	-0.23754200
H	5.70447900	-1.25019700	-0.71177500
C	4.51073300	0.54008700	-0.15196600
H	4.46395800	1.25138700	-0.99459900
H	4.54134200	1.16700700	0.74993600
C	3.23524700	-0.30273000	-0.14755600
H	3.26574300	-0.99243300	0.70355900
H	3.21518400	-0.92538400	-1.04991800
C	1.96030500	0.53339800	-0.08227200
H	1.93399100	1.22264200	-0.93515000
H	1.98023400	1.15874400	0.81862400
C	0.69119100	-0.31545500	-0.07993800
H	0.71616200	-1.00154100	0.77536600
H	0.67608200	-0.94478800	-0.97814700
C	-0.58991500	0.51314400	-0.02417800
H	-0.61471400	1.19975300	-0.87914500
H	-0.57779900	1.14139900	0.87478700
C	-1.85523100	-0.34140500	-0.02654500
H	-1.83210700	-1.02525300	0.83067400
H	-1.86302400	-0.97308700	-0.92320700
C	-3.13991700	0.48222200	0.02021700
H	-3.16239400	1.16689500	-0.83636800
H	-3.13491100	1.11258200	0.91778600
C	-4.40244400	-0.37640300	0.01278100
H	-4.38162600	-1.05887200	0.87115400
H	-4.40409500	-1.00942200	-0.88295600
C	-5.68959800	0.44385900	0.05206100
H	-5.70968000	1.12721600	-0.80565300
H	-5.69023700	1.07562200	0.94868200
C	-6.95014800	-0.41726300	0.04009700
H	-6.93239800	-1.09918500	0.89917700
H	-6.94782200	-1.05141900	-0.85502000
C	-8.23984900	0.39982300	0.07345000

H	-8.25558000	1.08071700	-0.78452700
H	-8.24226500	1.03141200	0.96851700
C	-9.48961500	-0.47703500	0.05772600
H	-9.50636200	-1.14477600	0.92312300
H	-10.40246100	0.12163500	0.07807000
H	-9.51572200	-1.09885200	-0.84110000

TS68: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + CH₃(CH₂)₂CH(CH₂)₁₁CH₃

C	9.18574800	-0.48587700	-0.23090800
H	9.18489700	-0.58695900	-1.31924500
H	9.30688100	-1.48520700	0.19562700
H	10.05906600	0.10623500	0.04939900
C	7.89094000	0.16077000	0.25321500
H	7.91824900	0.27319600	1.34301700
H	7.79879200	1.16826000	-0.16570100
C	6.65269200	-0.64373200	-0.13661700
H	6.73217400	-1.65995500	0.27295900
H	6.61563300	-0.75093900	-1.22687300
C	5.35743600	-0.01729400	0.34880500
H	5.30773600	1.04024200	-0.10221700
H	5.37320300	0.13146400	1.43510800
C	4.08416900	-0.72266100	-0.08656600
H	4.08749000	-1.74404500	0.31738500
H	4.08366700	-0.82098000	-1.17818500
C	2.81872300	0.00475800	0.36098500
H	2.84311700	1.02726700	-0.03271900
H	2.81791100	0.09172000	1.45461300
C	1.53608500	-0.68775800	-0.09165600
H	1.50847800	-1.70810500	0.31011400
H	1.54531500	-0.78683300	-1.18385900
C	0.27459800	0.05902500	0.33465200
H	0.30849400	1.07926100	-0.06618300
H	0.26295700	0.15852000	1.42698200
C	-1.01337600	-0.61969500	-0.12430400
H	-1.05632000	-1.63600200	0.28604700
H	-0.99571000	-0.72930500	-1.21550700
C	-2.27023900	0.14459800	0.28463200
H	-2.22207400	1.16160200	-0.12338500
H	-2.29023400	0.25271000	1.37600300
C	-3.56167600	-0.52333600	-0.18031900
H	-3.61643700	-1.53772400	0.23336700
H	-3.53822600	-0.63727200	-1.27099800
C	-4.81435800	0.25321600	0.21838100

H	-4.75522800	1.26864700	-0.19217500
H	-4.84011200	0.36457800	1.30929700
C	-6.10834300	-0.40562400	-0.25247800
H	-6.17146000	-1.41978100	0.16065000
H	-6.08096800	-0.51948000	-1.34310600
C	-7.35793100	0.37811100	0.14118600
H	-7.29204900	1.39392100	-0.26784500
H	-7.38875200	0.48869300	1.23221600
C	-8.65429500	-0.27243100	-0.33558200
H	-8.71985100	-1.28666600	0.07319700
H	-8.62225500	-0.38100700	-1.42521500
C	-9.89260300	0.52515200	0.06613700
H	-9.85544300	1.53531200	-0.35026300
H	-10.81031600	0.05052100	-0.28683100
H	-9.95931300	0.61774900	1.15348200
O	5.27052300	2.46656300	-0.57143100
H	5.53108000	2.86452000	0.27491400



C	9.42423900	0.86641100	0.38212100
H	9.20595800	1.75009100	0.98761100
H	9.57044400	1.19959200	-0.64874700
H	10.36671500	0.44277800	0.73472100
C	8.28417500	-0.14492500	0.46957300
H	8.52971300	-1.03100800	-0.12617300
H	8.17525300	-0.48969300	1.50367300
C	6.95407500	0.43072900	-0.00895100
H	7.05866000	0.77518200	-1.04482200
H	6.70316400	1.31598900	0.58676500
C	5.80085600	-0.56890600	0.07341900
H	5.70218800	-0.93213200	1.10577700
H	6.06114500	-1.46182900	-0.52080500
C	4.49586300	-0.01101300	-0.38283200
H	4.50349700	0.79358000	-1.11369600
C	3.21736400	-0.73881100	-0.14149400
H	3.20171200	-1.11713600	0.88990400
H	3.16676500	-1.63877900	-0.77850900
C	1.97348600	0.11385700	-0.39147800
H	1.98937200	0.47908400	-1.42523400
H	2.01422100	1.00102800	0.25079500
C	0.67012600	-0.63849100	-0.13848100
H	0.66890300	-1.02411900	0.88843500

H	0.62164300	-1.51510800	-0.79610200
C	-0.57011000	0.22579700	-0.35046000
H	-0.57195200	0.61531700	-1.37575500
H	-0.51713200	1.10000300	0.30994900
C	-1.87636700	-0.52055900	-0.09043100
H	-1.85557300	-0.94243700	0.92191600
H	-1.95209900	-1.37238000	-0.77717200
C	-3.11151900	0.36436400	-0.23905700
H	-3.13149500	0.79677500	-1.24688900
H	-3.03399800	1.20920200	0.45619500
C	-4.41996900	-0.37904100	0.01839600
H	-4.38107100	-0.84542400	1.01050900
H	-4.52118900	-1.19876400	-0.70312000
C	-5.64859600	0.52379700	-0.06402500
H	-5.68611400	0.99919800	-1.05186600
H	-5.54679400	1.33710600	0.66481300
C	-6.95845500	-0.21799100	0.18954800
H	-6.91115700	-0.71280600	1.16757500
H	-7.07454800	-1.01674300	-0.55322600
C	-8.18395600	0.69226700	0.14608200
H	-8.22927000	1.18930100	-0.82917000
H	-8.06661600	1.48622400	0.89162200
C	-9.48555400	-0.06422000	0.39912800
H	-9.46852400	-0.54967200	1.37855200
H	-10.35098600	0.60078700	0.36979100
H	-9.63477900	-0.84279800	-0.35365900

TS69: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + CH₃(CH₂)₃CH(CH₂)₁₀CH₃

C	-9.24264800	0.17355600	0.11533300
H	-9.19556300	1.19924900	-0.25951300
H	-9.33119600	0.22199800	1.20398500
H	-10.15335200	-0.28499800	-0.27489900
C	-7.99751000	-0.60906700	-0.29420900
H	-8.07062300	-1.63872800	0.07299500
H	-7.94510200	-0.67324000	-1.38646500
C	-6.71157800	0.02472600	0.23045900
H	-6.76045400	0.09054000	1.32466300
H	-6.63146900	1.05310600	-0.14030500
C	-5.45592700	-0.74358800	-0.17429700
H	-5.41389900	-0.82738900	-1.26643900
H	-5.50884300	-1.76964300	0.21431600
C	-4.17660100	-0.09303800	0.32360100
H	-4.20243500	0.04733900	1.41076700

H	-4.16598800	0.96895700	-0.11927200
C	-2.88648100	-0.76621800	-0.11128500
H	-2.88603000	-0.87325100	-1.20197600
H	-2.85961100	-1.78372400	0.30131900
C	-1.63858800	-0.00299400	0.32607700
H	-1.64761800	0.11347800	1.41710800
H	-1.67814500	1.00717900	-0.09820900
C	-0.33822700	-0.67999600	-0.09852400
H	-0.33704300	-0.80780900	-1.18768200
H	-0.29366200	-1.68856400	0.33030400
C	0.90463500	0.10271200	0.31816600
H	0.90621800	0.22856100	1.40784100
H	0.85352000	1.11218500	-0.10770200
C	2.20909100	-0.56094600	-0.11540700
H	2.20331900	-0.69286100	-1.20420600
H	2.26673200	-1.56784300	0.31583800
C	3.44831300	0.23396200	0.28911200
H	3.45756700	0.36230400	1.37840300
H	3.38511400	1.24230300	-0.13803900
C	4.75497300	-0.41927200	-0.15357600
H	4.74264100	-0.55219900	-1.24223600
H	4.82352400	-1.42542100	0.27783900
C	5.99124900	0.38492000	0.24175400
H	6.00647000	0.51477000	1.33081000
H	5.91865800	1.39228200	-0.18629200
C	7.29915200	-0.26051600	-0.20796200
H	7.28293100	-0.39353900	-1.29673500
H	7.37598400	-1.26664500	0.22254300
C	8.53463100	0.54854300	0.18098900
H	8.55117200	0.67895900	1.26854700
H	8.45475400	1.55330500	-0.24829900
C	9.83439800	-0.10626800	-0.27911100
H	9.84682000	-0.22385900	-1.36591600
H	10.70652600	0.48670700	0.00371000
H	9.94713700	-1.10005600	0.16246800
O	-4.12470800	2.39522200	-0.58967600
H	-3.82368200	2.77569000	0.25141300

OH-R70: $\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_9\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2)_9\text{CH}_3$

C	9.57124400	-0.00762900	0.26349100
H	9.60401300	0.50356700	1.22924400
H	9.72976700	0.74411400	-0.51429100

H	10.40725600	-0.70885300	0.22720500
C	8.23304800	-0.71568800	0.06841200
H	8.23278200	-1.24736800	-0.88937400
H	8.10119300	-1.47825600	0.84368900
C	7.04870400	0.24741300	0.10620500
H	7.17882000	1.01001300	-0.67163900
H	7.04874700	0.78306100	1.06354500
C	5.70372800	-0.44707400	-0.08524800
H	5.56546400	-1.20152200	0.69763500
H	5.70611400	-0.98770700	-1.03917900
C	4.52074000	0.51971900	-0.06249500
H	4.66922300	1.28484600	-0.84362200
H	4.52081700	1.07890400	0.88431700
C	3.19987100	-0.14595000	-0.24748400
H	3.17183300	-1.13615400	-0.69443900
C	1.93021800	0.62881600	-0.14922700
H	1.85406300	1.33412600	-0.99479300
H	1.95388500	1.26244200	0.74850600
C	0.67789800	-0.24728400	-0.12457100
H	0.73019400	-0.92429000	0.73564000
H	0.66772800	-0.88220800	-1.01848700
C	-0.61583800	0.55987700	-0.06348200
H	-0.66131600	1.23598500	-0.92609500
H	-0.60443000	1.19897700	0.82787000
C	-1.86760700	-0.31393300	-0.04192400
H	-1.82874000	-0.98297200	0.82627500
H	-1.87289100	-0.96013100	-0.92816700
C	-3.16268300	0.49361600	0.00027900
H	-3.19944500	1.16292400	-0.86793600
H	-3.15889700	1.13975500	0.88656300
C	-4.41522600	-0.37924400	0.01706900
H	-4.38305700	-1.04391500	0.88895400
H	-4.41467300	-1.03005100	-0.86581600
C	-5.71039200	0.42884000	0.04618600
H	-5.74103500	1.09411700	-0.82536500
H	-5.71249200	1.07907800	0.92950300
C	-6.96306000	-0.44360400	0.05869000
H	-6.93601600	-1.10638800	0.93239900
H	-6.95901300	-1.09703100	-0.82244100
C	-8.25947700	0.36327000	0.07970300
H	-8.28459000	1.02440100	-0.79342000
H	-8.26287000	1.01498800	0.96021800
C	-9.50212800	-0.52365500	0.09024600

H	-9.50927100	-1.17171800	0.97065200
H	-10.41957700	0.06816300	0.10188300
H	-9.52781800	-1.16583200	-0.79413800

TS70: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + CH₃(CH₂)₄CH(CH₂)₉CH₃

C	-9.34449600	-0.32829200	-0.27416400
H	-9.46887700	-1.32410600	0.15965600
H	-9.34514500	-0.43842800	-1.36175400
H	-10.21566400	0.26881300	0.00267100
C	-8.04589400	0.31490100	0.20507400
H	-7.95330600	1.32090500	-0.21845400
H	-8.07457300	0.43955300	1.29315900
C	-6.81181300	-0.50104800	-0.17361500
H	-6.78285100	-0.62731000	-1.26274500
H	-6.90052200	-1.50881900	0.25074600
C	-5.50632700	0.13559800	0.29451100
H	-5.53216600	0.25647100	1.38485100
H	-5.41841600	1.14197200	-0.13161300
C	-4.26980100	-0.67109100	-0.09500400
H	-4.23622900	-0.78566400	-1.18445700
H	-4.34526600	-1.68425000	0.32240200
C	-2.97389100	-0.03809100	0.38053600
H	-2.98365200	0.11537100	1.46619700
H	-2.93028200	1.01773000	-0.07487800
C	-1.69996100	-0.73882700	-0.06033700
H	-1.70731400	-0.84336100	-1.15137200
H	-1.69339300	-1.75784800	0.34950300
C	-0.43594100	-0.00007300	0.37279300
H	-0.42457000	0.08928400	1.46615500
H	-0.47326900	1.02138500	-0.02264400
C	0.84791500	-0.68208600	-0.09201600
H	0.82774900	-0.78386700	-1.18384400
H	0.88965900	-1.70115100	0.31184900
C	2.10692000	0.07766700	0.31863700
H	2.13088600	0.17770700	1.41073300
H	2.05763000	1.09733400	-0.08208200
C	3.39595400	-0.58807500	-0.15595600
H	3.36660100	-0.69700900	-1.24699700
H	3.45360900	-1.60424000	0.25299700
C	4.65021700	0.18783200	0.23900100
H	4.68239900	0.29442600	1.33024700
H	4.58748000	1.20491700	-0.16681300
C	5.94209200	-0.46732800	-0.24266300

H	5.90714800	-0.57833100	-1.33338100
H	6.01023700	-1.48241400	0.16738600
C	7.19278100	0.31815800	0.14395500
H	7.23141300	0.42599000	1.23503700
H	7.12154900	1.33483100	-0.26199800
C	8.48710300	-0.32801900	-0.34417300
H	8.44678000	-0.43451800	-1.43375300
H	8.55857100	-1.34285200	0.06212700
C	9.72632700	0.47224000	0.04932300
H	9.80157900	0.56271200	1.13630300
H	10.64254300	0.00111500	-0.31211300
H	9.68283300	1.48315600	-0.36462300
O	-2.90887900	2.43991400	-0.55953700
H	-3.20925400	2.84039600	0.27238400

OH-R71: $\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_8\text{CH}_3$
 $\text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_8\text{CH}_3$

C	9.45274400	0.80800300	0.26566600
H	9.32145300	1.67387800	0.91988700
H	9.54558400	1.17801000	-0.75877000
H	10.39422800	0.32479400	0.53407100
C	8.27154200	-0.15107300	0.39134800
H	8.43365400	-1.02287400	-0.25174300
H	8.21211700	-0.53136700	1.41687400
C	6.94220000	0.50369300	0.02232000
H	7.00068500	0.88684000	-1.00382200
H	6.77797900	1.37607900	0.66656600
C	5.75071900	-0.44335800	0.14090200
H	5.69525300	-0.82865700	1.16631300
H	5.91388300	-1.31376800	-0.50627600
C	4.42330700	0.21595400	-0.22300700
H	4.47696400	0.60046400	-1.24838200
H	4.25474300	1.08369500	0.42466100
C	3.22998200	-0.73245800	-0.10648100
H	3.17565700	-1.13161200	0.91578900
H	3.41082900	-1.61182800	-0.74838100
C	1.92862100	-0.09795200	-0.46177400
H	1.93376800	0.74172000	-1.15187800
C	0.63381700	-0.78620200	-0.19337800
H	0.65573600	-1.22924700	0.81155300
H	0.50836400	-1.63978300	-0.88169700
C	-0.58249200	0.13144200	-0.32212300
H	-0.59564200	0.57051000	-1.32671800

H	-0.47580300	0.96656000	0.37928800
C	-1.90469400	-0.58642800	-0.06592500
H	-1.88681100	-1.03407000	0.93521200
H	-2.00928600	-1.41836700	-0.77300400
C	-3.11782500	0.33293900	-0.18516300
H	-3.13353000	0.78407600	-1.18471600
H	-3.01447800	1.16246200	0.52472300
C	-4.44248000	-0.38369300	0.06560500
H	-4.42579500	-0.83773800	1.06382400
H	-4.54738900	-1.21110500	-0.64660500
C	-5.65477300	0.53746700	-0.04918500
H	-5.66965600	0.99405300	-1.04630800
H	-5.55117200	1.36316500	0.66522100
C	-6.98008600	-0.17912500	0.19702300
H	-6.96578300	-0.63727700	1.19358400
H	-7.08528200	-1.00404800	-0.51827300
C	-8.19309300	0.74182500	0.08439800
H	-8.20568700	1.19911700	-0.91089600
H	-8.08731400	1.56431400	0.80005600
C	-9.51024500	0.01051400	0.33167000
H	-9.52753800	-0.43141700	1.33137500
H	-10.36633500	0.68282100	0.24760200
H	-9.64686000	-0.79869500	-0.39048800

TS71: $\text{HO}_2 + \text{CH}_3(\text{CH}_2)_{14}\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2)_8\text{CH}_3$

C	-9.39510300	0.31611600	0.06434100
H	-9.34680600	1.32644600	-0.35044900
H	-9.47722400	0.40770900	1.15074000
H	-10.30988800	-0.15344400	-0.30257000
C	-8.15521300	-0.48716500	-0.32068300
H	-8.23093600	-1.50132700	0.08651800
H	-8.10847300	-0.59487700	-1.40983900
C	-6.86276900	0.15771800	0.17401900
H	-6.90746700	0.26725800	1.26477000
H	-6.78710200	1.17323600	-0.23379500
C	-5.61146500	-0.63053600	-0.20466400
H	-5.57235400	-0.74578300	-1.29459900
H	-5.68121900	-1.64353900	0.21024200
C	-4.32229600	0.02925900	0.27717200
H	-4.35785400	0.14181900	1.36811800
H	-4.25262000	1.04022800	-0.14127400
C	-3.06645100	-0.74817300	-0.10976200
H	-3.02594500	-0.85832800	-1.19946800

H	-3.12024200	-1.76412200	0.30413500
C	-1.78737400	-0.08653800	0.37257600
H	-1.80500800	0.06462900	1.45845400
H	-1.76713200	0.97090300	-0.08073400
C	-0.49562900	-0.75614200	-0.06459100
H	-0.49817100	-0.86264000	-1.15545400
H	-0.46411700	-1.77399800	0.34707400
C	0.74881400	0.01470100	0.36966200
H	0.75386400	0.10952500	1.46261700
H	0.68848100	1.03306600	-0.03089800
C	2.05035300	-0.63861700	-0.08694300
H	2.03633700	-0.74759200	-1.17816800
H	2.11565500	-1.65388000	0.32341200
C	3.28923200	0.15400700	0.32307600
H	3.30571300	0.26336700	1.41441000
H	3.21780000	1.16898700	-0.08618300
C	4.59561400	-0.48536400	-0.14007200
H	4.57444200	-0.60338800	-1.23032400
H	4.67432400	-1.49680300	0.27707500
C	5.83015400	0.32155500	0.25520700
H	5.85249400	0.43981300	1.34549900
H	5.74850500	1.33293100	-0.16148300
C	7.13861700	-0.31112000	-0.21070500
H	7.11437400	-0.43509000	-1.30041800
H	7.22577300	-1.32025100	0.21073100
C	8.37170600	0.50315700	0.17498000
H	8.39524900	0.62624600	1.26329000
H	8.28234800	1.51025400	-0.24684900
C	9.67229000	-0.14013800	-0.29890200
H	9.67772800	-0.25012200	-1.38656400
H	10.54270900	0.45629600	-0.01806300
H	9.79422300	-1.13623300	0.13499600
O	-1.77534700	2.39314600	-0.56598600
H	-2.08754800	2.78722200	0.26467800

OH-R72: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + CH₃(CH₂)₆CH(CH₂)₇CH₃
CH₃(CH₂)₆CH(CH₂)₇CH₃

C	-6.91709300	2.03957000	-0.02453500
H	-6.69795700	0.97196900	-0.10945600
H	-6.53106500	2.52925500	-0.92241900
H	-8.00223300	2.15945600	-0.01770300
C	-6.27756700	2.62663400	1.23131800
H	-6.53031800	3.68938200	1.31223000

H	-6.69614400	2.14190400	2.11997500
C	-4.75852000	2.47064900	1.24422600
H	-4.50390300	1.40678900	1.16282600
H	-4.33801500	2.95550800	0.35466100
C	-4.10351700	3.05292600	2.49424800
H	-4.52444300	2.56783100	3.38330100
H	-4.35829700	4.11658500	2.57489500
C	-2.58490400	2.89567200	2.50495500
H	-2.16455900	3.38097700	1.61569700
H	-2.33014700	1.83191700	2.42388700
C	-1.93027000	3.47808600	3.75454300
H	-2.34460100	2.98903900	4.64410100
H	-2.18212300	4.54113600	3.83995500
C	-0.40928800	3.32329400	3.76095100
H	0.01361800	3.80864500	2.87071600
H	-0.16122300	2.25356400	3.65000200
C	0.24156500	3.87469200	4.98351500
H	-0.32683800	3.89065800	5.90975500
C	1.71943800	4.05716800	5.05398100
H	2.07268200	4.54039900	4.13261700
H	2.22159700	3.07452400	5.07306800
C	2.17911100	4.86797100	6.26573400
H	1.82992800	4.37510300	7.18077000
H	1.69795700	5.85219900	6.24104800
C	3.69413700	5.04054500	6.32962000
H	4.04220000	5.53045600	5.41210500
H	4.17146800	4.05325200	6.35099300
C	4.15549500	5.85002100	7.53911800
H	3.80954700	5.35932200	8.45693200
H	3.67694400	6.83657500	7.51893100
C	5.67096900	6.02548400	7.60122400
H	6.01636100	6.51799400	6.68411900
H	6.14949800	5.03875100	7.61891500
C	6.13406700	6.83205500	8.81179700
H	5.79038600	6.33938800	9.72961700
H	5.65533500	7.81884400	8.79568500
C	7.64963600	7.00928500	8.87346100
H	7.99112600	7.50248700	7.95693500
H	8.12623400	6.02312600	8.88859000
C	8.09747500	7.81608000	10.08971900
H	7.78883700	7.32550500	11.01658900
H	9.18255600	7.93344600	10.11790600
H	7.65224800	8.81441400	10.07933100

TS72: HO₂ + CH₃(CH₂)₁₄CH₃ → H₂O₂ + CH₃(CH₂)₆CH(CH₂)₇CH₃

C	-9.50991300	-0.22256400	-0.29568100
H	-9.63403900	-1.22073500	0.13279700
H	-9.50999500	-0.32720000	-1.38388000
H	-10.38163600	0.37261200	-0.01622100
C	-8.21164300	0.41832000	0.18773800
H	-8.12014700	1.42741300	-0.22872500
H	-8.24049100	0.53601100	1.27654000
C	-6.97673400	-0.39406000	-0.19609900
H	-6.94688500	-0.51174000	-1.28636400
H	-7.06620900	-1.40553300	0.21925900
C	-5.67075400	0.23616700	0.27992900
H	-5.69813700	0.34748900	1.37087400
H	-5.58670700	1.24978800	-0.13030700
C	-4.43439000	-0.56794500	-0.11521100
H	-4.40948800	-0.67896800	-1.20605600
H	-4.51374000	-1.58189200	0.29597400
C	-3.13159000	0.07327500	0.35470300
H	-3.14882200	0.17252000	1.44713400
H	-3.05477400	1.08929000	-0.04889200
C	-1.89126600	-0.71422700	-0.06124100
H	-1.87645200	-0.82476200	-1.15162800
H	-1.94095000	-1.73017200	0.35347900
C	-0.59658800	-0.05977900	0.38976900
H	-0.59102600	0.09625100	1.47504800
H	-0.59818800	0.99607500	-0.06780500
C	0.67938700	-0.74129300	-0.07283700
H	0.65097300	-0.85757500	-1.16223700
H	0.71424600	-1.75529900	0.34772000
C	1.94072900	0.02146100	0.32504700
H	1.96333400	0.14253400	1.41539000
H	1.89085700	1.02986700	-0.10254200
C	3.22740600	-0.65885100	-0.13441500
H	3.19978500	-0.78485600	-1.22345100
H	3.28013400	-1.66822100	0.29157600
C	4.48314900	0.11932700	0.25106100
H	4.51615700	0.23848600	1.34102200
H	4.42182300	1.13145400	-0.16711300
C	5.77332900	-0.54391200	-0.22392500
H	5.73795000	-0.66532400	-1.31345400
H	5.83920200	-1.55507600	0.19604300
C	7.02570800	0.24267500	0.15485800

H	7.06573300	0.35953800	1.24496400
H	6.95572000	1.25599300	−0.25960700
C	8.31830200	−0.40985600	−0.32932800
H	8.27671900	−0.52485500	−1.41797500
H	8.38834300	−1.42158100	0.08489200
C	9.55931400	0.39128800	0.05660800
H	9.63569000	0.49047900	1.14274800
H	10.47426500	−0.08458300	−0.30172200
H	9.51739000	1.39884700	−0.36559800
O	−0.56523200	2.41540800	−0.55987000
H	−0.19545900	2.80030300	0.25121900