

Supplementary Materials: The Diels-Alder Cycloaddition Reaction of Substituted Hemifullerenes with 1,3-butadiene: Effect of Electron-Donating and Electron-Withdrawing Substituents

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Table S1. Activation energy E_a , standard activation Gibbs energy $\Delta^\ddagger G^\circ$, standard activation enthalpy $\Delta^\ddagger H^\circ$, and standard activation entropy $T\Delta^\ddagger S^\circ$ for the Diels-Alder reaction between ethylene and butadiene. Comparison between the experimental values and the calculated values using the B3LYP, PBE, M06L, M06, PBE0 and MP2 methods. The experimental values are taken from K. N. Houk, R. J. Loncharich, J. F. Blake, W. L. Jorgensen, J. Am.Chem. Soc. 1989, 111, 9172, and V. Guner, K. S. Khuong, A. G. Leach, P. S. Lee, M. D. Bartberger, K. N. Houk, J. Phys. Chem. A 2003, 107, 11445.

Method	E_a kcal·mol ⁻¹	$\Delta^\ddagger G^\circ$ kcal·mol ⁻¹	$\Delta^\ddagger H^\circ$ kcal·mol ⁻¹	$T\Delta^\ddagger S^\circ$ kcal·mol ⁻¹
B3LYP	24.80	36.35	23.41	-12.93
PBE	15.72	27.09	14.47	-12.62
M06L	19.87	31.28	18.56	-12.71
M06	20.89	32.35	19.53	-12.82
PBE0	19.34	30.85	18.00	-12.85
MP2	19.39	30.98	18.00	-12.98
M06-2X	17.47	29.54	16.06	-13.48
Exp	27.5 ^a 24.2–26.7 ^b	-	24.2 ^d	-13.32 ^f
Calculated	25.9 ^c	-	24.9 ^e	-12.76 ^g

^a E_a Experimental; ^b E_a Experimental from the cyclohexane cycloreversion and the experimental heat of reaction; ^c E_a calculated; ^d $\Delta^\ddagger H^\circ$ Experimental; ^e $\Delta^\ddagger H^\circ$ calculated; ^f $T\Delta^\ddagger S^\circ$ Experimental; ^g $T\Delta^\ddagger S^\circ$ calculated.

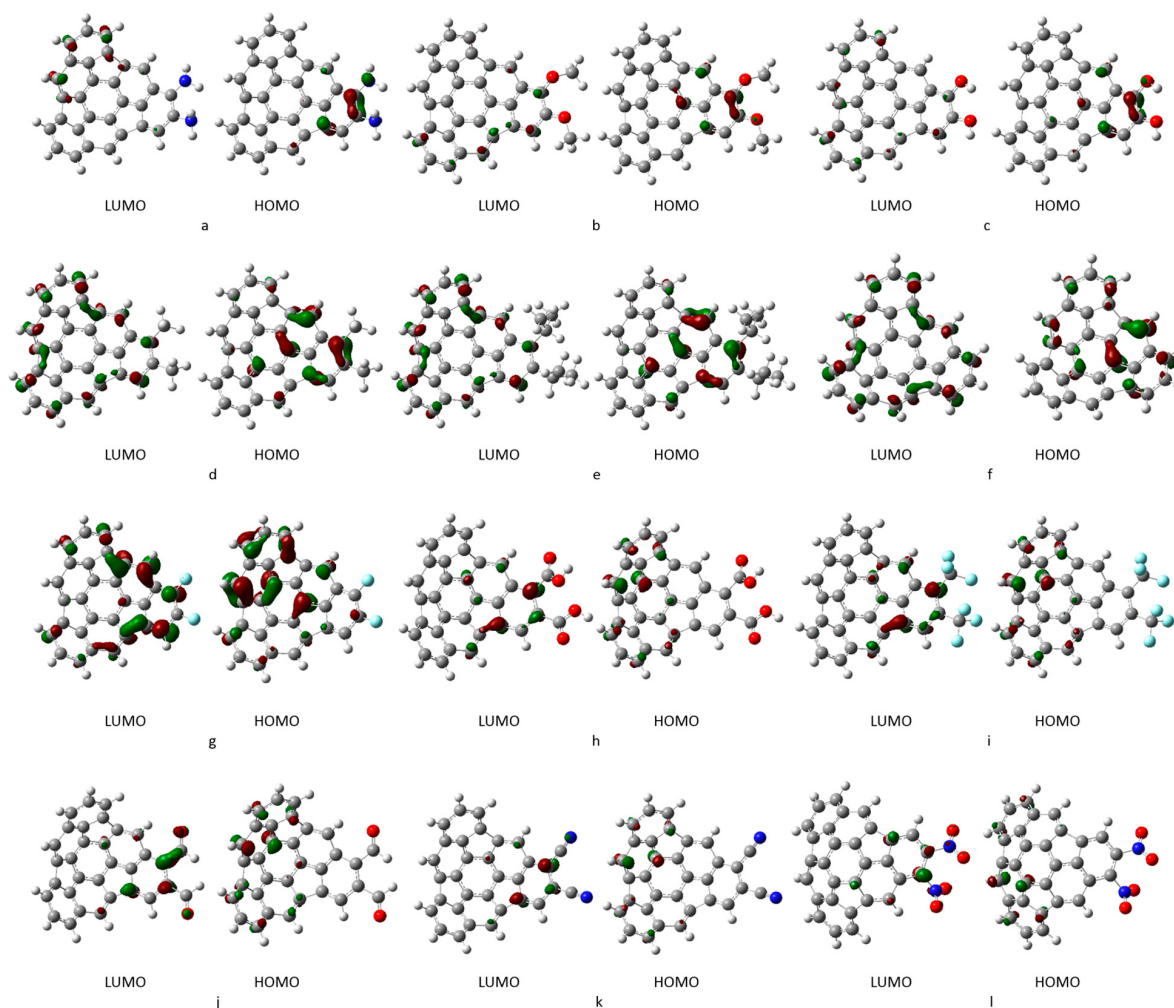


Figure S1. Frontier molecular orbitals HOMO and LUMO of the fragment 1 substituted with two equal molecular groups: (a) NH_2 ; (b) Ome; (c) OH; (d) Me; (e) *i*-Pr; (f) H; (g) F; (h) COOH; (i) CF_3 ; (j) CHO; (k) CN; (l) NO_2 . The substituent molecules are on the right side of the fragment. The large grey, blue and red spheres represent carbon, nitrogen and oxygen atoms, respectively, and hydrogen atoms are represented by the small grey spheres. The dark red and green surfaces represent the positive and negative lobes of the calculated molecular orbitals respectively, plotted at 0.08 au.

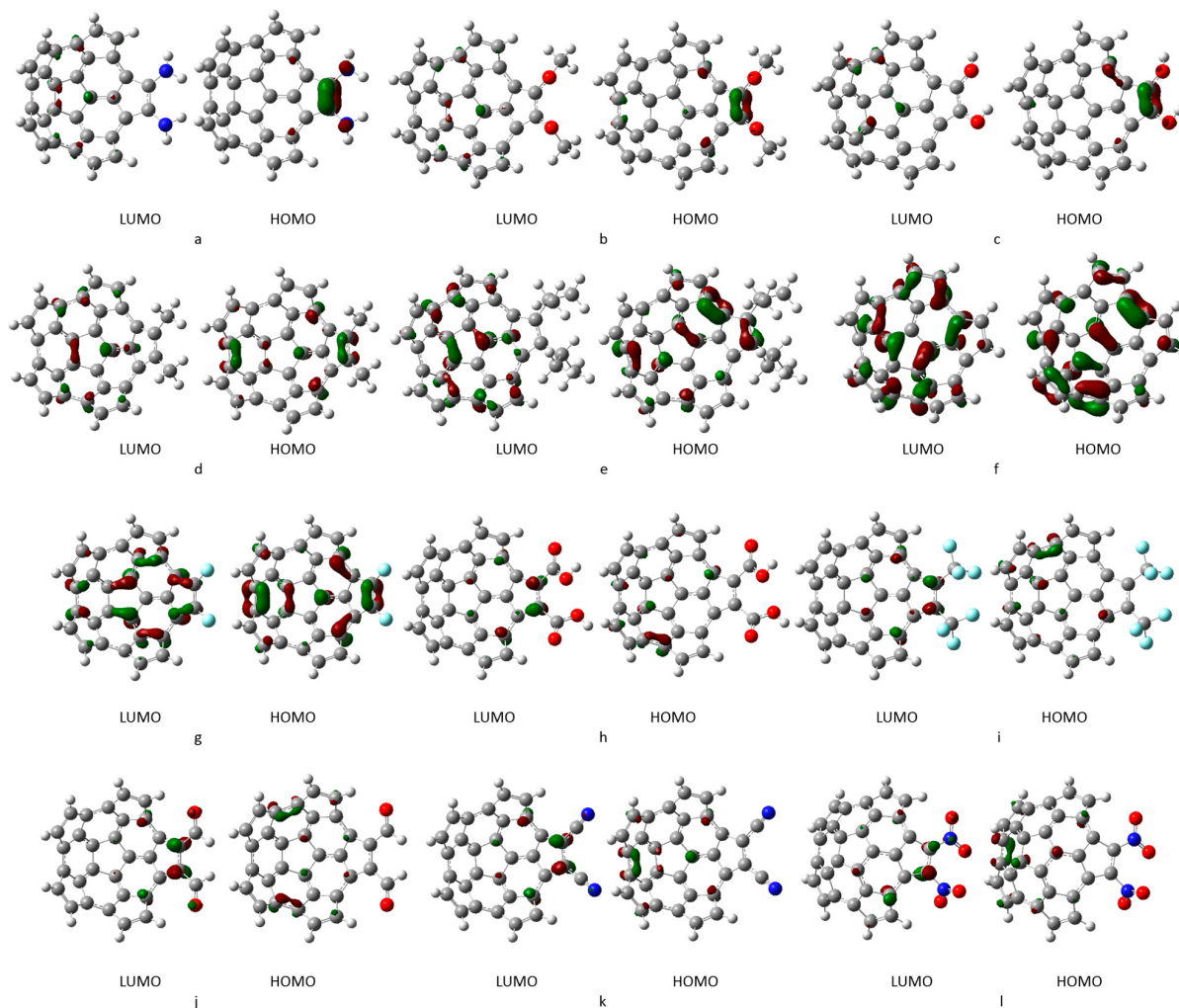


Figure S2. Frontier molecular orbitals HOMO and LUMO of the fragment 2 substituted with two equal molecular groups: (a) NH_2 ; (b) OMe ; (c) OH ; (d) Me ; (e) $i\text{-Pr}$; (f) H ; (g) F ; (h) COOH ; (i) CF_3 ; (j) CHO ; (k) CN ; (l) NO_2 . The substituent molecules are on the right side of the fragment. The large grey, blue and red spheres represent carbon, nitrogen and oxygen atoms, respectively, and hydrogen atoms are represented by the small grey spheres. The dark red and green surfaces represent the positive and negative lobes of the calculated molecular orbitals respectively, plotted at 0.08 au.

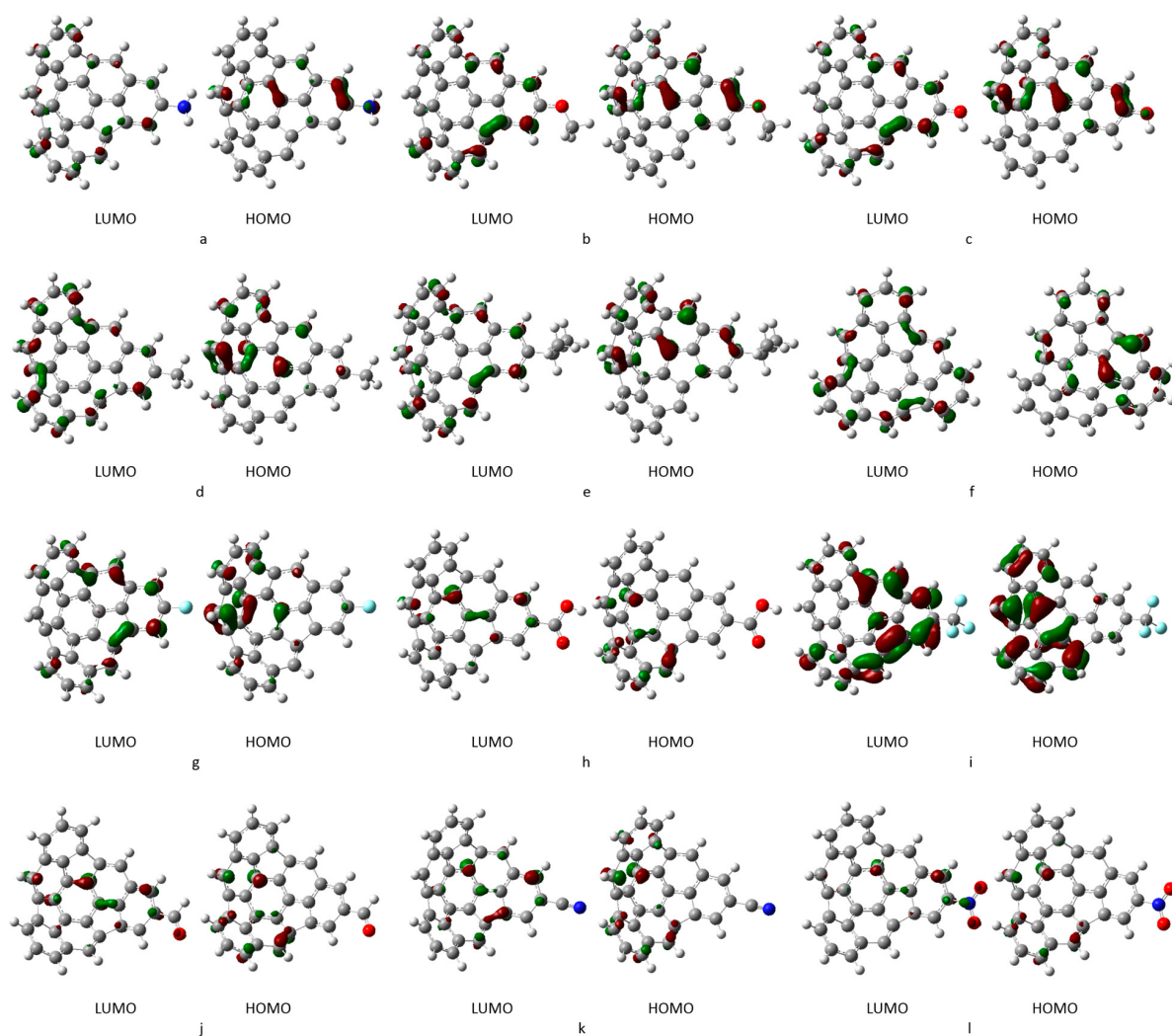


Figure S3. Frontier molecular orbitals HOMO and LUMO of the fragment **1** substituted with one molecular group: (a) NH₂; (b) OMe; (c) OH; (d) Me; (e) *i*-Pr; (f) H; (g) F; (h) COOH; (i) CF₃; (j) CHO; (k) CN; (l) NO₂. The substituent molecules are on the right side of the fragment. The large grey, blue and red spheres represent carbon, nitrogen and oxygen atoms, respectively, and hydrogen atoms are represented by the small grey spheres. The dark red and green surfaces represent the positive and negative lobes of the calculated molecular orbitals respectively, plotted at 0.08 au.

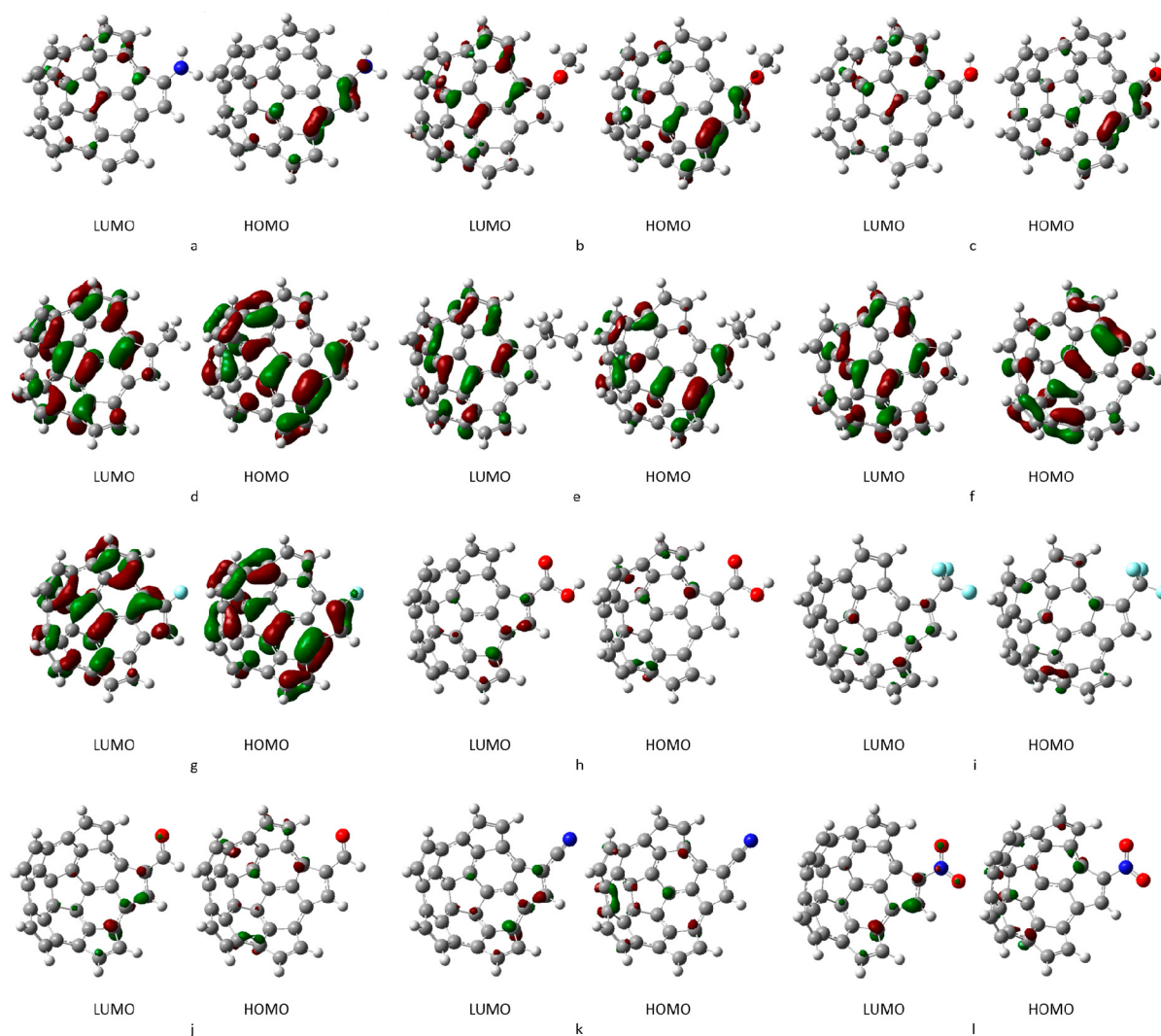


Figure S4. Frontier molecular orbitals HOMO and LUMO of the fragment **2** substituted with one molecular group: (a) NH_2 ; (b) OMe ; (c) OH ; (d) Me ; (e) $i\text{-Pr}$; (f) H ; (g) F ; (h) COOH ; (i) CF_3 ; (j) CHO ; (k) CN ; (l) NO_2 . The substituent molecules are on the right side of the fragment. The large grey, blue and red spheres represent carbon, nitrogen and oxygen atoms, respectively, and hydrogen atoms are represented by the small grey spheres. The dark red and green surfaces represent the positive and negative lobes of the calculated molecular orbitals respectively, plotted at 0.08 au.

Table S2. HOMO and LUMO energies (in eV) of the di-substituted ($R^1 = R^2$) and mono-substituted fragment **1**, and HOMO-LUMO gaps ΔE , for the NEDDA and IEDDA reactions with 1,3-butadiene. $\Delta E_{NEDDA} = ELUMO_{dienophile} - EHOMO_{diene}$ and $\Delta E_{IEDDA} = ELUMO_{diene} - EHOMO_{dienophile}$. Also, $\delta\Delta E = \Delta E_{IEDDA} - \Delta E_{NEDDA}$. Results for the reaction with the non-substituted fragment (row for H in the middle of the Table) are included for comparison.

Substituent R^1	EHOMO		ELUMO		ΔE_{NEDDA}		ΔE_{IEDDA}		$\delta\Delta E$	
	$R^2 = R^1$	$R^2 = H$	$R^2 = R^1$	$R^2 = H$	$R^2 = R^1$		$R^2 = R^1$	$R^2 = H$	$R^2 = R^1$	$R^2 = H$
NH ₂	-6.70	-6.95	1.48	1.38	10.26	10.16	10.15	10.40	-0.11	0.25
OMe	-7.01	-7.10	1.39	1.31	10.16	10.09	10.46	10.55	0.29	0.46
OH	-7.02	-7.17	1.38	1.27	10.16	10.04	10.47	10.62	0.31	0.58
Me	-7.13	-7.23	1.42	1.38	10.20	10.16	10.58	10.67	0.39	0.52
<i>i</i> -Pr	-7.15	-7.21	1.47	1.38	10.18	10.15	10.60	10.66	0.42	0.50
H	-7.28	-7.28	1.38	1.38	10.15	10.15	10.73	10.73	0.58	0.58
F	-7.50	-7.38	1.08	1.16	9.42	9.87	10.96	10.83	1.53	0.96
COOH	-7.53	-7.43	0.71	1.09	9.48	9.86	10.98	10.88	1.50	1.02
CF ₃	-7.67	-7.51	0.65	1.10	9.42	9.87	11.12	10.96	1.70	1.08
CHO	-7.57	-7.48	0.32	1.02	9.10	9.80	11.02	10.92	1.92	1.13
CN	-7.85	-7.61	0.17	0.90	8.94	9.67	11.29	11.05	2.35	1.38
NO ₂	-7.94	-7.67	-0.03	0.67	8.75	9.44	11.39	11.11	2.64	1.67

EHOMO butadieno = -8.77, ELUMO butadieno = 3.45.

Table S3. Standard Gibbs energies $\Delta_r G^\circ$, enthalpies $\Delta_r H^\circ$, and entropies $T\Delta_r S^\circ$ for the reaction of butadiene with the substituted fragment **1**.

Substituent R^1	$\Delta_r G^\circ$ (kcal·mol ⁻¹)		$\Delta_r H^\circ$ (kcal·mol ⁻¹)		$T\Delta_r S^\circ$ (kcal·mol ⁻¹)	
	$R^2 = R^1$	$R^2 = H$	$R^2 = R^1$	$R^2 = H$	$R^2 = R^1$	$R^2 = H$
NH ₂	25.06	17.78	9.56	2.83	-15.50	-15.88
OMe	22.26	15.45	6.18	0.58	-16.08	-14.87
OH	15.05	12.03	-0.62	-2.74	-15.67	-14.78
Me	16.03	12.19	-0.27	-3.69	-16.30	-15.88
<i>i</i> -Pr	26.27	16.40	9.25	0.49	-17.01	-15.91
H	10.34	10.34	-4.28	-4.28	-14.62	-14.62
F	5.97	7.88	-9.00	-6.74	-14.97	-14.62
COOH	15.33	15.24	-0.33	0.51	-15.65	-14.74
CF ₃	11.32	10.73	-5.16	-5.13	-16.48	-15.86
CHO	17.05	16.27	2.18	1.56	-14.87	-14.71
CN	23.95	16.52	9.14	1.91	-14.82	-14.61
NO ₂	3.83	10.55	-12.19	-4.59	-16.02	-15.14

Table S4. Standard Gibbs energies $\Delta_r G^\circ$, enthalpies $\Delta_r H^\circ$, and entropies $T\Delta_r S^\circ$ for the aromatization reaction of the DA cycloadduct 3 in Scheme 1.

Substituent R^1	$\Delta_r G^\circ$ (kcal·mol ⁻¹)		$\Delta_r H^\circ$ (kcal·mol ⁻¹)		$T\Delta_r S^\circ$ (kcal·mol ⁻¹)	
	$R^2 = R^1$	$R^2 = H$	$R^2 = R^1$	$R^2 = H$	$R^2 = R^1$	$R^2 = H$
NH ₂	-65.89	-46.18	-41.55	-25.75	24.33	20.43
OMe	-68.02	-44.73	-42.34	-23.76	25.68	20.97
OH	-54.80	-40.80	-31.14	-20.85	23.66	19.95
Me	-64.19	-42.89	-39.18	-21.85	25.01	21.04
<i>i</i> -Pr	-83.86	-47.47	-55.81	-25.55	28.05	21.92
H	-26.56	-26.56	-9.80	-9.80	16.77	16.77
F	-43.77	-32.55	-22.97	-13.84	20.79	18.71
COOH	-38.94	-29.87	-12.84	-8.86	26.10	21.02
CF ₃	-49.38	-32.76	-22.94	-11.30	26.43	21.47
CHO	-39.14	-31.57	-15.01	-10.88	24.14	20.69
CN	-45.23	-33.42	-23.57	-14.24	21.66	19.17
NO ₂	-45.84	-31.90	-20.39	-10.91	25.45	20.99

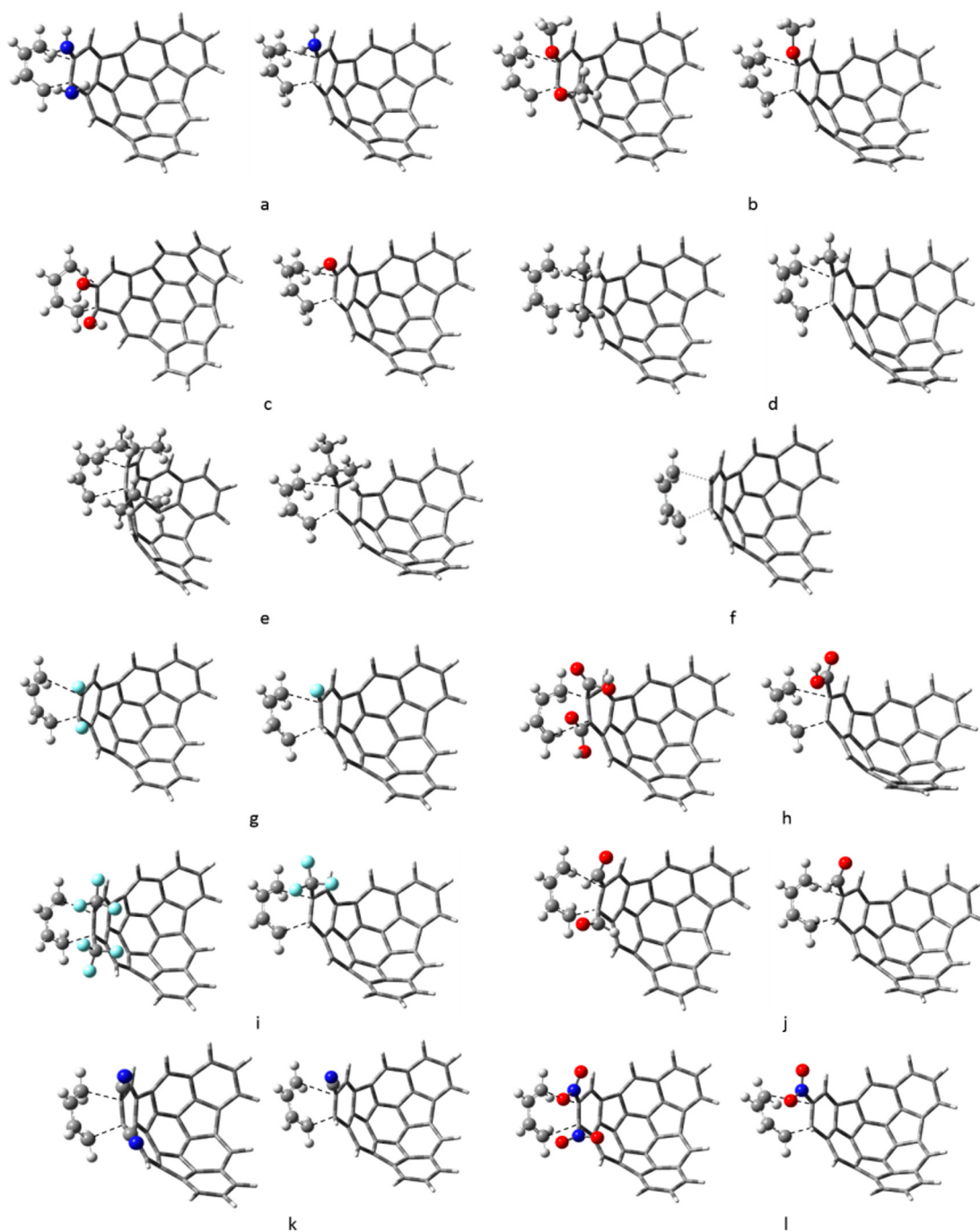


Figure S5. Transition state structures for the reaction of butadiene with fragment 1 substituted with two and one groups: (a) NH₂; (b) OMe; (c) OH; (d) Me; (e) *i*-Pr; (f) H; (g) F; (h) COOH; (i) CF₃; (j) CHO; (k) CN; (l) NO₂.

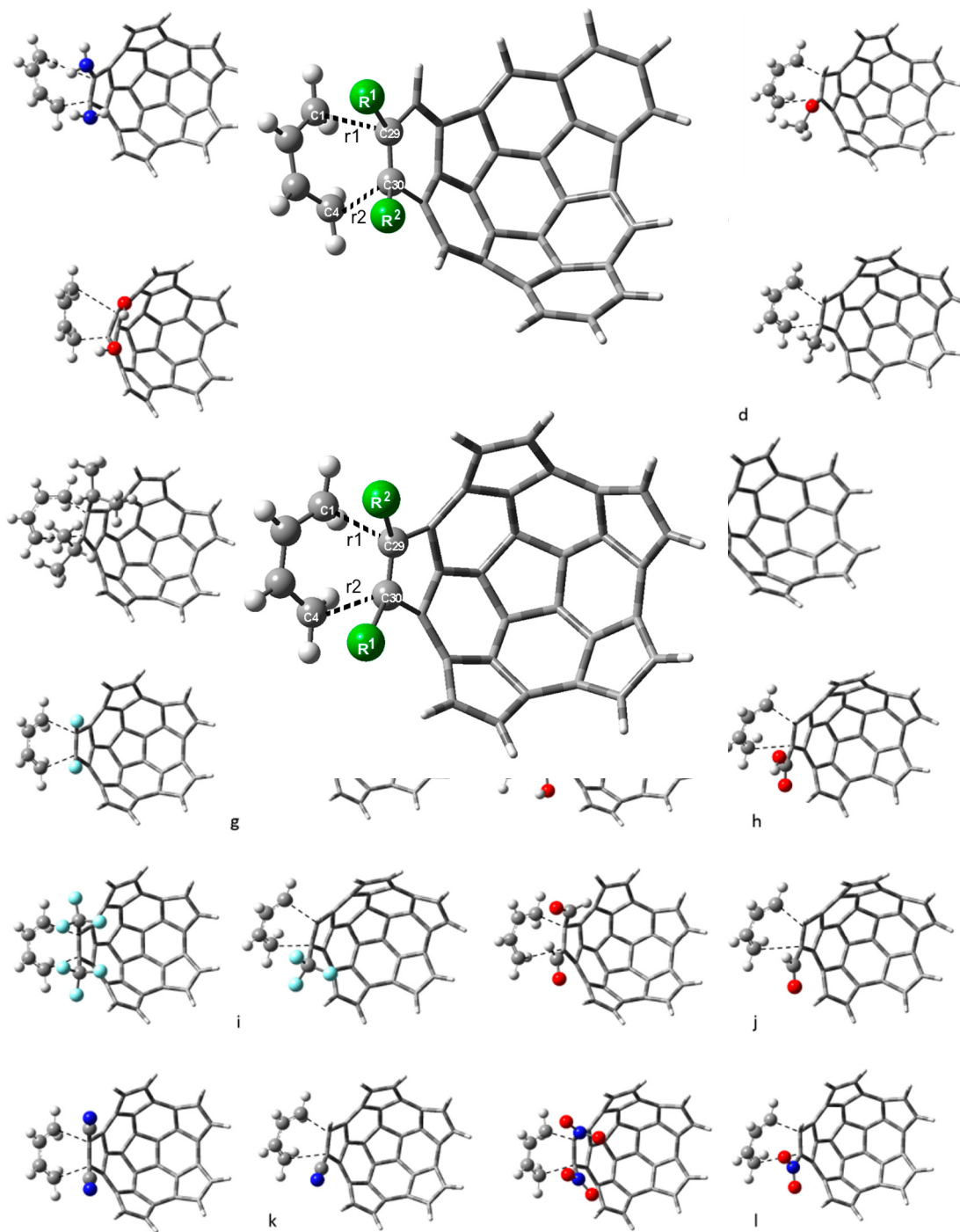


Figure S6. Transition state structures for the reaction of butadiene with fragment 2 substituted with two and one groups: (a) NH₂; (b) OMe; (c) OH; (d) Me; (e) *i*-Pr; (f) H; (g) F; (h) COOH; (i) CF₃; (j) CHO; (k) CN; (l) NO₂.

Figure S7. Definition of the transition distances r1 and r2.

Table S5. Distances r_1 and r_2 , in Å, for the transition states of reactions of fragment **1** shown in Figure S5. Also $\Delta r = r_1 - r_2$.

Substituent R^1	r_1		r_2		Δr	
	$R^2 = R^1$	$R^2 = H$	$R^2 = R^1$	$R^2 = H$	$R^2 = R^1$	$R^2 = H$
NH ₂	2.61	2.59	1.67	1.87	0.74	0.72
OMe	2.63	2.63	1.67	1.70	0.96	0.93
OH	2.76	2.72	1.68	1.71	1.08	1.01
Me	2.55	2.58	1.86	1.86	0.69	0.72
<i>i</i> -Pr	2.36	2.66	1.99	1.80	0.37	0.86
H	2.36	2.36	2.02	2.02	0.34	0.34
F	2.84	2.36	1.72	2.01	1.12	0.35
COOH	2.74	2.61	1.76	1.84	0.98	0.77
CF ₃	2.36	2.36	2.04	2.03	0.32	0.33
CHO	2.67	2.61	1.83	1.85	0.84	0.76
CN	2.23	2.64	2.08	1.84	0.15	0.80
NO ₂	2.55	3.20	2.42	1.73	0.13	1.47

Table S6. Activation energy E_a , standard activation Gibbs energy $\Delta^\ddagger G^\circ$, standard activation enthalpy $\Delta^\ddagger H^\circ$, and standard activation entropy $T\Delta^\ddagger S^\circ$ for the Diels-Alder reactions of butadiene with the substituted fragment **1**. Data for the reaction with the non-substituted fragment (H) are given as reference.

Substituent R^1	E_a (kcal·mol ⁻¹)		$\Delta^\ddagger G^\circ$ (kcal·mol ⁻¹)		$\Delta^\ddagger H^\circ$ (kcal·mol ⁻¹)		$T\Delta^\ddagger S^\circ$ (kcal·mol ⁻¹)	
	$R^2 = R^1$	$R^2 = H$	$R^2 = R^1$	$R^2 = H$	$R^2 = R^1$	$R^2 = H$	$R^2 = R^1$	$R^2 = H$
NH ₂	38.94	31.29	53.03	45.14	37.73	30.15	-15.29	-14.99
OMe	34.82	32.51	49.55	46.44	33.59	31.55	-15.97	-14.90
OH	35.06	31.24	49.16	45.05	33.85	30.13	-15.31	-14.92
Me	40.37	35.51	54.30	49.08	39.31	34.68	-14.99	-14.39
<i>i</i> -Pr	54.40	36.88	68.53	50.79	53.41	36.09	-15.12	-14.70
H	33.11	33.11	46.03	46.03	32.47	32.47	-13.56	-13.56
F	33.50	34.23	47.08	47.03	32.73	33.67	-14.35	-13.36
COOH	35.98	32.61	50.39	46.25	35.07	31.90	-15.32	-14.35
CF ₃	37.65	34.10	51.87	47.79	36.80	33.40	-15.06	-14.39
CHO	35.96	32.58	49.66	45.98	35.16	31.88	-14.51	-14.10
CN	38.52	33.64	51.80	46.77	37.87	33.03	-13.93	-13.74
NO ₂	32.79	28.71	47.19	42.52	31.88	27.90	-15.31	-14.62

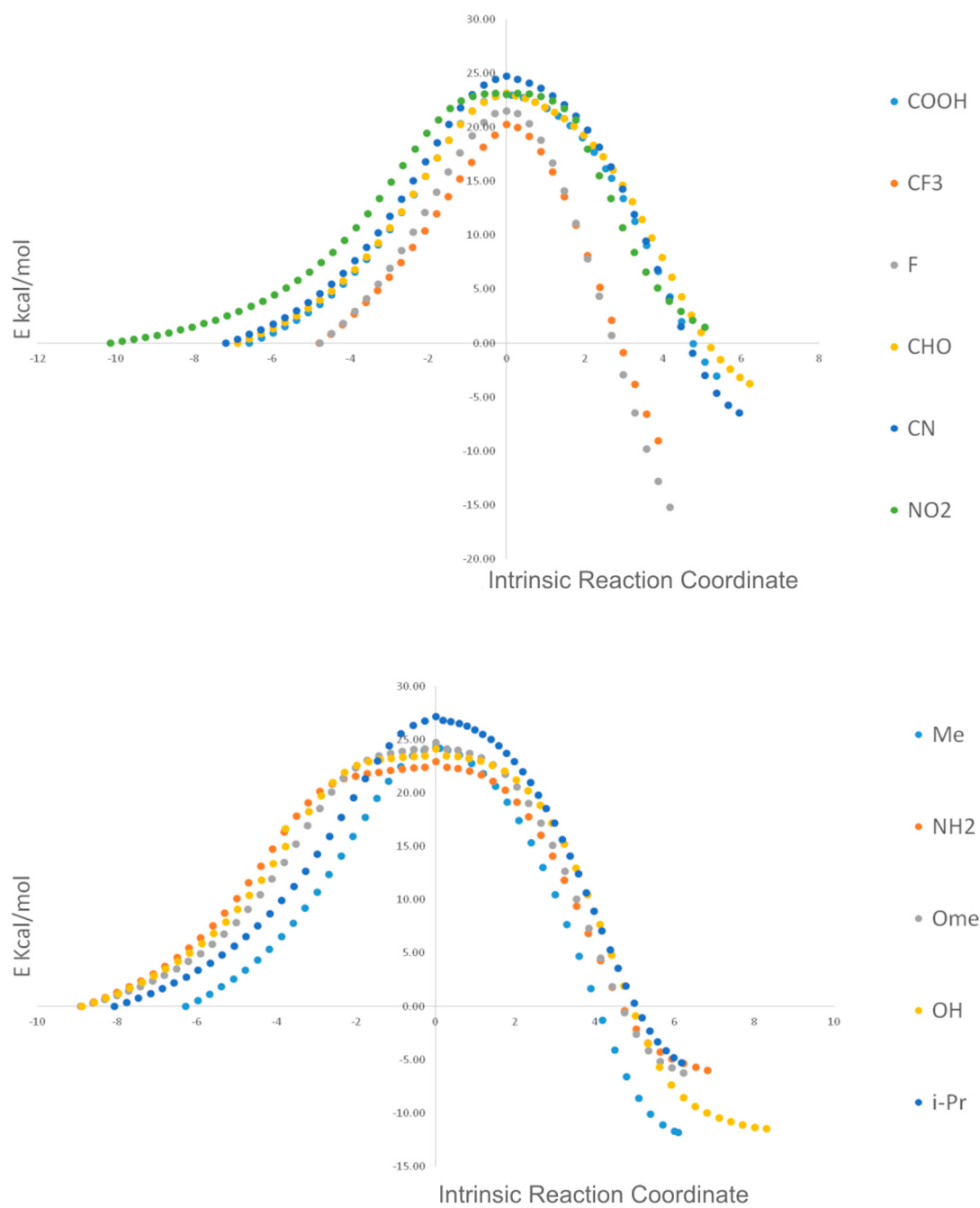


Figure S8. Intrinsic Reaction Coordinate for the reaction of 1,3-butadiene with mono-substituted fragment 1.

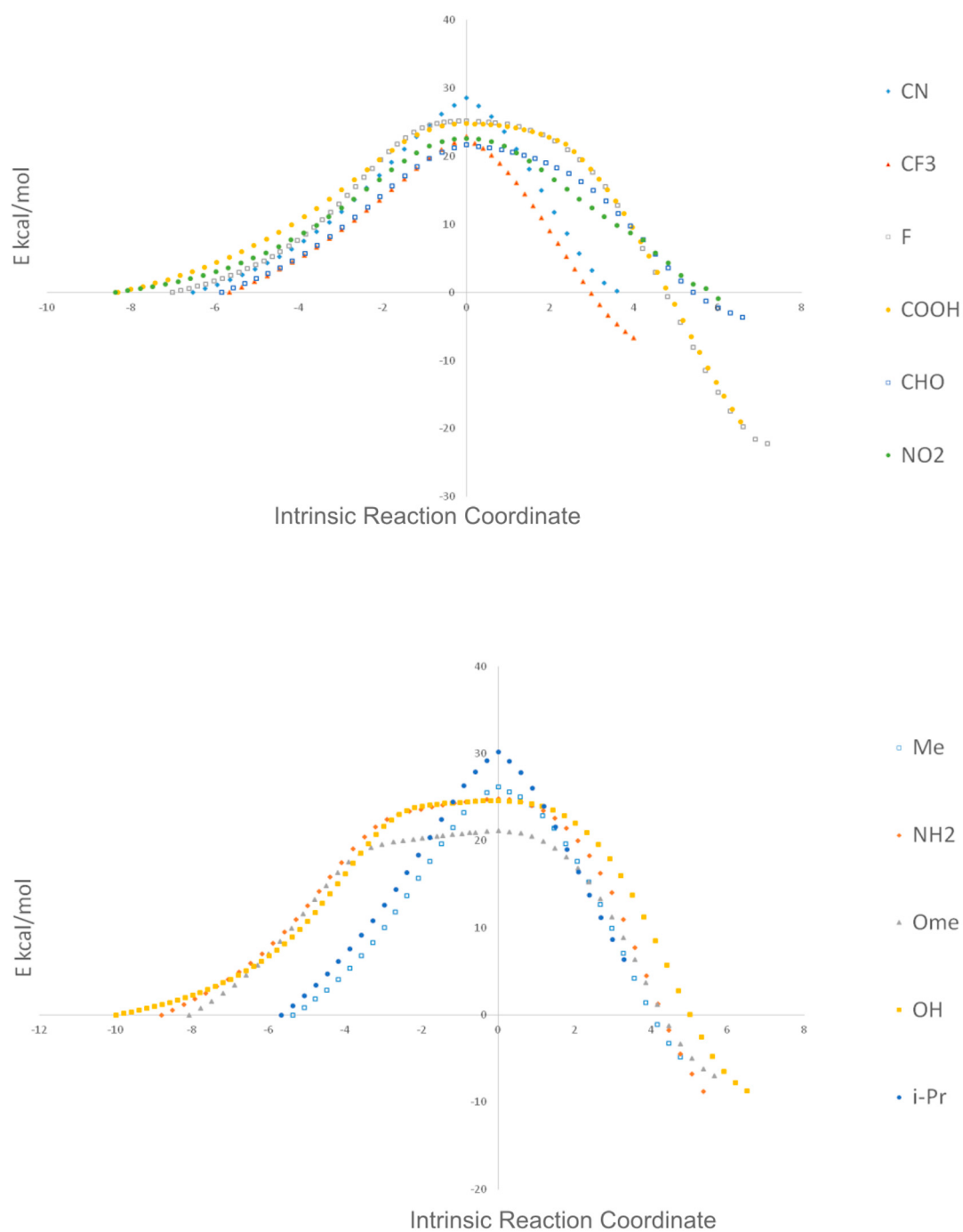


Figure S9. Intrinsic Reaction Coordinate for the reaction of 1,3-butadiene with di-substituted fragment 1.

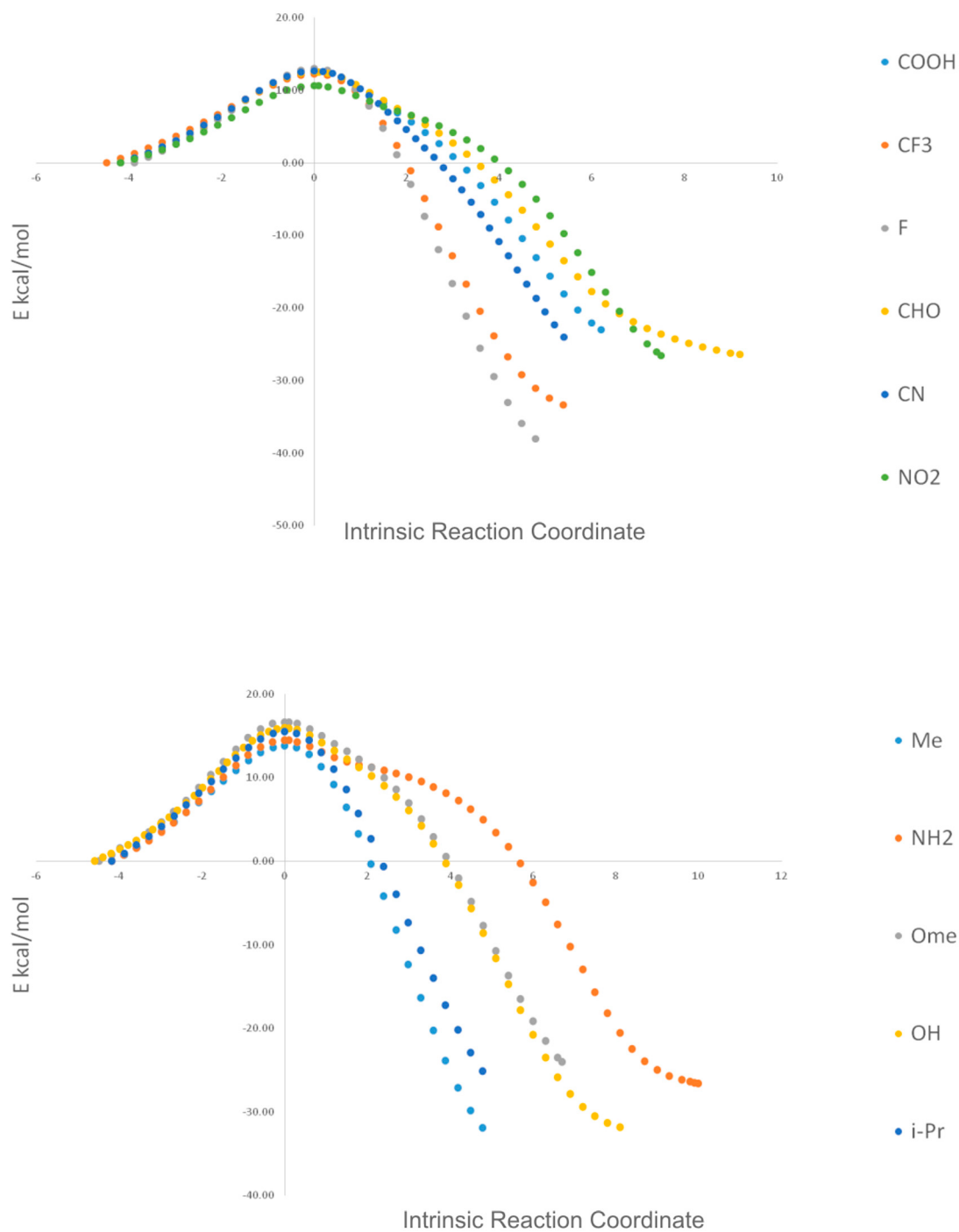


Figure S10. Intrinsic Reaction Coordinate for the reaction of 1,3-butadiene with mono-substituted fragment 2.

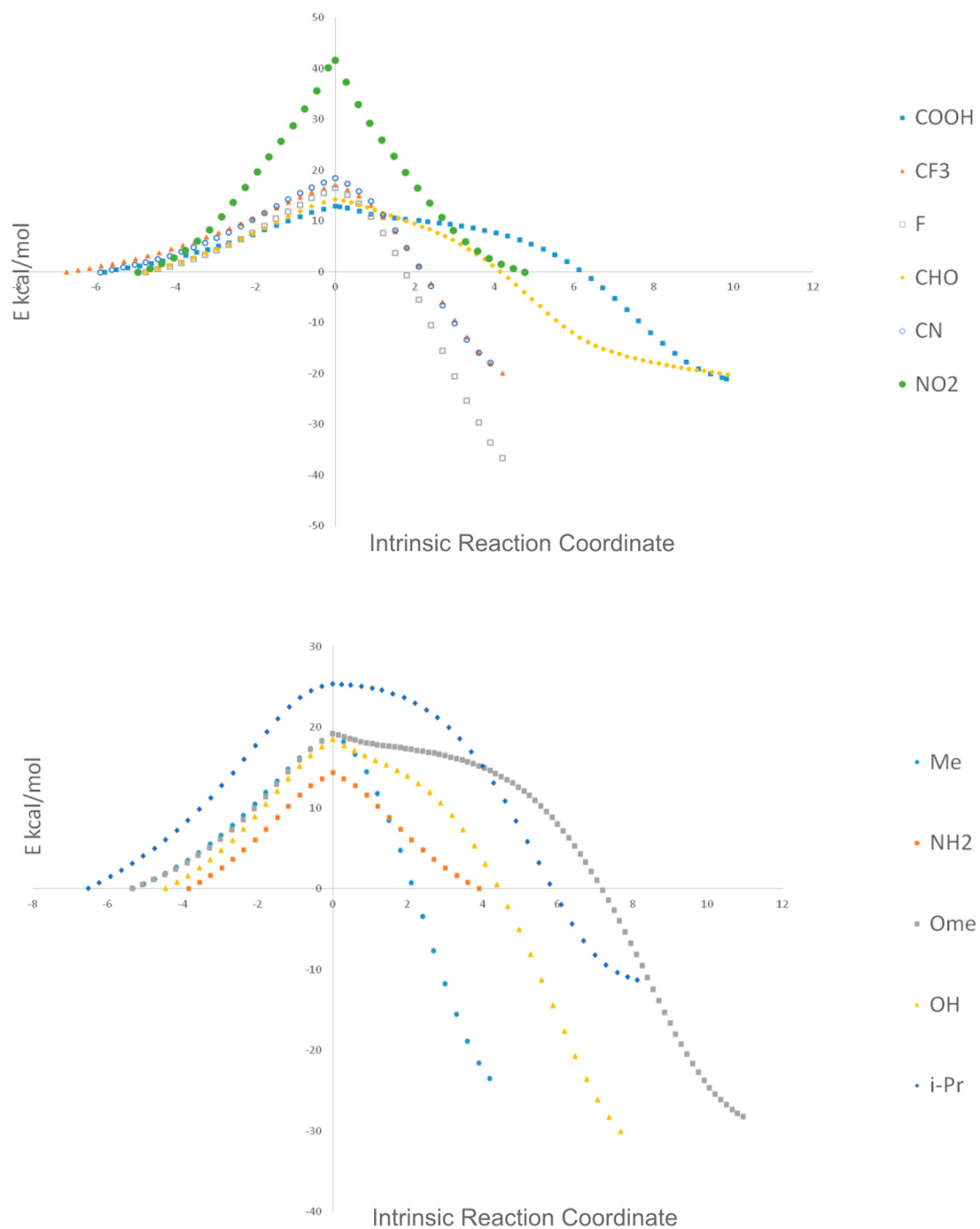


Figure S11. Intrinsic Reaction Coordinate for the reaction of 1,3-butadiene with di-substituted fragment 2.

Fragment 1

Molecular formula: C30H12

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.332792

Thermal correction to Enthalpy= 0.333736

Thermal correction to Gibbs Free Energy= 0.273526

Sum of electronic and zero-point Energies= -1150.083705

Sum of electronic and thermal Energies= -1150.066947

Sum of electronic and thermal Enthalpies= -1150.066003

Sum of electronic and thermal Free Energies= -1150.126213

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

208.830 77.395 126.723

Cartesian coordinates

Atom X Y Z

C	-1.297727	-0.504713	-1.324324	H	3.545519	-4.086661	1.906669
C	-1.082265	0.905737	-1.312770	H	1.267288	-4.615444	1.134267
C	0.211558	1.376136	-1.325430	H	-1.560575	-3.811829	0.714113
C	1.325136	0.483986	-1.313755	H	-4.633942	1.212866	1.128690
C	1.085804	-0.871716	-1.325130	H	-5.315016	-1.023718	1.903758
C	-0.243607	-1.389970	-1.311253	H	-3.979909	-3.017536	1.449613
C	2.406165	1.052915	-0.547839	H	-2.521789	3.256338	0.712629
C	3.302233	0.179565	0.054601	H	-0.625018	4.948161	1.457077
C	3.056302	-1.253963	0.070946	H	1.769647	5.108261	1.910776
C	1.897092	-1.737282	-0.571430	H	3.366599	3.403534	1.130490
C	3.678563	-2.188937	0.943734				
C	3.059574	-3.400721	1.221635				
C	1.764289	-3.734658	0.742442				
C	1.142516	-2.878878	-0.148395				
C	-0.291047	-2.607928	-0.541360				
C	-1.495784	-2.947461	0.060062				
C	-2.615134	-2.018597	0.072353				
C	-2.453983	-0.773961	-0.571986				
C	-3.066006	0.450874	-0.151234				
C	-4.118835	0.341635	0.738875				
C	-4.477207	-0.946474	1.219594				
C	-3.736991	-2.088767	0.943948				
C	0.556478	2.511620	-0.572282				
C	-0.440924	3.271637	0.074141				
C	-1.805706	2.768924	0.057703				
C	-2.114651	1.556658	-0.545263				
C	0.058526	4.276223	0.948552				
C	1.417859	4.346206	1.224113				
C	2.354608	3.393681	0.740456				
C	1.923205	2.428849	-0.151667				
H	4.082100	0.556490	0.709534				
H	4.604849	-1.934185	1.448158				

Fragment 1 substituted with one NH₂ groupMolecular formula: C₃₀H₁₃N

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.350028

Thermal correction to Enthalpy= 0.350972

Thermal correction to Gibbs Free Energy= 0.287968

Sum of electronic and zero-point Energies= -1205.425543

Sum of electronic and thermal Energies= -1205.407307

Sum of electronic and thermal Enthalpies= -1205.406363

Sum of electronic and thermal Free Energies= -1205.469367

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

219.646 83.408 132.603

Cartesian coordinates

Atom X Y Z

C	-1.181905	1.241735	-1.319929	H	-3.894975	-4.036169	2.091999
C	0.238482	1.182979	-1.462992	H	-4.741651	-1.812736	1.445725
C	0.839948	-0.054590	-1.555559	H	-4.289367	1.111487	1.033729
C	0.075840	-1.259820	-1.486927	H	0.415877	4.702775	1.049537
C	-1.293207	-1.167811	-1.355024	H	-1.793522	5.124669	2.059749
C	-1.948898	0.097744	-1.253030	H	-3.676160	3.590812	1.764326
C	0.833189	-2.288202	-0.814692	H	2.620768	2.818404	0.376287
C	0.124673	-3.288778	-0.157987	H	3.429126	-3.028496	0.580793
C	-1.319767	-3.198928	0.010936	N	5.354885	-1.387222	1.313934
C	-1.986384	-2.082711	-0.542146	H	5.788006	-0.670729	1.880547
C	-2.094264	-3.939577	0.948226	H	5.291000	-2.268527	1.805163
C	-3.334003	-3.462135	1.359932	H	4.570611	1.108512	0.887051
C	-3.851823	-2.199938	0.957027				
C	-3.158305	-1.465905	0.008977				
C	-3.083448	-0.002242	-0.367155				
C	-3.488530	1.150572	0.298589				
C	-2.680554	2.361812	0.258531				
C	-1.492618	2.346103	-0.506367				
C	-0.300260	3.079771	-0.193095				
C	-0.431653	4.100802	0.733384				
C	-1.697849	4.310182	1.347263				
C	-2.780153	3.456360	1.163809				
C	2.081258	-0.290477	-0.942530				
C	2.797092	0.764117	-0.333891				
C	2.150097	2.068326	-0.255571				
C	0.854570	2.259792	-0.726675				
C	3.933450	0.363280	0.416217				
C	4.197069	-0.994574	0.638533				
C	3.278049	-2.012985	0.221672				
C	2.188647	-1.666108	-0.551805				
H	0.647238	-4.042363	0.427329				
H	-1.693669	-4.845436	1.395977				

Fragment 1 substituted with one OMe group

Molecular formula: C31H14O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.367124

Thermal correction to Enthalpy= 0.368069

Thermal correction to Gibbs Free Energy= 0.301971

Sum of electronic and zero-point Energies= -1264.575106

Sum of electronic and thermal Energies= -1264.555693

Sum of electronic and thermal Enthalpies= -1264.554749

Sum of electronic and thermal Free Energies= -1264.620847

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

230.374 86.586 139.115

Cartesian coordinates

Atom X Y Z

C	-1.235628	1.270262	-1.323159	H	-3.645578	-4.100755	2.169325
C	0.176081	1.243715	-1.538419	H	-4.575218	-1.891491	1.592118
C	0.798306	0.022222	-1.679771	H	-4.209511	1.045302	1.189415
C	0.066761	-1.200361	-1.584877	H	0.405602	4.745876	0.996303
C	-1.295193	-1.140919	-1.379360	H	-1.756711	5.106370	2.125150
C	-1.972179	0.107973	-1.228758	H	-3.616208	3.531231	1.912871
C	0.882151	-2.216211	-0.962718	H	2.616066	2.921784	0.185950
C	0.231804	-3.238694	-0.279656	H	3.546532	-2.916192	0.289834
C	-1.203495	-3.184549	-0.035076	O	5.446376	-1.099721	0.986457
C	-1.923800	-2.079337	-0.540907	C	5.809836	-2.438565	1.279736
C	-1.910401	-3.951831	0.933735	H	6.793917	-2.385183	1.747771
C	-3.137257	-3.507168	1.414797	H	5.107757	-2.909981	1.979904
C	-3.704089	-2.253565	1.053130	H	5.876087	-3.050922	0.371414
C	-3.078498	-1.495021	0.077536	H	4.640458	1.226457	0.584411
C	-3.056246	-0.026483	-0.286022				
C	-3.450261	1.110146	0.413131				
C	-2.673456	2.340355	0.343853				
C	-1.527395	2.359614	-0.482394				
C	-0.337824	3.118516	-0.224332				
C	-0.443458	4.127489	0.718498				
C	-1.680048	4.301270	1.399897				
C	-2.750361	3.423649	1.264666				
C	2.075169	-0.191524	-1.130622				
C	2.798254	0.876721	-0.551206				
C	2.127868	2.167123	-0.426428				
C	0.806018	2.330428	-0.824814				
C	3.978239	0.495148	0.131870				
C	4.272610	-0.859386	0.324740				
C	3.372199	-1.901091	-0.047080				
C	2.233276	-1.564021	-0.762826				
H	0.801194	-3.984155	0.271402				
H	-1.466111	-4.852109	1.350339				

Fragment 1 substituted with one OH groupMolecular formula: C₃₀H₁₂O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.337274

Thermal correction to Enthalpy= 0.338219

Thermal correction to Gibbs Free Energy= 0.275539

Sum of electronic and zero-point Energies= -1225.299321

Sum of electronic and thermal Energies= -1225.281305

Sum of electronic and thermal Enthalpies= -1225.280361

Sum of electronic and thermal Free Energies= -1225.343041

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

211.643 82.163 131.921

Cartesian coordinates

Atom X Y Z

C -1.232684 1.239518 -1.350418
C 0.184885 1.201158 -1.522097
C 0.804986 -0.026784 -1.609077
C 0.064190 -1.243234 -1.502763
C -1.302909 -1.172070 -1.340394
C -1.977516 0.083718 -1.245335
C 0.854151 -2.246226 -0.829850
C 0.178393 -3.246483 -0.138600
C -1.263014 -3.178274 0.061774
C -1.961371 -2.083770 -0.495588
C -2.002458 -3.914604 1.030308
C -3.240299 -3.450532 1.462235
C -3.789053 -2.204887 1.048818
C -3.130796 -1.476913 0.071475
C -3.090173 -0.019377 -0.332513
C -3.499544 1.138508 0.321616
C -2.714563 2.362793 0.241006
C -1.544027 2.353575 -0.550297
C -0.358575 3.114055 -0.277967
C -0.487062 4.149495 0.632726
C -1.742683 4.348022 1.271317
C -2.813276 3.472011 1.128305
C 2.063764 -0.230050 -1.017444
C 2.774807 0.851009 -0.448312
C 2.108186 2.146248 -0.380392
C 0.798471 2.304120 -0.821500
C 3.937783 0.487246 0.279185
C 4.212331 -0.859608 0.515745
C 3.318855 -1.908156 0.147580
C 2.202399 -1.596178 -0.608200
H 0.726987 -3.979917 0.448473
H -1.575870 -4.804932 1.485014

H -3.774008 -4.020041 2.217761
H -4.673732 -1.823798 1.551386
H -4.282497 1.099269 1.075740
H 0.3565060 4.771654 0.918703
H -1.836713 5.173524 1.971111
H -3.697651 3.601857 1.746715
H 2.582827 2.916461 0.223150
H 3.496154 -2.911415 0.531010
O 5.351650 -1.138054 1.222842
H 5.422160 -2.092852 1.349472
H 4.589802 1.230595 0.726622

Fragment 1 substituted with one Me group

Molecular formula: C31H14

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.361318

Thermal correction to Enthalpy= 0.362262

Thermal correction to Gibbs Free Energy= 0.298181

Sum of electronic and zero-point Energies= -1189.377335

Sum of electronic and thermal Energies= -1189.358806

Sum of electronic and thermal Enthalpies= -1189.357862

Sum of electronic and thermal Free Energies= -1189.421944

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

226.731 83.364 134.871

Cartesian coordinates

Atom X Y Z

C -1.207174 1.241183 -1.330697
C 0.214144 1.194210 -1.464549
C 0.828055 -0.037830 -1.550610
C 0.077221 -1.250367 -1.470801
C -1.293554 -1.171043 -1.343351
C -1.960524 0.088771 -1.252899
C 0.843323 -2.264530 -0.787113
C 0.142078 -3.266785 -0.124249
C -1.303386 -3.189828 0.039980
C -1.980051 -2.085277 -0.524393
C -2.072828 -3.929643 0.982268
C -3.317944 -3.460616 1.387128
C -3.847354 -2.207138 0.972008
C -3.159179 -1.475094 0.018683
C -3.097576 -0.014244 -0.370368
C -3.515908 1.141558 0.281769
C -2.721940 2.361739 0.230855
C -1.531697 2.351100 -0.530405
C -0.348739 3.101957 -0.222689
C -0.494560 4.131535 0.692185
C -1.764706 4.332913 1.300510
C -2.836661 3.464662 1.123987
C 2.067552 -0.253787 -0.923904
C 2.770825 0.817922 -0.334703
C 2.114669 2.116505 -0.271796
C 0.816442 2.289098 -0.743598
C 3.913043 0.428839 0.421669
C 4.188458 -0.914756 0.671601
C 3.284159 -1.943828 0.259437
C 2.190217 -1.625482 -0.523628
H 0.670625 -4.009383 0.469515
H -1.664291 -4.827259 1.439210

H -3.874660 -4.033365 2.123381
H -4.741805 -1.824344 1.455664
H -4.318515 1.101800 1.014967
H 0.344986 4.746644 1.004201
H -1.871391 5.153824 2.003910
H -3.735560 3.595212 1.720946
H 2.582296 2.879965 0.346128
H 3.445079 -2.953769 0.629589
C 5.410928 -1.306144 1.470265
H 6.149932 -1.814723 0.839012
H 5.899098 -0.433146 1.911455
H 5.155219 -1.996417 2.281951
H 4.549324 1.188423 0.869946

Fragment 1 substituted with one *i*-Pr groupMolecular formula: C₃₃H₁₈

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.420864

Thermal correction to Enthalpy= 0.421808

Thermal correction to Gibbs Free Energy= 0.351429

Sum of electronic and zero-point Energies= -1267.951792

Sum of electronic and thermal Energies= -1267.930592

Sum of electronic and thermal Enthalpies= -1267.929647

Sum of electronic and thermal Free Energies= -1268.000027

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

264.096 93.604 148.126

Cartesian coordinates

Atom X Y Z

C -1.236467 1.265149 -1.240615
C 0.183188 1.222130 -1.389888
C 0.795267 -0.006036 -1.524075
C 0.044989 -1.220243 -1.478599
C -1.324510 -1.145050 -1.335212
C -1.989896 0.110863 -1.195173
C 0.817589 -2.256847 -0.836439
C 0.121987 -3.281181 -0.201843
C -1.321961 -3.209978 -0.021801
C -2.003639 -2.086765 -0.541505
C -2.082823 -3.981851 0.901540
C -3.323902 -3.526983 1.334025
C -3.856630 -2.259800 0.967584
C -3.177151 -1.495437 0.033547
C -3.118237 -0.022009 -0.305459
C -3.528895 1.110673 0.390547
C -2.734817 2.331800 0.373735
C -1.552312 2.347127 -0.399421
C -0.366361 3.087497 -0.078535
C -0.502796 4.085724 0.871884
C -1.766630 4.265987 1.499604
C -2.840303 3.403756 1.304874
C 2.040112 -0.243886 -0.914518
C 2.750801 0.807367 -0.296128
C 2.095538 2.104807 -0.185096
C 0.793517 2.292756 -0.637926
C 3.896972 0.394659 0.436939
C 4.176576 -0.958935 0.642182
C 3.270137 -1.969457 0.199097
C 2.165773 -1.625783 -0.562530
H 0.655633 -4.043454 0.361670
H -1.670332 -4.894812 1.323180

H -3.873941 -4.124863 2.055163
H -4.746279 -1.893810 1.472615
H -4.324086 1.045799 1.130014
H 0.339933 4.690193 1.195845
H -1.866146 5.062651 2.231372
H -3.733071 3.513747 1.915032
H 2.569120 2.847052 0.453836
H 3.437284 -2.993077 0.525978
C 5.412132 -1.378748 1.435614
H 5.396910 -2.474860 1.493195
C 5.391304 -0.846752 2.880841
H 5.438566 0.247330 2.905483
H 4.479619 -1.152570 3.403127
H 6.250924 -1.226571 3.443702
C 6.713336 -0.977279 0.716121
H 6.802199 0.111650 0.636666
H 7.587970 -1.344002 1.264434
H 6.748809 -1.388409 -0.297334
H 4.531277 1.145043 0.902450

Fragment 1 substituted with one F groupMolecular formula: C₃₀H₁₁F

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.324600

Thermal correction to Enthalpy= 0.325544

Thermal correction to Gibbs Free Energy= 0.263507

Sum of electronic and zero-point Energies= -1249.323965

Sum of electronic and thermal Energies= -1249.306372

Sum of electronic and thermal Enthalpies= -1249.305428

Sum of electronic and thermal Free Energies= -1249.367465

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

203.690 80.350 130.569

Cartesian coordinates

Atom X Y Z

C -1.204229 1.232581 -1.335716
C 0.215604 1.179869 -1.479982
C 0.825019 -0.054080 -1.560479
C 0.070771 -1.263693 -1.470423
C -1.298266 -1.178834 -1.331940
C -1.960860 0.083498 -1.244457
C 0.837887 -2.277501 -0.788780
C 0.140091 -3.272772 -0.111972
C -1.303549 -3.189680 0.063705
C -1.980737 -2.085963 -0.501662
C -2.066913 -3.921035 1.017410
C -3.306897 -3.445055 1.429575
C -3.835551 -2.192464 1.010754
C -3.153399 -1.468529 0.046947
C -3.090822 -0.010366 -0.352070
C -3.499965 1.150929 0.296131
C -2.702646 2.368228 0.230395
C -1.518728 2.349047 -0.540401
C -0.331595 3.098824 -0.247423
C -0.466297 4.134723 0.661867
C -1.730901 4.344029 1.278890
C -2.806625 3.477632 1.116834
C 2.069943 -0.270404 -0.944656
C 2.781650 0.806968 -0.369377
C 2.129052 2.108167 -0.310826
C 0.826890 2.277871 -0.770545
C 3.932766 0.428160 0.376220
C 4.162952 -0.918962 0.603129
C 3.290230 -1.971153 0.230221
C 2.187934 -1.642602 -0.539879
H 0.671588 -4.013914 0.480829
H -1.657449 -4.817020 1.476500

H -3.859247 -4.010914 2.174279
H -4.724678 -1.803818 1.499444
H -4.296640 1.118691 1.036053
H 0.377606 4.749277 0.962814
H -1.829573 5.169855 1.977557
H -3.700273 3.615088 1.720009
H 2.604502 2.875101 0.296109
H 3.483169 -2.965690 0.618638
F 5.251385 -1.264501 1.328908
H 4.593201 1.156967 0.834338

Fragment 1 substituted with one COOH group

Molecular formula: C31H12O2

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.349992

Thermal correction to Enthalpy= 0.350936

Thermal correction to Gibbs Free Energy= 0.283834

Sum of electronic and zero-point Energies= -1338.646976

Sum of electronic and thermal Energies= -1338.627331

Sum of electronic and thermal Enthalpies= -1338.626386

Sum of electronic and thermal Free Energies= -1338.693489

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

219.623 87.424 141.229

Cartesian coordinates

Atom X Y Z

C	-2.045402	1.213422	-1.313051	H	-4.297149	-4.043832	2.453551
C	-0.655302	1.149523	-1.628804	H	-5.217708	-1.822261	1.911314
C	-0.072267	-0.089530	-1.800111	H	-4.819581	1.102797	1.423238
C	-0.819253	-1.294394	-1.622512	H	-0.164002	4.703469	0.793114
C	-2.160327	-1.199020	-1.315447	H	-2.224418	5.130650	2.077634
C	-2.793089	0.067947	-1.135104	H	-4.123658	3.589387	2.045477
C	0.017080	-2.319947	-1.049438	H	1.953819	2.818317	-0.165808
C	-0.602451	-3.316054	-0.300713	H	2.814002	-3.035738	-0.003716
C	-2.012412	-3.222554	0.052252	C	4.802750	-1.431251	0.567556
C	-2.744003	-2.107826	-0.415082	O	5.091852	-2.581994	0.834700
C	-2.659828	-3.957059	1.086173	O	5.650577	-0.403005	0.832416
C	-3.835098	-3.474858	1.651930	H	6.432071	-0.810364	1.240654
C	-4.399282	-2.213378	1.313331	H	3.957620	1.095832	0.093967
C	-3.833842	-1.485734	0.279426				
C	-3.805983	-0.024353	-0.111586				
C	-4.120544	1.135203	0.590424				
C	-3.328355	2.347772	0.434681				
C	-2.249716	2.326478	-0.477526				
C	-1.030289	3.066379	-0.329974				
C	-1.043218	4.096544	0.595709				
C	-2.219569	4.309447	1.366728				
C	-3.313157	3.450846	1.334771				
C	1.233222	-0.318918	-1.335887				
C	2.021882	0.750248	-0.854668				
C	1.395607	2.058512	-0.707959				
C	0.047893	2.241456	-0.997834				
C	3.250839	0.355353	-0.264438				
C	3.529232	-1.000343	-0.065940				
C	2.580249	-2.032511	-0.343726				
C	1.392855	-1.696076	-0.961648				
H	-0.008639	-4.066933	0.215533				
H	-2.205628	-4.861178	1.482860				

Fragment 1 substituted with one CF₃ groupMolecular formula: C₃₁H₁₁F₃

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.340468

Thermal correction to Enthalpy= 0.341412

Thermal correction to Gibbs Free Energy= 0.272006

Sum of electronic and zero-point Energies= -1487.116059

Sum of electronic and thermal Energies= -1487.095653

Sum of electronic and thermal Enthalpies= -1487.094708

Sum of electronic and thermal Free Energies= -1487.164114

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

213.647 89.920 146.077

Cartesian coordinates

Atom X Y Z

C 2.088414 -1.050182 -1.263137
C 0.714272 -1.327799 -1.530559
C -0.148815 -0.269261 -1.724426
C 0.297759 1.083590 -1.616845
C 1.631027 1.318775 -1.355005
C 2.550197 0.244722 -1.154218
C -0.740445 1.907319 -1.048245
C -0.354001 3.051519 -0.357114
C 1.047262 3.307440 -0.053607
C 2.007945 2.376637 -0.508716
C 1.530958 4.216551 0.929712
C 2.801960 4.048261 1.468192
C 3.638517 2.941541 1.152707
C 3.232772 2.058128 0.166247
C 3.540293 0.615859 -0.172513
C 4.139143 -0.406293 0.557624
C 3.650172 -1.776040 0.474910
C 2.571784 -2.047033 -0.396566
C 1.565433 -3.044747 -0.178100
C 1.845890 -4.002458 0.782342
C 3.060499 -3.900943 1.515916
C 3.920252 -2.812684 1.412919
C -1.460117 -0.333132 -1.223626
C -1.958948 -1.533320 -0.672517
C -1.039060 -2.649669 -0.500593
C 0.305454 -2.524427 -0.834194
C -3.231099 -1.411260 -0.049029
C -3.805488 -0.154846 0.114069
C -3.140370 1.058613 -0.233089
C -1.927390 0.982762 -0.889720
H -1.093615 3.663006 0.154848
H 0.887387 5.004668 1.311515

H 3.138597 4.743289 2.231988
H 4.542452 2.779702 1.733275
H 4.834241 -0.175253 1.361803
H 1.140081 -4.789157 1.033762
H 3.278311 -4.666998 2.254472
H 4.760390 -2.727397 2.097091
H -1.386662 -3.493868 0.090345
H -3.570022 2.002052 0.087595
C -5.164959 -0.036901 0.750354
F -5.562065 -1.182385 1.346211
F -6.113629 0.285584 -0.160801
F -5.192525 0.936374 1.692663
H -3.733062 -2.280543 0.361616

Fragment 1 substituted with one CHO group

Molecular formula: C31H12O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.343395

Thermal correction to Enthalpy= 0.344340

Thermal correction to Gibbs Free Energy= 0.279544

Sum of electronic and zero-point Energies= -1263.400880

Sum of electronic and thermal Energies= -1263.382126

Sum of electronic and thermal Enthalpies= -1263.381181

Sum of electronic and thermal Free Energies= -1263.445977

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

215.484 83.976 136.373

Cartesian coordinates

Atom X Y Z

C 1.598977 -0.971084 -1.271930
C 0.236939 -1.360032 -1.441082
C -0.718790 -0.374911 -1.587122
C -0.374882 1.010740 -1.527435
C 0.950363 1.353976 -1.360970
C 1.962171 0.358112 -1.208974
C -1.435390 1.762176 -0.903901
C -1.095047 2.945574 -0.255523
C 0.298817 3.313734 -0.048537
C 1.298052 2.452670 -0.555168
C 0.772717 4.273594 0.890385
C 2.085177 4.213015 1.345898
C 2.983919 3.169644 0.988277
C 2.585603 2.241494 0.040656
C 2.982740 0.822029 -0.300803
C 3.708041 -0.138136 0.398234
C 3.326310 -1.543478 0.363050
C 2.217345 -1.913056 -0.430164
C 1.311197 -2.984191 -0.133998
C 1.731862 -3.901630 0.814532
C 2.980652 -3.692212 1.462899
C 3.741032 -2.540465 1.291056
C -1.982276 -0.532371 -0.996760
C -2.348945 -1.764204 -0.407881
C -1.333593 -2.802683 -0.288065
C -0.027419 -2.575517 -0.708899
C -3.586235 -1.727160 0.287239
C -4.257025 -0.515253 0.472518
C -3.709298 0.743057 0.067829
C -2.533716 0.751522 -0.652588
H -1.845960 3.507306 0.295346
H 0.095399 5.015466 1.304986

H 2.414955 4.944218 2.078252
H 3.933414 3.087709 1.509918
H 4.434644 0.159740 1.150933
H 1.110519 -4.738556 1.120867
H 3.308420 -4.427087 2.192452
H 4.615223 -2.377952 1.915986
H -1.574459 -3.665066 0.329307
H -4.218802 1.641746 0.401086
C -5.527867 -0.525171 1.228231
H -5.864997 -1.535467 1.550960
O -6.182689 0.464854 1.498319
H -3.995432 -2.629574 0.737339

Fragment 1 substituted with one CN group

Molecular formula: C31H11N

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.332444

Thermal correction to Enthalpy= 0.333389

Thermal correction to Gibbs Free Energy= 0.268969

Sum of electronic and zero-point Energies= -1242.327866

Sum of electronic and thermal Energies= -1242.309293

Sum of electronic and thermal Enthalpies= -1242.308349

Sum of electronic and thermal Free Energies= -1242.372768

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

208.612 83.358 135.582

Cartesian coordinates

Atom X Y Z

C	1.466879	-1.049333	-1.280654	H	2.758658	4.746583	2.128947
C	0.077924	-1.326004	-1.450924	H	4.123094	2.781254	1.537573
C	-0.796089	-0.266957	-1.585090	H	4.388287	-0.175405	1.147014
C	-0.342527	1.085789	-1.510985	H	0.682246	-4.791811	1.072865
C	1.005810	1.320062	-1.342373	H	2.900343	-4.669313	2.141573
C	1.935718	0.245534	-1.204297	H	4.366492	-2.728541	1.883809
C	-1.338053	1.911663	-0.874667	H	-1.907360	-3.496146	0.305703
C	-0.904240	3.056344	-0.212822	H	-4.099278	2.011204	0.433486
C	0.514700	3.310939	-0.006717	C	-5.561824	-0.058539	1.212196
C	1.440904	2.378339	-0.525101	N	-6.564693	0.021755	1.797327
C	1.065244	4.220701	0.940204	H	-4.232301	-2.281582	0.734265
C	2.369830	4.051283	1.390687				
C	3.181718	2.943284	1.020040				
C	2.708787	2.059252	0.064507				
C	2.991382	0.616551	-0.293717				
C	3.638757	-0.406056	0.393251				
C	3.145398	-1.775884	0.344167				
C	2.008832	-2.046646	-0.449818				
C	1.020970	-3.045163	-0.162927				
C	1.368124	-4.004056	0.774230				
C	2.630969	-3.902493	1.421152				
C	3.480699	-2.813377	1.259903				
C	-2.068563	-0.329824	-0.994045				
C	-2.529613	-1.532701	-0.412451				
C	-1.599834	-2.650838	-0.305271				
C	-0.281847	-2.523867	-0.728497				
C	-3.755726	-1.413351	0.289878				
C	-4.326715	-0.149101	0.488014				
C	-3.681686	1.068620	0.094993				
C	-2.511151	0.987716	-0.632478				
H	-1.606242	3.670110	0.347038				
H	0.450260	5.010037	1.364112				

Fragment 1 substituted with one NO₂ groupMolecular formula: C₃₀H₁₁NO₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.337170

Thermal correction to Enthalpy= 0.338115

Thermal correction to Gibbs Free Energy= 0.271542

Sum of electronic and zero-point Energies= -1354.582741

Sum of electronic and thermal Energies= -1354.563420

Sum of electronic and thermal Enthalpies= -1354.562476

Sum of electronic and thermal Free Energies= -1354.629049

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

211.578 85.828 140.115

Cartesian coordinates

Atom X Y Z

C	-1.996410	1.228916	-1.311518	H	-4.316895	-4.047351	2.386284
C	-0.600193	1.168807	-1.595929	H	-5.229603	-1.825786	1.832835
C	-0.010887	-0.068387	-1.761263	H	-4.828888	1.102233	1.362853
C	-0.758816	-1.275988	-1.604828	H	-0.170242	4.716819	0.847220
C	-2.106073	-1.184232	-1.325645	H	-2.259308	5.134158	2.087858
C	-2.744906	0.080880	-1.153788	H	-4.153141	3.588170	2.008761
C	0.065943	-2.302061	-1.017720	H	1.973586	2.841435	-0.073270
C	-0.566509	-3.302146	-0.285020	H	2.841150	-3.018428	0.092501
C	-1.983776	-3.213208	0.037177	O	4.996386	-2.540825	0.902860
C	-2.706847	-2.097658	-0.441355	O	5.578342	-0.443547	0.988816
C	-2.651182	-3.953068	1.054470	N	4.792268	-1.344140	0.691250
C	-3.838916	-3.474834	1.596753	H	3.987199	1.102306	0.235261
C	-4.397947	-2.212960	1.250872				
C	-3.812513	-1.480300	0.231774				
C	-3.779542	-0.017491	-0.153211				
C	-4.111693	1.139014	0.545894				
C	-3.319705	2.354192	0.411516				
C	-2.221404	2.338854	-0.476801				
C	-1.008252	3.081913	-0.300395				
C	-1.043332	4.108455	0.628690				
C	-2.236778	4.315621	1.374414				
C	-3.326994	3.454134	1.315540				
C	1.283677	-0.295781	-1.269106				
C	2.058348	0.774838	-0.765660				
C	1.427770	2.082353	-0.628214				
C	0.086345	2.260941	-0.945559				
C	3.273812	0.383464	-0.149579				
C	3.526881	-0.971970	0.036308				
C	2.609647	-2.018676	-0.252759				
C	1.436849	-1.675052	-0.896007				
H	0.017752	-4.053899	0.240668				
H	-2.203986	-4.857936	1.457106				

Fragment 2

Molecular formula: C30H10

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.307666

Thermal correction to Enthalpy= 0.308610

Thermal correction to Gibbs Free Energy= 0.250112

Sum of electronic and zero-point Energies= -1148.792523

Sum of electronic and thermal Energies= -1148.776376

Sum of electronic and thermal Enthalpies= -1148.775432

Sum of electronic and thermal Free Energies= -1148.833930

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

193.063 75.571 123.120

Cartesian coordinates

Atom X Y Z

C	1.213429	-0.121090	1.521538	H	-2.397373	3.882573	-1.595244
C	0.490188	1.116732	1.521531	H	-4.132308	1.935960	-1.595019
C	-0.910536	0.811348	1.521541	H	-4.436084	-1.080778	-1.592243
C	-1.052951	-0.615231	1.521457	H	-3.118440	-3.331088	-1.595471
C	0.259685	-1.191490	1.521377	H	-0.342920	-4.548544	-1.596869
C	0.949599	2.162708	0.758602	H	2.205111	-3.993892	-1.596046
C	0.049767	3.051981	0.048236	H	4.223140	-1.732804	-1.593252
C	-1.315222	2.754645	0.048352	H	4.480976	0.862242	-1.594948
C	-1.763302	1.571364	0.758462				
C	-2.887511	0.990394	0.048720				
C	-3.026633	-0.399643	0.049068				
C	-2.039518	-1.191491	0.758775				
C	-1.834237	-2.439818	0.048344				
C	-0.555086	-3.001364	0.048017				
C	0.502913	-2.307666	0.758376				
C	1.753998	-2.498475	0.048761				
C	2.683695	-1.455744	0.049361				
C	2.350356	-0.234914	0.758921				
C	2.213302	2.101832	0.048309				
C	2.917850	0.895530	0.048324				
C	0.900872	3.750147	-0.923546				
C	2.152271	3.201769	-0.922535				
C	-2.379825	3.035617	-0.923055				
C	-3.288754	2.015531	-0.922989				
C	-3.624124	-1.325667	-0.921228				
C	-2.933583	-2.504617	-0.922935				
C	0.140981	-3.853845	-0.924005				
C	1.476009	-3.563238	-0.923391				
C	3.710769	-1.057614	-0.921597				
C	3.845692	0.301984	-0.922628				
H	0.564549	4.527574	-1.595857				
H	2.952779	3.480713	-1.594048				

Fragment 2 substituted with one NH₂ groupMolecular formula: C₃₀H₁₁N

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.325372

Thermal correction to Enthalpy= 0.326316

Thermal correction to Gibbs Free Energy= 0.265089

Sum of electronic and zero-point Energies= -1204.139813

Sum of electronic and thermal Energies= -1204.122226

Sum of electronic and thermal Enthalpies= -1204.121282

Sum of electronic and thermal Free Energies= -1204.182509

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

204.174 81.369 128.863

Cartesian coordinates

Atom X Y Z

C -0.722401 -0.000984 1.707659
C 0.120469 -1.165435 1.632549
C 1.474872 -0.720265 1.500948
C 1.473927 0.715190 1.497923
C 0.115152 1.159827 1.624642
C -0.306146 -2.243229 0.891960
C 0.609257 -3.044488 0.097325
C 1.939724 -2.613952 -0.019314
C 2.329917 -1.393209 0.654764
C 3.323496 -0.701133 -0.148981
C 3.320785 0.699057 -0.150592
C 2.323583 1.387285 0.649025
C 1.931263 2.611414 -0.028027
C 0.605352 3.044481 0.096283
C -0.307865 2.249677 0.896398
C -1.635498 2.315872 0.312710
C -2.456294 1.186932 0.416537
C -1.930128 -0.000118 1.054764
C -1.636805 -2.315000 0.308370
C -2.455277 -1.179833 0.376285
C -0.253746 -3.826199 -0.792469
C -1.551041 -3.400358 -0.672796
C 2.936881 -2.788951 -1.084942
C 3.739671 -1.683365 -1.158851
C 3.732785 1.682574 -1.161156
C 2.929906 2.788535 -1.090199
C -0.261204 3.821018 -0.800408
C -1.557689 3.402174 -0.676054
C -3.565271 0.692375 -0.428089
C -3.553462 -0.689783 -0.445961
H 0.095110 -4.567382 -1.501418
H -2.378045 -3.756332 -1.275803

H 2.976645 -3.632804 -1.763427
H 4.510068 -1.519979 -1.902713
H 4.503762 1.520374 -1.904891
H 2.970663 3.632153 -1.768654
H 0.088350 4.554027 -1.517552
H -2.381485 3.744358 -1.289478
N -4.360429 1.540841 -1.168573
H -5.169861 1.123636 -1.606835
H -4.559666 2.436656 -0.745620
H -4.201245 -1.303657 -1.059971

Fragment 2 substituted with one OMe group

Molecular formula: C31H12O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.342257

Thermal correction to Enthalpy= 0.343202

Thermal correction to Gibbs Free Energy= 0.278452

Sum of electronic and zero-point Energies= -1263.283836

Sum of electronic and thermal Energies= -1263.264848

Sum of electronic and thermal Enthalpies= -1263.263904

Sum of electronic and thermal Free Energies= -1263.328654

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

214.770 84.792 136.276

Cartesian coordinates

Atom X Y Z

C -0.902509 0.001918 1.657082
C -0.057523 -1.159764 1.603299
C 1.301904 -0.714664 1.510213
C 1.300026 0.720348 1.506383
C -0.062644 1.163142 1.596097
C -0.460688 -2.243266 0.857925
C 0.475939 -3.043395 0.087947
C 1.806643 -2.611755 0.004203
C 2.177532 -1.387576 0.687406
C 3.193021 -0.697622 -0.089395
C 3.189823 0.702494 -0.093085
C 2.171043 1.391158 0.678756
C 1.796027 2.613418 -0.011228
C 0.466598 3.043734 0.075303
C -0.466949 2.249058 0.852789
C -1.779267 2.313700 0.235396
C -2.609142 1.189129 0.322335
C -2.096735 0.000858 0.976087
C -1.772325 -2.313145 0.235246
C -2.595253 -1.182344 0.286607
C -0.363758 -3.826466 -0.825940
C -1.662815 -3.401941 -0.742449
C 2.833570 -2.788680 -1.031871
C 3.636671 -1.682216 -1.085305
C 3.628728 1.684813 -1.093530
C 2.823051 2.789844 -1.046159
C -0.376697 3.816405 -0.845833
C -1.675505 3.395444 -0.754734
C -3.683019 0.675119 -0.557759
C -3.666634 -0.697370 -0.580768
H 0.004863 -4.568586 -1.523774
H -2.474508 -3.758227 -1.365357

H 2.893057 -3.633833 -1.707119
H 4.427039 -1.519878 -1.808153
H 4.419792 1.522081 -1.815657
H 2.880966 3.632244 -1.724811
H -0.009269 4.546922 -1.556467
H -2.483569 3.734750 -1.390161
O -4.480693 1.434435 -1.350436
C -5.189180 2.491869 -0.694303
H -5.704241 3.046917 -1.479756
H -5.925619 2.084333 0.008197
H -4.513311 3.162340 -0.153937
H -4.300493 -1.301773 -1.216179

Fragment 2 substituted with one OH groupMolecular formula: C₃₀H₁₀O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.312579

Thermal correction to Enthalpy= 0.313524

Thermal correction to Gibbs Free Energy= 0.252498

Sum of electronic and zero-point Energies= -1224.009417

Sum of electronic and thermal Energies= -1223.992003

Sum of electronic and thermal Enthalpies= -1223.991059

Sum of electronic and thermal Free Energies= -1224.052084

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

196.147 80.165 128.438

Cartesian coordinates

Atom X Y Z

C	-0.713692	-0.015102	1.740359	H	2.957015	-3.652858	-1.754005
C	0.140625	-1.169801	1.663799	H	4.461412	-1.524915	-1.954346
C	1.487875	-0.710986	1.499158	H	4.421381	1.516228	-1.998009
C	1.469398	0.724272	1.475619	H	2.867458	3.612374	-1.859532
C	0.108144	1.154213	1.623245	H	-0.020357	4.500489	-1.567517
C	-0.287370	-2.263733	0.948734	H	-2.469804	3.673186	-1.282694
C	0.620462	-3.064748	0.145812	O	-4.438806	1.361428	-1.087004
C	1.942065	-2.620775	-0.005029	H	-4.384884	2.276032	-0.780967
C	2.331668	-1.385245	0.644366	H	-4.230798	-1.387918	-0.956305
C	3.301226	-0.693827	-0.189116				
C	3.282927	0.705776	-0.209456				
C	2.294213	1.393904	0.600917				
C	1.874090	2.603352	-0.085492				
C	0.545806	3.022764	0.059399				
C	-0.341916	2.229225	0.888713				
C	-1.680914	2.270512	0.330248				
C	-2.486665	1.133521	0.469179				
C	-1.936980	-0.039160	1.116426				
C	-1.628394	-2.357894	0.392039				
C	-2.460460	-1.234644	0.465020				
C	-0.252466	-3.869115	-0.715461				
C	-1.551450	-3.457588	-0.575085				
C	2.920474	-2.799899	-1.086951				
C	3.708207	-1.686093	-1.192666				
C	3.663446	1.679886	-1.241390				
C	2.849644	2.777623	-1.169329				
C	-0.346134	3.773745	-0.833186				
C	-1.634705	3.340553	-0.677542				
C	-3.589588	0.602872	-0.352263				
C	-3.575092	-0.770639	-0.357175				
H	0.090441	-4.616519	-1.420702				
H	-2.387311	-3.831490	-1.154198				

Fragment 2 substituted with one Me group

Molecular formula: C31H12

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.336471

Thermal correction to Enthalpy= 0.337415

Thermal correction to Gibbs Free Energy= 0.275551

Sum of electronic and zero-point Energies= -1188.088599

Sum of electronic and thermal Energies= -1188.070799

Sum of electronic and thermal Enthalpies= -1188.069855

Sum of electronic and thermal Free Energies= -1188.131719

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

211.139 81.391 130.204

Cartesian coordinates

Atom X Y Z

C -0.676292 0.005583 1.730159
C 0.160441 -1.158682 1.641731
C 1.517119 -0.717970 1.492023
C 1.520216 0.717002 1.490229
C 0.164493 1.163673 1.636925
C -0.276704 -2.243414 0.917055
C 0.623160 -3.045299 0.106916
C 1.948911 -2.616036 -0.036777
C 2.353074 -1.392352 0.630507
C 3.335742 -0.704812 -0.188864
C 3.338847 0.695452 -0.189450
C 2.358300 1.386845 0.628414
C 1.960305 2.613708 -0.038578
C 0.637407 3.050039 0.106490
C -0.267672 2.250744 0.912791
C -1.605093 2.324733 0.348900
C -2.424826 1.191574 0.437475
C -1.893603 0.009245 1.090675
C -1.614116 -2.309593 0.353182
C -2.428512 -1.174359 0.440053
C -0.259131 -3.828574 -0.767753
C -1.552204 -3.403120 -0.625398
C 2.929696 -2.795064 -1.116368
C 3.732140 -1.690340 -1.203958
C 3.739601 1.679651 -1.203998
C 2.943134 2.788995 -1.116354
C -0.240164 3.846191 -0.760583
C -1.536501 3.431380 -0.618283
C 3.532388 0.698145 -0.410891
C -3.522122 -0.674024 -0.397298
H 0.076273 -4.573350 -1.479425
H -2.392468 -3.761260 -1.208016

H 2.958374 -3.640159 -1.793665
H 4.490749 -1.529860 -1.960516
H 4.497508 1.515977 -1.960629
H 2.976737 3.634131 -1.793334
H 0.098455 4.597967 -1.463358
H -2.374842 3.814437 -1.186181
C -4.441926 1.564548 -1.224936
H -4.940642 2.316885 -0.602663
H -3.884011 2.108851 -1.997233
H -5.211212 0.970369 -1.724903
H -4.182996 -1.294752 -0.991457

Fragment 2 substituted with one *i*-Pr groupMolecular formula: C₃₃H₁₆

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.396077

Thermal correction to Enthalpy= 0.397022

Thermal correction to Gibbs Free Energy= 0.328986

Sum of electronic and zero-point Energies= -1266.662030

Sum of electronic and thermal Energies= -1266.641484

Sum of electronic and thermal Enthalpies= -1266.640539

Sum of electronic and thermal Free Energies= -1266.708575

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

248.542 91.677 143.194

Cartesian coordinates

Atom X Y Z

C -0.649938 0.018231 1.729010
C 0.192130 -1.142906 1.653934
C 1.549002 -0.696920 1.522223
C 1.546549 0.738182 1.519423
C 0.187139 1.179486 1.646745
C -0.231182 -2.230031 0.924744
C 0.682314 -3.029076 0.127268
C 2.008113 -2.594312 0.000411
C 2.398509 -1.368405 0.671979
C 3.389865 -0.677730 -0.134519
C 3.387883 0.722532 -0.135630
C 2.393657 1.410466 0.668597
C 1.999823 2.635311 -0.004058
C 0.673175 3.066175 0.122488
C -0.240622 2.263231 0.915226
C -1.570998 2.331167 0.332502
C -2.389112 1.194335 0.411460
C -1.857764 0.016518 1.072655
C -1.561276 -2.302687 0.344764
C -2.381207 -1.170070 0.420220
C -0.185660 -3.817209 -0.757169
C -1.482361 -3.397083 -0.631404
C 3.003913 -2.770235 -1.065637
C 3.803335 -1.662425 -1.143370
C 3.798464 1.708074 -1.144993
C 2.996545 2.814340 -1.068432
C -0.194411 3.858915 -0.756910
C -1.490917 3.438710 -0.633691
C -3.494253 0.695690 -0.439230
C -3.473191 -0.678431 -0.422939
H 0.161684 -4.561286 -1.463833
H -2.313560 -3.759524 -1.224312

H 3.044778 -3.615568 -1.742021
H 4.571317 -1.499683 -1.889929
H 4.567140 1.547173 -1.891286
H 3.035921 3.659386 -1.745216
H 0.151064 4.611895 -1.455035
H -2.320029 3.817240 -1.217382
C -4.412602 1.568147 -1.267524
H -4.359543 2.582619 -0.852324
C -3.947535 1.634498 -2.738200
H -4.016622 0.647308 -3.207274
H -4.574720 2.326618 -3.310975
H -2.908916 1.968192 -2.817945
C -5.880000 1.113628 -1.179472
H -6.527096 1.798385 -1.737675
H -6.013671 0.113658 -1.605894
H -6.226002 1.084741 -0.142171
H -4.124936 -1.313186 -1.011644

Fragment 2 substituted with one F groupMolecular formula: C₃₀H₉F

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.299916

Thermal correction to Enthalpy= 0.300860

Thermal correction to Gibbs Free Energy= 0.240400

Sum of electronic and zero-point Energies= -1248.031202

Sum of electronic and thermal Energies= -1248.014177

Sum of electronic and thermal Enthalpies= -1248.013233

Sum of electronic and thermal Free Energies= -1248.073693

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

188.200 78.367 127.250

Cartesian coordinates

Atom X Y Z

C -0.681966 0.000687 1.748224
C 0.157012 -1.161616 1.655593
C 1.512109 -0.717809 1.500213
C 1.512049 0.717171 1.498120
C 0.155208 1.161413 1.650599
C -0.281575 -2.244986 0.930174
C 0.617475 -3.045929 0.117696
C 1.942299 -2.614822 -0.029632
C 2.346076 -1.390312 0.635801
C 3.323852 -0.700688 -0.187953
C 3.322364 0.699404 -0.189733
C 2.343351 1.388607 0.631608
C 1.939051 2.614712 -0.036765
C 0.617741 3.050330 0.114971
C -0.279171 2.253890 0.933766
C -1.614184 2.322140 0.372042
C -2.429218 1.191355 0.480465
C -1.905352 0.000185 1.119036
C -1.620630 -2.314193 0.367989
C -2.439104 -1.182655 0.456128
C -0.264964 -3.830289 -0.754800
C -1.558456 -3.406352 -0.610726
C 2.919654 -2.792249 -1.112457
C 3.719204 -1.685676 -1.203649
C 3.715606 1.683265 -1.207484
C 2.916373 2.790355 -1.118993
C -0.268217 3.830050 -0.761953
C -1.561556 3.408676 -0.613648
C -3.498576 0.671351 -0.370785
C -3.528082 -0.693518 -0.395379
H 0.070035 -4.574359 -1.467308
H -2.399001 -3.765210 -1.192419

H 2.947795 -3.637510 -1.789508
H 4.474585 -1.523865 -1.963069
H 4.470830 1.520452 -1.966948
H 2.944772 3.634456 -1.797340
H 0.066539 4.568500 -1.480410
H -2.408371 3.752809 -1.193652
F -4.276151 1.476983 -1.104980
H -4.179234 -1.290668 -1.018889

Fragment 2 substituted with one COOH group

Molecular formula: C31H10O2

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.325077

Thermal correction to Enthalpy= 0.326021

Thermal correction to Gibbs Free Energy= 0.260775

Sum of electronic and zero-point Energies= -1337.357226

Sum of electronic and thermal Energies= -1337.338190

Sum of electronic and thermal Enthalpies= -1337.337245

Sum of electronic and thermal Free Energies= -1337.402491

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

203.989 85.489 137.321

Cartesian coordinates

Atom X Y Z

C 1.264660 -0.128374 1.424697
C 0.548347 1.112440 1.438792
C -0.855581 0.816549 1.504927
C -1.005521 -0.609015 1.527831
C 0.306488 -1.192802 1.477134
C 0.980484 2.156803 0.652278
C 0.056198 3.050008 -0.024800
C -1.310128 2.755462 0.028744
C -1.734030 1.574104 0.765028
C -2.890228 0.993928 0.109028
C -3.036449 -0.399274 0.128905
C -2.022800 -1.188002 0.806082
C -1.854566 -2.451490 0.107764
C -0.577174 -3.020359 0.062021
C 0.514769 -2.314698 0.712333
C 1.738044 -2.529924 -0.043996
C 2.678407 -1.490393 -0.091789
C 2.367780 -0.257841 0.609503
C 2.214673 2.089191 -0.101578
C 2.916907 0.872114 -0.116668
C 0.876661 3.743740 -1.027903
C 2.127101 3.189188 -1.070812
C -2.417128 3.037237 -0.894682
C -3.329132 2.018272 -0.849500
C -3.681450 -1.337780 -0.799093
C -2.998683 -2.523813 -0.810897
C 0.079639 -3.908434 -0.905705
C 1.418122 -3.630597 -0.965152
C 3.697546 -1.090377 -1.085797
C 3.817975 0.283787 -1.096746
H 0.518463 4.522798 -1.689943
H 2.906492 3.462048 -1.771829

H -2.461116 3.882920 -1.570150
H -4.203106 1.937555 -1.484616
H -4.521575 -1.097489 -1.439419
H -3.217708 -3.361036 -1.462502
H -0.433837 -4.623801 -1.536801
H 2.137759 -4.077630 -1.636181
C 4.426382 -1.999464 -1.978593
O 4.284706 -3.208670 -2.033299
O 5.320383 -1.351455 -2.772579
H 5.740133 -2.043188 -3.309976
H 4.449546 0.830815 -1.784454

Fragment 2 substituted with one CF₃ groupMolecular formula: C₃₁H₉F₃

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.315591

Thermal correction to Enthalpy= 0.316535

Thermal correction to Gibbs Free Energy= 0.248700

Sum of electronic and zero-point Energies= -1485.825741

Sum of electronic and thermal Energies= -1485.805896

Sum of electronic and thermal Enthalpies= -1485.804952

Sum of electronic and thermal Free Energies= -1485.872787

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

198.036 88.012 142.770

Cartesian coordinates

Atom X Y Z

C -0.528563 0.064392 -1.977097
C -1.340576 -1.102267 -1.790905
C -2.664725 -0.670855 -1.441295
C -2.669492 0.763218 -1.411647
C -1.347219 1.216833 -1.741924
C -0.805457 -2.205794 -1.166673
C -1.578598 -3.028882 -0.253195
C -2.865866 -2.604708 0.094429
C -3.362758 -1.365255 -0.480679
C -4.215722 -0.699645 0.486801
C -4.219812 0.700584 0.516585
C -3.370949 1.411613 -0.422482
C -2.881759 2.628990 0.203160
C -1.596053 3.073562 -0.123939
C -0.816211 2.290818 -1.067537
C 0.586342 2.358047 -0.695308
C 1.386761 1.230992 -0.927966
C 0.770544 0.057955 -1.519195
C 0.596795 -2.281236 -0.804021
C 1.390975 -1.140460 -0.987306
C -0.577342 -3.831590 0.463479
C 0.681309 -3.400989 0.143168
C -3.680910 -2.810757 1.299120
C -4.460158 -1.709273 1.526328
C -4.470550 1.664257 1.596917
C -3.697946 2.779015 1.415433
C -0.601574 3.856129 0.621896
C 0.660629 3.445703 0.291315
C 2.595112 0.702943 -0.267365
C 2.592607 -0.666500 -0.300077
H -0.805180 -4.595563 1.196925
H 1.598071 -3.771992 0.584999

H -3.612296 -3.670897 1.953969
H -5.100449 -1.568072 2.388687
H -5.109036 1.482960 2.453066
H -3.633767 3.610737 2.106472
H -0.835075 4.591283 1.382454
H 1.573218 3.798604 0.750920
C 3.629265 1.524813 0.423194
F 4.706846 0.791129 0.771727
F 3.152364 2.093189 1.563190
F 4.058647 2.543701 -0.356595
H 3.340722 -1.292098 0.169048

Fragment 2 substituted with one CHO group

Molecular formula: C31H10O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.318537

Thermal correction to Enthalpy= 0.319481

Thermal correction to Gibbs Free Energy= 0.256587

Sum of electronic and zero-point Energies= -1262.111620

Sum of electronic and thermal Energies= -1262.093506

Sum of electronic and thermal Enthalpies= -1262.092562

Sum of electronic and thermal Free Energies= -1262.155456

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

199.885 81.999 132.372

Cartesian coordinates

Atom X Y Z

C -0.310293 0.010313 1.839270
C 0.514147 -1.151919 1.691467
C 1.865340 -0.716429 1.471923
C 1.873406 0.716963 1.478098
C 0.527196 1.166166 1.704026
C 0.037034 -2.243072 0.999652
C 0.888451 -3.047022 0.139495
C 2.200033 -2.616821 -0.084791
C 2.644981 -1.390504 0.560576
C 3.577912 -0.705014 -0.312357
C 3.584276 0.695960 -0.309787
C 2.657629 1.386935 0.568590
C 2.224678 2.619896 -0.068341
C 0.915084 3.058148 0.154642
C 0.056921 2.254578 1.010182
C -1.309429 2.337014 0.521825
C -2.129114 1.208604 0.655710
C -1.564395 0.020425 1.267070
C -1.325171 -2.308469 0.515078
C -2.134472 -1.167200 0.655308
C -0.046020 -3.830949 -0.680854
C -1.328080 -3.405514 -0.461207
C 3.117934 -2.797054 -1.217345
C 3.912526 -1.691280 -1.349931
C 3.928773 1.683625 -1.341115
C 3.143114 2.795374 -1.201485
C -0.013122 3.862983 -0.651253
C -1.300218 3.450943 -0.436954
C -3.280758 0.704376 -0.124191
C -3.264929 -0.678226 -0.117951
H 0.244874 -4.578684 -1.408710
H -2.202967 -3.764698 -0.989257

H 3.108511 -3.642154 -1.894831
H 4.625825 -1.530879 -2.149382
H 4.639487 1.520845 -2.142275
H 3.139512 3.642934 -1.876088
H 0.285420 4.616924 -1.369607
H -2.185859 3.809055 -0.943430
C -4.263362 1.472378 -0.882953
H -5.044079 0.849114 -1.371232
O -4.277206 2.687907 -1.004908
H -3.961958 -1.296990 -0.672443

Fragment 2 substituted with one CN group

Molecular formula: C31H9N

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.307535

Thermal correction to Enthalpy= 0.308479

Thermal correction to Gibbs Free Energy= 0.245711

Sum of electronic and zero-point Energies= -1241.039190

Sum of electronic and thermal Energies= -1241.021217

Sum of electronic and thermal Enthalpies= -1241.020273

Sum of electronic and thermal Free Energies= -1241.083040

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

192.981 81.383 132.106

Cartesian coordinates

Atom X Y Z

C	0.324900	-0.004275	1.866258	H	-3.019839	3.642774	-1.937910
C	-0.499992	1.156209	1.702975	H	-4.525850	1.528513	-2.230284
C	-1.843666	0.715952	1.450314	H	-4.528196	-1.522289	-2.231413
C	-1.846040	-0.718267	1.451604	H	-3.025445	-3.638942	-1.939361
C	-0.504208	-1.163273	1.707571	H	-0.179245	-4.587651	-1.388682
C	-0.009299	2.247015	1.021242	H	2.265158	-3.779889	-0.918900
C	-0.843390	3.049871	0.143335	C	4.230860	-1.506658	-0.764674
C	-2.149099	2.616870	-0.109997	N	4.958047	-2.204435	-1.349690
C	-2.604283	1.388663	0.522823	H	4.013053	1.306393	-0.600216
C	-3.515918	0.701606	-0.372934				
C	-3.517314	-0.698742	-0.373456				
C	-2.607435	-1.388683	0.523329				
C	-2.155128	-2.617296	-0.109083				
C	-0.849889	-3.052786	0.143585				
C	-0.015991	-2.252413	1.024100				
C	1.359418	-2.324706	0.565716				
C	2.165948	-1.191855	0.727059				
C	1.593397	-0.005989	1.326907				
C	1.364382	2.316232	0.564366				
C	2.173340	1.178365	0.720299				
C	0.106137	3.836731	-0.655958				
C	1.384250	3.413184	-0.411161				
C	-3.042190	2.796481	-1.262240				
C	-3.830944	1.688997	-1.414902				
C	-3.834410	-1.684619	-1.415495				
C	-3.047353	-2.793419	-1.262672				
C	0.099240	-3.841868	-0.654121				
C	1.378823	-3.423026	-0.409918				
C	3.320705	-0.687935	-0.044135				
C	3.314734	0.692888	-0.045231				
H	-0.171120	4.584331	-1.389189				
H	2.268889	3.774236	-0.921260				

Fragment 2 substituted with one NO₂ groupMolecular formula: C₃₀H₉NO₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.312266

Thermal correction to Enthalpy= 0.313210

Thermal correction to Gibbs Free Energy= 0.248552

Sum of electronic and zero-point Energies= -1353.290164

Sum of electronic and thermal Energies= -1353.271446

Sum of electronic and thermal Enthalpies= -1353.270502

Sum of electronic and thermal Free Energies= -1353.335160

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

195.950 83.884 136.085

Cartesian coordinates

Atom X Y Z

C	1.234291	-0.137662	1.471472	H	-2.409527	3.908976	-1.577251
C	0.517380	1.102528	1.478704	H	-4.151124	1.962057	-1.562916
C	-0.888070	0.806411	1.505274	H	-4.468369	-1.076478	-1.561331
C	-1.037688	-0.619123	1.508076	H	-3.164718	-3.339847	-1.571406
C	0.276306	-1.202057	1.485683	H	-0.381072	-4.601067	-1.581719
C	0.970252	2.157377	0.718665	H	2.186891	-4.063203	-1.603638
C	0.064888	3.059078	0.027317	O	4.342323	-3.124658	-1.718818
C	-1.301377	2.762588	0.038092	O	5.300995	-1.368544	-2.598522
C	-1.744834	1.571604	0.748931	N	4.507299	-1.902862	-1.818639
C	-2.881709	0.999079	0.054289	H	4.514190	0.853834	-1.641121
C	-3.027735	-0.394188	0.054653				
C	-2.033296	-1.189743	0.751578				
C	-1.845574	-2.446492	0.044753				
C	-0.568207	-3.015703	0.030256				
C	0.505932	-2.317309	0.717489				
C	1.749396	-2.527615	-0.005775				
C	2.693754	-1.488894	-0.008689				
C	2.360710	-0.257761	0.687200				
C	2.224244	2.100420	-0.000863				
C	2.929541	0.883404	-0.009234				
C	0.913748	3.765697	-0.942843				
C	2.165726	3.212658	-0.957019				
C	-2.383028	3.055138	-0.911372				
C	-3.294865	2.035172	-0.903347				
C	-3.646401	-1.323304	-0.900366				
C	-2.963796	-2.509478	-0.905539				
C	0.114355	-3.893583	-0.927917				
C	1.454557	-3.618137	-0.946087				
C	3.732041	-1.052465	-0.955028				
C	3.858831	0.317089	-0.969538				
H	0.574707	4.553148	-1.604908				
H	2.964899	3.494481	-1.631458				

Fragment 1 substituted with two NH₂ groupMolecular formula: C₃₀H₁₄N₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.368809

Thermal correction to Enthalpy= 0.369753

Thermal correction to Gibbs Free Energy= 0.304012

Sum of electronic and zero-point Energies= -1260.766890

Sum of electronic and thermal Energies= -1260.747312

Sum of electronic and thermal Enthalpies= -1260.746368

Sum of electronic and thermal Free Energies= -1260.812109

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

231.431 88.349 138.364

Cartesian coordinates

Atom X Y Z

C -1.183429 1.241633 -1.317784
C 0.237414 1.183446 -1.460948
C 0.838906 -0.054381 -1.550560
C 0.077307 -1.259559 -1.479397
C -1.291848 -1.169272 -1.348039
C -1.947154 0.095761 -1.245221
C 0.839442 -2.286148 -0.806456
C 0.127776 -3.291593 -0.156927
C -1.315738 -3.200567 0.014143
C -1.985505 -2.084925 -0.537288
C -2.091321 -3.942850 0.949971
C -3.330450 -3.465755 1.363826
C -3.849599 -2.202886 0.963958
C -3.156796 -1.468686 0.015722
C -3.081538 -0.004489 -0.359272
C -3.485848 1.149319 0.305287
C -2.679495 2.361664 0.262560
C -1.493222 2.346587 -0.505119
C -0.300808 3.082229 -0.195833
C -0.431904 4.104576 0.729612
C -1.696641 4.312230 1.346878
C -2.778361 3.456751 1.167208
C 2.081965 -0.291145 -0.935673
C 2.802765 0.779671 -0.360477
C 2.152595 2.077730 -0.272567
C 0.852708 2.267042 -0.736214
C 3.980784 0.390111 0.352318
C 4.196452 -0.977777 0.631319
C 3.278164 -1.986424 0.245687
C 2.192004 -1.666484 -0.556712
H 0.648795 -4.047696 0.426602
H -1.690945 -4.849598 1.396274

H -3.890333 -4.041228 2.095727
H -4.738492 -1.816185 1.454712
H -4.285609 1.110645 1.041693
H 0.415298 4.708217 1.043625
H -1.791304 5.126848 2.059382
H -3.672683 3.590082 1.770473
H 2.611650 2.826208 0.369157
H 3.426786 -2.992076 0.633858
N 4.869128 1.327085 0.878056
H 5.795257 0.935456 1.018667
H 4.907532 2.195584 0.360519
N 5.367708 -1.291312 1.379459
H 5.346459 -0.880310 2.310849
H 5.501316 -2.291567 1.473948

Fragment 1 substituted with two OMe groupMolecular formula: C₃₂H₁₆O₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.402319

Thermal correction to Enthalpy= 0.403263

Thermal correction to Gibbs Free Energy= 0.330565

Sum of electronic and zero-point Energies= -1379.060592

Sum of electronic and thermal Energies= -1379.038253

Sum of electronic and thermal Enthalpies= -1379.037308

Sum of electronic and thermal Free Energies= -1379.110006

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

252.459 95.893 153.006

Cartesian coordinates

Atom X Y Z

C	-1.238018	1.271928	-1.319845	H	-3.635269	-4.109486	2.166764
C	0.172851	1.245685	-1.540095	H	-4.566474	-1.897828	1.600725
C	0.793761	0.024270	-1.686847	H	-4.200507	1.040692	1.204976
C	0.063311	-1.198347	-1.591749	H	0.414169	4.740571	1.001799
C	-1.297954	-1.139595	-1.381443	H	-1.743259	5.098397	2.141285
C	-1.973765	0.109011	-1.224629	H	-3.603943	3.524152	1.932814
C	0.881946	-2.215869	-0.975270	H	2.630865	2.913949	0.174922
C	0.232939	-3.241392	-0.294747	H	3.556216	-2.908567	0.268751
C	-1.201255	-3.187054	-0.044196	O	4.757212	1.477648	0.692782
C	-1.923802	-2.080349	-0.543749	O	5.444755	-1.098018	0.982159
C	-1.905114	-3.957263	0.924665	C	6.015481	1.729513	0.058179
C	-3.129825	-3.513592	1.412077	H	6.475703	2.550765	0.611180
C	-3.697798	-2.258586	1.056917	H	6.663816	0.849554	0.102686
C	-3.075693	-1.497375	0.081216	H	5.873300	2.030602	-0.987309
C	-3.054158	-0.027708	-0.278157	C	5.774743	-2.433270	1.327259
C	-3.444673	1.107427	0.425486	H	6.745264	-2.382022	1.822863
C	-2.668369	2.337945	0.355946	H	5.042600	-2.867430	2.020072
C	-1.525911	2.359445	-0.475345	H	5.855788	-3.075520	0.440863
C	-0.335204	3.117953	-0.220925				
C	-0.436700	4.124175	0.725355				
C	-1.670187	4.295811	1.412855				
C	-2.741224	3.418670	1.280094				
C	2.073304	-0.192602	-1.142821				
C	2.796232	0.881758	-0.576041				
C	2.129918	2.170914	-0.438009				
C	0.805989	2.332512	-0.829124				
C	3.984197	0.506982	0.106633				
C	4.276037	-0.859589	0.309526				
C	3.375199	-1.893599	-0.065479				
C	2.232687	-1.564537	-0.782339				
H	0.803566	-3.989314	0.251727				
H	-1.459657	-4.859075	1.336754				

Fragment 1 substituted with two OH group

Molecular formula: C30H12O2

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.342936

Thermal correction to Enthalpy= 0.343880

Thermal correction to Gibbs Free Energy= 0.278371

Sum of electronic and zero-point Energies= -1300.517189

Sum of electronic and thermal Energies= -1300.497814

Sum of electronic and thermal Enthalpies= -1300.496870

Sum of electronic and thermal Free Energies= -1300.562379

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

215.195 86.714 137.875

Cartesian coordinates

Atom X Y Z

C	-1.232034	1.239949	-1.343764	H	-3.780644	-4.028955	2.207672
C	0.185289	1.198950	-1.515804	H	-4.675763	-1.826486	1.554146
C	0.802210	-0.030296	-1.608318	H	-4.277742	1.100298	1.086394
C	0.059891	-1.244843	-1.503653	H	0.364999	4.770029	0.923051
C	-1.306942	-1.171846	-1.339375	H	-1.825383	5.171599	1.981637
C	-1.978022	0.084787	-1.238941	H	-3.687976	3.601293	1.760795
C	0.850677	-2.251397	-0.834911	H	2.601117	2.911520	0.209833
C	0.170974	-3.255665	-0.151298	H	3.513237	-2.921253	0.509708
C	-1.269473	-3.183440	0.052600	O	4.745163	1.442383	0.779379
C	-1.967304	-2.085283	-0.498663	H	5.415680	0.991317	1.316969
C	-2.010831	-3.922566	1.018006	O	5.359571	-1.091997	1.225176
C	-3.246554	-3.456899	1.454234	H	5.370848	-1.997303	1.559058
C	-3.793122	-2.207670	1.048084				
C	-3.134258	-1.477604	0.072887				
C	-3.090076	-0.018373	-0.325630				
C	-3.495701	1.139388	0.331242				
C	-2.709320	2.363026	0.251440				
C	-1.540098	2.353509	-0.542001				
C	-0.353357	3.113139	-0.272434				
C	-0.479594	4.148448	0.638962				
C	-1.733560	4.346604	1.280888				
C	-2.805239	3.471405	1.140031				
C	2.063298	-0.240590	-1.019800				
C	2.773560	0.853497	-0.470906				
C	2.113272	2.147188	-0.387733				
C	0.801161	2.304372	-0.821353				
C	3.938125	0.484236	0.253921				
C	4.202147	-0.873510	0.499543				
C	3.320895	-1.916410	0.137984				
C	2.199535	-1.608588	-0.622575				
H	0.717197	-3.994945	0.430773				
H	-1.586740	-4.816773	1.467585				

Fragment 1 substituted with two Me groupMolecular formula: C₃₂H₁₆

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.390766

Thermal correction to Enthalpy= 0.391710

Thermal correction to Gibbs Free Energy= 0.324589

Sum of electronic and zero-point Energies= -1228.666860

Sum of electronic and thermal Energies= -1228.646756

Sum of electronic and thermal Enthalpies= -1228.645812

Sum of electronic and thermal Free Energies= -1228.712933

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

245.209 89.211 141.268

Cartesian coordinates

Atom X Y Z

C -1.207936 1.233281 -1.336258
C 0.213717 1.182912 -1.465094
C 0.827676 -0.048839 -1.534497
C 0.074645 -1.259327 -1.451109
C -1.296673 -1.178360 -1.331332
C -1.963046 0.082422 -1.252590
C 0.837354 -2.269472 -0.758123
C 0.132372 -3.267502 -0.092535
C -1.313647 -3.187560 0.065681
C -1.987487 -2.086544 -0.509141
C -2.087741 -3.920087 1.009871
C -3.333912 -3.447056 1.406951
C -3.860488 -2.195934 0.981419
C -3.167879 -1.471431 0.025519
C -3.102912 -0.013212 -0.372926
C -3.521012 1.147358 0.270879
C -2.724328 2.365614 0.215343
C -1.531955 2.348198 -0.542576
C -0.347752 3.097475 -0.234987
C -0.493963 4.132368 0.673832
C -1.765389 4.340069 1.277380
C -2.838971 3.473555 1.102290
C 2.065719 -0.262041 -0.900871
C 2.782224 0.812760 -0.329123
C 2.114123 2.109865 -0.276471
C 0.816645 2.279533 -0.749991
C 3.954787 0.442763 0.408126
C 4.200410 -0.919217 0.663494
C 3.283314 -1.940658 0.277689
C 2.182597 -1.629891 -0.499385
H 0.657549 -4.007050 0.507996
H -1.681884 -4.814911 1.474671

H -3.893875 -4.014261 2.145072
H -4.756183 -1.808689 1.459216
H -4.325676 1.113466 1.002139
H 0.346068 4.747225 0.985221
H -1.872127 5.164956 1.976148
H -3.739250 3.609347 1.696011
H 2.563747 2.883731 0.339139
H 3.449818 -2.948942 0.648827
C 4.889671 1.492497 0.961206
H 4.834265 1.556414 2.055784
H 5.931544 1.262249 0.713469
H 4.674592 2.483009 0.556750
C 5.423156 -1.326388 1.457306
H 6.351431 -1.059659 0.937077
H 5.459815 -0.836382 2.437506
H 5.440963 -2.406035 1.625404

Fragment 1 substituted with two *i*-Pr groupMolecular formula: C₃₆H₂₄

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.510365

Thermal correction to Enthalpy= 0.511309

Thermal correction to Gibbs Free Energy= 0.432609

Sum of electronic and zero-point Energies= -1385.803049

Sum of electronic and thermal Energies= -1385.777484

Sum of electronic and thermal Enthalpies= -1385.776540

Sum of electronic and thermal Free Energies= -1385.855240

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

320.259 110.006 165.638

Cartesian coordinates

Atom X Y Z

C -1.264163 1.272354 -1.262781
C 0.160461 1.257668 -1.365555
C 0.807388 0.045058 -1.449495
C 0.081680 -1.184318 -1.412107
C -1.293352 -1.139681 -1.318426
C -1.992193 0.102122 -1.220894
C 0.855090 -2.194507 -0.733152
C 0.163329 -3.226583 -0.107212
C -1.286931 -3.184916 0.025906
C -1.976509 -2.085269 -0.532711
C -2.060337 -3.960425 0.935669
C -3.324580 -3.527570 1.321315
C -3.873172 -2.278310 0.918866
C -3.180934 -1.512498 -0.004572
C -3.144177 -0.043167 -0.364295
C -3.600271 1.090448 0.301625
C -2.831700 2.327897 0.291667
C -1.626886 2.358255 -0.445964
C -0.464941 3.124426 -0.096904
C -0.650355 4.130782 0.836494
C -1.936407 4.293715 1.422777
C -2.986744 3.408441 1.205994
C 2.038672 -0.153582 -0.797522
C 2.728891 0.913196 -0.181745
C 2.017510 2.190412 -0.116259
C 0.725912 2.344542 -0.611853
C 3.928892 0.552468 0.539823
C 4.210469 -0.819866 0.733061
C 3.287211 -1.836336 0.321593
C 2.179941 -1.529700 -0.438565
H 0.695454 -3.969779 0.482559
H -1.641711 -4.857661 1.384199

H -3.884311 -4.127414 2.033338
H -4.786674 -1.925303 1.389412
H -4.416198 1.018788 1.017541
H 0.169889 4.755390 1.179658
H -2.073633 5.096738 2.141423
H -3.899636 3.507626 1.787567
H 2.428183 2.969205 0.513191
H 3.469902 -2.855673 0.652168
C 4.858114 1.637853 1.091727
H 5.778784 1.139009 1.389403
C 5.473719 -1.380422 1.416852
H 5.323702 -2.466498 1.414552
C 4.329357 2.314729 2.377589
H 4.055762 1.569669 3.129669
H 5.107322 2.957512 2.804946
H 3.450840 2.940414 2.203888
C 5.282359 2.672436 0.029021
H 5.728209 2.176793 -0.838996
H 4.447597 3.277435 -0.332675
H 6.029648 3.354666 0.449155
C 5.655947 -1.016587 2.904832
H 5.958278 0.020949 3.064884
H 4.729974 -1.185369 3.463565
H 6.433053 -1.650994 3.345698
C 6.762297 -1.161123 0.595987
H 7.066780 -0.111902 0.548574
H 7.590985 -1.722540 1.042035
H 6.630582 -1.513821 -0.431432

Fragment 1 substituted with two F groupMolecular formula: C₃₀H₁₀F₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.317497

Thermal correction to Enthalpy= 0.318441

Thermal correction to Gibbs Free Energy= 0.254240

Sum of electronic and zero-point Energies= -1348.556578

Sum of electronic and thermal Energies= -1348.537999

Sum of electronic and thermal Enthalpies= -1348.537054

Sum of electronic and thermal Free Energies= -1348.601256

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

199.233 83.332 135.124

Cartesian coordinates

Atom X Y Z

C	-1.200753	1.233071	-1.331807	H	-3.862671	-4.014542	2.167797
C	0.218778	1.179400	-1.473406	H	-4.725560	-1.805209	1.497144
C	0.826579	-0.055300	-1.555895	H	-4.295217	1.119387	1.036383
C	0.072694	-1.264871	-1.467831	H	0.378725	4.751660	0.966110
C	-1.296303	-1.178773	-1.329956	H	-1.829313	5.171414	1.979561
C	-1.957511	0.083899	-1.241228	H	-3.699078	3.615719	1.721407
C	0.839185	-2.279980	-0.787068	H	2.614281	2.875697	0.298408
C	0.139045	-3.276706	-0.114100	H	3.487550	-2.964279	0.628329
C	-1.304482	-3.191983	0.060855	F	4.711745	1.344261	0.930440
C	-1.980706	-2.086663	-0.502624	F	5.244688	-1.236978	1.364360
C	-2.069660	-3.924521	1.012368				
C	-3.309282	-3.447782	1.424583				
C	-3.836607	-2.193726	1.008128				
C	-3.153155	-1.468904	0.046054				
C	-3.088666	-0.010058	-0.350642				
C	-3.497506	1.151389	0.297600				
C	-2.700216	2.368830	0.232774				
C	-1.515626	2.349822	-0.536941				
C	-0.329579	3.100749	-0.243964				
C	-0.464843	4.136848	0.665042				
C	-1.729896	4.345567	1.281127				
C	-2.805071	3.478451	1.118786				
C	2.071781	-0.275928	-0.941317				
C	2.776962	0.813014	-0.376871				
C	2.131148	2.114445	-0.306657				
C	0.829218	2.279939	-0.765441				
C	3.913211	0.418221	0.369763				
C	4.162257	-0.926914	0.623118				
C	3.289348	-1.970114	0.241098				
C	2.189078	-1.646973	-0.538174				
H	0.668683	-4.020073	0.477515				
H	-1.661836	-4.822016	1.469897				

Fragment 1 substituted with two COOH group

Molecular formula: C32H12O4

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.367529

Thermal correction to Enthalpy= 0.368473

Thermal correction to Gibbs Free Energy= 0.294526

Sum of electronic and zero-point Energies= -1527.193562

Sum of electronic and thermal Energies= -1527.170913

Sum of electronic and thermal Enthalpies= -1527.169968

Sum of electronic and thermal Free Energies= -1527.243916

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

230.628 97.723 155.635

Cartesian coordinates

Atom X Y Z

C -2.031219 1.218094 -1.316102
C -0.632090 1.164224 -1.588579
C -0.030449 -0.066876 -1.737661
C -0.772829 -1.277028 -1.578894
C -2.123452 -1.194193 -1.313142
C -2.774246 0.066792 -1.157094
C 0.053576 -2.292874 -0.977253
C -0.576112 -3.291928 -0.240535
C -1.996559 -3.211245 0.069088
C -2.723966 -2.105479 -0.425662
C -2.666170 -3.947371 1.087512
C -3.862136 -3.474127 1.615986
C -4.427899 -2.219950 1.254103
C -3.839766 -1.491267 0.233498
C -3.815282 -0.031539 -0.163113
C -4.159618 1.127031 0.526552
C -3.373449 2.345766 0.391014
C -2.268237 2.331309 -0.488835
C -1.059249 3.080169 -0.305503
C -1.106547 4.111169 0.617889
C -2.307299 4.317040 1.352384
C -3.393185 3.450480 1.289196
C 1.264491 -0.282355 -1.234071
C 2.034045 0.791444 -0.731595
C 1.381637 2.092727 -0.600729
C 0.044090 2.259224 -0.935966
C 3.264666 0.403257 -0.109624
C 3.549536 -0.965921 0.059832
C 2.599969 -1.988403 -0.222521
C 1.416282 -1.655605 -0.851562
H 0.010255 -4.034155 0.296237
H -2.214528 -4.844664 1.502052

H -4.341975 -4.043318 2.406841
H -5.267239 -1.833957 1.825809
H -4.881966 1.090569 1.339037
H -0.237179 4.723347 0.840373
H -2.339440 5.139266 2.061322
H -4.225585 3.584179 1.975042
H 1.918170 2.868308 -0.065747
H 2.838987 -2.995088 0.103194
C 4.133654 1.477623 0.460680
C 4.861420 -1.472801 0.570481
O 4.345290 2.550317 -0.066633
O 4.997054 -2.477770 1.237391
O 4.602990 1.173250 1.694387
H 5.164478 1.922390 1.956942
O 5.915852 -0.748025 0.127998
H 6.704877 -1.163367 0.515095

Fragment 1 substituted with two CF₃ groupMolecular formula: C₃₂H₁₀F₆

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.348680

Thermal correction to Enthalpy= 0.349625

Thermal correction to Gibbs Free Energy= 0.272412

Sum of electronic and zero-point Energies= -1824.133455

Sum of electronic and thermal Energies= -1824.109478

Sum of electronic and thermal Enthalpies= -1824.108534

Sum of electronic and thermal Free Energies= -1824.185746

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

218.800 102.568 162.507

Cartesian coordinates

Atom X Y Z

C -2.418721 1.246415 -1.291169
C -1.024788 1.194188 -1.590616
C -0.429477 -0.034207 -1.775271
C -1.172901 -1.245423 -1.630026
C -2.518958 -1.164926 -1.341796
C -3.163369 0.094290 -1.146911
C -0.340573 -2.274521 -1.061511
C -0.960861 -3.288182 -0.337355
C -2.376630 -3.212723 -0.006501
C -3.108169 -2.094428 -0.465536
C -3.033034 -3.970692 1.004455
C -4.219813 -3.506761 1.561047
C -4.786960 -2.243017 1.236674
C -4.211844 -1.492618 0.224425
C -4.188237 -0.024275 -0.138363
C -4.515444 1.117872 0.585985
C -3.725051 2.335503 0.468719
C -2.635177 2.338272 -0.430055
C -1.418812 3.074225 -0.245823
C -1.442774 4.079064 0.706812
C -2.629665 4.272616 1.466521
C -3.722369 3.415230 1.397071
C 0.874469 -0.263788 -1.300409
C 1.663746 0.792952 -0.797158
C 1.011707 2.091211 -0.616907
C -0.331876 2.267081 -0.919756
C 2.926053 0.387041 -0.245350
C 3.166323 -0.981302 -0.014419
C 2.198089 -1.984755 -0.302606
C 1.024516 -1.640208 -0.941563
H -0.368714 -4.043179 0.174757
H -2.578015 -4.878511 1.391389

H -4.689779 -4.092815 2.345429
H -5.616632 -1.868081 1.829388
H -5.223949 1.063858 1.409542
H -0.565349 4.678445 0.932366
H -2.644095 5.074591 2.198721
H -4.542367 3.535067 2.100141
H 1.539666 2.847327 -0.048978
H 2.387861 -2.995417 0.034018
C 3.905456 1.477827 0.155398
C 4.448696 -1.487289 0.633931
F 3.750704 2.575871 -0.624543
F 3.707217 1.878965 1.432798
F 5.193484 1.117517 0.032232
F 4.780401 -0.780311 1.734259
F 5.496584 -1.458347 -0.213713
F 4.320505 -2.774731 1.036922

Fragment 1 substituted with two CHO group

Molecular formula: C32H12O2

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.354849

Thermal correction to Enthalpy= 0.355793

Thermal correction to Gibbs Free Energy= 0.285566

Sum of electronic and zero-point Energies= -1376.705199

Sum of electronic and thermal Energies= -1376.684159

Sum of electronic and thermal Enthalpies= -1376.683215

Sum of electronic and thermal Free Energies= -1376.753442

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

222.671 90.953 147.805

Cartesian coordinates

Atom X Y Z

C	1.612312	1.207289	1.312005	H	3.951363	-4.164776	-2.232737
C	0.200012	1.199022	1.512175	H	4.911050	-1.977365	-1.626771
C	-0.447541	-0.011644	1.639867	H	4.590103	0.962595	-1.190996
C	0.266004	-1.245343	1.531699	H	0.033671	4.730243	-0.978824
C	1.630436	-1.206892	1.337844	H	2.207556	5.070580	-2.093756
C	2.326730	0.032286	1.202935	H	4.041424	3.464715	-1.889599
C	-0.556963	-2.243406	0.898821	H	-2.219431	2.957788	-0.158647
C	0.078455	-3.270262	0.206141	H	-3.295305	-2.882286	-0.319437
C	1.514664	-3.236400	-0.028796	C	-4.565033	1.582709	-0.675202
C	2.247956	-2.146386	0.491799	H	-5.417870	1.227786	-1.280491
C	2.213185	-4.004282	-1.003355	C	-5.238951	-1.315451	-0.932740
C	3.448440	-3.572551	-1.473859	H	-6.041521	-0.571493	-1.078897
C	4.031845	-2.331446	-1.095822	O	-4.417139	2.783086	-0.510072
C	3.414205	-1.573414	-0.114506	O	-5.436500	-2.477884	-1.239261
C	3.413978	-0.109180	0.265587				
C	3.828247	1.030357	-0.417568				
C	3.073356	2.273227	-0.336335				
C	1.924735	2.302519	0.485305				
C	0.749108	3.082657	0.230218				
C	0.873035	4.098292	-0.703158				
C	2.115520	4.259984	-1.376793				
C	3.171350	3.364337	-1.246157				
C	-1.718814	-0.191181	1.069577				
C	-2.433865	0.899258	0.522805				
C	-1.733380	2.177050	0.411542				
C	-0.408302	2.303240	0.813204				
C	-3.665427	0.537630	-0.131913				
C	-3.961817	-0.839905	-0.324032				
C	-3.045127	-1.878897	0.007995				
C	-1.889385	-1.567433	0.691947				
H	-0.502558	-4.001284	-0.351344				
H	1.756819	-4.892830	-1.431216				

Fragment 1 substituted with two CN group

Molecular formula: C32H10N2

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.332688

Thermal correction to Enthalpy= 0.333633

Thermal correction to Gibbs Free Energy= 0.264780

Sum of electronic and zero-point Energies= -1334.566040

Sum of electronic and thermal Energies= -1334.545526

Sum of electronic and thermal Enthalpies= -1334.544582

Sum of electronic and thermal Free Energies= -1334.613434

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

208.765 89.480 144.912

Cartesian coordinates

Atom X Y Z

C -1.511957 1.243194 -1.318337
C -0.106065 1.164292 -1.542291
C 0.476653 -0.079735 -1.667519
C -0.291058 -1.277400 -1.532314
C -1.647344 -1.168171 -1.310989
C -2.279607 0.105437 -1.180533
C 0.495055 -2.306164 -0.900013
C -0.177409 -3.291159 -0.181365
C -1.605367 -3.183703 0.079065
C -2.294202 -2.065377 -0.442063
C -2.321864 -3.904386 1.076464
C -3.525472 -3.406767 1.563093
C -4.055007 -2.143281 1.179122
C -3.419952 -1.428580 0.176848
C -3.355858 0.028964 -0.223239
C -3.703227 1.196163 0.450265
C -2.892154 2.400667 0.337393
C -1.758300 2.364221 -0.503997
C -0.545034 3.094465 -0.282246
C -0.604362 4.128430 0.637251
C -1.825563 4.357032 1.329694
C -2.923168 3.508703 1.231286
C 1.747088 -0.316916 -1.118314
C 2.505838 0.750197 -0.591955
C 1.888949 2.064919 -0.491672
C 0.564858 2.252977 -0.870155
C 3.706619 0.344993 0.073691
C 3.954844 -1.030305 0.293857
C 3.009528 -2.046173 -0.037358
C 1.862904 -1.692808 -0.723836
H 0.376110 -4.043338 0.375946
H -1.901846 -4.808975 1.507736

H -4.042375 -3.964073 2.338708
H -4.905979 -1.740626 1.721180
H -4.454083 1.175790 1.236903
H 0.267279 4.726058 0.887991
H -1.867491 5.181406 2.035267
H -3.776009 3.659020 1.887768
H 2.422038 2.822392 0.076095
H 3.199022 -3.056636 0.308501
C 4.603862 1.336213 0.578916
C 5.155685 -1.435916 0.962712
N 5.297020 2.184801 0.971863
N 6.118674 -1.804113 1.501726

Fragment 1 substituted with two NO₂ groupMolecular formula: C₃₀H₁₀N₂O₄

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.341972

Thermal correction to Enthalpy= 0.342917

Thermal correction to Gibbs Free Energy= 0.269799

Sum of electronic and zero-point Energies= -1559.057042

Sum of electronic and thermal Energies= -1559.034948

Sum of electronic and thermal Enthalpies= -1559.034004

Sum of electronic and thermal Free Energies= -1559.107121

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

214.591 94.643 153.888

Cartesian coordinates

Atom X Y Z

C	-1.992009	1.234272	-1.310717	H	-4.328905	-4.051157	2.362872
C	-0.593433	1.178085	-1.576838	H	-5.244959	-1.834776	1.797462
C	0.005257	-0.053452	-1.735313	H	-4.851005	1.094037	1.333537
C	-0.739874	-1.263969	-1.590020	H	-0.198547	4.722532	0.876846
C	-2.090409	-1.178386	-1.326227	H	-2.303833	5.132741	2.093678
C	-2.737885	0.083157	-1.162103	H	-4.191767	3.581418	1.989722
C	0.080306	-2.286843	-0.993921	H	1.957080	2.876038	-0.041223
C	-0.553955	-3.289896	-0.265396	H	2.857353	-3.003454	0.115293
C	-1.974683	-3.207962	0.039134	O	4.381342	2.406876	-0.178831
C	-2.696390	-2.095078	-0.448124	O	4.850776	-2.423649	1.319807
C	-2.649020	-3.950803	1.049673	O	4.485762	1.246861	1.670668
C	-3.844700	-3.477466	1.578193	O	5.833473	-0.766133	0.291445
C	-4.405040	-2.218223	1.225115	N	4.133960	1.417759	0.508167
C	-3.812162	-1.482816	0.212082	N	4.843684	-1.411291	0.622278
C	-3.782539	-0.020117	-0.173065				
C	-4.125581	1.134431	0.524146				
C	-3.336920	2.352758	0.399768				
C	-2.229217	2.342890	-0.476471				
C	-1.021355	3.089912	-0.284512				
C	-1.068103	4.113633	0.646996				
C	-2.270837	4.316057	1.378786				
C	-3.357467	3.451168	1.305736				
C	1.296717	-0.276203	-1.229231				
C	2.063342	0.800663	-0.721169				
C	1.419221	2.104260	-0.580636				
C	0.082282	2.269496	-0.913294				
C	3.274179	0.388384	-0.100535				
C	3.540673	-0.971172	0.089141				
C	2.616084	-1.998233	-0.208398				
C	1.440800	-1.652312	-0.851159				
H	0.028461	-4.038577	0.266495				
H	-2.201888	-4.853139	1.457653				

Fragment 2 substituted with two NH₂ groupMolecular formula: C₃₀H₁₂N₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.343503

Thermal correction to Enthalpy= 0.344447

Thermal correction to Gibbs Free Energy= 0.278754

Sum of electronic and zero-point Energies= -1259.478192

Sum of electronic and thermal Energies= -1259.458633

Sum of electronic and thermal Enthalpies= -1259.457689

Sum of electronic and thermal Free Energies= -1259.523381

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

215.551 87.523 138.261

Cartesian coordinates

Atom X Y Z

C	-0.725530	-0.000051	1.706445	H	2.980949	-3.627670	-1.764547
C	0.116774	-1.163523	1.625039	H	4.518295	-1.516906	-1.893358
C	1.472234	-0.717747	1.499597	H	4.518293	1.517022	-1.893275
C	1.472244	0.717703	1.499687	H	2.980914	3.627762	-1.764352
C	0.116790	1.163468	1.625178	H	0.099150	4.544798	-1.526893
C	-0.306263	-2.245896	0.887861	H	-2.372031	3.730379	-1.309915
C	0.609020	-3.041598	0.091141	N	-4.359040	-1.544956	-1.198600
C	1.939941	-2.610476	-0.022593	H	-4.594593	-2.412334	-0.730835
C	2.329354	-1.391346	0.655814	H	-5.189714	-1.123662	-1.595393
C	3.328395	-0.699946	-0.141544	N	-4.356712	1.545023	-1.200738
C	3.328384	0.699974	-0.141512	H	-5.179492	1.121720	-1.611232
C	2.329349	1.391345	0.655910	H	-4.601883	2.408613	-0.730936
C	1.939935	2.610499	-0.022425				
C	0.608987	3.041572	0.091274				
C	-0.306270	2.245770	0.887944				
C	-1.636270	2.314251	0.300741				
C	-2.454324	1.181984	0.393016				
C	-1.928705	-0.000023	1.053076				
C	-1.636246	-2.314329	0.300671				
C	-2.454344	-1.182086	0.393086				
C	-0.252403	-3.814184	-0.808468				
C	-1.551338	-3.393053	-0.689552				
C	2.940209	-2.785310	-1.084281				
C	3.745007	-1.680478	-1.152451				
C	3.745006	1.680554	-1.152359				
C	2.940194	2.785374	-1.084119				
C	-0.252484	3.814258	-0.808196				
C	-1.551427	3.393095	-0.689296				
C	-3.568938	0.695092	-0.422544				
C	-3.569393	-0.695234	-0.421930				
H	0.099253	-4.544609	-1.527271				
H	-2.371753	-3.730380	-1.310439				

Fragment 2 substituted with two OMe groupMolecular formula: C₃₂H₁₄O₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.377448

Thermal correction to Enthalpy= 0.378392

Thermal correction to Gibbs Free Energy= 0.306973

Sum of electronic and zero-point Energies= -1377.769856

Sum of electronic and thermal Energies= -1377.747870

Sum of electronic and thermal Enthalpies= -1377.746926

Sum of electronic and thermal Free Energies= -1377.818345

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

236.852 94.165 150.315

Cartesian coordinates

Atom X Y Z

C -0.901397 0.002768 1.654578
C -0.057827 -1.159153 1.598708
C 1.302769 -0.715079 1.509435
C 1.302870 0.719949 1.507807
C -0.057661 1.164426 1.596096
C -0.459964 -2.243662 0.853537
C 0.475805 -3.040164 0.080413
C 1.807184 -2.610301 -0.000228
C 2.179011 -1.388339 0.687669
C 3.198826 -0.699477 -0.084019
C 3.198917 0.700482 -0.085608
C 2.179204 1.391226 0.684527
C 1.807540 2.611682 -0.006123
C 0.476235 3.041934 0.073596
C -0.459657 2.247323 0.848504
C -1.771411 2.313100 0.226686
C -2.600745 1.188883 0.306261
C -2.096508 0.002103 0.978176
C -1.771712 -2.310620 0.231836
C -2.600821 -1.186086 0.308826
C -0.363545 -3.812814 -0.842226
C -1.663181 -3.389855 -0.757449
C 2.836233 -2.787486 -1.033426
C 3.642137 -1.682694 -1.081277
C 3.642340 1.681380 -1.085100
C 2.836595 2.786394 -1.039736
C -0.362989 3.812659 -0.850753
C -1.662695 3.390124 -0.765016
C -3.686099 0.691011 -0.552314
C -3.686037 -0.690026 -0.550891
H 0.006308 -4.543531 -1.551384
H -2.469106 -3.726670 -1.397028

H 2.895445 -3.630951 -1.710742
H 4.434887 -1.520501 -1.801587
H 4.435056 1.517447 -1.805054
H 2.895909 3.628322 -1.718953
H 0.006987 4.541726 -1.561545
H -2.468538 3.725727 -1.405334
O -4.473136 1.444874 -1.362692
O -4.472875 -1.445838 -1.359727
C -5.215163 2.477608 -0.706553
H -5.745206 3.018675 -1.492010
H -5.940720 2.049358 -0.004575
H -4.560050 3.168444 -0.164419
C -5.215940 -2.476077 -0.700879
H -5.939941 -2.045389 0.001218
H -5.747822 -3.017646 -1.484747
H -4.561351 -3.167101 -0.158283

Fragment 2 substituted with two OH group

Molecular formula: C30H10O2

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.318192

Thermal correction to Enthalpy= 0.319137

Thermal correction to Gibbs Free Energy= 0.255233

Sum of electronic and zero-point Energies= -1299.224756

Sum of electronic and thermal Energies= -1299.205927

Sum of electronic and thermal Enthalpies= -1299.204983

Sum of electronic and thermal Free Energies= -1299.268886

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

199.669 84.824 134.496

Cartesian coordinates

Atom X Y Z

C -0.711664 -0.009373 1.737115
C 0.139281 -1.164877 1.654993
C 1.489056 -0.708917 1.494878
C 1.475375 0.726152 1.477146
C 0.118273 1.160687 1.627202
C -0.286480 -2.265522 0.948110
C 0.617339 -3.064760 0.141164
C 1.937610 -2.620113 -0.012779
C 2.330306 -1.385047 0.639833
C 3.304501 -0.696144 -0.189243
C 3.293129 0.703619 -0.205612
C 2.307004 1.396134 0.606526
C 1.892860 2.605277 -0.076629
C 0.562333 3.027532 0.063427
C -0.328517 2.232733 0.888977
C -1.669783 2.284242 0.330240
C -2.477410 1.147275 0.450128
C -1.932561 -0.030629 1.113256
C -1.625635 -2.357055 0.391046
C -2.451970 -1.234170 0.480982
C -0.260715 -3.865098 -0.722228
C -1.559700 -3.456142 -0.578041
C 2.916466 -2.799870 -1.093249
C 3.707446 -1.687706 -1.194944
C 3.679483 1.676560 -1.235782
C 2.868466 2.776351 -1.161592
C -0.325222 3.783132 -0.825911
C -1.616876 3.351312 -0.673897
C -3.572449 0.624471 -0.357227
C -3.555442 -0.754262 -0.347722
H 0.080810 -4.609637 -1.431306
H -2.403331 -3.817030 -1.152213

H 2.951515 -3.651462 -1.762067
H 4.461825 -1.527482 -1.955778
H 4.437321 1.510903 -1.991968
H 2.888446 3.611747 -1.851167
H 0.003829 4.509587 -1.559146
H -2.453660 3.679356 -1.278567
O -4.405738 1.324049 -1.193828
H -4.657125 2.153551 -0.766321
O -4.343448 -1.573407 -1.081873
H -4.939437 -1.015735 -1.606034

Fragment 2 substituted with two Me group

Molecular formula: C32H14

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.365958

Thermal correction to Enthalpy= 0.366903

Thermal correction to Gibbs Free Energy= 0.301307

Sum of electronic and zero-point Energies= -1227.382263

Sum of electronic and thermal Energies= -1227.362682

Sum of electronic and thermal Enthalpies= -1227.361738

Sum of electronic and thermal Free Energies= -1227.427333

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

229.642 87.352 138.058

Cartesian coordinates

Atom X Y Z

C -0.682252 -0.000154 1.720404
C 0.156810 -1.161382 1.632915
C 1.513062 -0.717564 1.489746
C 1.513011 0.717442 1.489840
C 0.156727 1.161146 1.633065
C -0.275979 -2.245749 0.905602
C 0.629846 -3.047369 0.102653
C 1.955200 -2.614611 -0.036856
C 2.353776 -1.389744 0.631134
C 3.338026 -0.700035 -0.184104
C 3.337977 0.700262 -0.184012
C 2.353677 1.389794 0.631316
C 1.955016 2.614721 -0.036513
C 0.629631 3.047365 0.103049
C -0.276138 2.245576 0.905892
C -1.612926 2.316514 0.338150
C -2.427924 1.179686 0.421314
C -1.894955 -0.000155 1.074137
C -1.612762 -2.316710 0.337853
C -2.427840 -1.179951 0.421162
C -0.246302 -3.841062 -0.767133
C -1.542370 -3.422725 -0.629468
C 2.940501 -2.791934 -1.112527
C 3.740010 -1.684767 -1.197883
C 3.739892 1.685155 -1.197660
C 2.940306 2.792255 -1.112160
C -0.246573 3.841108 -0.766636
C -1.542611 3.422658 -0.629028
C -3.539363 0.689731 -0.418894
C -3.539313 -0.689965 -0.418986
H 0.092791 -4.593186 -1.469326
H -2.378804 -3.802949 -1.202013

H 2.973850 -3.637202 -1.789418
H 4.500729 -1.522575 -1.951991
H 4.500624 1.523116 -1.951789
H 2.973597 3.637615 -1.788939
H 0.092465 4.593349 -1.468729
H -2.379071 3.802897 -1.201526
C -4.432348 -1.595743 -1.210373
H -3.880387 -2.077351 -2.027968
H -4.835795 -2.398094 -0.582157
H -5.274226 -1.060516 -1.654887
C -4.432464 1.595548 -1.210162
H -4.835956 2.397798 -0.581844
H -3.880541 2.077290 -2.027703
H -5.274314 1.060322 -1.654733

Fragment 2 substituted with two *i*-Pr groupMolecular formula: C₃₆H₂₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.485546

Thermal correction to Enthalpy= 0.486490

Thermal correction to Gibbs Free Energy= 0.409757

Sum of electronic and zero-point Energies= -1384.521415

Sum of electronic and thermal Energies= -1384.496493

Sum of electronic and thermal Enthalpies= -1384.495549

Sum of electronic and thermal Free Energies= -1384.572282

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

304.685 107.997 161.498

Cartesian coordinates

Atom X Y Z

C -0.720947 -0.037768 1.584779
C 0.145186 -1.176893 1.572803
C 1.499779 -0.706320 1.550745
C 1.468464 0.728148 1.548183
C 0.095515 1.142192 1.575074
C -0.204808 -2.264408 0.810940
C 0.786406 -3.059237 0.108838
C 2.109350 -2.598463 0.078945
C 2.423209 -1.360979 0.768919
C 3.457943 -0.653011 0.036841
C 3.426760 0.747361 0.031288
C 2.362763 1.416429 0.759567
C 1.994338 2.631572 0.057410
C 0.652997 3.035904 0.086866
C -0.299219 2.216832 0.814382
C -1.591643 2.263733 0.149691
C -2.395840 1.113066 0.180640
C -1.873625 -0.064766 0.839008
C -1.490064 -2.370533 0.133610
C -2.342043 -1.249549 0.140817
C 0.004818 -3.899645 -0.802531
C -1.307827 -3.513093 -0.780254
C 3.187755 -2.760122 -0.905835
C 3.965838 -1.634272 -0.931951
C 3.889882 1.740027 -0.948113
C 3.061707 2.829402 -0.932871
C -0.166072 3.810217 -0.851920
C -1.461328 3.369364 -0.814487
C -3.486166 0.623076 -0.685829
C -3.452396 -0.761144 -0.726750
H 0.413503 -4.669835 -1.445531
H -2.081276 -3.955050 -1.391962

H 3.297203 -3.607500 -1.571967
H 4.783372 -1.459034 -1.620915
H 4.714005 1.594014 -1.636005
H 3.132484 3.674182 -1.607502
H 0.213467 4.562867 -1.532500
H -2.247498 3.728600 -1.466082
C -4.455860 1.592294 -1.345093
H -4.093300 2.591956 -1.083407
C -4.381525 -1.640598 -1.541023
H -5.255169 -1.031033 -1.790546
C -4.492119 1.532068 -2.884447
H -4.952447 0.610635 -3.250655
H -5.078627 2.369320 -3.278825
H -3.484849 1.595916 -3.307710
C -5.872699 1.498052 -0.737743
H -6.510800 2.291104 -1.143051
H -6.354183 0.540928 -0.958577
H -5.839734 1.611710 0.349750
C -3.764601 -2.074798 -2.889564
H -4.471963 -2.700752 -3.445100
H -3.523621 -1.205266 -3.506563
H -2.841957 -2.643096 -2.760047
C -4.909543 -2.840877 -0.731993
H -5.623437 -3.416989 -1.330330
H -4.109427 -3.518139 -0.422016
H -5.421887 -2.504254 0.174621

Fragment 2 substituted with two F groupMolecular formula: C₃₀H₈F₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.292878

Thermal correction to Enthalpy= 0.293822

Thermal correction to Gibbs Free Energy= 0.231059

Sum of electronic and zero-point Energies= -1347.262148

Sum of electronic and thermal Energies= -1347.244081

Sum of electronic and thermal Enthalpies= -1347.243137

Sum of electronic and thermal Free Energies= -1347.305900

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

183.783 81.361 132.096

Cartesian coordinates

Atom X Y Z

C	-0.685281	-0.000002	1.744210	H	2.947601	-3.635421	-1.792507
C	0.153541	-1.161873	1.650688	H	4.474327	-1.521480	-1.961673
C	1.509339	-0.717440	1.498497	H	4.474360	1.521549	-1.961630
C	1.509330	0.717463	1.498495	H	2.947460	3.635376	-1.792627
C	0.153525	1.161879	1.650690	H	0.069047	4.567383	-1.480161
C	-0.280828	-2.251254	0.930961	H	-2.405895	3.752023	-1.199395
C	0.617047	-3.049293	0.114915	F	-4.275569	-1.459503	-1.149869
C	1.940149	-2.614840	-0.033310	F	-4.275564	1.459435	-1.149905
C	2.343144	-1.389701	0.634398				
C	3.322650	-0.699961	-0.186879				
C	3.322640	0.700000	-0.186880				
C	2.343120	1.389729	0.634386				
C	1.940100	2.614854	-0.033338				
C	0.617003	3.049311	0.114933				
C	-0.280863	2.251257	0.930971				
C	-1.616967	2.321563	0.367493				
C	-2.433575	1.191951	0.469877				
C	-1.909448	-0.000010	1.118655				
C	-1.616932	-2.321579	0.367491				
C	-2.433558	-1.191981	0.469880				
C	-0.266662	-3.828767	-0.762385				
C	-1.561017	-3.407304	-0.616797				
C	2.918632	-2.790929	-1.114655				
C	3.718141	-1.684037	-1.203219				
C	3.718145	1.684088	-1.203200				
C	2.918530	2.790912	-1.114738				
C	-0.266720	3.828841	-0.762298				
C	-1.561050	3.407264	-0.616823				
C	-3.500228	0.684579	-0.383885				
C	-3.500231	-0.684629	-0.383868				
H	0.069114	-4.567267	-1.480288				
H	-2.405873	-3.752097	-1.199333				

Fragment 2 substituted with two COOH group

Molecular formula: C32H10O4

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.342768

Thermal correction to Enthalpy= 0.343712

Thermal correction to Gibbs Free Energy= 0.270970

Sum of electronic and zero-point Energies= -1525.907750

Sum of electronic and thermal Energies= -1525.885632

Sum of electronic and thermal Enthalpies= -1525.884687

Sum of electronic and thermal Free Energies= -1525.957429

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

215.090 95.747 153.097

Cartesian coordinates

Atom X Y Z

C	1.262188	-0.111436	1.426220	H	-2.470386	3.888227	-1.564851
C	0.537881	1.122709	1.444261	H	-4.197519	1.929319	-1.506349
C	-0.865997	0.815909	1.502883	H	-4.490976	-1.112489	-1.483683
C	-1.004335	-0.610250	1.514025	H	-3.171327	-3.366571	-1.507970
C	0.313479	-1.181859	1.464427	H	-0.373830	-4.617577	-1.557682
C	0.969532	2.167109	0.662052	H	2.192057	-4.065966	-1.622183
C	0.041779	3.061946	-0.010385	C	4.881892	1.110860	-1.797479
C	-1.322298	2.759410	0.034647	C	4.403704	-2.046304	-1.924558
C	-1.743116	1.569070	0.759092	O	4.629348	2.125364	-2.416729
C	-2.889517	0.984171	0.090001	O	4.473578	-3.240433	-1.698770
C	-3.024425	-0.410732	0.100861	O	6.137429	0.630425	-1.676464
C	-2.010715	-1.194099	0.781043	H	6.698902	1.210150	-2.219484
C	-1.826751	-2.454221	0.076424	O	4.895890	-1.500405	-3.061198
C	-0.546365	-3.015206	0.040666	H	5.325408	-2.228614	-3.540613
C	0.535103	-2.302800	0.700581				
C	1.763570	-2.506010	-0.042781				
C	2.699532	-1.455912	-0.073310				
C	2.371877	-0.227267	0.617421				
C	2.212899	2.118342	-0.085201				
C	2.930134	0.906140	-0.092511				
C	0.864518	3.774751	-0.995358				
C	2.120619	3.233572	-1.039700				
C	-2.425212	3.038975	-0.894006				
C	-3.329595	2.012305	-0.863346				
C	-3.654192	-1.349835	-0.837860				
C	-2.963360	-2.531048	-0.850730				
C	0.126667	-3.896418	-0.922833				
C	1.464387	-3.610122	-0.965783				
C	3.739818	-1.070525	-1.037335				
C	3.893589	0.309981	-1.029095				
H	0.503803	4.555438	-1.654098				
H	2.901340	3.496288	-1.738392				

Fragment 2 substituted with two CF₃ groupMolecular formula: C₃₂H₈F₆

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.323897

Thermal correction to Enthalpy= 0.324841

Thermal correction to Gibbs Free Energy= 0.249359

Sum of electronic and zero-point Energies= -1822.849031

Sum of electronic and thermal Energies= -1822.825557

Sum of electronic and thermal Enthalpies= -1822.824613

Sum of electronic and thermal Free Energies= -1822.900095

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

203.248 100.654 158.865

Cartesian coordinates

Atom X Y Z

C	-0.490278	0.044726	-1.923504	H	-3.701969	-3.657147	1.932590
C	-1.310631	-1.115159	-1.752578	H	-5.192507	-1.546256	2.313412
C	-2.645618	-0.677978	-1.449116	H	-5.189648	1.509529	2.360934
C	-2.644462	0.755288	-1.427301	H	-3.695209	3.628317	2.045140
C	-1.308300	1.200012	-1.717665	H	-0.872118	4.586204	1.398694
C	-0.797137	-2.213641	-1.105324	H	1.546081	3.805087	0.824741
C	-1.601359	-3.033245	-0.215036	C	3.575714	-1.619160	0.449584
C	-2.896125	-2.603487	0.091272	C	3.760847	1.551671	0.317691
C	-3.371948	-1.363816	-0.504675	F	3.707244	-2.758107	-0.272783
C	-4.249367	-0.690368	0.434275	F	3.112348	-1.988947	1.670641
C	-4.248461	0.710327	0.455897	F	4.805249	-1.111739	0.626150
C	-3.370230	1.411180	-0.461863	F	4.915213	1.339688	-0.345738
C	-2.891553	2.629824	0.171835	F	3.994851	1.325670	1.627876
C	-1.595083	3.063831	-0.119871	F	3.482876	2.870650	0.184876
C	-0.788640	2.272999	-1.034410				
C	0.606866	2.344753	-0.635311				
C	1.421167	1.216849	-0.865013				
C	0.797351	0.038052	-1.434019				
C	0.593432	-2.294980	-0.703984				
C	1.398804	-1.156335	-0.884330				
C	-0.624080	-3.841948	0.525381				
C	0.646119	-3.420971	0.239898				
C	-3.747936	-2.800507	1.271360				
C	-4.528448	-1.694313	1.470448				
C	-4.525542	1.682405	1.522752				
C	-3.742949	2.792677	1.357663				
C	-0.621121	3.847816	0.646901				
C	0.649451	3.440038	0.347650				
C	2.643448	0.700520	-0.220922				
C	2.618153	-0.679622	-0.222149				
H	-0.874315	-4.607103	1.250124				
H	1.547153	-3.798191	0.701957				

Fragment 2 substituted with two CHO group

Molecular formula: C32H10O2

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.329986

Thermal correction to Enthalpy= 0.330930

Thermal correction to Gibbs Free Energy= 0.263235

Sum of electronic and zero-point Energies= -1375.422947

Sum of electronic and thermal Energies= -1375.402657

Sum of electronic and thermal Enthalpies= -1375.401712

Sum of electronic and thermal Free Energies= -1375.469408

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

207.069 88.860 142.478

Cartesian coordinates

Atom X Y Z

C -0.326030 0.000002 1.801401
C 0.505783 -1.156428 1.670298
C 1.860506 -0.715903 1.470054
C 1.860518 0.715869 1.470060
C 0.505801 1.156418 1.670303
C 0.040339 -2.246435 0.974885
C 0.907686 -3.055818 0.133738
C 2.218997 -2.620831 -0.076455
C 2.650699 -1.387780 0.567794
C 3.588786 -0.700916 -0.297843
C 3.588800 0.700862 -0.297835
C 2.650725 1.387738 0.567806
C 2.219047 2.620801 -0.076433
C 0.907743 3.055809 0.133760
C 0.040375 2.246434 0.974894
C -1.318387 2.328437 0.477900
C -2.140581 1.190092 0.609383
C -1.572646 0.000015 1.210421
C -1.318421 -2.328409 0.477896
C -2.140586 -1.190049 0.609369
C -0.014436 -3.862018 -0.676552
C -1.303639 -3.449213 -0.472042
C 3.150875 -2.800252 -1.197320
C 3.940433 -1.690097 -1.326651
C 3.940469 1.690048 -1.326632
C 3.150931 2.800215 -1.197293
C -0.014360 3.862038 -0.676521
C -1.303571 3.449249 -0.472031
C -3.305201 0.702665 -0.138073
C -3.305165 -0.702614 -0.138129
H 0.287554 -4.621283 -1.387765
H -2.184306 -3.817234 -0.977995

H 3.153048 -3.647600 -1.871970
H 4.660937 -1.529291 -2.119472
H 4.660972 1.529235 -2.119453
H 3.153120 3.647568 -1.871936
H 0.287650 4.621308 -1.387721
H -2.184222 3.817295 -0.977986
C -4.298651 -1.546696 -0.809881
H -5.142031 -1.016069 -1.290998
C -4.298746 1.546735 -0.809764
H -5.142411 1.016123 -1.290396
O -4.247468 -2.766670 -0.855343
O -4.247391 2.766689 -0.855576

Fragment 2 substituted with two CN groupMolecular formula: C₃₂H₈N₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.307912

Thermal correction to Enthalpy= 0.308856

Thermal correction to Gibbs Free Energy= 0.241636

Sum of electronic and zero-point Energies= -1333.280452

Sum of electronic and thermal Energies= -1333.260538

Sum of electronic and thermal Enthalpies= -1333.259594

Sum of electronic and thermal Free Energies= -1333.326814

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

193.218 87.407 141.477

Cartesian coordinates

Atom X Y Z

C	0.327816	-0.000001	1.861134	H	-3.025194	3.644559	-1.935871
C	-0.498252	1.158450	1.699606	H	-4.526599	1.527888	-2.229208
C	-1.843758	0.716697	1.450251	H	-4.526609	-1.528116	-2.229158
C	-1.843718	-0.716822	1.450238	H	-3.024804	-3.644547	-1.936126
C	-0.498184	-1.158498	1.699593	H	-0.175710	-4.594838	-1.384495
C	-0.011085	2.250846	1.019400	H	2.268545	-3.784366	-0.918694
C	-0.846855	3.055264	0.143187	C	4.215032	1.525544	-0.772005
C	-2.150487	2.619119	-0.110332	C	4.215232	-1.525337	-0.771828
C	-2.602990	1.387720	0.521878	N	4.927435	2.243980	-1.349526
C	-3.513611	0.700207	-0.374106	N	4.927711	-2.243743	-1.349293
C	-3.513570	-0.700387	-0.374114				
C	-2.602900	-1.387865	0.521840				
C	-2.150312	-2.619216	-0.110412				
C	-0.846676	-3.055316	0.143162				
C	-0.010954	-2.250862	1.019382				
C	1.360513	-2.324753	0.559151				
C	2.168259	-1.185575	0.718517				
C	1.596417	0.000039	1.317158				
C	1.360377	2.324826	0.559181				
C	2.168189	1.185690	0.718512				
C	0.101956	3.845911	-0.653015				
C	1.382311	3.426071	-0.410640				
C	-3.045360	2.797904	-1.260778				
C	-3.831686	1.688631	-1.413983				
C	-3.831641	-1.688825	-1.413974				
C	-3.045075	-2.797954	-1.260958				
C	0.102182	-3.845980	-0.652959				
C	1.382500	-3.425952	-0.410726				
C	3.314220	-0.697779	-0.053757				
C	3.314110	0.697948	-0.053866				
H	-0.175977	4.594723	-1.384583				
H	2.268348	3.784572	-0.918562				

Fragment 2 substituted with two NO₂ groupMolecular formula: C₃₀H₈N₂O₄

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.317190

Thermal correction to Enthalpy= 0.318134

Thermal correction to Gibbs Free Energy= 0.246460

Sum of electronic and zero-point Energies= -1557.767231

Sum of electronic and thermal Energies= -1557.745639

Sum of electronic and thermal Enthalpies= -1557.744694

Sum of electronic and thermal Free Energies= -1557.816368

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

199.039 92.723 150.850

Cartesian coordinates

Atom X Y Z

C	1.256887	-0.103013	1.438463	H	-2.459882	3.892407	-1.570946
C	0.528788	1.128755	1.458689	H	-4.181797	1.929016	-1.532389
C	-0.874412	0.817552	1.503434	H	-4.472134	-1.117936	-1.512244
C	-1.009102	-0.608681	1.509660	H	-3.151701	-3.370752	-1.526698
C	0.312182	-1.175810	1.462165	H	-0.353869	-4.603432	-1.573034
C	0.963564	2.177237	0.685429	H	2.193911	-4.030529	-1.651900
C	0.040611	3.072516	0.006942	O	4.924254	2.248510	-1.654761
C	-1.322553	2.763468	0.035807	O	3.873035	-2.571809	-2.691286
C	-1.745985	1.569793	0.753349	O	5.325717	0.407011	-2.767476
C	-2.884929	0.983126	0.072326	O	5.651872	-2.201029	-1.473118
C	-3.016907	-0.411815	0.080863	N	4.771023	1.041416	-1.868173
C	-2.006847	-1.192661	0.767459	N	4.489626	-2.002235	-1.794013
C	-1.816534	-2.454674	0.062680				
C	-0.537280	-3.015497	0.038574				
C	0.539152	-2.301142	0.704678				
C	1.767858	-2.501425	-0.033840				
C	2.700621	-1.443578	-0.048701				
C	2.376286	-0.208481	0.641177				
C	2.215531	2.139874	-0.047788				
C	2.940176	0.933909	-0.051228				
C	0.873567	3.796617	-0.960851				
C	2.135022	3.265175	-0.987586				
C	-2.417925	3.041655	-0.901985				
C	-3.319733	2.012429	-0.881840				
C	-3.639036	-1.353515	-0.861156				
C	-2.948024	-2.534576	-0.869334				
C	0.141783	-3.889471	-0.926741				
C	1.478468	-3.596736	-0.967947				
C	3.732851	-1.046107	-0.989464				
C	3.879753	0.327146	-0.995423				
H	0.520786	4.585671	-1.613683				
H	2.934958	3.561559	-1.650697				

Transition state structure for the reaction of butadiene with Fragment 1

Molecular formula: C34H18

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.424186

Thermal correction to Enthalpy= 0.425130

Thermal correction to Gibbs Free Energy= 0.354540

Sum of electronic and zero-point Energies= -1305.947309

Sum of electronic and thermal Energies= -1305.926010

Sum of electronic and thermal Enthalpies= -1305.925066

Sum of electronic and thermal Free Energies= -1305.995656

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

266.180 95.050 148.570

Cartesian coordinates

Atom X Y Z

C	-1.484501	-0.455318	-1.124694	H	-5.659630	-1.205181	1.852843
C	-1.328754	0.964926	-1.080600	H	-4.220722	-3.138421	1.437012
C	-0.055532	1.486766	-1.026965	H	-2.966200	3.230814	0.897283
C	1.100112	0.641538	-0.985957	H	-1.168499	4.977766	1.770287
C	0.919047	-0.731496	-1.036977	H	1.196523	5.210138	2.352222
C	-0.394321	-1.298410	-1.075821	H	2.894876	3.578875	1.623941
C	2.109780	1.231285	-0.159777	H	-1.726175	-3.826972	0.815465
C	3.016781	0.362538	0.464880	H	1.030477	-4.403874	1.505173
C	2.841029	-1.063059	0.415716	H	4.160192	-1.623166	2.050072
C	1.741989	-1.584087	-0.287965	H	3.184850	-3.785729	2.451068
C	3.583183	-2.036661	1.227269	C	4.080384	-4.994678	0.428870
C	2.892095	-3.286604	1.536364	H	3.606507	-5.930962	0.708262
C	1.567913	-3.571799	1.056991	H	3.666626	-4.518834	-0.450344
C	0.988808	-2.768499	0.106796	C	5.188531	-2.403499	0.069060
C	-0.432366	-2.532664	-0.331263	H	4.575583	-2.652051	-0.791715
C	-1.659161	-2.938622	0.191213	H	5.646130	-1.420580	-0.013010
C	-2.811465	-2.052700	0.168748	C	5.922793	-3.430448	0.686727
C	-2.664483	-0.784148	-0.436885	H	6.834246	-3.180427	1.224982
C	-3.352308	0.408768	-0.033046	C	5.357005	-4.694864	0.877680
C	-4.452009	0.235663	0.790183	H	5.852967	-5.388756	1.553839
C	-4.784285	-1.079495	1.221811				
C	-3.983418	-2.186975	0.968019				
C	0.204953	2.619235	-0.236615				
C	-0.853611	3.332048	0.369144				
C	-2.197187	2.778625	0.274755				
C	-2.426765	1.560611	-0.357919				
C	-0.435147	4.337971	1.286242				
C	0.906903	4.448861	1.633371				
C	1.903006	3.538734	1.181922				
C	1.554331	2.575038	0.249785				
H	3.761055	0.752568	1.156785				
H	-5.028626	1.076876	1.164901				

Transition state structure for the reaction of butadiene with Fragment 1 substituted with one NH₂ groupMolecular formula: C₃₄H₁₉N

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.442493

Thermal correction to Enthalpy= 0.443437

Thermal correction to Gibbs Free Energy= 0.372330

Sum of electronic and zero-point Energies= -1361.292056

Sum of electronic and thermal Energies= -1361.270065

Sum of electronic and thermal Enthalpies= -1361.269120

Sum of electronic and thermal Free Energies= -1361.340227

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

277.669 99.638 149.657

Cartesian coordinates

Atom X Y Z

C -1.756577 -0.513229 -0.934914
C -1.634541 0.911415 -0.934984
C -0.374290 1.465485 -0.925561
C 0.803692 0.649146 -0.884166
C 0.653302 -0.729620 -0.888692
C -0.646038 -1.327648 -0.884709
C 1.812730 1.284645 -0.098117
C 2.752083 0.448908 0.535248
C 2.611022 -0.973162 0.524966
C 1.510372 -1.541326 -0.132590
C 3.438409 -1.910731 1.352091
C 2.712738 -3.182993 1.715618
C 1.413220 -3.529920 1.237966
C 0.787921 -2.732819 0.305175
C -0.638514 -2.542453 -0.104608
C -1.849134 -2.964041 0.449598
C -3.020232 -2.105537 0.426313
C -2.915321 -0.850214 -0.216092
C -3.623670 0.336968 0.167705
C -4.704182 0.161489 1.015589
C -4.997309 -1.149176 1.488095
C -4.175923 -2.244672 1.249194
C -0.125363 2.625195 -0.172274
C -1.187995 3.328679 0.436974
C -2.519429 2.741652 0.386047
C -2.732265 1.500826 -0.207281
C -0.775425 4.367883 1.319416
C 0.570158 4.518016 1.636717
C 1.578188 3.619265 1.188980
C 1.234250 2.623399 0.288933
H 3.501862 0.877257 1.198133

H -5.293817 0.999015 1.378032
H -5.858419 -1.277934 2.137883
H -4.383601 -3.188418 1.746989
H -3.286398 3.193230 1.011553
H -1.514008 5.003104 1.801529
H 0.856011 5.304111 2.329969
H 2.577122 3.693453 1.610265
H -1.885180 -3.837802 1.096648
H 0.911833 -4.376575 1.701916
C 3.777347 -4.707002 -0.124972
H 3.284826 -5.658388 -0.299250
H 3.411767 -3.878842 -0.717104
C 4.913234 -2.187953 0.586283
H 4.648527 -2.163942 -0.473052
H 5.519769 -1.306944 0.804019
C 5.567546 -3.446672 0.949165
H 6.460140 -3.439410 1.568333
C 4.981335 -4.648730 0.564964
H 5.415967 -5.578528 0.931727
N 3.219895 -3.777140 2.847533
H 2.886123 -4.720617 3.012452
H 4.242714 -3.741418 2.874754
H 3.743313 -1.437454 2.290187

Transition state structure for the reaction of butadiene with Fragment 1 substituted with one OMe group

Molecular formula: C35H20O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.459333

Thermal correction to Enthalpy= 0.460277

Thermal correction to Gibbs Free Energy= 0.385924

Sum of electronic and zero-point Energies= -1420.439673

Sum of electronic and thermal Energies= -1420.416224

Sum of electronic and thermal Enthalpies= -1420.415280

Sum of electronic and thermal Free Energies= -1420.489634

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

288.236 103.774 156.490

Cartesian coordinates

Atom X Y Z

C	-1.752516	-0.529316	-0.959794	H	-5.256201	0.901501	1.454438
C	-1.649255	0.896636	-0.940729	H	-5.773059	-1.393665	2.193557
C	-0.396155	1.467102	-0.949609	H	-4.281574	-3.277806	1.742656
C	0.792650	0.665791	-0.946779	H	-3.286770	3.126486	1.077053
C	0.660315	-0.714365	-0.974134	H	-1.520951	4.948477	1.855313
C	-0.630162	-1.329404	-0.948396	H	0.856128	5.272664	2.336394
C	1.811015	1.303160	-0.172829	H	2.581526	3.695705	1.555118
C	2.775722	0.471101	0.426177	H	-1.790045	-3.883252	1.026865
C	2.652680	-0.951898	0.395481	H	0.979772	-4.338222	1.621177
C	1.545083	-1.526560	-0.249059	C	3.840559	-4.866565	-0.103764
C	3.511550	-1.900366	1.169216	H	3.396683	-5.856424	-0.141417
C	2.786521	-3.145930	1.583304	H	3.399062	-4.135397	-0.767219
C	1.485192	-3.503873	1.147179	C	4.903880	-2.225482	0.249032
C	0.849255	-2.725686	0.195294	H	4.504830	-2.324234	-0.762207
C	-0.587393	-2.553462	-0.182833	H	5.487126	-1.305024	0.304391
C	-1.780097	-2.999702	0.392045	C	5.630686	-3.407962	0.680671
C	-2.962676	-2.157585	0.407678	H	6.527601	-3.297176	1.282880
C	-2.889614	-0.892109	-0.219361	C	5.075670	-4.667545	0.500962
C	-3.605039	0.279551	0.197671	H	5.571471	-5.521601	0.960528
C	-4.663719	0.077381	1.066778	O	3.373612	-3.660936	2.689190
C	-4.928438	-1.243877	1.526804	C	2.921430	-4.910407	3.193897
C	-4.097844	-2.324287	1.254055	H	2.945108	-5.670517	2.404040
C	-0.145650	2.618340	-0.183838	H	3.610751	-5.180516	3.994514
C	-1.203502	3.298788	0.458898	H	1.907232	-4.833943	3.601881
C	-2.528028	2.694913	0.427809	H	3.927492	-1.447049	2.071945
C	-2.737873	1.460619	-0.179907				
C	-0.785079	4.330154	1.347751				
C	0.565166	4.493156	1.637820				
C	1.574590	3.614577	1.154688				
C	1.223797	2.627511	0.247491				
H	3.536352	0.898174	1.077411				

Transition state structure for the reaction of butadiene with Fragment 1 substituted with one OH group

Molecular formula: C34H18O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.428917

Thermal correction to Enthalpy= 0.429861

Thermal correction to Gibbs Free Energy= 0.358955

Sum of electronic and zero-point Energies= -1381.165906

Sum of electronic and thermal Energies= -1381.144092

Sum of electronic and thermal Enthalpies= -1381.143148

Sum of electronic and thermal Free Energies= -1381.214054

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

269.150 98.500 149.235

Cartesian coordinates

Atom X Y Z

C	-1.780624	-0.554002	-0.923812	H	-5.293081	0.953525	1.429507
C	-1.658726	0.870351	-0.922337	H	-5.848460	-1.323766	2.193660
C	-0.398195	1.424397	-0.924073	H	-4.377061	-3.233617	1.784311
C	0.778854	0.607389	-0.893019	H	-3.291368	3.148574	1.044343
C	0.629035	-0.770295	-0.898330	H	-1.512436	4.958677	1.817782
C	-0.670196	-1.368573	-0.886404	H	0.862227	5.261389	2.323169
C	1.795817	1.242927	-0.113961	H	2.577285	3.652015	1.585586
C	2.739310	0.408826	0.510911	H	-1.886203	-3.881603	1.105084
C	2.597945	-1.015611	0.502023	H	0.959852	-4.483255	1.629473
C	1.491594	-1.583834	-0.148425	C	3.904320	-4.716036	-0.287675
C	3.399110	-1.945008	1.355453	H	3.445485	-5.659408	-0.562721
C	2.701814	-3.234176	1.657151	H	3.538310	-3.841862	-0.810434
C	1.417176	-3.603301	1.187989	C	4.949556	-2.217185	0.696140
C	0.773318	-2.777284	0.287339	H	4.764781	-2.141470	-0.376543
C	-0.655541	-2.585186	-0.109952	H	5.543751	-1.357934	1.009109
C	-1.858950	-3.007374	0.458536	C	5.548775	-3.500174	1.058533
C	-3.030592	-2.148823	0.448471	H	6.396232	-3.532227	1.737473
C	-2.932130	-0.892634	-0.193074	C	5.019838	-4.684644	0.523586
C	-3.636253	0.293612	0.199793	H	5.430826	-5.631058	0.872785
C	-4.707267	0.116568	1.059710	O	3.243220	-3.924460	2.668078
C	-4.995005	-1.194311	1.534132	H	4.229923	-3.899983	2.525682
C	-4.175972	-2.289418	1.284915	H	3.655044	-1.487850	2.315949
C	-0.141941	2.583240	-0.171284				
C	-1.198948	3.285539	0.449026				
C	-2.530618	2.698084	0.410589				
C	-2.749190	1.458314	-0.182635				
C	-0.778209	4.324261	1.328104				
C	0.570272	4.475540	1.632315				
C	1.574276	3.577671	1.174266				
C	1.221681	2.582643	0.276754				
H	3.491883	0.836968	1.170523				

Transition state structure for the reaction of butadiene with Fragment 1 substituted with one Me group

Molecular formula: C35H20

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.453321

Thermal correction to Enthalpy= 0.454265

Thermal correction to Gibbs Free Energy= 0.381126

Sum of electronic and zero-point Energies= -1345.237117

Sum of electronic and thermal Energies= -1345.214338

Sum of electronic and thermal Enthalpies= -1345.213393

Sum of electronic and thermal Free Energies= -1345.286533

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

284.463 100.895 153.935

Cartesian coordinates

Atom	X	Y	Z	
C	-1.462914	-0.483206	-1.131567	H -5.023370 1.041491 1.137875
C	-1.318463	0.938705	-1.099887	H -5.638074 -1.239688 1.844261
C	-0.049730	1.471817	-1.049494	H -4.183336 -3.164986 1.448621
C	1.112953	0.636062	-0.998606	H -2.977125 3.208173 0.855909
C	0.941949	-0.738783	-1.038680	H -1.195052 4.976305 1.717863
C	-0.365896	-1.316674	-1.073754	H 1.167216 5.231782 2.301959
C	2.116510	1.241427	-0.177373	H 2.879580 3.608560 1.589459
C	3.029255	0.382878	0.457869	H -1.681948 -3.838461 0.840406
C	2.862532	-1.040368	0.421325	H 1.054996 -4.361690 1.571315
C	1.768729	-1.577649	-0.276856	C 4.030850 -5.031250 0.156581
C	3.623804	-2.010151	1.238824	H 3.561712 -6.002873 0.275877
C	2.892800	-3.234193	1.630956	H 3.568591 -4.376085 -0.568029
C	1.599480	-3.538926	1.113112	C 5.123478 -2.391957 0.195997
C	1.024020	-2.758486	0.131852	H 4.597703 -2.555082 -0.742320
C	-0.393390	-2.543393	-0.313725	H 5.645900 -1.437001 0.190993
C	-1.620176	-2.955375	0.208152	C 5.853982 -3.508155 0.691148
C	-2.778751	-2.079452	0.174646	H 6.764859 -3.342736 1.261002
C	-2.641417	-0.815068	-0.442803	C 5.289549 -4.789148 0.668933
C	-3.339521	0.375719	-0.050887	H 5.796426 -5.586707 1.209344
C	-4.439490	0.201527	0.771718	C 3.328320 -3.852084 2.934066
C	-4.762259	-1.112574	1.214142	H 3.058204 -3.197598 3.774734
C	-3.952246	-2.215821	0.971931	H 2.867537 -4.828909 3.103876
C	0.200434	2.612725	-0.268110	H 4.417579 -3.970998 2.962714
C	-0.864581	3.321935	0.330363	H 4.144652 -1.561661 2.085569
C	-2.203484	2.756991	0.238374	
C	-2.422440	1.531917	-0.384315	
C	-0.455794	4.338486	1.240231	
C	0.884759	4.462520	1.588729	
C	1.888805	3.556838	1.146136	
C	1.549520	2.582568	0.221226	
H	3.771148	0.785395	1.145403	

Transition state structure for the reaction of butadiene with Fragment 1 substituted with one *i*-Pr group

Molecular formula: C37H24

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.512928

Thermal correction to Enthalpy= 0.513872

Thermal correction to Gibbs Free Energy= 0.434915

Sum of electronic and zero-point Energies= -1423.809393

Sum of electronic and thermal Energies= -1423.783877

Sum of electronic and thermal Enthalpies= -1423.782933

Sum of electronic and thermal Free Energies= -1423.861890

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

321.867 111.265 166.180

Cartesian coordinates

Atom X Y Z

C -1.625121 -0.337956 -0.785264
C -1.458579 1.081828 -0.761619
C -0.182158 1.597210 -0.799323
C 0.969477 0.744936 -0.830627
C 0.776198 -0.627412 -0.862181
C -0.538801 -1.186821 -0.806073
C 2.034732 1.332818 -0.077991
C 2.975717 0.458151 0.493574
C 2.785383 -0.960472 0.464817
C 1.641533 -1.480027 -0.160890
C 3.598814 -1.952524 1.213332
C 2.859444 -3.157527 1.685942
C 1.535637 -3.437793 1.246992
C 0.911548 -2.649949 0.298019
C -0.529595 -2.414702 -0.046831
C -1.723010 -2.810604 0.559473
C -2.868329 -1.918473 0.608737
C -2.756849 -0.654812 -0.015640
C -3.409030 0.544695 0.425335
C -4.451394 0.384293 1.322449
C -4.760847 -0.926090 1.785091
C -3.985109 -2.039972 1.486077
C 0.137612 2.732289 -0.034950
C -0.873072 3.455365 0.636505
C -2.223032 2.909681 0.636883
C -2.501440 1.688752 0.029948
C -0.387727 4.463551 1.517738
C 0.975210 4.566454 1.774207
C 1.932768 3.646795 1.262883
C 1.516337 2.680377 0.361384
H 3.768715 0.848153 1.129471
H -4.996467 1.231644 1.729139

H -5.592466 -1.042219 2.474448
H -4.195713 -2.986807 1.976717
H -2.945596 3.370437 1.306995
H -1.082863 5.111138 2.045824
H 1.317237 5.329600 2.467680
H 2.952090 3.682047 1.637877
H -1.752873 -3.694641 1.192804
H 0.994747 -4.244514 1.732808
C 3.920847 -4.992893 0.075662
H 3.491756 -5.984173 0.177847
H 3.381445 -4.316736 -0.571694
C 4.958048 -2.330744 0.085441
H 4.387619 -2.501744 -0.826190
H 5.485268 -1.379456 0.026557
C 5.749132 -3.444953 0.511027
H 6.702010 -3.270736 1.003948
C 5.206594 -4.732490 0.508383
H 5.770907 -5.534755 0.980847
C 2.888992 -5.169650 3.316899
H 3.070528 -5.864629 2.494601
H 3.406288 -5.546881 4.204837
H 1.817467 -5.181691 3.544588
C 3.384461 -3.755796 2.985350
H 4.479859 -3.795389 2.881499
C 3.074805 -2.821261 4.182064
H 1.994300 -2.750807 4.347312
H 3.531085 -3.214228 5.097154
H 3.453668 -1.806874 4.030515
H 4.176277 -1.504098 2.021792

Transition state structure for the reaction of butadiene with Fragment 1 substituted with one F groupMolecular formula: C₃₄H₁₇F

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.416451

Thermal correction to Enthalpy= 0.417396

Thermal correction to Gibbs Free Energy= 0.344646

Sum of electronic and zero-point Energies= -1405.185798

Sum of electronic and thermal Energies= -1405.163522

Sum of electronic and thermal Enthalpies= -1405.162578

Sum of electronic and thermal Free Energies= -1405.235328

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

261.327 98.237 153.115

Cartesian coordinates

Atom X Y Z

C -1.761349 -0.509530 -0.989239

C -1.638755 0.914192 -0.967772

C -0.377232 1.465891 -0.940824

C 0.797439 0.647712 -0.904845

C 0.648973 -0.729047 -0.936348

C -0.651365 -1.326327 -0.947060

C 1.804552 1.272593 -0.099549

C 2.738622 0.435588 0.524790

C 2.602766 -0.996077 0.490655

C 1.505218 -1.554277 -0.191817

C 3.377959 -1.927813 1.314539

C 2.733571 -3.207231 1.567054

C 1.401676 -3.538032 1.165992

C 0.781599 -2.746954 0.230851

C -0.649571 -2.550369 -0.184992

C -1.857907 -2.977517 0.363196

C -3.030633 -2.118858 0.346742

C -2.922800 -0.856011 -0.278748

C -3.632431 0.326073 0.118579

C -4.714694 0.139233 0.961668

C -5.008998 -1.176913 1.417149

C -4.186465 -2.269057 1.166399

C -0.131360 2.615121 -0.169867

C -1.197315 3.312063 0.441375

C -2.528832 2.726371 0.375139

C -2.739415 1.494468 -0.236812

C -0.789019 4.341208 1.336975

C 0.555009 4.488815 1.662169

C 1.565289 3.595148 1.209671

C 1.225202 2.609878 0.297133

H 3.480001 0.852642 1.203560

H -5.305080 0.972016 1.333677

H -5.871000 -1.313698 2.063961

H -4.393806 -3.218788 1.652628

H -3.298770 3.169585 1.002896

H -1.529964 4.971182 1.822264

H 0.837210 5.267656 2.364894

H 2.562433 3.665122 1.635697

H -1.894235 -3.858610 1.000083

H 0.928812 -4.385044 1.653285

C 3.776513 -4.682587 0.046285

H 3.215577 -5.611855 0.059971

H 3.462430 -3.970370 -0.707256

C 5.110220 -2.199133 0.333612

H 4.622325 -2.219437 -0.635353

H 5.632040 -1.263345 0.519719

C 5.689200 -3.390499 0.804470

H 6.533813 -3.341389 1.487274

C 5.018615 -4.610090 0.650758

H 5.390205 -5.477410 1.191325

F 3.183691 -3.823742 2.692706

H 3.857511 -1.519992 2.200272

Transition state structure for the reaction of butadiene with Fragment 1 substituted with one COOH group

Molecular formula: C35H18O2

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.442060

Thermal correction to Enthalpy= 0.443004

Thermal correction to Gibbs Free Energy= 0.366776

Sum of electronic and zero-point Energies= -1494.511390

Sum of electronic and thermal Energies= -1494.487305

Sum of electronic and thermal Enthalpies= -1494.486360

Sum of electronic and thermal Free Energies= -1494.562589

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

277.397 105.209 160.436

Cartesian coordinates

Atom	X	Y	Z
C	-1.694340	-0.352471	-0.940508
C	-1.546981	1.068104	-0.871373
C	-0.277390	1.599866	-0.831421
C	0.884797	0.762591	-0.824882
C	0.711794	-0.611202	-0.900092
C	-0.597690	-1.188256	-0.925725
C	1.904186	1.344212	-0.006938
C	2.831382	0.468463	0.583446
C	2.659030	-0.951793	0.510157
C	1.552947	-1.468784	-0.180104
C	3.451573	-1.950368	1.271265
C	2.695160	-3.154566	1.683441
C	1.390397	-3.455735	1.176884
C	0.813932	-2.663113	0.214168
C	-0.613417	-2.434811	-0.201540
C	-1.828193	-2.859806	0.335896
C	-2.986506	-1.982792	0.347973
C	-2.859318	-0.702427	-0.237642
C	-3.548195	0.477698	0.199929
C	-4.631863	0.281472	1.039067
C	-4.947319	-1.043693	1.452615
C	-4.143212	-2.140370	1.165377
C	-0.011046	2.718831	-0.024021
C	-1.063729	3.411583	0.613898
C	-2.404511	2.849737	0.532275
C	-2.636593	1.642005	-0.119081
C	-0.636589	4.402013	1.543922
C	0.710302	4.515436	1.870804
C	1.704658	3.621488	1.384672
C	1.346734	2.674580	0.438762
H	3.590128	0.849767	1.264250
H	-5.207570	1.111460	1.439274
H	-5.810195	-1.186859	2.096824
H	-4.364544	-3.101584	1.621780
H	-3.165798	3.284285	1.176443
H	-1.365918	5.026644	2.053111
H	1.006794	5.263923	2.600133
H	2.703314	3.659304	1.811280
H	-1.876139	-3.759153	0.94567
H	0.861432	-4.273349	1.656364
C	4.016176	-5.080943	0.516614
H	3.647231	-6.038812	0.867743
H	3.430572	-4.603654	-0.256184
C	4.800304	-2.351923	0.082705
H	4.177603	-2.683808	-0.746493
H	5.234280	-1.375179	-0.121661
C	5.689908	-3.321213	0.625331
H	6.626472	-2.987042	1.064130
C	5.273808	-4.634096	0.864428
H	5.904639	-5.272050	1.479395
C	3.060321	-3.851789	2.935447
O	2.424218	-4.742479	3.473747
O	4.207603	-3.368313	3.497565
H	4.331217	-3.893864	4.304975
H	4.039323	-1.531373	2.083393

Transition state structure for the reaction of butadiene with Fragment 1 substituted with one CF₃ groupMolecular formula: C₃₅H₁₇F₃

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.432470

Thermal correction to Enthalpy= 0.433414

Thermal correction to Gibbs Free Energy= 0.354921

Sum of electronic and zero-point Energies= -1642.978103

Sum of electronic and thermal Energies= -1642.953235

Sum of electronic and thermal Enthalpies= -1642.952290

Sum of electronic and thermal Free Energies= -1643.030784

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

271.379 107.723 165.203

Cartesian coordinates

Atom X Y Z

C -1.855695 -0.151851 -0.832289
C -1.684616 1.265951 -0.763118
C -0.405802 1.776019 -0.737519
C 0.741978 0.919937 -0.747666
C 0.546269 -0.450226 -0.822103
C -0.773057 -1.005908 -0.833192
C 1.780555 1.482923 0.061446
C 2.698601 0.594537 0.640381
C 2.505213 -0.827543 0.566041
C 1.383304 -1.323039 -0.116147
C 3.266758 -1.825685 1.325025
C 2.568759 -3.068932 1.658017
C 1.218273 -3.326798 1.206069
C 0.630983 -2.508093 0.281783
C -0.801627 -2.254329 -0.114208
C -2.014588 -2.659654 0.438888
C -3.158842 -1.763530 0.468141
C -3.017447 -0.484341 -0.115790
C -3.681211 0.706162 0.332758
C -4.757000 0.525750 1.185395
C -5.088866 -0.794861 1.600383
C -4.306778 -1.904076 1.300372
C -0.111109 2.889414 0.067939
C -1.144525 3.598655 0.719341
C -2.495244 3.058900 0.654015
C -2.754974 1.856119 0.003910
C -0.689587 4.581369 1.644218
C 0.662981 4.673098 1.954075
C 1.636507 3.763452 1.455174
C 1.251091 2.823564 0.513336
H 3.466875 0.962775 1.317413

H -5.313844 1.364122 1.594667
H -5.945483 -0.925205 2.255541
H -4.538200 -2.862539 1.757582
H -3.241149 3.504862 1.308252
H -1.402164 5.217383 2.162923
H 0.980612 5.416255 2.679886
H 2.640965 3.784698 1.869026
H -2.070418 -3.559571 1.047307
H 0.682008 -4.149980 1.668302
C 3.662793 -4.762637 0.427807
H 3.198689 -5.692535 0.738080
H 3.177445 -4.259669 -0.397964
C 4.774597 -2.188506 0.011655
H 4.074689 -2.409519 -0.787680
H 5.230506 -1.206587 -0.085290
C 5.546738 -3.236490 0.533298
H 6.506535 -3.010891 0.991972
C 4.983722 -4.498226 0.750943
H 5.527929 -5.209862 1.366738
C 2.876205 -3.634561 3.023613
F 2.201316 -2.953449 3.989362
F 2.506584 -4.930944 3.157147 F
4.185242 -3.548563 3.349291
H 3.908898 -1.441579 2.111464

Transition state structure for the reaction of butadiene with Fragment 1 substituted with one CHO group

Molecular formula: C35H18O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.435629

Thermal correction to Enthalpy= 0.436574

Thermal correction to Gibbs Free Energy= 0.362254

Sum of electronic and zero-point Energies= -1419.265331

Sum of electronic and thermal Energies= -1419.242131

Sum of electronic and thermal Enthalpies= -1419.241187

Sum of electronic and thermal Free Energies= -1419.315506

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

273.362 101.622 156.418

Cartesian coordinates

Atom X Y Z

C -1.669247 0.128279 -0.978713
C -1.550645 1.549281 -0.869526
C -0.293394 2.101583 -0.766625
C 0.882466 1.284387 -0.734420
C 0.737666 -0.089826 -0.849985
C -0.559383 -0.688840 -0.942143
C 1.858114 1.862553 0.137907
C 2.779089 0.989621 0.741946
C 2.633373 -0.430717 0.627785
C 1.565441 -0.949963 -0.118938
C 3.411774 -1.444801 1.382651
C 2.649340 -2.649271 1.770285
C 1.380906 -2.970979 1.188652
C 0.833155 -2.167441 0.218925
C -0.580894 -1.953319 -0.250714
C -1.806289 -2.411551 0.231590
C -2.980207 -1.555433 0.219898
C -2.853669 -0.259191 -0.329591
C -3.579998 0.897621 0.109174
C -4.690435 0.662086 0.902004
C -4.997027 -0.677759 1.272263
C -4.162964 -1.753051 0.989725
C -0.079019 3.204365 0.077718
C -1.168130 3.862597 0.690437
C -2.494167 3.280028 0.542636
C -2.678714 2.085193 -0.146601
C -0.795639 4.836452 1.660611
C 0.535083 4.964777 2.043311
C 1.563563 4.100333 1.575239
C 1.260009 3.171943 0.592743
H 3.504344 1.367472 1.459990

H -5.295581 1.472083 1.299672
H -5.880237 -0.851209 1.880363
H -4.383103 -2.728627 1.415014
H -3.287685 3.685131 1.166723
H -1.555553 5.435464 2.155590
H 0.789183 5.699452 2.802010
H 2.543811 4.144317 2.041998
H -1.860168 -3.325979 0.817872
H 0.841555 -3.798358 1.640498
C 4.179107 -4.569496 0.884881
H 3.881757 -5.504299 1.347711
H 3.567686 -4.236280 0.058151
C 4.753452 -1.844107 0.165854
H 4.120528 -2.287214 -0.601531
H 5.108135 -0.861918 -0.139026
C 5.722068 -2.691074 0.771379
H 6.644656 -2.249183 1.140042
C 5.401709 -3.991881 1.167832
H 6.081226 -4.511957 1.840067
C 2.981925 -3.317548 3.046740
O 2.272670 -4.128768 3.622706
H 3.948220 -2.991951 3.490205
H 4.003177 -1.037052 2.201754

Transition state structure for the reaction of butadiene with Fragment 1 substituted with one CN group

Molecular formula: C35H17N

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.424467

Thermal correction to Enthalpy= 0.425411

Thermal correction to Gibbs Free Energy= 0.350895

Sum of electronic and zero-point Energies= -1398.190637

Sum of electronic and thermal Energies= -1398.167457

Sum of electronic and thermal Enthalpies= -1398.166513

Sum of electronic and thermal Free Energies= -1398.241029

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

266.357 101.224 156.832

Cartesian coordinates

Atom X Y Z

C -1.728426 -0.431132 -0.976118
 C -1.597400 0.991380 -0.917989
 C -0.333764 1.537456 -0.883392
 C 0.837151 0.713111 -0.871014
 C 0.680021 -0.662709 -0.936161
 C -0.622703 -1.254429 -0.957498
 C 1.850898 1.313138 -0.058412
 C 2.789523 0.453388 0.535527
 C 2.635286 -0.969697 0.470346
 C 1.532473 -1.506615 -0.212130
 C 3.447127 -1.949712 1.232010
 C 2.708722 -3.177993 1.629701
 C 1.397356 -3.494093 1.146377
 C 0.805041 -2.705432 0.188188
 C -0.624304 -2.496080 -0.225090
 C -1.834207 -2.931177 0.316224
 C -3.001968 -2.067061 0.323615
 C -2.889021 -0.789220 -0.270265
 C -3.590786 0.386146 0.159232
 C -4.671599 0.183431 1.000460
 C -4.972186 -1.142420 1.423045
 C -4.156535 -2.232214 1.142651
 C -0.078994 2.665520 -0.084793
 C -1.138906 3.351005 0.548919
 C -2.473306 2.773387 0.473099
 C -2.692724 1.558438 -0.169207
 C -0.722112 4.353420 1.470764
 C 0.623724 4.485080 1.795124
 C 1.627771 3.598917 1.314880
 C 1.279498 2.640913 0.376598
 H 3.545312 0.848434 1.211647

H -5.256444 1.009476 1.395397
 H -5.833066 -1.290639 2.068683
 H -4.367522 -3.192764 1.605245
 H -3.238733 3.204290 1.114723
 H -1.457968 4.973588 1.975885
 H 0.912323 5.242439 2.518300
 H 2.626321 3.651621 1.739985
 H -1.873391 -3.827737 0.930832
 H 0.872448 -4.320792 1.615840
 C 4.014755 -5.051307 0.312146
 H 3.631062 -6.032126 0.573013
 H 3.461688 -4.511969 -0.444266
 C 4.841359 -2.308859 0.092022
 H 4.258984 -2.589991 -0.783439
 H 5.292804 -1.327204 -0.038734
 C 5.693845 -3.318387 0.622676
 H 6.609830 -3.023272 1.128134
 C 5.253284 -4.639156 0.756632
 H 5.845020 -5.322643 1.360483
 C 3.136330 -3.801224 2.843006
 N 3.492263 -4.259943 3.854592
 H 4.000726 -1.518823 2.064242

Transition state structure for the reaction of butadiene with Fragment 1 substituted with one NO₂ groupMolecular formula: C₃₄H₁₇NO₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.429267

Thermal correction to Enthalpy= 0.430211

Thermal correction to Gibbs Free Energy= 0.354935

Sum of electronic and zero-point Energies= -1510.453371

Sum of electronic and thermal Energies= -1510.429763

Sum of electronic and thermal Enthalpies= -1510.428819

Sum of electronic and thermal Free Energies= -1510.504094

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

269.369 103.405 158.431

Cartesian coordinates

Atom X Y Z

C	-1.518358	-0.451393	-1.108588	H	-5.043985	1.129242	1.175521
C	-1.356548	0.968818	-1.086598	H	-5.680584	-1.138972	1.901503
C	-0.082243	1.489689	-1.051377	H	-4.252864	-3.084770	1.506979
C	1.070162	0.641300	-0.997687	H	-2.976576	3.272395	0.860250
C	0.883314	-0.732437	-1.023381	H	-1.170406	5.027306	1.695896
C	-0.431409	-1.297058	-1.050338	H	1.197975	5.262787	2.262007
C	2.085989	1.243637	-0.190259	H	2.888071	3.615922	1.551019
C	2.995153	0.380108	0.444575	H	-1.765185	-3.792584	0.884753
C	2.809823	-1.039539	0.422162	H	1.008199	-4.388739	1.582014
C	1.703451	-1.571838	-0.257978	C	4.524654	-5.343309	0.005416
C	3.578118	-2.003177	1.263817	H	4.327644	-6.408022	-0.056863
C	2.786763	-3.200102	1.634828	H	3.890556	-4.700164	-0.593152
C	1.512487	-3.544602	1.125749	C	5.012038	-2.432079	0.392595
C	0.943814	-2.747682	0.155361	H	4.634122	-2.695877	-0.594156
C	-0.470515	-2.519414	-0.286311	H	5.553048	-1.487430	0.345391
C	-1.698436	-2.914082	0.247133	C	5.766153	-3.485449	1.025207
C	-2.845941	-2.024289	0.214820	H	6.569368	-3.219144	1.702790
C	-2.696794	-0.765173	-0.410784	C	5.530412	-4.866451	0.784882
C	-3.377462	0.436222	-0.021996	H	6.141228	-5.573240	1.340182
C	-4.473099	0.280126	0.810214	O	4.488203	-3.623089	3.066831
C	-4.808728	-1.026970	1.263352	O	2.749169	-4.974880	3.124966
C	-4.014534	-2.141790	1.022143	N	3.338719	-3.981217	2.667433
C	0.186183	2.634704	-0.281672	H	4.022174	-1.556226	2.153167
C	-0.867076	3.359275	0.318732				
C	-2.212265	2.807383	0.241504				
C	-2.449394	1.579533	-0.369214				
C	-0.441219	4.378420	1.217913				
C	0.902847	4.491572	1.556328				
C	1.894149	3.571894	1.114240				
C	1.537846	2.595072	0.198543				
H	3.748059	0.779507	1.121424				

Transition state structure for the reaction of butadiene with Fragment 2

Molecular formula: C34H16

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.399111

Thermal correction to Enthalpy= 0.400055

Thermal correction to Gibbs Free Energy= 0.331085

Sum of electronic and zero-point Energies= -1304.672868

Sum of electronic and thermal Energies= -1304.652091

Sum of electronic and thermal Enthalpies= -1304.651146

Sum of electronic and thermal Free Energies= -1304.720117

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

250.446 93.382 145.160

Cartesian coordinates

Atom X Y Z

C	1.237558	-0.175533	2.401603	H	-4.113914	1.911990	-0.727846
C	0.523254	1.070295	2.385807	H	-4.442979	-1.114857	-0.703189
C	-0.880014	0.776329	2.383144	H	-3.143127	-3.382130	-0.690629
C	-1.035143	-0.650319	2.394850	H	-0.358101	-4.627172	-0.689826
C	0.272363	-1.238852	2.404440	H	2.199525	-4.095153	-0.689221
C	0.989910	2.100369	1.599973	H	4.303630	0.753026	-0.874177
C	0.097929	2.996555	0.884516	H	3.013184	3.396900	-0.749286
C	-1.273365	2.713802	0.892481	H	4.027408	-1.792281	-0.853273
C	-1.729218	1.537931	1.611747	C	5.883695	0.754808	1.085151
C	-2.863317	0.962516	0.912382	H	5.962380	1.830768	0.960292
C	-3.014804	-0.429709	0.923907	C	5.575269	-2.099239	1.107487
C	-2.029331	-1.224056	1.634136	H	5.422880	-3.169145	0.999756
C	-1.837962	-2.481762	0.934449	C	6.799422	-0.085117	0.474580
C	-0.559224	-3.052169	0.932877	H	7.536384	0.344640	-0.200886
C	0.505611	-2.357266	1.635601	C	6.648211	-1.483841	0.485603
C	1.757637	-2.570649	0.936474	H	7.275398	-2.071419	-0.181936
C	2.696466	-1.535035	0.934549	H	5.125245	-1.668605	1.993922
C	2.379528	-0.305577	1.638437	H	5.352441	0.443409	1.976219
C	2.257496	2.029014	0.900000				
C	2.951902	0.815931	0.915740				
C	0.958353	3.685624	-0.086552				
C	2.206425	3.125172	-0.078906				
C	-2.343526	3.001215	-0.072845				
C	-3.263104	1.988433	-0.061513				
C	-3.627159	-1.361257	-0.034250				
C	-2.946737	-2.548019	-0.027785				
C	0.131605	-3.925419	-0.025519				
C	1.470950	-3.645961	-0.024727				
C	3.799535	-1.191618	0.016458				
C	3.953144	0.229181	0.004523				
H	0.629103	4.465079	-0.762992				
H	-2.357239	3.847165	-0.749519				

Transition state structure for the reaction of butadiene with Fragment 2 substituted with one NH₂ groupMolecular formula: C₃₄H₁₇N

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.417150

Thermal correction to Enthalpy= 0.418095

Thermal correction to Gibbs Free Energy= 0.345692

Sum of electronic and zero-point Energies= -1360.017897

Sum of electronic and thermal Energies= -1359.995513

Sum of electronic and thermal Enthalpies= -1359.994569

Sum of electronic and thermal Free Energies= -1360.066971

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

261.766 99.189 152.383

Cartesian coordinates

Atom X Y Z

C	0.982654	-0.315396	2.247161	H	-2.697844	3.843455	-0.610136
C	0.258917	0.923668	2.313020	H	-4.444410	1.899407	-0.656739
C	-1.141403	0.619223	2.322377	H	-4.761779	-1.122947	-0.784896
C	-1.288343	-0.806284	2.259360	H	-3.450645	-3.380600	-0.920339
C	0.020262	-1.384660	2.205100	H	-0.663485	-4.600810	-1.048475
C	0.702286	1.999825	1.579713	H	1.883018	-4.053478	-1.082486
C	-0.205972	2.926289	0.931949	H	2.682456	3.446976	-0.720768
C	-1.576676	2.632370	0.948777	C	5.452299	0.596681	0.535083
C	-2.010986	1.417739	1.611906	H	5.603830	1.585413	0.106903
C	-3.157014	0.872648	0.906050	C	5.765966	-2.014125	1.960558
C	-3.302399	-0.518956	0.846871	H	5.914645	-2.983654	2.423718
C	-2.299285	-1.346061	1.492754	C	6.418000	-0.383083	0.199017
C	-2.117356	-2.561401	0.724260	H	7.070980	-0.214024	-0.653981
C	-0.834604	-3.126846	0.664627	C	6.542876	-1.610262	0.917301
C	0.243874	-2.462360	1.377647	H	7.315041	-2.296859	0.568590
C	1.483966	-2.641098	0.649503	H	5.001962	-1.383311	2.400719
C	2.430139	-1.595864	0.695652	H	5.176108	0.652681	1.586237
C	2.102800	-0.391213	1.453212	N	4.108187	-1.936756	-1.146755
C	1.960814	1.974846	0.854245	H	4.140363	-2.929173	-0.950470
C	2.662202	0.772153	0.797721	H	5.022247	-1.564896	-1.407751
C	0.634532	3.674222	-0.012835	H	3.825740	0.756588	-1.094574
C	1.888422	3.127596	-0.056281				
C	-2.666540	2.963168	0.020674				
C	-3.580927	1.945320	-0.004094				
C	-3.930862	-1.400250	-0.147501				
C	-3.244526	-2.581938	-0.217895				
C	-0.164087	-3.938780	-0.351549				
C	1.178653	-3.652514	-0.363440				
C	3.463950	-1.178222	-0.222174				
C	3.699141	0.249100	-0.141220				
H	0.288955	4.487575	-0.639581				

Transition state structure for the reaction of butadiene with Fragment 2 substituted with one OMe group

Molecular formula: C35H18O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.434131

Thermal correction to Enthalpy= 0.435075

Thermal correction to Gibbs Free Energy= 0.358628

Sum of electronic and zero-point Energies= -1419.157970

Sum of electronic and thermal Energies= -1419.134094

Sum of electronic and thermal Enthalpies= -1419.133150

Sum of electronic and thermal Free Energies= -1419.209598

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

272.421 103.064 160.898

Cartesian coordinates

Atom X Y Z

C	1.024156	-0.415179	2.176191	H	-2.778212	3.835424	-0.371560
C	0.277724	0.801310	2.324410	H	-4.490218	1.865265	-0.507216
C	-1.116200	0.469207	2.336087	H	-4.754770	-1.148396	-0.814055
C	-1.236124	-0.952719	2.189540	H	-3.397372	-3.363028	-1.114503
C	0.083239	-1.499471	2.080482	H	-0.597344	-4.474522	-1.386646
C	0.688566	1.928289	1.651757	H	1.917834	-3.873870	-1.437033
C	-0.245003	2.874082	1.072723	H	2.614784	3.549553	-0.575512
C	-1.608967	2.553879	1.092405	C	5.371683	0.846875	0.755536
C	-2.010880	1.292758	1.688963	H	5.408433	1.891872	0.454059
C	-3.159148	0.770793	0.970603	C	5.912769	-1.867293	1.852355
C	-3.279791	-0.617199	0.828965	H	6.158740	-2.860718	2.212403
C	-2.250125	-1.461986	1.406618	C	6.490944	0.058930	0.405644
C	-2.054944	-2.619439	0.558706	H	7.143797	0.395394	-0.395209
C	-0.759669	-3.144352	0.437424	C	6.725426	-1.222030	0.960814
C	0.321563	-2.507605	1.173825	H	7.604916	-1.756073	0.602290
C	1.560415	-2.619141	0.424367	H	5.042530	-1.397898	2.295941
C	2.515919	-1.578361	0.555392	H	5.016590	0.739110	1.778409
C	2.143016	-0.421977	1.378410	O	4.316900	-1.684177	-1.217256
C	1.938351	1.972616	0.917286	C	4.664273	-3.065012	-1.076920
C	2.667287	0.792037	0.793830	H	5.295149	-3.299114	-1.935243
C	0.570808	3.693769	0.165057	H	5.220115	-3.200168	-0.142200
C	1.834716	3.176760	0.077564	H	3.790130	-3.715438	-1.077313
C	-2.720646	2.919773	0.204625	H	3.938637	0.896863	-1.044140
C	-3.616943	1.888150	0.133555				
C	-3.907437	-1.447445	-0.208960				
C	-3.197043	-2.606331	-0.365451				
C	-0.097145	-3.864252	-0.644631				
C	1.239600	-3.551593	-0.658598				
C	3.593809	-1.077445	-0.266436				
C	3.765415	0.355109	-0.117791				
H	0.202766	4.535719	-0.408889				

Transition state structure for the reaction of butadiene with Fragment 2 substituted with one OH groupMolecular formula: C₃₄H₁₆O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.403500

Thermal correction to Enthalpy= 0.404444

Thermal correction to Gibbs Free Energy= 0.332131

Sum of electronic and zero-point Energies= -1379.887495

Sum of electronic and thermal Energies= -1379.865405

Sum of electronic and thermal Enthalpies= -1379.864461

Sum of electronic and thermal Free Energies= -1379.936774

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

253.200 97.556 152.196

Cartesian coordinates

Atom X Y Z

C	0.953272	-0.305689	2.300777	H	-2.739648	3.768092	-0.657171
C	0.202624	0.917170	2.348778	H	-4.437827	1.783749	-0.748926
C	-1.191816	0.582820	2.323486	H	-4.684252	-1.249632	-0.877042
C	-1.306336	-0.845285	2.260910	H	-3.325416	-3.480492	-0.964638
C	0.016704	-1.395374	2.242059	H	-0.508879	-4.655355	-1.002222
C	0.641123	2.003603	1.627689	H	2.041059	-4.040664	-0.960907
C	-0.270692	2.909178	0.954354	H	2.648605	3.494123	-0.621152
C	-1.633220	2.584245	0.933028	C	5.484696	0.585749	0.514299
C	-2.057965	1.359485	1.586291	H	5.655383	1.559483	0.061494
C	-3.170944	0.787957	0.850239	C	5.865797	-1.983946	2.017772
C	-3.283303	-0.607061	0.790774	H	6.036637	-2.935052	2.509488
C	-2.281219	-1.409017	1.467555	C	6.384517	-0.444617	0.128460
C	-2.053405	-2.627007	0.710380	H	7.027818	-0.285514	-0.733810
C	-0.761315	-3.167891	0.691728	C	6.563629	-1.638768	0.905684
C	0.282538	-2.476035	1.431433	H	7.301133	-2.347783	0.530261
C	1.539861	-2.630450	0.732689	H	5.129051	-1.331593	2.473977
C	2.455187	-1.561956	0.783181	H	5.271713	0.664811	1.578426
C	2.093107	-0.359421	1.529798	O	4.168261	-1.856699	-0.976812
C	1.916488	2.005102	0.933357	H	5.096571	-1.471989	-0.979877
C	2.647100	0.818311	0.893115	H	3.786419	0.822223	-1.016041
C	0.578088	3.676074	0.031465				
C	1.843978	3.157358	0.021566				
C	-2.704886	2.889235	-0.024685				
C	-3.593955	1.850190	-0.072831				
C	-3.865754	-1.506607	-0.215523				
C	-3.154440	-2.674454	-0.261323				
C	-0.042276	-3.975100	-0.300123				
C	1.292060	-3.659216	-0.278501				
C	3.469951	-1.110618	-0.136039				
C	3.679858	0.314005	-0.061244				
H	0.231212	4.481670	-0.604439				

Transition state structure for the reaction of butadiene with Fragment 2 substituted with one Me group

Molecular formula: C35H18

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.428556

Thermal correction to Enthalpy= 0.429500

Thermal correction to Gibbs Free Energy= 0.357960

Sum of electronic and zero-point Energies= -1343.962589

Sum of electronic and thermal Energies= -1343.940313

Sum of electronic and thermal Enthalpies= -1343.939369

Sum of electronic and thermal Free Energies= -1344.010909

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

268.923 99.202 150.569

Cartesian coordinates

Atom X Y Z

C 0.960759 -0.262930 2.320594
C 0.238343 0.977273 2.347031
C -1.162828 0.673696 2.354872
C -1.308445 -0.753713 2.331159
C 0.002460 -1.332796 2.306913
C 0.687573 2.031329 1.583378
C -0.218510 2.939289 0.902479
C -1.587693 2.646947 0.920192
C -2.026892 1.449800 1.614873
C -3.166636 0.885405 0.915908
C -3.309752 -0.507660 0.893236
C -2.309858 -1.313777 1.569323
C -2.119898 -2.550954 0.835946
C -0.836461 -3.111350 0.800943
C 0.235100 -2.424899 1.502227
C 1.482306 -2.616380 0.784564
C 2.421072 -1.575801 0.803683
C 2.093856 -0.365311 1.541989
C 1.947335 1.986521 0.868163
C 2.649636 0.779183 0.847884
C 0.626322 3.659193 -0.060608
C 1.878392 3.108462 -0.081153
C -2.672257 2.952338 -0.023215
C -3.585214 1.933510 -0.026012
C -3.929421 -1.418341 -0.080142
C -3.241340 -2.600392 -0.112668
C -0.155404 -3.961469 -0.181228
C 1.183210 -3.675640 -0.192815
C 3.527728 -1.204975 -0.099943
C 3.667952 0.226315 -0.070919
H 0.284029 4.453589 -0.712791

H -2.700148 3.815391 -0.677490
H -4.444234 1.868797 -0.683021
H -4.755741 -1.160473 -0.731613
H -3.441325 -3.418636 -0.794002
H -0.649008 -4.654583 -0.851674
H 1.899867 -4.114557 -0.874876
H 2.675685 3.404142 -0.752766
C 5.517625 0.827495 0.893404
H 5.592212 1.876542 0.620629
C 5.263854 -1.983086 1.332909
H 5.125243 -3.058751 1.386761
C 6.482108 -0.069042 0.445030
H 7.231837 0.270427 -0.266487
C 6.354857 -1.450941 0.673738
H 7.031459 -2.122801 0.149613
H 4.726250 -1.416710 2.082583
H 5.023291 0.654726 1.842712
C 3.912471 -1.992685 -1.324433
H 4.028382 -3.058480 -1.112965
H 3.150028 -1.887031 -2.108423
H 4.859262 -1.627467 -1.732357
H 3.948237 0.753802 -0.975104

Transition state structure for the reaction of butadiene with Fragment 2 substituted with one *i*-Pr group

Molecular formula: C37H22

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.488329

Thermal correction to Enthalpy= 0.489273

Thermal correction to Gibbs Free Energy= 0.412596

Sum of electronic and zero-point Energies= -1422.528457

Sum of electronic and thermal Energies= -1422.503654

Sum of electronic and thermal Enthalpies= -1422.502710

Sum of electronic and thermal Free Energies= -1422.579387

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

306.431 109.291 161.381

Cartesian coordinates

Atom X Y Z

C 0.959080 -0.528331 2.328942
C 0.265071 0.724946 2.418204
C -1.136945 0.448476 2.532336
C -1.311751 -0.975385 2.511247
C -0.017859 -1.578237 2.379958
C 0.673896 1.774657 1.626912
C -0.263050 2.704119 1.021185
C -1.632326 2.439090 1.144114
C -2.040163 1.246359 1.865308
C -3.241843 0.709440 1.254576
C -3.414401 -0.680436 1.235995
C -2.380639 -1.509781 1.826910
C -2.271810 -2.743938 1.073231
C -1.004918 -3.324240 0.931319
C 0.133134 -2.662876 1.547175
C 1.320661 -2.875585 0.736811
C 2.290587 -1.858472 0.700599
C 2.030027 -0.648081 1.468741
C 1.875399 1.710721 0.820833
C 2.551065 0.491295 0.746537
C 0.520830 3.413257 0.000139
C 1.757266 2.839550 -0.116236
C -2.780360 2.771720 0.289061
C -3.711080 1.771243 0.352580
C -4.126456 -1.572763 0.309645
C -3.465590 -2.767062 0.216351
C -0.421527 -4.183200 -0.101220
C 0.918405 -3.927344 -0.214934
C 3.358778 -1.500652 -0.266058
C 3.525120 -0.062633 -0.222144
H 0.145864 4.217512 -0.621256
H -2.841192 3.639043 -0.357285

H -4.619533 1.727221 -0.236112
H -4.996662 -1.295050 -0.272875
H -3.733767 -3.576677 -0.451752
H -0.979014 -4.864663 -0.732319
H 1.564951 -4.391878 -0.946297
H 2.507290 3.124309 -0.844686
C 5.313549 0.594965 0.682264
H 5.347512 1.640000 0.385295
C 5.184299 -2.199225 1.194800
H 5.104706 -3.274983 1.302904
C 6.333452 -0.263292 0.268073
H 7.074747 0.092350 -0.444292
C 6.261332 -1.638713 0.532052
H 6.983921 -2.295870 0.052183
H 4.601059 -1.626202 1.903204
H 4.865442 0.440567 1.657844
C 4.170385 -3.722453 -1.341336
H 4.001527 -4.330915 -2.236968
H 5.249397 -3.671742 -1.175661
H 3.726912 -4.243782 -0.490090
C 3.577779 -2.313458 -1.544542
H 2.562035 -2.462056 -1.945528
C 4.379041 -1.577368 -2.631342
H 5.378761 -1.309629 -2.277166
H 4.497852 -2.225320 -3.505818
H 3.878566 -0.665225 -2.969073
H 3.739197 0.473381 -1.137097

Transition state structure for the reaction of butadiene with Fragment 2 substituted with one F groupMolecular formula: C₃₄H₁₅F

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.391645

Thermal correction to Enthalpy= 0.392589

Thermal correction to Gibbs Free Energy= 0.321655

Sum of electronic and zero-point Energies= -1403.908262

Sum of electronic and thermal Energies= -1403.886505

Sum of electronic and thermal Enthalpies= -1403.885560

Sum of electronic and thermal Free Energies= -1403.956494

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

245.761 96.568 149.293

Cartesian coordinates

Atom X Y Z

C 0.972280 -0.268470 2.389011
C 0.238062 0.965617 2.383863
C -1.160328 0.649818 2.359754
C -1.293306 -0.778881 2.343028
C 0.022981 -1.347967 2.358834
C 0.697484 2.016279 1.620723
C -0.201419 2.912050 0.912954
C -1.568333 2.608942 0.902181
C -2.013373 1.413023 1.594276
C -3.130414 0.833598 0.871194
C -3.258694 -0.560738 0.852513
C -2.268145 -1.353189 1.558026
C -2.048512 -2.593130 0.834840
C -0.761148 -3.143476 0.838068
C 0.280892 -2.448718 1.573145
C 1.546155 -2.632759 0.888913
C 2.465128 -1.587359 0.935440
C 2.126909 -0.366757 1.641897
C 1.971113 1.976160 0.929108
C 2.684902 0.773045 0.927966
C 0.655890 3.629343 -0.039385
C 1.911646 3.085828 -0.032205
C -2.632468 2.898733 -0.068893
C -3.536096 1.871858 -0.086946
C -3.844288 -1.481726 -0.131833
C -3.144208 -2.656969 -0.142047
C -0.041850 -3.982140 -0.131431
C 1.293126 -3.684240 -0.106287
C 3.588472 -1.200376 0.066085
C 3.682348 0.221539 0.002237
H 0.320649 4.415390 -0.705116
H -2.652054 3.757263 -0.729323

H -4.378444 1.795099 -0.763859
H -4.656035 -1.234620 -0.805385
H -3.318565 -3.480003 -0.824536
H -0.512454 -4.670223 -0.823240
H 2.041985 -4.089100 -0.774832
H 2.719516 3.379414 -0.691905
C 5.736636 0.857152 0.908813
H 5.857720 1.892824 0.605296
C 5.238259 -1.930437 1.354823
H 5.027147 -2.993651 1.420052
C 6.567794 -0.120999 0.398625
H 7.297455 0.152751 -0.360480
C 6.331840 -1.490681 0.627109
H 6.895201 -2.211816 0.040009
H 4.842026 -1.341553 2.174887
H 5.212123 0.717142 1.845579
F 3.881327 -1.945350 -1.030176
H 3.981410 0.714455 -0.911502

Transition state structure for the reaction of butadiene with Fragment 2 substituted with one COOH group

Molecular formula: C35H16O2

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.417255

Thermal correction to Enthalpy= 0.418199

Thermal correction to Gibbs Free Energy= 0.343411

Sum of electronic and zero-point Energies= -1493.237137

Sum of electronic and thermal Energies= -1493.213528

Sum of electronic and thermal Enthalpies= -1493.212584

Sum of electronic and thermal Free Energies= -1493.287371

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

261.831 103.456 157.404

Cartesian coordinates

Atom X Y Z

C 0.940695 -0.240259 2.292286
C 0.227547 1.003683 2.317000
C -1.175714 0.710280 2.373173
C -1.330139 -0.714849 2.384955
C -0.021310 -1.301768 2.329980
C 0.660142 2.045444 1.528667
C -0.256862 2.946262 0.854836
C -1.625433 2.659661 0.909086
C -2.052990 1.476646 1.638603
C -3.212074 0.905747 0.981524
C -3.363959 -0.487516 0.992664
C -2.352477 -1.284302 1.661247
C -2.190610 -2.543115 0.954453
C -0.914062 -3.112980 0.896031
C 0.184350 -2.410331 1.543434
C 1.404289 -2.629958 0.789200
C 2.353405 -1.590318 0.749062
C 2.049068 -0.363873 1.478513
C 1.903331 1.984577 0.789134
C 2.598542 0.774510 0.779654
C 0.572620 3.649464 -0.135594
C 1.823799 3.098170 -0.171057
C -2.732728 2.952796 -0.011311
C -3.648770 1.937618 0.029119
C -4.016216 -1.417658 0.059995
C -3.338256 -2.606086 0.038912
C -0.265173 -4.002519 -0.071849
C 1.074082 -3.726841 -0.134771
C 3.422584 -1.212569 -0.184320
C 3.641465 0.218186 -0.124936
H 0.219911 4.434582 -0.793429

H -2.773900 3.803064 -0.681268
H -4.524058 1.863864 -0.605113
H -4.857163 -1.169466 -0.576304
H -3.562009 -3.438428 -0.617394
H -0.781838 -4.716191 -0.702074
H 1.786214 -4.167647 -0.816511
H 2.608574 3.382182 -0.861932
C 5.297340 0.701646 0.872334
H 5.298153 1.782227 0.756226
C 5.547169 -2.173228 1.129684
H 5.556745 -3.256039 1.066050
C 6.375337 -0.016376 0.336720
H 7.044572 0.482482 -0.359740
C 6.473206 -1.417111 0.457930
H 7.229475 -1.925635 -0.135516
H 4.874431 -1.749456 1.862931
H 4.895312 0.379283 1.828640
O 3.671590 -3.195416 -1.530885
O 4.730363 -1.302070 -2.129657
C 3.917015 -2.021958 -1.295863
H 5.005793 -1.933788 -2.814054
H 3.904049 0.729309 -1.042953

Transition state structure for the reaction of butadiene with Fragment 2 substituted with one CF₃ groupMolecular formula: C₃₅H₁₅F₃

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.407660

Thermal correction to Enthalpy= 0.408604

Thermal correction to Gibbs Free Energy= 0.332393

Sum of electronic and zero-point Energies= -1641.705110

Sum of electronic and thermal Energies= -1641.680850

Sum of electronic and thermal Enthalpies= -1641.679905

Sum of electronic and thermal Free Energies= -1641.756116

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

255.810 105.933 160.399

Cartesian coordinates

Atom X Y Z

C 0.946430 -0.241081 2.279703
C 0.219839 0.996157 2.287592
C -1.180560 0.687459 2.318658
C -1.320058 -0.740074 2.329415
C -0.004946 -1.313555 2.301555
C 0.656091 2.037241 1.499525
C -0.260580 2.926839 0.808369
C -1.627185 2.627158 0.843323
C -2.053956 1.442119 1.568133
C -3.196402 0.857133 0.892209
C -3.332904 -0.537056 0.902841
C -2.323507 -1.321656 1.588926
C -2.135341 -2.577978 0.884450
C -0.851654 -3.133773 0.851238
C 0.224041 -2.422986 1.521719
C 1.462142 -2.627074 0.791672
C 2.392411 -1.580065 0.774524
C 2.070718 -0.355402 1.487244
C 1.909256 1.985640 0.775046
C 2.617236 0.780829 0.774208
C 0.573416 3.632570 -0.174952
C 1.828890 3.089888 -0.193773
C -2.722105 2.906519 -0.096086
C -3.628789 1.882612 -0.068618
C -3.958053 -1.474894 -0.040991
C -3.266544 -2.655281 -0.050463
C -0.174649 -4.011545 -0.111085
C 1.161157 -3.722983 -0.146282
C 3.504897 -1.205957 -0.131785
C 3.635476 0.222972 -0.135506
H 0.221625 4.411332 -0.840674

H -2.760660 3.754778 -0.768752
H -4.492797 1.798676 -0.716789
H -4.790949 -1.236451 -0.691428
H -3.469758 -3.490579 -0.709600
H -0.671744 -4.727020 -0.754772
H 1.877015 -4.171079 -0.820244
H 2.619125 3.376123 -0.877488
C 5.474818 0.822711 0.937245
H 5.513452 1.892781 0.755439
C 5.306269 -2.029071 1.123795
H 5.192753 -3.105816 1.067935
C 6.456588 -0.003748 0.411181
H 7.191727 0.419408 -0.269825
C 6.373090 -1.404382 0.506382
H 7.052159 -2.000734 -0.097619
H 4.773090 -1.553307 1.937462
H 4.956323 0.543619 1.846869
C 3.794935 -1.952364 -1.397217
F 4.045691 -3.274206 -1.205830
F 2.744909 -1.898164 -2.258783
F 4.859237 -1.435690 -2.051912
H 3.957417 0.742998 -1.027365

Transition state structure for the reaction of butadiene with Fragment 2 substituted with one CHO group

Molecular formula: C35H16O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.410814

Thermal correction to Enthalpy= 0.411758

Thermal correction to Gibbs Free Energy= 0.338820

Sum of electronic and zero-point Energies= -1417.991376

Sum of electronic and thermal Energies= -1417.968663

Sum of electronic and thermal Enthalpies= -1417.967719

Sum of electronic and thermal Free Energies= -1418.040657

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

257.790 99.886 153.512

Cartesian coordinates

Atom X Y Z

C	0.957187	-0.200850	2.318331	H	-2.673055	3.847425	-0.752309
C	0.242149	1.042574	2.325457	H	-4.422702	1.906466	-0.732509
C	-1.161883	0.747987	2.339731	H	-4.753476	-1.127969	-0.720548
C	-1.315555	-0.677076	2.343674	H	-3.456935	-3.396238	-0.728750
C	-0.004187	-1.262674	2.323067	H	-0.676110	-4.666784	-0.741969
C	0.696405	2.086337	1.552465	H	1.893033	-4.100116	-0.792769
C	-0.201005	2.988531	0.854884	H	2.714713	3.436727	-0.771954
C	-1.570344	2.700647	0.867867	C	5.317236	0.685426	1.123716
C	-2.017887	1.515490	1.581458	H	5.260678	1.769838	1.168464
C	-3.156383	0.945230	0.889170	C	5.746079	-2.182632	0.969058
C	-3.307098	-0.448234	0.892463	H	5.821978	-3.239486	0.737516
C	-2.314850	-1.245416	1.588361	C	6.455763	0.116460	0.533159
C	-2.132079	-2.503764	0.883719	H	7.116374	0.754593	-0.049416
C	-0.854868	-3.072847	0.861376	C	6.631280	-1.277151	0.437067
C	0.224170	-2.371038	1.542154	H	7.426037	-1.646452	-0.207605
C	1.462453	-2.583531	0.817504	H	5.046248	-1.918803	1.750635
C	2.411617	-1.542468	0.806949	H	4.899038	0.205661	2.004397
C	2.087779	-0.321284	1.534590	O	3.672130	-3.044640	-1.603856
C	1.961966	2.029956	0.850411	C	4.010987	-1.921880	-1.248472
C	2.657481	0.820540	0.857914	H	4.769925	-1.360609	-1.835467
C	0.657152	3.696702	-0.107025	H	4.053706	0.801181	-0.892835
C	1.909969	3.147834	-0.106542				
C	-2.650563	2.995354	-0.083800				
C	-3.566341	1.979292	-0.072899				
C	-3.931360	-1.377084	-0.060472				
C	-3.252749	-2.565264	-0.064478				
C	-0.177707	-3.957088	-0.092917				
C	1.161536	-3.677026	-0.120213				
C	3.493411	-1.162539	-0.113706				
C	3.736813	0.264739	-0.004619				
H	0.323643	4.484097	-0.772099				

Transition state structure for the reaction of butadiene with Fragment 2 substituted with one CN group

Molecular formula: C35H15N

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.399695

Thermal correction to Enthalpy= 0.400639

Thermal correction to Gibbs Free Energy= 0.327478

Sum of electronic and zero-point Energies= -1396.918032

Sum of electronic and thermal Energies= -1396.895326

Sum of electronic and thermal Enthalpies= -1396.894382

Sum of electronic and thermal Free Energies= -1396.967543

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

250.812 99.424 153.981

Cartesian coordinates

Atom X Y Z

C	0.965871	-0.246719	2.324630	H	-2.659342	3.796090	-0.764239
C	0.240978	0.990742	2.327165	H	-4.395250	1.843054	-0.779888
C	-1.160825	0.684316	2.320265	H	-4.698437	-1.189304	-0.803585
C	-1.302532	-0.743035	2.309719	H	-3.379581	-3.445186	-0.822247
C	0.011650	-1.318961	2.308638	H	-0.587530	-4.666110	-0.836234
C	0.697526	2.042110	1.564562	H	1.964154	-4.096441	-0.839245
C	-0.199735	2.941782	0.862522	H	2.722422	3.411517	-0.744819
C	-1.566773	2.644277	0.858844	C	5.413981	0.746695	0.975188
C	-2.013274	1.450359	1.558003	H	5.423049	1.825078	0.840828
C	-3.140113	0.877322	0.847364	C	5.586975	-2.127342	1.251377
C	-3.279099	-0.516406	0.836211	H	5.570714	-3.210630	1.195178
C	-2.288819	-1.312894	1.536990	C	6.466883	0.000774	0.434894
C	-2.085691	-2.559263	0.818916	H	7.142481	0.478947	-0.270394
C	-0.802918	-3.118590	0.809061	C	6.522669	-1.402466	0.556906
C	0.256678	-2.421511	1.521323	H	7.247097	-1.937407	-0.052289
C	1.507197	-2.614442	0.816163	H	4.950860	-1.683782	2.005915
C	2.438118	-1.565469	0.833219	H	4.997599	0.438695	1.929581
C	2.110958	-0.350014	1.559183	C	3.906931	-1.957124	-1.209623
C	1.968001	1.996791	0.868844	N	4.203073	-2.583450	-2.148708
C	2.672864	0.792528	0.874092	H	3.986835	0.766280	-0.940760
C	0.660022	3.659150	-0.090731				
C	1.914920	3.116139	-0.085749				
C	-2.638272	2.938842	-0.102384				
C	-3.546944	1.916408	-0.110077				
C	-3.882397	-1.438947	-0.136291				
C	-3.192208	-2.619977	-0.145984				
C	-0.104706	-3.970834	-0.160521				
C	1.232427	-3.677457	-0.160617				
C	3.517115	-1.184707	-0.083439				
C	3.727359	0.247082	-0.025512				
H	0.325947	4.447453	-0.754348				

Transition state structure for the reaction of butadiene with Fragment 2 substituted with one NO₂ groupMolecular formula: C₃₄H₁₅NO₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.404398

Thermal correction to Enthalpy= 0.405343

Thermal correction to Gibbs Free Energy= 0.330467

Sum of electronic and zero-point Energies= -1509.176222

Sum of electronic and thermal Energies= -1509.152750

Sum of electronic and thermal Enthalpies= -1509.151806

Sum of electronic and thermal Free Energies= -1509.226682

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

253.764 102.065 157.589

Cartesian coordinates

Atom X Y Z

C	0.939102	-0.271331	2.282290	H	-2.739922	3.853447	-0.621816
C	0.221489	0.967850	2.332393	H	-4.482088	1.906320	-0.638339
C	-1.181984	0.668524	2.358608	H	-4.803719	-1.127580	-0.712584
C	-1.331045	-0.756703	2.323724	H	-3.500382	-3.390447	-0.801535
C	-0.019742	-1.337986	2.273477	H	-0.717860	-4.652764	-0.880278
C	0.663072	2.039151	1.589260	H	1.849758	-4.101472	-0.927234
C	-0.246461	2.958149	0.930119	H	2.645025	3.458897	-0.725453
C	-1.613472	2.663242	0.949409	C	5.363093	0.733932	0.750117
C	-2.048616	1.454720	1.633559	H	5.395038	1.794551	0.516783
C	-3.193973	0.901631	0.938967	C	5.814720	-2.095433	1.493300
C	-3.341022	-0.491551	0.903507	H	5.948675	-3.158497	1.661395
C	-2.339017	-1.306363	1.565218	C	6.372635	-0.073967	0.208279
C	-2.160990	-2.541654	0.822606	H	6.962328	0.307572	-0.619399
C	-0.882089	-3.107461	0.770254	C	6.582592	-1.430969	0.592134
C	0.202536	-2.424127	1.460731	H	7.338948	-1.985151	0.042924
C	1.436720	-2.621759	0.723753	H	5.066788	-1.604729	2.104785
C	2.381075	-1.577118	0.731986	H	5.047157	0.529417	1.768726
C	2.060831	-0.364710	1.483766	N	4.105930	-1.888667	-1.148702
C	1.915674	2.005677	0.866095	O	3.871849	-3.101478	-1.288413
C	2.618177	0.798484	0.830019	O	4.953934	-1.267350	-1.834882
C	0.596412	3.695784	-0.023855	H	3.880399	0.783765	-1.032230
C	1.850069	3.150304	-0.057344				
C	-2.706263	2.982128	0.020791				
C	-3.618107	1.962456	0.012906				
C	-3.973630	-1.393427	-0.069343				
C	-3.291329	-2.578602	-0.115482				
C	-0.214234	-3.961872	-0.215250				
C	1.126094	-3.682986	-0.243858				
C	3.440951	-1.143672	-0.162913				
C	3.656310	0.279670	-0.099847				
H	0.251552	4.500779	-0.661433				

Transition state structure for the reaction of butadiene with Fragment 1 substituted with two NH₂ groupMolecular formula: C₃₄H₂₀N₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.460535

Thermal correction to Enthalpy= 0.461479

Thermal correction to Gibbs Free Energy= 0.388109

Sum of electronic and zero-point Energies= -1416.621211

Sum of electronic and thermal Energies= -1416.597981

Sum of electronic and thermal Enthalpies= -1416.597037

Sum of electronic and thermal Free Energies= -1416.670406

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

288.990 105.093 154.419

Cartesian coordinates

Atom X Y Z

C	-1.347409	-0.526112	-1.103618	H	-4.889589	1.076556	1.139620
C	-1.198957	0.895872	-1.117037	H	-5.508977	-1.180957	1.914679
C	0.071563	1.425423	-1.093045	H	-4.065161	-3.123240	1.565666
C	1.232679	0.587356	-1.023248	H	-2.835318	3.229195	0.780636
C	1.057852	-0.787740	-1.014529	H	-1.040894	5.014793	1.576935
C	-0.252920	-1.359851	-1.026012	H	1.326296	5.275665	2.138430
C	2.242951	1.211627	-0.230717	H	3.026773	3.623314	1.462788
C	3.159078	0.369591	0.426629	H	-1.570144	-3.826993	0.959338
C	2.989324	-1.050262	0.432218	H	1.193419	-4.398107	1.624900
C	1.888487	-1.607239	-0.235548	C	4.058020	-4.925258	-0.108337
C	3.822662	-1.993814	1.265636	H	3.562553	-5.888290	-0.183940
C	3.032925	-3.267469	1.631232	H	3.673747	-4.151969	-0.758809
C	1.726570	-3.576430	1.150541	C	5.186037	-2.362068	0.366166
C	1.134619	-2.778760	0.198657	H	4.821467	-2.441952	-0.659435
C	-0.281836	-2.566646	-0.235331	H	5.793212	-1.458877	0.449326
C	-1.507697	-2.960299	0.304769	C	5.877791	-3.579665	0.796588
C	-2.662120	-2.080163	0.254653	H	6.803001	-3.517821	1.362468
C	-2.522947	-0.833966	-0.398742	C	5.284531	-4.810624	0.536307
C	-3.214188	0.370527	-0.037921	H	5.736900	-5.708371	0.957763
C	-4.310553	0.224164	0.795141	N	3.480004	-3.867317	2.788615
C	-4.635909	-1.075458	1.276762	H	3.092457	-4.791360	2.944574
C	-3.832091	-2.188820	1.061521	H	4.499888	-3.888181	2.847380
C	0.331655	2.588812	-0.349297	N	4.369206	-1.301598	2.440842
C	-0.726589	3.319130	0.235747	H	3.681328	-1.279994	3.189416
C	-2.067915	2.756505	0.171409	H	5.185011	-1.792573	2.797674
C	-2.295795	1.513579	-0.412239				
C	-0.307495	4.360222	1.113076				
C	1.035839	4.487698	1.449154				
C	2.033309	3.565036	1.026593				
C	1.684298	2.566124	0.131990				
H	3.906935	0.772993	1.101941				

Transition state structure for the reaction of butadiene with Fragment 1 substituted with two OMe group

Molecular formula: C₃₆H₂₂O₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.493990

Thermal correction to Enthalpy= 0.494934

Thermal correction to Gibbs Free Energy= 0.415684

Sum of electronic and zero-point Energies= -1534.921484

Sum of electronic and thermal Energies= -1534.895533

Sum of electronic and thermal Enthalpies= -1534.894589

Sum of electronic and thermal Free Energies= -1534.973839

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

309.984 113.022 166.796

Cartesian coordinates

	H	-5.526073	-0.948341	2.041029
	H	-4.093303	-2.915226	1.807510
Atom	X	Y	Z	
C	-1.391664	-0.511880	-1.051599	H
C	-1.238373	0.905127	-1.161406	H
C	0.033810	1.430997	-1.186928	H
C	1.192366	0.594903	-1.070661	H
C	1.011561	-0.775534	-0.968658	H
C	-0.299631	-1.343649	-0.930715	C
C	2.214051	1.269493	-0.334650	H
C	3.134043	0.468746	0.368201	H
C	2.949707	-0.944256	0.482316	C
C	1.842197	-1.543102	-0.137100	H
C	3.775026	-1.832923	1.377081	H
C	3.004055	-3.081661	1.809544	C
C	1.697615	-3.420095	1.376450	H
C	1.095600	-2.681768	0.374064	C
C	-0.322708	-2.495466	-0.059160	H
C	-1.546946	-2.847840	0.514694	O
C	-2.697830	-1.967321	0.418210	O
C	-2.561357	-0.767129	-0.317185	C
C	-3.244956	0.461339	-0.030784	H
C	-4.333765	0.375421	0.820296	H
C	-4.658613	-0.888490	1.389665	H
C	-3.861017	-2.017072	1.240926	C
C	0.305472	2.641371	-0.527126	H
C	-0.744581	3.413214	0.017989	H
C	-2.088255	2.852061	0.006039	H
C	-2.326153	1.573306	-0.489295	
C	-0.313500	4.510714	0.817200	
C	1.033889	4.657343	1.128661	
C	2.024679	3.705265	0.759291	
C	1.663469	2.647859	-0.060429	
H	3.899632	0.922123	0.991710	
H	-4.906632	1.251066	1.112726	

Transition state structure for the reaction of butadiene with Fragment 1 substituted with two OH groupMolecular formula: C₃₄H₁₈O₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.434778

Thermal correction to Enthalpy= 0.435722

Thermal correction to Gibbs Free Energy= 0.362613

Sum of electronic and zero-point Energies= -1456.377685

Sum of electronic and thermal Energies= -1456.354677

Sum of electronic and thermal Enthalpies= -1456.353732

Sum of electronic and thermal Free Energies= -1456.426841

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

272.827 103.342 153.871

Cartesian coordinates

Atom X Y Z

C -1.359166 -0.482182 -1.134269
C -1.211777 0.939699 -1.114275
C 0.057784 1.470301 -1.068470
C 1.218144 0.631805 -1.004550
C 1.043654 -0.742971 -1.031043
C -0.264805 -1.317476 -1.069532
C 2.224264 1.246891 -0.196813
C 3.142223 0.391890 0.442036
C 2.965032 -1.025806 0.422296
C 1.864841 -1.580873 -0.259274
C 3.761837 -1.998846 1.228674
C 2.937223 -3.198941 1.653757
C 1.676158 -3.548013 1.138710
C 1.112344 -2.756570 0.146556
C -0.296010 -2.540200 -0.301162
C -1.527668 -2.945998 0.220066
C -2.681300 -2.065895 0.180323
C -2.539931 -0.805515 -0.445694
C -3.235092 0.390156 -0.063670
C -4.336329 0.225311 0.759056
C -4.663520 -1.085183 1.210005
C -3.857444 -2.192826 0.976322
C 0.310812 2.619279 -0.300834
C -0.752906 3.336724 0.290048
C -2.092857 2.772973 0.204404
C -2.314729 1.541781 -0.405754
C -0.341612 4.363573 1.187487
C 0.999782 4.490185 1.532306
C 2.002667 3.578616 1.099219
C 1.660970 2.592482 0.187215
H 3.904644 0.795633 1.103684

H -4.918214 1.069454 1.118587
H -5.540658 -1.205216 1.839661
H -4.093051 -3.138073 1.458461
H -2.865769 3.232662 0.816519
H -1.079245 5.008348 1.658161
H 1.284253 5.268358 2.234988
H 2.994798 3.636508 1.538847
H -1.594224 -3.826379 0.855498
H 1.143126 -4.357329 1.628281
C 4.066083 -5.111885 0.019970
H 3.596618 -6.089767 0.028121
H 3.661977 -4.399370 -0.685798
C 5.113411 -2.450558 0.343601
H 4.725125 -2.614137 -0.663383
H 5.719055 -1.543383 0.355468
C 5.789873 -3.615599 0.892196
H 6.647713 -3.479848 1.543294
C 5.229710 -4.883022 0.731095
H 5.669296 -5.713987 1.280175
O 3.377370 -3.783945 2.778857
H 4.132896 -3.246371 3.083845
O 4.381647 -1.437214 2.404538
H 3.696077 -0.929082 2.866024

Transition state structure for the reaction of butadiene with Fragment 1 substituted with two Me groupMolecular formula: C₃₆H₂₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.482865

Thermal correction to Enthalpy= 0.483809

Thermal correction to Gibbs Free Energy= 0.408575

Sum of electronic and zero-point Energies= -1384.518909

Sum of electronic and thermal Energies= -1384.494908

Sum of electronic and thermal Enthalpies= -1384.493963

Sum of electronic and thermal Free Energies= -1384.569197

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

303.002 106.580 158.342

Cartesian coordinates

Atom	X	Y	Z	
C	-1.426328	-0.479561	-1.122724	H -5.038043 1.032256 1.072823
C	-1.293531	0.943871	-1.098027	H -5.648834 -1.249147 1.782076
C	-0.030131	1.486851	-1.028955	H -4.173498 -3.166044 1.424230
C	1.137089	0.659264	-0.950118	H -3.002346 3.212686 0.814394
C	0.978644	-0.716638	-0.978370	H -1.248033 4.997375 1.698962
C	-0.324222	-1.303800	-1.036872	H 1.101454 5.269888 2.325500
C	2.120256	1.272333	-0.116170	H 2.836161 3.653472 1.654050
C	3.030471	0.424163	0.539738	H -1.657428 -3.826454 0.863393
C	2.883419	-1.003607	0.515585	H 1.080731 -4.337902 1.619443
C	1.798063	-1.543181	-0.196184	C 3.981351 -5.049325 0.251328
C	3.683911	-1.984466	1.317969	H 3.529581 -6.012675 0.467342
C	2.925146	-3.226359	1.693517	H 3.472344 -4.453454 -0.492117
C	1.626105	-3.509369	1.172974	C 5.017056 -2.411192 0.096719
C	1.054532	-2.729657	0.193839	H 4.383777 -2.626500 -0.761181
C	-0.357195	-2.526822	-0.273036	H 5.525895 -1.456704 -0.028042
C	-1.590117	-2.945662	0.228501	C 5.825945 -3.495748 0.548056
C	-2.753906	-2.077986	0.169158	H 6.795187 -3.295033 0.996660
C	-2.614611	-0.816258	-0.453549	C 5.280051 -4.777367 0.644710
C	-3.328435	0.371810	-0.081515	H 5.840145 -5.544957 1.176167
C	-4.441652	0.194397	0.722303	C 3.303706 -3.915015 2.985380
C	-4.762799	-1.119384	1.166948	H 4.372369 -4.142236 3.033697
C	-3.940639	-2.218072	0.946005	H 3.072219 -3.279303 3.851095
C	0.198738	2.633266	-0.249492	H 2.752877 -4.851570 3.103114
C	-0.881652	3.338256	0.325903	C 4.481792 -1.362723 2.471932
C	-2.214747	2.763394	0.213319	H 5.090069 -0.526837 2.118399
C	-2.414247	1.533013	-0.405822	H 3.815090 -0.983658 3.254192
C	-0.496166	4.361896	1.238192	H 5.163952 -2.084638 2.922514
C	0.836863	4.495539	1.610893	
C	1.854488	3.593585	1.191815	
C	1.538891	2.612629	0.265603	
H	3.752176	0.856125	1.226068	

Transition state structure for the reaction of butadiene with Fragment 1 substituted with two *i*-Pr group

Molecular formula: C40H30

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.602601

Thermal correction to Enthalpy= 0.603545

Thermal correction to Gibbs Free Energy= 0.516945

Sum of electronic and zero-point Energies= -1541.632735

Sum of electronic and thermal Energies= -1541.603174

Sum of electronic and thermal Enthalpies= -1541.602230

Sum of electronic and thermal Free Energies= -1541.688830

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

378.138 127.440 182.264

Cartesian coordinates			
Atom	X	Y	Z
C	-1.371835	-0.660600	-1.065945
C	-1.211033	0.753132	-1.200571
C	0.065230	1.270203	-1.209809
C	1.214277	0.429679	-1.061501
C	1.031779	-0.936128	-0.932773
C	-0.286204	-1.495874	-0.907850
C	2.221582	1.102305	-0.303585
C	3.113553	0.316337	0.435381
C	2.944363	-1.116050	0.584869
C	1.850205	-1.694541	-0.085039
C	3.700744	-1.992393	1.497814
C	3.155614	-3.389189	1.679423
C	1.725635	-3.614365	1.324578
C	1.093669	-2.838192	0.414720
C	-0.334876	-2.633452	-0.026690
C	-1.561235	-2.966038	0.541408
C	-2.709014	-2.081014	0.411206
C	-2.554100	-0.897345	-0.344757
C	-3.236595	0.339697	-0.093004
C	-4.338077	0.274939	0.743553
C	-4.676734	-0.974700	1.334391
C	-3.881002	-2.109153	1.220260
C	0.332448	2.489388	-0.562897
C	-0.723007	3.277260	-0.051724
C	-2.069995	2.724393	-0.079678
C	-2.305769	1.438605	-0.557363
C	-0.299934	4.385148	0.736818
C	1.041720	4.528421	1.073235
C	2.032222	3.562377	0.741131
C	1.679553	2.495083	-0.068349
H	3.851035	0.812417	1.052970
H	-4.911105	1.158887	1.009705
H	-5.553005	-1.017332	1.975131
H	-4.123465	-2.994125	1.802982
H	-2.836601	3.254356	0.481441
H	-1.030174	5.084178	1.136320
H	1.334729	5.369920	1.694730
H	3.022750	3.649184	1.179565
H	-1.633321	-3.773679	1.266534
H	1.226557	-4.457111	1.795554
C	3.864025	-4.516969	0.189211
H	3.308527	-5.446602	0.295077
H	3.431471	-3.869381	-0.569856
C	5.412414	-2.215624	-0.113606
H	4.576759	-2.198191	-0.796326
H	5.978294	-1.291549	-0.078411
C	6.029523	-3.429744	0.174906
H	7.069277	-3.444586	0.498427
C	5.272256	-4.594576	0.261820
H	5.742064	-5.515262	0.597679
C	2.607228	-3.879705	4.181552
H	1.548401	-3.762689	3.935428
H	2.688796	-4.662690	4.944113
H	2.947553	-2.947173	4.637815
C	3.411370	-0.484303	3.541959
H	3.823240	-0.297894	4.540344
H	3.219679	0.486611	3.080181
H	2.445475	-0.981078	3.661419
C	3.461590	-4.266530	2.953317
H	3.098994	-5.254076	2.642234
C	4.914426	-4.502352	3.426260
H	4.978021	-5.491362	3.893638
H	5.638805	-4.472532	2.615405
H	5.230910	-3.783316	4.187938
C	4.404441	-1.347778	2.719550
H	4.683639	-2.168876	3.372434
C	5.718610	-0.572331	2.501944
H	6.040993	-0.138851	3.455416
H	6.515179	-1.233655	2.154981
H	5.632037	0.249179	1.786306

Transition state structure for the reaction of butadiene with Fragment 1 substituted with two COOH group

Molecular formula: C36H18O4

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.459196

Thermal correction to Enthalpy= 0.460140

Thermal correction to Gibbs Free Energy= 0.378617

Sum of electronic and zero-point Energies= -1683.052598

Sum of electronic and thermal Energies= -1683.025833

Sum of electronic and thermal Enthalpies= -1683.024889

Sum of electronic and thermal Free Energies= -1683.106412

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

288.150 115.796 171.580

Cartesian coordinates

Atom X Y Z

C -1.500710 -0.456006 -1.143204
C -1.361408 0.966676 -1.137277
C -0.098045 1.501522 -1.011194
C 1.056722 0.670969 -0.865013
C 0.894546 -0.704565 -0.870989
C -0.410544 -1.284932 -0.987244
C 1.998573 1.288709 0.018589
C 2.867768 0.464776 0.736876
C 2.727004 -0.982380 0.724774
C 1.673806 -1.520708 -0.046416
C 3.394037 -1.937637 1.584562
C 2.861292 -3.335995 1.699376
C 1.456947 -3.559904 1.206718
C 0.906278 -2.716989 0.307767
C -0.494106 -2.497906 -0.220024
C -1.744827 -2.899460 0.237566
C -2.901454 -2.025825 0.108352
C -2.722226 -0.776477 -0.526444
C -3.445473 0.421694 -0.210108
C -4.597126 0.263419 0.542448
C -4.947048 -1.039486 0.995101
C -4.121478 -2.146368 0.833089
C 0.098501 2.660015 -0.238619
C -1.005373 3.381165 0.268222
C -2.334748 2.812198 0.098458
C -2.510356 1.572532 -0.509909
C -0.659416 4.418831 1.180250
C 0.653673 4.552214 1.618056
C 1.684964 3.636722 1.267723
C 1.409287 2.643601 0.342692
H 3.544903 0.892687 1.463734

H -5.204816 1.110457 0.848619
H -5.861283 -1.153153 1.570605
H -4.380967 -3.083993 1.317579
H -3.148575 3.275740 0.651693
H -1.429484 5.066732 1.590838
H 0.886221 5.337390 2.331795
H 2.642045 3.696413 1.778409
H -1.844600 -3.768902 0.883370
H 0.935841 -4.432825 1.590122
C 3.791743 -4.490828 0.749878
H 3.307281 -5.436089 0.981211
H 3.552611 -4.154977 -0.258794
C 5.540164 -2.357131 -0.073503
H 4.622465 -2.407090 -0.641184
H 6.145608 -1.470141 -0.229232
C 6.016290 -3.419585 0.660744
H 7.022379 -3.367422 1.069462
C 5.189730 -4.468686 1.073636
H 5.566820 -5.189894 1.790229
C 2.906909 -3.923071 3.127382
C 4.472375 -1.644463 2.519372
O 4.961242 -2.488871 3.267459
O 3.263687 -5.041193 3.422408
O 2.293421 -3.098574 4.006270
H 2.334573 -3.552701 4.864676
O 4.953318 -0.367956 2.529419
H 5.650730 -0.375484 3.205025

Transition state structure for the reaction of butadiene with Fragment 1 substituted with two CF₃ groupMolecular formula: C₃₆H₁₆F₆

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.440664

Thermal correction to Enthalpy= 0.441608

Thermal correction to Gibbs Free Energy= 0.356404

Sum of electronic and zero-point Energies= -1979.989832

Sum of electronic and thermal Energies= -1979.961633

Sum of electronic and thermal Enthalpies= -1979.960689

Sum of electronic and thermal Free Energies= -1980.045893

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

276.521 120.397 179.326

Cartesian coordinates

Atom X Y Z

C	-1.398424	-0.467746	-1.135493	H	3.740414	0.853647	1.299252
C	-1.267673	0.955741	-1.092970	H	-5.037293	1.015780	1.032861
C	-0.005805	1.499440	-1.000404	H	-5.653099	-1.271995	1.713549
C	1.158620	0.671060	-0.914380	H	-4.170332	-3.183662	1.354456
C	1.005425	-0.703470	-0.960251	H	-3.003411	3.198251	0.825364
C	-0.296921	-1.292228	-1.042218	H	-1.263936	4.970017	1.759792
C	2.127555	1.269467	-0.053127	H	1.074845	5.231335	2.428556
C	3.033644	0.423836	0.602415	H	2.818276	3.620887	1.762647
C	2.894165	-1.011850	0.553516	H	-1.646668	-3.831759	0.819806
C	1.818612	-1.534990	-0.179808	H	1.054338	-4.335039	1.587209
C	3.681634	-2.026154	1.320690	C	3.974033	-5.020199	0.453490
C	2.952300	-3.283458	1.674016	H	3.531056	-5.925660	0.855483
C	1.614930	-3.514792	1.158676	H	3.435964	-4.572989	-0.370673
C	1.069966	-2.724778	0.191829	C	5.033368	-2.476836	-0.139194
C	-0.341139	-2.521102	-0.294874	H	4.237608	-2.737053	-0.828976
C	-1.575203	-2.946269	0.192242	H	5.473062	-1.506442	-0.341068
C	-2.740988	-2.080969	0.124087	C	5.862808	-3.506023	0.337218
C	-2.594402	-0.813572	-0.484252	H	6.866049	-3.266539	0.677407
C	-3.314214	0.369744	-0.108780	C	5.320396	-4.751210	0.657750
C	-4.436073	0.182226	0.680541	H	5.911143	-5.438129	1.257535
C	-4.761018	-1.135768	1.108953	C	4.615037	-1.393671	2.360222
C	-3.934833	-2.231143	0.887137	C	3.153145	-3.982264	3.027179
C	0.212270	2.634773	-0.200831	F	5.431599	-0.460060	1.797876
C	-0.876738	3.331499	0.368323	F	3.911647	-0.749107	3.318143
C	-2.207312	2.757555	0.229300	F	5.434254	-2.260710	2.974391
C	-2.397884	1.535270	-0.408751	F	2.835153	-3.147783	4.046758
C	-0.505068	4.341339	1.301387	F	2.328338	-5.057299	3.143361
C	0.821669	4.468839	1.697586	F	4.385517	-4.456172	3.284082
C	1.845023	3.571770	1.282289				
C	1.543036	2.607323	0.335115				

Transition state structure for the reaction of butadiene with Fragment 1 substituted with two CHO groupMolecular formula: C₃₆H₁₈O₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.476638

Thermal correction to Enthalpy= 0.477582

Thermal correction to Gibbs Free Energy= 0.402143

Sum of electronic and zero-point Energies= -1522.843870

Sum of electronic and thermal Energies= -1522.820649

Sum of electronic and thermal Enthalpies= -1522.819705

Sum of electronic and thermal Free Energies= -1522.895144

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

299.095 99.664 158.774

Cartesian coordinates

Atom	X	Y	Z	
C	-1.815819	0.006933	-0.742634	H -5.383419 1.721147 1.300774
C	-1.618409	1.417211	-0.755971	H -6.106002 -0.500203 2.046235
C	-0.353245	1.895996	-0.690287	H -4.727942 -2.467667 1.772093
C	0.765818	1.021284	-0.571048	H -3.240632 3.803185 1.027364
C	0.551696	-0.326225	-0.559725	H -1.408386 5.551886 1.848315
C	-0.773623	-0.852618	-0.622289	H 0.917360 5.736452 2.483724
C	1.766288	1.606099	0.244813	H 2.571212 4.021679 1.906263
C	2.617342	0.757603	0.926633	H -2.222986 -3.253628 1.285689
C	2.411696	-0.675574	0.934829	H 0.569045 -4.014435 1.907937
C	1.329492	-1.166438	0.227147	C 3.411020 -4.247114 0.581774
C	3.117980	-1.669151	1.775185	H 2.859848 -5.165340 0.691135
C	2.492439	-2.991594	1.914836	H 3.076238 -3.643833 -0.240537
C	1.092371	-3.185135	1.473978	C 4.941671 -1.906957 0.440884
C	0.540226	-2.341111	0.604546	H 4.220920 -1.916840 -0.348806
C	-0.877776	-2.057863	0.142784	H 5.491790 -0.985872 0.527998
C	-2.109096	-2.400172	0.639222	C 5.510203 -3.088290 0.889557
C	-3.234738	-1.479502	0.536735	H 6.462701 -3.059661 1.389425
C	-3.026653	-0.258095	-0.094898	C 4.768420 -4.251093 0.926384
C	-3.698253	0.963587	0.218544	H 5.176161 -5.114238 1.423531
C	-4.820708	0.859635	0.986416	C 2.819961 -3.860900 3.115136
C	-5.208894	-0.427508	1.457021	C 4.010831 -1.154706 2.838932
C	-4.439587	-1.550002	1.289368	O 4.398822 -1.752534 3.798418
C	-0.078758	3.055072	0.044129	O 1.997276 -4.538269 3.648071
C	-1.115769	3.821004	0.564441	H 3.853593 -3.884772 3.425507
C	-2.475701	3.300828	0.459700	H 4.333886 -0.124489 2.695975
C	-2.718329	2.079770	-0.113842	
C	-0.692754	4.862299	1.434954	
C	0.624398	4.952615	1.807779	
C	1.603102	3.987485	1.437697	
C	1.250960	3.002244	0.561599	
H	3.332737	1.188244	1.600576	

Transition state structure for the reaction of butadiene with Fragment 1 substituted with two CN groupMolecular formula: C₃₆H₁₆N₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.424532

Thermal correction to Enthalpy= 0.425476

Thermal correction to Gibbs Free Energy= 0.346820

Sum of electronic and zero-point Energies= -1490.421025

Sum of electronic and thermal Energies= -1490.395979

Sum of electronic and thermal Enthalpies= -1490.395035

Sum of electronic and thermal Free Energies= -1490.473691

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

266.398 107.478 165.546

Cartesian coordinates

Atom	X	Y	Z			
				H	-5.022974	1.071971 1.115018
				H	-5.660007	-1.197596 1.833752
				H	-4.216196	-3.137138 1.465892
C	-1.451363	-0.492097	-1.106597	H	-2.960838	3.224229 0.835745
C	-1.297412	0.929218	-1.083933	H	-1.177702	4.984080 1.706220
C	-0.025790	1.454283	-1.024813	H	1.177785	5.224356 2.321124
C	1.128077	0.610382	-0.952246	H	2.885531	3.581314 1.642241
C	0.951299	-0.763906	-0.983321	H	-1.714664	-3.832842 0.884183
C	-0.362328	-1.333668	-1.030397	H	1.040666	-4.423221 1.579947
C	2.123754	1.213322	-0.119240	C	3.992467	-4.865168 0.342534
C	3.025390	0.360768	0.531830	H	3.475768	-5.788206 0.586388
C	2.850407	-1.065338	0.494394	H	3.595796	-4.339054 -0.517345
C	1.767713	-1.602887	-0.215491	C	5.233140	-2.362653 0.062581
C	3.610418	-2.036811	1.314226	H	4.573825	-2.533563 -0.781115
C	2.934844	-3.343194	1.587457	H	5.704251	-1.384102 0.053735
C	1.571399	-3.594881	1.121507	C	5.938234	-3.449966 0.606042
C	1.005138	-2.785652	0.185823	H	6.874629	-3.269738 1.126555
C	-0.412568	-2.555491	-0.272017	C	5.318332	-4.689294 0.740398
C	-1.642090	-2.954398	0.247108	H	5.790160	-5.449596 1.356471
C	-2.794729	-2.070424	0.195082	C	4.355625	-1.466974 2.415841
C	-2.639302	-0.811653	-0.428052	C	3.251581	-3.980193 2.841404
C	-3.332696	0.387061	-0.052745	N	3.479595	-4.523798 3.844539
C	-4.441386	0.225558	0.760625	N	4.969007	-0.958360 3.262911
C	-4.778289	-1.082415	1.210065			
C	-3.974679	-2.193592	0.983922			
C	0.224446	2.599488	-0.248738			
C	-0.842664	3.319751	0.332376			
C	-2.183749	2.762975	0.230375			
C	-2.405013	1.534642	-0.385731			
C	-0.437292	4.338450	1.241387			
C	0.899236	4.454798	1.607217			
C	1.901564	3.538312	1.183928			
C	1.565570	2.564812	0.257660			
H	3.754511	0.760303	1.231616			

Transition state structure for the reaction of butadiene with Fragment 1 substituted with two NO₂ groupMolecular formula: C₃₄H₁₆N₂O₄

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.466964

Thermal correction to Enthalpy= 0.467908

Thermal correction to Gibbs Free Energy= 0.393973

Sum of electronic and zero-point Energies= -1704.430568

Sum of electronic and thermal Energies= -1704.407805

Sum of electronic and thermal Enthalpies= -1704.406861

Sum of electronic and thermal Free Energies= -1704.480797

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

293.024 99.592 155.610

Cartesian coordinates

Atom X Y Z

C	-1.159847	-0.689594	-1.170665	H	-4.644804	1.300783	0.761167
C	-0.918713	0.708789	-1.302796	H	-5.423008	-0.824763	1.701539
C	0.359598	1.155085	-1.298510	H	-4.109878	-2.851376	1.578446
C	1.455510	0.259512	-1.113849	H	-2.447335	3.286006	0.283970
C	1.201925	-1.082378	-0.999762	H	-0.556832	5.038751	0.937519
C	-0.144086	-1.568248	-0.993741	H	1.780352	5.202453	1.536102
C	2.478514	0.883338	-0.365995	H	3.373764	3.394270	1.087851
C	3.306625	0.060954	0.384459	H	-1.638638	-3.757815	1.122983
C	3.051279	-1.341175	0.486840	H	1.198464	-4.689182	1.623255
C	1.962114	-1.873981	-0.157134	C	3.952854	-4.374954	0.155585
C	3.697649	-2.223127	1.560414	H	3.981537	-5.445003	0.332506
C	3.207962	-3.720804	1.357206	H	3.331551	-4.231163	-0.718201
C	1.703799	-3.883705	1.130049	C	5.231320	-2.121070	1.601857
C	1.136459	-3.026553	0.304473	H	5.505131	-1.075909	1.587800
C	-0.279152	-2.706010	-0.135939	H	5.601664	-2.516332	2.537426
C	-1.509604	-2.964038	0.407444	C	5.884853	-2.845175	0.461759
C	-2.607073	-2.018163	0.244960	H	6.872441	-2.518957	0.185849
C	-2.368648	-0.861024	-0.487761	C	5.328481	-3.865205	-0.150275
C	-2.998115	0.402816	-0.271784	H	5.847297	-4.374523	-0.944639
C	-4.112687	0.398749	0.514763	O	1.988590	-1.748704	3.087514
C	-4.533185	-0.830786	1.097218	O	2.750321	-4.668667	3.435227
C	-3.801236	-1.987427	1.015991	O	4.721881	-4.855665	2.705224
C	0.676484	2.363230	-0.668723	O	3.940679	-1.173531	3.642167
C	-0.330541	3.200996	-0.203017	N	3.158455	-1.678903	2.897377
C	-1.704764	2.714249	-0.246420	N	3.590829	-4.488583	2.612678
C	-1.990766	1.455731	-0.709461				
C	0.133345	4.296726	0.575010				
C	1.456534	4.376605	0.927927				
C	2.400893	3.354143	0.630117				
C	2.009208	2.313362	-0.160818				
H	4.036544	0.498277	1.042542				

Transition state structure for the reaction of butadiene with Fragment 2 substituted with two NH₂ groupMolecular formula: C₃₄H₁₈N₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.435154

Thermal correction to Enthalpy= 0.436098

Thermal correction to Gibbs Free Energy= 0.360891

Sum of electronic and zero-point Energies= -1415.349855

Sum of electronic and thermal Energies= -1415.325970

Sum of electronic and thermal Enthalpies= -1415.325026

Sum of electronic and thermal Free Energies= -1415.400233

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

273.063 104.938 158.286

Cartesian coordinates

Atom X Y Z

C	1.198103	-0.335793	2.316520	H	-2.602309	3.574382	-0.744503
C	0.454268	0.894673	2.301390	H	-4.312991	1.599908	-0.637159
C	-0.940132	0.573259	2.362182	H	-4.569761	-1.432631	-0.567587
C	-1.064536	-0.854623	2.399633	H	-3.220928	-3.671474	-0.572106
C	0.253568	-1.417605	2.369569	H	-0.405528	-4.871577	-0.638632
C	0.870322	1.930163	1.493685	H	2.149915	-4.279406	-0.728534
C	-0.069271	2.800868	0.806337	H	2.761532	3.233289	-0.953548
C	-1.434661	2.484980	0.868710	C	6.554669	0.693227	1.842815
C	-1.836587	1.309056	1.616667	H	7.041166	1.610682	2.155899
C	-2.981593	0.699076	0.966733	C	5.348358	-1.883107	0.807321
C	-3.100492	-0.696382	0.998642	H	5.233102	-2.947799	0.607554
C	-2.072805	-1.460957	1.682785	C	7.072484	-0.064091	0.838248
C	-1.879929	-2.723465	0.995123	H	7.993172	0.288290	0.371317
C	-0.589387	-3.269530	0.957997	C	6.535121	-1.282989	0.313631
C	0.481413	-2.541157	1.611608	H	7.081290	-1.773719	-0.488950
C	1.719194	-2.743514	0.875508	H	5.076929	-1.630403	1.830728
C	2.637115	-1.696569	0.839841	H	5.659673	0.411170	2.386883
C	2.306788	-0.458443	1.512185	N	4.530879	0.724694	-1.091566
C	2.114509	1.886846	0.755588	H	4.755869	1.691829	-0.896925
C	2.847981	0.678328	0.771856	H	5.346284	0.186509	-1.385104
C	0.734300	3.491622	-0.202655	N	3.892159	-2.141688	-1.301908
C	1.999212	2.957308	-0.234781	H	3.294771	-1.753632	-2.028668
C	-2.544803	2.736893	-0.059611	H	4.848159	-2.133699	-1.648207
C	-3.440065	1.703307	-0.003910				
C	-3.725750	-1.652463	0.075059				
C	-3.019505	-2.824802	0.073187				
C	0.091342	-4.149177	-0.002022				
C	1.425997	-3.849351	-0.050006				
C	3.774863	-1.368571	-0.080330				
C	3.773883	0.094305	-0.157891				
H	0.363284	4.249879	-0.881489				

Transition state structure for the reaction of butadiene with Fragment 2 substituted with two OMe groupMolecular formula: C₃₆H₂₀O₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.469135

Thermal correction to Enthalpy= 0.470080

Thermal correction to Gibbs Free Energy= 0.389330

Sum of electronic and zero-point Energies= -1533.639687

Sum of electronic and thermal Energies= -1533.613411

Sum of electronic and thermal Enthalpies= -1533.612467

Sum of electronic and thermal Free Energies= -1533.693217

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

294.387 112.298 169.953

Cartesian coordinates

Atom X Y Z

C	1.107474	-0.300792	2.385539	H	-3.013114	3.482040	-0.404476
C	0.306947	0.894245	2.440401	H	-4.620965	1.425261	-0.263936
C	-1.066199	0.503196	2.555044	H	-4.733584	-1.619402	-0.247230
C	-1.120412	-0.929667	2.561015	H	-3.286732	-3.792959	-0.360744
C	0.219884	-1.426476	2.454423	H	-0.416271	-4.876251	-0.568559
C	0.633900	1.962360	1.634900	H	2.098706	-4.176865	-0.764076
C	-0.376789	2.802317	1.010421	H	2.362909	3.401834	-0.851299
C	-1.720294	2.419259	1.129196	C	6.419128	0.729996	1.256764
C	-2.030044	1.209052	1.867051	H	6.920800	1.684553	1.374468
C	-3.173823	0.557250	1.255742	C	5.092630	-1.871129	0.735480
C	-3.226104	-0.842883	1.262671	H	4.814633	-2.915284	0.609469
C	-2.132069	-1.569545	1.879480	C	6.959523	-0.258761	0.482754
C	-1.914074	-2.809065	1.156753	H	7.907383	-0.051247	-0.013305
C	-0.602851	-3.292327	1.048011	C	6.348047	-1.505320	0.201453
C	0.462295	-2.522005	1.659802	H	6.799215	-2.138690	-0.556925
C	1.669413	-2.650230	0.861294	H	4.875087	-1.507730	1.738574
C	2.516911	-1.547597	0.791850	H	5.503884	0.593777	1.820768
C	2.178175	-0.349796	1.522103	O	3.896169	1.123334	-1.227648
C	1.840927	1.997415	0.837705	O	3.736392	-1.826312	-1.390540
C	2.623102	0.824334	0.780804	C	5.089679	0.875280	-1.979319
C	0.348990	3.558068	-0.013267	H	4.949835	1.381178	-2.936118
C	1.633991	3.085665	-0.117004	H	5.938584	1.308781	-1.442156
C	-2.883874	2.634552	0.257983	H	5.261362	-0.192852	-2.128288
C	-3.725345	1.558039	0.330949	C	2.686256	-1.566355	-2.332768
C	-3.850123	-1.810883	0.349920	H	1.709724	-1.862457	-1.936022
C	-3.092537	-2.949136	0.290385	H	2.653448	-0.511051	-2.621986
C	0.072174	-4.129215	0.045689	H	2.917049	-2.175510	-3.209408
C	1.387252	-3.764897	-0.059981				
C	3.614325	-1.14709	-0.166240				
C	3.526905	0.320943	-0.212625				
H	-0.088200	4.315896	-0.652082				

Transition state structure for the reaction of butadiene with Fragment 2 substituted with two OH groupMolecular formula: C₃₄H₁₆O₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.442374

Thermal correction to Enthalpy= 0.443318

Thermal correction to Gibbs Free Energy= 0.377938

Sum of electronic and zero-point Energies= -1446.002006

Sum of electronic and thermal Energies= -1445.982636

Sum of electronic and thermal Enthalpies= -1445.981692

Sum of electronic and thermal Free Energies= -1446.047072

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

277.594 89.133 137.604

Cartesian coordinates

Atom X Y Z

C 1.477698 -0.412786 2.604413
C 0.773273 0.824236 2.632653
C -0.626766 0.539634 2.574361
C -0.785359 -0.875636 2.507068
C 0.513541 -1.467052 2.529322
C 1.260584 1.882067 1.932959
C 0.393698 2.809348 1.234981
C -0.947419 2.535608 1.181012
C -1.434639 1.332942 1.824405
C -2.528646 0.798969 1.052544
C -2.679857 -0.565412 0.984718
C -1.737889 -1.397713 1.690118
C -1.520924 -2.611234 0.932791
C -0.272063 -3.177339 0.949561
C 0.762173 -2.527490 1.722903
C 2.035966 -2.721506 1.073652
C 2.968975 -1.728816 1.170593
C 2.630003 -0.515552 1.875791
C 2.528281 1.823861 1.255242
C 3.204692 0.628754 1.224297
C 1.297863 3.549919 0.322549
C 2.514022 2.987347 0.329955
C -1.998639 2.882988 0.194476
C -2.898519 1.892523 0.120419
C -3.272651 -1.457259 -0.042561
C -2.612952 -2.623691 -0.070790
C 0.468583 -4.040656 -0.003730
C 1.783297 -3.786785 0.069013
C 4.268332 -1.446992 0.426113
C 4.203864 0.125560 0.177137
H 1.000589 4.374759 -0.296085

H -2.000354 3.769187 -0.410540
H -3.732231 1.863409 -0.554727
H -4.072638 -1.181840 -0.702705
H -2.802818 -3.426313 -0.757288
H 0.008296 -4.724623 -0.690690
H 2.541239 -4.222177 -0.550356
H 3.339349 3.286509 -0.285903
C 5.571813 0.847458 0.158980
H 5.636603 1.375135 -0.785334
C 5.454197 -1.856778 1.310933
H 5.510708 -2.939293 1.281858
C 6.783988 -0.029871 0.326763
H 7.724070 0.396654 0.018236
C 6.743329 -1.238725 0.844712
H 7.648831 -1.809923 0.959126
H 5.265206 -1.580940 2.345519
H 5.585458 1.608680 0.935034
O 4.397342 -2.141165 -0.772642
H 4.098585 -1.582035 -1.474672
O 3.643261 0.327423 -1.113795
H 2.700157 0.297146 -1.063543

Transition state structure for the reaction of butadiene with Fragment 2 substituted with two Me groupMolecular formula: C₃₆H₂₀

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.457977

Thermal correction to Enthalpy= 0.458921

Thermal correction to Gibbs Free Energy= 0.384520

Sum of electronic and zero-point Energies= -1383.249667

Sum of electronic and thermal Energies= -1383.225896

Sum of electronic and thermal Enthalpies= -1383.224951

Sum of electronic and thermal Free Energies= -1383.299352

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

287.385 105.060 156.589

Cartesian coordinates

Atom X Y Z

C 1.304335 -0.186839 2.311956
C 0.591687 1.058511 2.332105
C -0.810436 0.766208 2.387473
C -0.966042 -0.660152 2.396955
C 0.340003 -1.248901 2.347992
C 1.028143 2.087319 1.529386
C 0.107781 2.992354 0.863356
C -1.263084 2.712588 0.927595
C -1.690462 1.532824 1.656476
C -2.852812 0.962722 1.000849
C -3.004665 -0.429773 1.009964
C -1.991343 -1.228521 1.674238
C -1.828965 -2.481832 0.961021
C -0.550692 -3.051487 0.902941
C 0.543445 -2.358202 1.559837
C 1.771710 -2.574099 0.817179
C 2.718540 -1.541522 0.796640
C 2.416496 -0.313510 1.508305
C 2.271768 2.022977 0.783908
C 2.973635 0.810015 0.777908
C 0.929220 3.696202 -0.127287
C 2.177959 3.138875 -0.174482
C -2.372065 3.008315 0.009637
C -3.291193 1.995698 0.051144
C -3.656392 -1.356142 0.072835
C -2.976983 -2.543361 0.045474
C 0.099574 -3.929483 -0.076083
C 1.439394 -3.656176 -0.126644
C 3.846180 -1.213070 -0.108239
C 4.000056 0.233634 -0.122769
H 0.576375 4.487045 -0.778124

H -2.412574 3.858910 -0.660154
H -4.168507 1.924414 -0.580511
H -4.498835 -1.106066 -0.560828
H -3.200966 -3.373856 -0.613182
H -0.415395 -4.634299 -0.717649
H 2.133349 -4.119659 -0.815456
H 2.953232 3.433480 -0.869405
C 5.780738 0.754550 1.173561
H 5.864135 1.830591 1.051356
C 5.471655 -2.060601 1.207024
H 5.322169 -3.132398 1.114722
C 6.776177 -0.078975 0.682985
H 7.586364 0.348334 0.096082
C 6.623953 -1.474739 0.700882
H 7.322222 -2.081672 0.128511
H 4.949734 -1.608168 2.041650
H 5.177255 0.446974 2.018950
C 4.455639 0.947408 -1.373852
H 3.675425 0.917809 -2.146925
H 4.688969 1.995971 -1.177824
H 5.353080 0.485120 -1.791551
C 4.142665 -2.031402 -1.343559
H 4.157079 -3.101502 -1.125673
H 3.383215 -1.858561 -2.118483
H 5.114587 -1.770915 -1.768761

Transition state structure for the reaction of butadiene with Fragment 2 substituted with two *i*-Pr groupMolecular formula: C₄₀H₂₈

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.577703

Thermal correction to Enthalpy= 0.578647

Thermal correction to Gibbs Free Energy= 0.495174

Sum of electronic and zero-point Energies= -1540.363119

Sum of electronic and thermal Energies= -1540.334511

Sum of electronic and thermal Enthalpies= -1540.333567

Sum of electronic and thermal Free Energies= -1540.417039

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

362.514 125.307 175.683

Cartesian coordinates			
Atom	X	Y	Z
C	1.027636	-0.450098	2.116077
C	0.300684	0.767216	2.301757
C	-1.075092	0.435501	2.534597
C	1.199644	-0.991892	2.481793
C	0.097469	-1.538426	2.218547
C	0.605091	1.842566	1.504642
C	-0.413030	2.762499	1.035565
C	-1.757056	2.448467	1.268948
C	-2.060567	1.218262	1.977478
C	-3.291467	0.658117	1.455369
C	-3.414288	-0.736845	1.400863
C	-2.305189	-1.544922	1.872007
C	-2.216448	-2.747272	1.066767
C	-0.945882	-3.273396	0.795339
C	0.218809	-2.589062	1.338532
C	1.348783	-2.744791	0.448939
C	2.309548	-1.692458	0.386091
C	2.027899	-0.496962	1.172418
C	1.752242	1.859114	0.608859
C	2.486476	0.672312	0.463184
C	0.260724	3.559879	0.007386
C	1.507922	3.054595	-0.231894
C	-2.988219	2.771210	0.534128
C	-3.873954	1.733472	0.638763
C	-4.171405	-1.624696	0.506139
C	-3.477300	-2.788006	0.313174
C	-0.420256	-4.071707	-0.307200
C	0.903174	-3.765930	-0.508888
C	3.348965	-1.336839	-0.552185
C	3.612293	0.152202	-0.453655
H	-0.184806	4.386171	-0.533391
H	-3.136056	3.657925	-0.070431
H	-4.828441	1.676735	0.129228
H	-5.097907	-1.361518	0.010148
H	-3.771339	-3.584103	-0.360338
H	-1.001499	-4.746176	-0.924014
H	1.498683	-4.181704	-1.309294
H	2.172035	3.440836	-0.989887
C	4.984982	0.528907	0.642572
H	4.982305	1.615149	0.656991
C	5.559061	-2.242384	1.136451
H	5.740578	-3.307363	1.219427
C	6.237554	-0.059865	0.277737
H	6.959946	0.515173	-0.295442
C	6.463624	-1.421320	0.494614
H	7.365112	-1.870797	0.080439
H	4.734312	-1.856796	1.718809
H	4.582128	0.154241	1.582818
C	4.075622	-3.736547	-1.150340
H	3.853529	-4.495103	-1.910478
H	5.149884	-3.763607	-0.958015
H	3.561347	-4.013644	-0.230135
C	4.532687	2.298491	-1.676971
H	5.593634	2.245182	-1.418421
H	4.467972	2.802407	-2.647069
H	4.053615	2.943447	-0.939452
C	3.680346	-2.333339	-1.674805
H	2.713332	-2.464068	-2.190848
C	3.905607	0.891015	-1.789279
H	4.669976	0.297891	-2.285739
C	2.669233	0.897319	-2.709299
H	2.265169	-0.109883	-2.845463
H	1.862646	1.518101	-2.311832
H	2.934218	1.288480	-3.697764
C	4.706802	-1.979868	-2.769805
H	5.665210	-1.671159	-2.343874
H	4.893803	-2.880017	-3.364896
H	4.361853	-1.213479	-3.465092

Transition state structure for the reaction of butadiene with Fragment 2 substituted with two F groupMolecular formula: C₃₄H₁₄F₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.384305

Thermal correction to Enthalpy= 0.385249

Thermal correction to Gibbs Free Energy= 0.311638

Sum of electronic and zero-point Energies= -1503.137732

Sum of electronic and thermal Energies= -1503.114855

Sum of electronic and thermal Enthalpies= -1503.113910

Sum of electronic and thermal Free Energies= -1503.187521

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

241.155 99.740 154.927

Cartesian coordinates

Atom X Y Z

C 1.265646 -0.177497 2.388173
C 0.548948 1.069143 2.372539
C -0.854255 0.774181 2.380198
C -1.009075 -0.652098 2.392643
C 0.298451 -1.241299 2.392240
C 1.007066 2.099121 1.581814
C 0.110879 2.991683 0.868021
C -1.260509 2.710326 0.890248
C -1.709896 1.535989 1.616028
C -2.851100 0.960820 0.927769
C -3.002298 -0.431146 0.940101
C -2.009395 -1.225734 1.639926
C -1.823635 -2.481459 0.935115
C -0.544397 -3.050284 0.919860
C 0.523609 -2.358633 1.619765
C 1.770437 -2.573429 0.911309
C 2.708973 -1.543138 0.921253
C 2.407466 -0.307829 1.627559
C 2.269809 2.030151 0.872810
C 2.966016 0.822607 0.901357
C 0.962836 3.671300 -0.117044
C 2.211270 3.110915 -0.119548
C -2.339253 2.997394 -0.064935
C -3.259708 1.985572 -0.043098
C -3.622750 -1.361004 -0.013871
C -2.940877 -2.546953 -0.016663
C 0.140342 -3.913869 -0.051725
C 1.479769 -3.634342 -0.062004
C 3.810584 -1.194526 0.020995
C 3.960694 0.230728 0.007523
H 0.625191 4.440856 -0.800540

H -2.358227 3.842142 -0.742854
H -4.116815 1.908718 -0.701152
H -4.444773 -1.113824 -0.674771
H -3.141988 -3.379613 -0.679778
H -0.355316 -4.605641 -0.721962
H 2.206400 -4.060124 -0.742016
H 3.011354 3.358656 -0.805221
C 5.879967 0.749191 1.165341
H 5.937536 1.825842 1.037714
C 5.556339 -2.088293 1.166774
H 5.375869 -3.152000 1.044694
C 6.762544 -0.078160 0.501403
H 7.460882 0.358167 -0.208485
C 6.604473 -1.481446 0.502936
H 7.186852 -2.063816 -0.206701
H 5.140457 -1.656538 2.069924
H 5.368563 0.421803 2.063005
F 4.327304 0.841001 -1.142080
F 4.027016 -1.884770 -1.122796

Transition state structure for the reaction of butadiene with Fragment 2 substituted with two COOH group

Molecular formula: C36H16O4

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.434543

Thermal correction to Enthalpy= 0.435488

Thermal correction to Gibbs Free Energy= 0.353916

Sum of electronic and zero-point Energies= -1681.786522

Sum of electronic and thermal Energies= -1681.759807

Sum of electronic and thermal Enthalpies= -1681.758863

Sum of electronic and thermal Free Energies= -1681.840434

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

272.680 114.164 171.681

Cartesian coordinates

Atom X Y Z

C	-0.494110	0.084687	-1.815893	H	-4.143570	-3.642356	1.610980
C	-1.346640	-1.064589	-1.756420	H	-5.630566	-1.511901	1.885216
C	-2.695687	-0.609229	-1.575053	H	-5.592023	1.538722	1.998421
C	-2.674659	0.823141	-1.521939	H	-4.042050	3.639525	1.884914
C	-1.313568	1.252384	-1.670403	H	-1.154698	4.573204	1.547561
C	-0.922853	-2.186115	-1.082745	H	1.307288	3.741959	1.210417
C	-1.822585	-3.010805	-0.297620	H	1.215131	-3.885962	0.874124
C	-3.135157	-2.563616	-0.113348	C	3.883885	-1.391231	-1.144176
C	-3.527129	-1.303180	-0.725902	H	3.778818	-2.454408	-0.960697
C	-4.486574	-0.634866	0.130868	C	4.623765	1.384528	-1.808688
C	-4.468160	0.765488	0.183236	H	4.896819	2.424229	-1.954903
C	-3.490656	1.471977	-0.623367	C	5.110469	-0.807027	-0.805961
C	-3.064461	2.667887	0.080896	H	5.774308	-1.347224	-0.138758
C	-1.735752	3.085336	-0.060624	C	5.455990	0.527285	-1.157198
C	-0.849465	2.294326	-0.902289	H	6.403611	0.907169	-0.782930
C	0.496117	2.340973	-0.363466	H	3.685117	1.070684	-2.247838
C	1.309076	1.195281	-0.506352	H	3.388240	-1.034966	-2.042318
C	0.734838	0.041390	-1.190428	O	4.324343	0.675584	1.647319
C	0.420506	-2.307629	-0.556497	O	3.555826	-2.583383	1.397389
C	1.246804	-1.182384	-0.624128	O	3.349115	2.652893	1.173317
C	-0.935084	-3.863928	0.507662	O	2.139551	-1.171033	2.418124
C	0.364197	-3.466745	0.352989	C	3.437887	1.297673	1.066345
C	-4.107059	-2.770867	0.968673	C	2.844818	-1.602775	1.352307
C	-4.885675	-1.654964	1.111606	H	4.076776	2.905708	1.764588
C	-4.842281	1.718960	1.237527	H	2.395456	-1.747341	3.158429
C	-4.030796	2.819023	1.177628				
C	-0.837250	3.842331	0.813771				
C	0.451602	3.412938	0.639997				
C	2.452893	0.660464	0.219480				
C	2.492661	-0.786624	0.113731				
H	-1.268801	-4.646527	1.178297				

Transition state structure for the reaction of butadiene with Fragment 2 substituted with two CF₃ groupMolecular formula: C₃₆H₁₄F₆

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.415949

Thermal correction to Enthalpy= 0.416894

Thermal correction to Gibbs Free Energy= 0.333133

Sum of electronic and zero-point Energies= -1978.725199

Sum of electronic and thermal Energies= -1978.697452

Sum of electronic and thermal Enthalpies= -1978.696507

Sum of electronic and thermal Free Energies= -1978.780268

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

261.012 118.569 176.289

Cartesian coordinates

Atom X Y Z

C 1.323786 -0.187644 2.233089
C 0.615193 1.054441 2.279454
C -0.786835 0.763871 2.384508
C -0.941679 -0.661075 2.394993
C 0.365040 -1.247667 2.296403
C 1.028951 2.081712 1.466743
C 0.088413 2.992210 0.836620
C -1.278111 2.714581 0.940961
C -1.685335 1.530455 1.679089
C -2.865642 0.963816 1.056362
C -3.017264 -0.429397 1.066986
C 1.985023 -1.227128 1.699574
C -1.842667 -2.481585 0.979332
C -0.567744 -3.047478 0.880763
C 0.547177 -2.351360 1.499195
C 1.755814 -2.573652 0.725427
C 2.713017 -1.544735 0.698937
C 2.413449 -0.312085 1.397115
C 2.255562 2.028087 0.691484
C 2.969631 0.817161 0.681229
C 0.884352 3.708023 -0.165024
C 2.134522 3.162500 -0.247509
C -2.414821 3.015057 0.059550
C -3.331411 2.001502 0.124386
C -3.696934 -1.356682 0.150189
C -3.019425 -2.544184 0.101517
C 0.054814 -3.932349 -0.108721
C 1.392891 -3.669299 -0.196774
C 3.892722 -1.216749 -0.152230
C 4.048252 0.231624 -0.165026
H 0.513927 4.502620 -0.801162

H -2.474977 3.867516 -0.606089
H -4.226241 1.932295 -0.482351
H -4.557557 -1.106424 -0.458356
H -3.262915 -3.373812 -0.550975
H -0.478006 -4.638680 -0.733609
H 2.064284 -4.135229 -0.900653
H 2.888778 3.463469 -0.957362
C 5.789692 0.755441 1.201392
H 5.876285 1.827715 1.069703
C 5.475684 -2.068210 1.231053
H 5.326399 -3.136626 1.126578
C 6.801799 -0.085480 0.763153
H 7.635659 0.336378 0.208661
C 6.647689 -1.479686 0.778883
H 7.368301 -2.085848 0.236758
H 4.900765 -1.605479 2.023592
H 5.128963 0.448422 2.002889
C 4.214474 -2.104204 -1.332193
C 4.548343 1.010285 -1.359120
F 4.158032 -3.420467 -0.988414
F 5.433282 -1.916849 -1.864791
F 3.312568 -1.931387 -2.328866
F 5.696889 0.556455 -1.887817
F 3.627099 1.018859 -2.352857
F 4.777320 2.313479 -1.037906

Transition state structure for the reaction of butadiene with Fragment 2 substituted with two CHO groupMolecular formula: C₃₆H₁₆O₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.421895

Thermal correction to Enthalpy= 0.422839

Thermal correction to Gibbs Free Energy= 0.345468

Sum of electronic and zero-point Energies= -1531.295427

Sum of electronic and thermal Energies= -1531.270627

Sum of electronic and thermal Enthalpies= -1531.269683

Sum of electronic and thermal Free Energies= -1531.347054

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

264.743 106.979 162.841

Cartesian coordinates

Atom X Y Z

C 1.304360 -0.244931 2.390574
C 0.594761 0.996818 2.442687
C -0.808976 0.707303 2.503709
C -0.966580 -0.716743 2.489585
C 0.341568 -1.305176 2.416790
C 1.026907 2.051311 1.674407
C 0.109800 2.978499 1.038468
C -1.259129 2.691417 1.087485
C -1.686051 1.490616 1.788035
C -2.846619 0.936309 1.121053
C -3.000036 -0.457074 1.103108
C -1.990278 -1.268926 1.755139
C -1.833518 -2.516541 1.025462
C -0.560540 -3.091359 0.958040
C 0.541494 -2.402032 1.614042
C 1.760006 -2.615708 0.856978
C 2.715021 -1.577047 0.833465
C 2.403621 -0.356025 1.562265
C 2.269132 2.008992 0.928952
C 2.950777 0.787935 0.877058
C 0.942735 3.728071 0.088335
C 2.195889 3.181544 0.034255
C -2.369304 3.008747 0.178629
C -3.284477 1.991884 0.194910
C -3.656604 -1.368730 0.154598
C -2.983169 -2.558900 0.110935
C 0.086370 -3.972878 -0.019089
C 1.427422 -3.705151 -0.075679
C 3.810855 -1.216201 -0.073947
C 4.028667 0.238452 -0.018724
H 0.599674 4.554345 -0.522382

H -2.412229 3.875380 -0.469768
H -4.160714 1.934268 -0.439601
H -4.497761 -1.106446 -0.475638
H -3.211141 -3.378505 -0.559635
H -0.432243 -4.676770 -0.658524
H 2.142661 -4.141008 -0.756767
H 2.990594 3.530817 -0.612857
C 5.629428 0.753817 1.005616
H 5.582626 1.838834 0.955698
C 6.051176 -2.110124 1.134587
H 6.123250 -3.185684 1.015441
C 6.755794 0.128294 0.445310
H 7.405387 0.701372 -0.207809
C 6.928821 -1.268337 0.497308
H 7.713419 -1.705012 -0.116355
H 5.355865 -1.763724 1.887704
H 5.237428 0.362672 1.940326
O 4.044970 -3.232133 -1.347149
O 5.292070 0.765954 -2.013499
C 4.375214 -2.071767 -1.125058
C 4.299309 0.921676 -1.332511
H 5.140567 -1.580777 -1.750055
H 3.486793 1.597482 -1.666779

Transition state structure for the reaction of butadiene with Fragment 2 substituted with two CN groupMolecular formula: C₃₆H₁₄N₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.399884

Thermal correction to Enthalpy= 0.400828

Thermal correction to Gibbs Free Energy= 0.323964

Sum of electronic and zero-point Energies= -1489.153517

Sum of electronic and thermal Energies= -1489.129018

Sum of electronic and thermal Enthalpies= -1489.128074

Sum of electronic and thermal Free Energies= -1489.204938

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

250.931 105.544 161.774

Cartesian coordinates

Atom X Y Z

C 1.275011 -0.181418 2.351271
C 0.563201 1.062629 2.351434
C -0.842216 0.770481 2.380328
C -0.997385 -0.654940 2.390906
C 0.312354 -1.243049 2.368490
C 1.014131 2.096183 1.562766
C 0.110122 2.999057 0.870686
C -1.258613 2.715120 0.900946
C -1.701612 1.533194 1.623683
C -2.846640 0.961405 0.941918
C -2.998270 -0.431226 0.952271
C -2.001733 -1.225961 1.643852
C -1.824302 -2.485828 0.938967
C -0.548627 -3.057744 0.914969
C 0.529357 -2.360577 1.595507
C 1.765625 -2.577194 0.871088
C 2.704649 -1.541410 0.867005
C 2.404793 -0.309975 1.564197
C 2.266579 2.031169 0.836842
C 2.960977 0.817823 0.849236
C 0.955614 3.697750 -0.107280
C 2.204634 3.141873 -0.128492
C -2.346926 3.007263 -0.041976
C -3.264135 1.992865 -0.019333
C -3.629009 -1.362579 0.005180
C -2.951491 -2.550704 -0.001295
C 0.125678 -3.936961 -0.050358
C 1.465108 -3.663447 -0.077177
C 3.831794 -1.214639 -0.043099
C 3.989479 0.243456 -0.055432
H 0.614951 4.481389 -0.772774

H -2.373247 3.856010 -0.714352
H -4.125796 1.918610 -0.671617
H -4.455582 -1.114580 -0.649608
H -3.160784 -3.383634 -0.661244
H -0.375872 -4.639635 -0.704394
H 2.179599 -4.107445 -0.757483
H 2.996314 3.410744 -0.815092
C 5.833415 0.748251 1.105262
H 5.901844 1.822735 0.967906
C 5.529301 -2.078808 1.132797
H 5.367981 -3.145815 1.016486
C 6.792177 -0.086173 0.539892
H 7.551532 0.346961 -0.105604
C 6.642502 -1.478380 0.553929
H 7.291293 -2.075782 -0.080955
H 5.056199 -1.641368 2.004163
H 5.281988 0.437878 1.984947
C 4.080398 -1.987230 -1.222347
C 4.391676 0.925170 -1.247842
N 4.274049 -2.646856 -2.161916
N 4.717285 1.512222 -2.199062

Transition state structure for the reaction of butadiene with Fragment 2 substituted with two NO₂ groupMolecular formula: C₃₄H₁₄N₂O₄

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.409021

Thermal correction to Enthalpy= 0.409965

Thermal correction to Gibbs Free Energy= 0.328365

Sum of electronic and zero-point Energies= -1713.654808

Sum of electronic and thermal Energies= -1713.628471

Sum of electronic and thermal Enthalpies= -1713.627527

Sum of electronic and thermal Free Energies= -1713.709128

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

256.665 111.186 171.743

Cartesian coordinates

Atom X Y Z

C	0.953340	-0.395953	2.185942	H	-2.807249	3.622149	-0.756729
C	0.211092	0.827299	2.221103	H	-4.506234	1.638096	-0.756712
C	-1.187195	0.499930	2.256548	H	-4.763685	-1.406035	-0.799391
C	-1.306065	-0.927938	2.237646	H	-3.414852	-3.642440	-0.859928
C	0.018046	-1.482416	2.192054	H	-0.608362	-4.846342	-0.922221
C	0.630478	1.900526	1.469597	H	1.947705	-4.244719	-0.972300
C	-0.297753	2.797624	0.806138	H	2.590105	3.360020	-0.840224
C	-1.656974	2.471947	0.825883	C	5.396043	0.588319	0.849655
C	-2.067250	1.259103	1.521274	H	5.346197	1.652717	0.659681
C	-3.199738	0.675411	0.831205	C	6.183468	-2.214862	1.579464
C	-3.317714	-0.720852	0.811246	H	6.477499	-3.243223	1.758687
C	-2.300242	-1.506862	1.483881	C	6.423515	-0.134478	0.257166
C	-2.095758	-2.747657	0.755532	H	6.949716	0.314862	-0.578768
C	-0.806542	-3.289683	0.713780	C	6.793690	-1.474868	0.627007
C	0.262760	-2.576437	1.397151	H	7.588518	-1.932429	0.044024
C	1.500694	-2.757392	0.661912	H	5.385014	-1.826969	2.202855
C	2.419193	-1.688812	0.653156	H	5.013991	0.265383	1.812581
C	2.073466	-0.476393	1.385203	N	4.222159	-2.024606	-1.141873
C	1.883503	1.892602	0.746177	N	3.853790	0.940816	-1.467888
C	2.609697	0.694789	0.727629	O	5.117916	-1.421433	-1.777699
C	0.531595	3.550494	-0.146399	O	4.645671	1.877269	-1.501060
C	1.798872	3.036457	-0.176793	O	4.009240	-3.242924	-1.240454
C	-2.755895	2.758642	-0.105061	O	3.095456	0.627439	-2.373343
C	-3.645065	1.718871	-0.104448				
C	-3.929833	-1.647190	-0.151410				
C	-3.223711	-2.818905	-0.182824				
C	-0.119725	-4.139963	-0.262381				
C	1.215173	-3.834803	-0.293055				
C	3.459848	-1.250104	-0.256261				
C	3.656888	0.166266	-0.177155				
H	0.171734	4.345937	-0.787434				

Adduct of the reaction of butadiene with Fragment 1Molecular formula: C₃₄H₁₈

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.428248

Thermal correction to Enthalpy= 0.429192

Thermal correction to Gibbs Free Energy= 0.360282

Sum of electronic and zero-point Energies= -1306.005183

Sum of electronic and thermal Energies= -1305.984569

Sum of electronic and thermal Enthalpies= -1305.983625

Sum of electronic and thermal Free Energies= -1306.052535

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

268.729 93.207 145.033

Cartesian coordinates

Atom X Y Z

C -1.244710 -0.497274 -1.312506

C -1.054092 0.920163 -1.287819

C 0.229744 1.412999 -1.252332

C 1.369131 0.542380 -1.208971

C 1.155817 -0.831553 -1.229668

C -0.175291 -1.364856 -1.250827

C 2.388999 1.113132 -0.396825

C 3.277184 0.220659 0.236531

C 3.073678 -1.192933 0.195454

C 1.968838 -1.691154 -0.489869

C 3.876415 -2.182556 1.028346

C 3.180669 -3.601376 1.228614

C 1.738409 -3.745212 0.773253

C 1.177444 -2.883813 -0.090506

C -0.247527 -2.592581 -0.506316

C -1.479944 -2.963732 0.024042

C -2.609342 -2.047955 -0.001680

C -2.430165 -0.789606 -0.618769

C -3.087062 0.425061 -0.227303

C -4.189602 0.287863 0.598973

C -4.554100 -1.013849 1.044793

C -3.782506 -2.144257 0.800815

C 0.520299 2.549309 -0.479037

C -0.517342 3.293602 0.124636

C -1.874137 2.772019 0.044992

C -2.135114 1.550299 -0.568974

C -0.069864 4.296519 1.031734

C 1.275487 4.375052 1.374376

C 2.245927 3.434836 0.927820

C 1.869628 2.473726 0.003995

H 4.032065 0.602602 0.921540

H -4.745045 1.147029 0.964841

H -5.431393 -1.110755 1.678153

H -4.043862 -3.084742 1.278957

H -2.629214 3.251682 0.663989

H -0.784831 4.959080 1.512692

H 1.587084 5.134134 2.086314

H 3.239431 3.451699 1.367741

H -1.567252 -3.847852 0.651574

H 1.177404 -4.573697 1.201995

H 4.010228 -1.756390 2.029796

H 3.174206 -3.782736 2.310754

C 4.034953 -4.767178 0.633987

H 3.589203 -5.723711 0.925935

H 3.971201 -4.719077 -0.462858

C 5.310806 -2.319323 0.418964

H 5.205831 -2.452674 -0.667534

H 5.844267 -1.373776 0.556122

C 6.078764 -3.481054 0.990512

H 7.110301 -3.341900 1.304521

C 5.469668 -4.666383 1.078669

H 5.975918 -5.544267 1.472253

Adduct of the reaction of butadiene with Fragment 1 substituted with one NH₂ groupMolecular formula: C₃₄H₁₉N

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.446023

Thermal correction to Enthalpy= 0.446968

Thermal correction to Gibbs Free Energy= 0.375802

Sum of electronic and zero-point Energies= -1361.335476

Sum of electronic and thermal Energies= -1361.313607

Sum of electronic and thermal Enthalpies= -1361.312662

Sum of electronic and thermal Free Energies= -1361.383828

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

279.884 98.736 149.781

Cartesian coordinates

Atom X Y Z

C	-1.369100	-0.697969	-1.278014	H	-5.518475	-1.427659	1.738988
C	-1.222485	0.724895	-1.259979	H	-4.070888	-3.358766	1.342722
C	0.045812	1.257305	-1.232220	H	-2.858943	3.012271	0.693589
C	1.211579	0.422229	-1.192038	H	-1.064854	4.777094	1.529508
C	1.041252	-0.957494	-1.209026	H	1.303003	5.025957	2.092858
C	-0.272984	-1.531735	-1.218943	H	3.002700	3.393008	1.370919
C	2.216741	1.025982	-0.384583	H	-1.574507	-4.044695	0.707988
C	3.134287	0.163743	0.247899	H	1.178926	-4.660421	1.271587
C	2.976081	-1.255844	0.208225	C	4.019477	-4.758234	0.536056
C	1.885830	-1.789108	-0.472456	H	3.593694	-5.742532	0.760655
C	3.814901	-2.216194	1.036024	H	3.920328	-4.616778	-0.550228
C	3.166302	-3.659572	1.267673	C	5.248573	-2.299009	0.410059
C	1.718734	-3.830037	0.819051	H	5.136984	-2.384999	-0.680540
C	1.133324	-2.998520	-0.055157	H	5.763590	-1.349690	0.585378
C	-0.302640	-2.756183	-0.466426	C	6.052949	-3.469496	0.908735
C	-1.519146	-3.162922	0.073610	H	7.090018	-3.326251	1.202296
C	-2.677317	-2.283888	0.048494	C	5.466129	-4.669893	0.945565
C	-2.541024	-1.023907	-0.576091	H	5.995723	-5.559121	1.278250
C	-3.233642	0.171319	-0.186701	N	3.166917	-3.867420	2.734451
C	-4.327049	0.003634	0.646038	H	2.788024	-4.791649	2.942589
C	-4.648177	-1.306537	1.100192	H	4.136088	-3.890097	3.050986
C	-3.842459	-2.413179	0.857875	H	3.923231	-1.795359	2.041542
C	0.304981	2.404066	-0.462972				
C	-0.752179	3.117726	0.143792				
C	-2.092592	2.554713	0.071739				
C	-2.318852	1.323929	-0.537713				
C	-0.331834	4.135980	1.046683				
C	1.011829	4.256459	1.383490				
C	2.008539	3.345260	0.934843				
C	1.657909	2.371183	0.014554				
H	3.877285	0.570498	0.931368				
H	-4.907067	0.846774	1.011055				

Adduct of the reaction of butadiene with Fragment 1 substituted with one OMe groupMolecular formula: C₃₅H₂₀O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.462604

Thermal correction to Enthalpy= 0.463548

Thermal correction to Gibbs Free Energy= 0.389154

Sum of electronic and zero-point Energies= -1420.488800

Sum of electronic and thermal Energies= -1420.465567

Sum of electronic and thermal Enthalpies= -1420.464623

Sum of electronic and thermal Free Energies= -1420.539017

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

290.288 102.758 156.574

Cartesian coordinates

Atom X Y Z

C	-1.387668	-0.694445	-1.281367	H	-5.423114	-1.476978	1.874421
C	-1.244520	0.728487	-1.249577	H	-3.984486	-3.397890	1.401800
C	0.022699	1.264276	-1.259751	H	-2.816118	2.984124	0.792375
C	1.191153	0.432175	-1.272506	H	-0.998158	4.743116	1.587522
C	1.024479	-0.947402	-1.303160	H	1.387419	4.991486	2.070220
C	-0.287794	-1.525285	-1.273256	H	3.064625	3.373186	1.266621
C	2.222436	1.027767	-0.491488	H	-1.510435	-4.067146	0.667432
C	3.162197	0.160323	0.098449	H	1.253363	-4.684334	1.116007
C	3.008100	-1.259849	0.043045	C	4.096927	-4.763417	0.377047
C	1.897818	-1.787157	-0.609518	H	3.686696	-5.754656	0.590104
C	3.868530	-2.224738	0.839231	H	3.975556	-4.612743	-0.704809
C	3.234571	-3.668055	1.076818	C	5.291547	-2.297062	0.191592
C	1.778927	-3.848780	0.661242	H	5.165635	-2.395084	-0.896767
C	1.164291	-3.002836	-0.180134	H	5.793785	-1.337925	0.349715
C	0.286712	-2.758965	-0.535837	C	6.118023	-3.447833	0.698472
C	-1.481094	-3.176742	0.043375	H	7.154869	-3.284835	0.980846
C	-2.642254	-2.301616	0.071758	C	5.545564	-4.651406	0.768167
C	-2.532320	-1.033466	-0.541322	H	6.082545	-5.529310	1.117802
C	-3.213867	0.154207	-0.111680	O	3.293853	-3.788624	2.518704
C	-4.276085	-0.027889	0.757709	C	3.181415	-5.073297	3.099837
C	-4.576679	-1.344760	1.206423	H	4.062079	-5.700259	2.905492
C	-3.776718	-2.445368	0.921226	H	3.106314	-4.909587	4.177713
C	0.306126	2.401269	-0.484311	H	2.285120	-5.621603	2.776427
C	-0.730614	3.103553	0.169213	H	3.999092	-1.831214	1.852141
C	-2.071279	2.537488	0.137328				
C	-2.315723	1.314293	-0.480247				
C	-0.281085	4.110750	1.070426				
C	1.073329	4.230703	1.361237				
C	2.055755	3.328538	0.865418				
C	1.675047	2.366111	-0.055209				
H	3.925399	0.560009	0.763486				
H	-4.845166	0.808506	1.154089				

Adduct of the reaction of butadiene with Fragment 1 substituted with one OH groupMolecular formula: C₃₄H₁₈O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.433062

Thermal correction to Enthalpy= 0.434006

Thermal correction to Gibbs Free Energy= 0.362876

Sum of electronic and zero-point Energies= -1381.218216

Sum of electronic and thermal Energies= -1381.196482

Sum of electronic and thermal Enthalpies= -1381.195538

Sum of electronic and thermal Free Energies= -1381.266668

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

271.750 97.926 149.705

Cartesian coordinates

Atom X Y Z

C	-1.374990	-0.724374	-1.258632	H	-5.510143	-1.381121	1.794705
C	-1.217560	0.697203	-1.260792	H	-4.079612	-3.328472	1.415713
C	0.054963	1.220206	-1.247535	H	-2.825864	3.023842	0.669769
C	1.213966	0.376253	-1.201233	H	-1.014353	4.786897	1.470310
C	1.033754	-1.001954	-1.200114	H	1.358273	5.026156	2.017667
C	-0.285152	-1.565868	-1.195367	H	3.041738	3.369892	1.310499
C	2.227084	0.983193	-0.405150	H	-1.593216	-4.043972	0.772068
C	3.136095	0.123240	0.240706	H	1.204174	-4.716683	1.299178
C	2.968047	-1.296837	0.220253	C	4.026865	-4.709393	0.335792
C	1.875082	-1.831501	-0.455860	H	3.597982	-5.711727	0.422362
C	3.762321	-2.246563	1.105382	H	3.950615	-4.413396	-0.719786
C	3.175865	-3.724260	1.196842	C	5.272946	-2.230129	0.679612
C	1.712287	-3.882018	0.824311	H	5.314194	-2.092127	-0.409914
C	1.115620	-3.034513	-0.027764	H	5.755557	-1.346857	1.108861
C	-0.320275	-2.780578	-0.427198	C	6.034161	-3.486317	1.016524
C	-1.535924	-3.170541	0.126606	H	7.057342	-3.405411	1.376005
C	-2.687069	-2.282263	0.097421	C	5.459271	-4.675852	0.805485
C	-2.545052	-1.031934	-0.545028	H	5.987601	-5.606247	0.997605
C	-3.226313	0.173586	-0.168048	O	3.245471	-4.148035	2.565143
C	-4.315444	0.025757	0.674097	H	4.188023	-4.247968	2.768974
C	-4.643292	-1.275422	1.148568	H	3.706624	-1.880985	2.137636
C	-3.847495	-2.391439	0.916331				
C	0.326956	2.375496	-0.495344				
C	-0.721526	3.105714	0.106906				
C	-2.066495	2.551850	0.050167				
C	-2.305229	1.314366	-0.540475				
C	-0.288712	4.133425	0.992957				
C	1.057593	4.248652	1.321133				
C	2.044818	3.323426	0.880594				
C	1.681712	2.339144	-0.023890				
H	3.878885	0.535958	0.920602				
H	-4.886778	0.878278	1.030907				

Adduct of the reaction of butadiene with Fragment 1 substituted with one Me group

Molecular formula: C35H20

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.457294

Thermal correction to Enthalpy= 0.458238

Thermal correction to Gibbs Free Energy= 0.387461

Sum of electronic and zero-point Energies= -1345.297397

Sum of electronic and thermal Energies= -1345.275484

Sum of electronic and thermal Enthalpies= -1345.274540

Sum of electronic and thermal Free Energies= -1345.345317

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

286.956 99.065 148.963

Cartesian coordinates

Atom X Y Z

C -1.349993 -0.851123 -1.172476

C -1.156473 0.559099 -1.310141

C 0.129489 1.046891 -1.360239

C 1.265952 0.179081 -1.246746

C 1.050467 -1.187030 -1.115733

C -0.282407 -1.712742 -1.045079

C 2.302846 0.827402 -0.516045

C 3.186079 0.009872 0.213995

C 2.979502 -1.401104 0.336489

C 1.874085 -1.964162 -0.298176

C 3.612654 -2.268962 1.429311

C 3.243112 -3.794410 1.264144

C 1.739457 -3.981112 1.027854

C 1.098593 -3.124363 0.213907

C -0.338565 -2.854486 -0.170757

C -1.555332 -3.156578 0.432074

C -2.682769 -2.240916 0.337854

C -2.517312 -1.059572 -0.418809

C -3.161774 0.193413 -0.148467

C -4.242330 0.154431 0.716909

C -4.595830 -1.087083 1.315477

C -3.832296 -2.241209 1.178518

C 0.441077 2.258979 -0.720818

C -0.580197 3.070234 -0.178424

C -1.939697 2.549950 -0.168487

C -2.217708 1.269522 -0.637687

C -0.109654 4.163787 0.603503

C 1.243127 4.271890 0.906577

C 2.199637 3.282337 0.545398

C 1.799712 2.228865 -0.260204

H 3.928727 0.475854 0.857498

H -4.786829 1.051644 0.998071

H -5.455597 -1.108976 1.979161

H -4.081560 -3.121124 1.765916

H -2.678318 3.098160 0.412276

H -0.811992 4.878529 1.024617

H 1.572921 5.102397 1.524338

H 3.202544 3.340764 0.959676

H -1.627363 -3.967142 1.153713

H 1.240666 -4.820844 1.507009

C 4.014449 -4.385827 0.043550

H 3.939384 -5.481205 0.073066

H 3.516105 -4.082869 -0.886087

C 5.138520 -2.079677 1.588757

H 5.396970 -1.024534 1.441254

H 5.428793 -2.296072 2.627274

C 5.958471 -2.933652 0.659451

H 7.014978 -2.687420 0.570112

C 5.460289 -3.970684 -0.017295

H 6.111126 -4.550509 -0.669600

C 3.645433 -4.555865 2.542692

H 3.172528 -4.117990 3.428589

H 3.327292 -5.602107 2.477385

H 4.727960 -4.550422 2.691069

H 3.146389 -1.938483 2.371550

Adduct of the reaction of butadiene with Fragment 1 substituted with one *i*-Pr groupMolecular formula: C₃₇H₂₄

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.516960

Thermal correction to Enthalpy= 0.517904

Thermal correction to Gibbs Free Energy= 0.440875

Sum of electronic and zero-point Energies= -1423.865355

Sum of electronic and thermal Energies= -1423.840614

Sum of electronic and thermal Enthalpies= -1423.839670

Sum of electronic and thermal Free Energies= -1423.916699

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

324.397 109.509 162.121

Cartesian coordinates

Atom X Y Z

C -1.351829 -0.832431 -1.117533
C -1.116698 0.561282 -1.336022
C 0.180614 0.995882 -1.485646
C 1.289826 0.090665 -1.398172
C 1.033941 -1.258217 -1.187364
C -0.309978 -1.727783 -1.010964
C 2.392445 0.730887 -0.762999
C 3.289450 -0.085962 -0.048980
C 3.041397 -1.481153 0.153817
C 1.877954 -2.027912 -0.383870
C 3.710271 -2.316229 1.252652
C 3.271548 -3.839740 1.195048
C 1.748984 -3.968006 1.055712
C 1.095190 -3.128921 0.233367
C -0.352745 -2.822955 -0.078313
C -1.540754 -3.049033 0.609348
C -2.638586 -2.096216 0.536423
C -2.477764 -0.959469 -0.286682
C -3.059157 0.328932 -0.040832
C -4.085946 0.372682 0.887611
C -4.446235 -0.824476 1.566981
C -3.733944 -2.012304 1.442723
C 0.574486 2.223005 -0.925344
C -0.381570 3.097882 -0.363370
C -1.756060 2.632203 -0.248136
C -2.108412 1.343214 -0.637208
C 0.175371 4.207006 0.335427
C 1.547215 4.275973 0.551936
C 2.443371 3.234242 0.182752
C 1.956938 2.161095 -0.545591
H 4.086794 0.380557 0.524963
H -4.580199 1.302417 1.155648

H -5.264214 -0.781700 2.280607
H -3.977957 -2.852948 2.087096
H -2.437684 3.235070 0.347976
H -0.473336 4.967460 0.762482
H 1.944062 5.120585 1.108065
H 3.471272 3.272580 0.533228
H -1.597869 -3.820887 1.373565
H 1.232809 -4.753676 1.599809
C 3.929121 -4.462300 -0.079772
H 3.766017 -5.544007 -0.096932
H 3.403402 -4.081664 -0.964157
C 5.249856 -2.175403 1.304677
H 5.531254 -1.142122 1.069646
H 5.600452 -2.331257 2.335667
C 5.982997 -3.116833 0.387747
H 7.047315 -2.937279 0.246905
C 5.395757 -4.151493 -0.217415
H 5.981118 -4.798860 -0.868166
C 3.526092 -6.105973 2.466370
H 4.067071 -6.600301 1.656088
H 3.879323 -6.547084 3.404178
H 2.466297 -6.366730 2.369863
C 3.759527 -4.583097 2.493184
H 4.844784 -4.443451 2.545996
C 3.151945 -4.005214 3.785653
H 2.059086 -4.084635 3.789329
H 3.523945 -4.558132 4.654444
H 3.405236 -2.953232 3.941600
H 3.319457 -1.898459 2.190455

Adduct of the reaction of butadiene with Fragment 1 substituted with one F groupMolecular formula: C₃₄H₁₇F

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.420378

Thermal correction to Enthalpy= 0.421322

Thermal correction to Gibbs Free Energy= 0.350582

Sum of electronic and zero-point Energies= -1405.249395

Sum of electronic and thermal Energies= -1405.227912

Sum of electronic and thermal Enthalpies= -1405.226967

Sum of electronic and thermal Free Energies= -1405.297707

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

263.791 96.439 148.885

Cartesian coordinates

Atom X Y Z

C	-1.376242	-0.674744	-1.291200	H	-5.514031	-1.443428	1.732695
C	-1.228434	0.747716	-1.253223	H	-4.069400	-3.370178	1.304009
C	0.040438	1.278637	-1.221674	H	-2.856734	3.008554	0.737481
C	1.205019	0.441769	-1.195723	H	-1.058799	4.761275	1.591069
C	1.033815	-0.936872	-1.232716	H	1.310843	5.001426	2.150146
C	-0.280968	-1.510182	-1.248199	H	3.007297	3.377076	1.401362
C	2.213014	1.033586	-0.381799	H	-1.576296	-4.049179	0.648889
C	3.131612	0.162845	0.235865	H	1.190705	-4.675698	1.216409
C	2.973190	-1.256299	0.174098	C	4.027495	-4.800400	0.650669
C	1.880517	-1.779529	-0.511137	H	3.591406	-5.750223	0.973602
C	3.805423	-2.229187	0.991446	H	3.963260	-4.776658	-0.446658
C	3.146621	-3.655122	1.203105	C	5.242586	-2.330032	0.386329
C	1.709345	-3.837587	0.758425	H	5.146155	-2.474465	-0.699700
C	1.126060	-2.992728	-0.105842	H	5.745297	-1.367305	0.518270
C	-0.309790	-2.745050	-0.513682	C	6.040765	-3.460633	0.979237
C	-1.523480	-3.158253	0.027339	H	7.065719	-3.286836	1.296131
C	-2.681131	-2.278198	0.018499	C	5.457114	-4.654291	1.102413
C	-2.545769	-1.009850	-0.589062	H	5.973738	-5.509042	1.529369
C	-3.235915	0.180254	-0.180567	F	3.119958	-3.854757	2.607742
C	-4.325989	0.001558	0.654359	H	3.912510	-1.843422	2.010958
C	-4.646395	-1.314372	1.091945				
C	-3.842583	-2.418184	0.831269				
C	0.303093	2.414259	-0.437147				
C	-0.751729	3.120261	0.182522				
C	-2.092656	2.559123	0.107035				
C	-2.321814	1.337122	-0.518880				
C	-0.327783	4.126044	1.097636				
C	1.016991	4.241436	1.431791				
C	2.011652	3.335592	0.968138				
C	1.657241	2.374435	0.035816				
H	3.877386	0.559076	0.922331				
H	-4.904018	0.839913	1.033202				

Adduct of the reaction of butadiene with Fragment 1 substituted with one COOH group

Molecular formula: C35H18O2

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.445853

Thermal correction to Enthalpy= 0.446797

Thermal correction to Gibbs Free Energy= 0.371182

Sum of electronic and zero-point Energies= -1494.560790

Sum of electronic and thermal Energies= -1494.537323

Sum of electronic and thermal Enthalpies= -1494.536379

Sum of electronic and thermal Free Energies= -1494.611995

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

279.777 103.464 159.147

Cartesian coordinates

Atom X Y Z

C -1.310686 -0.887495 -1.094530

C -1.123848 0.523121 -1.238443

C 0.159066 1.012764 -1.331793

C 1.299629 0.146438 -1.256610

C 1.090146 -1.219188 -1.116393

C -0.238568 -1.747590 -1.002985

C 2.360523 0.796293 -0.561875

C 3.271615 -0.019228 0.134734

C 3.070143 -1.430519 0.265471

C 1.941998 -1.994041 -0.326282

C 3.745568 -2.288354 1.339201

C 3.364526 -3.808790 1.176859

C 1.847620 -4.015354 1.001818

C 1.184875 -3.153577 0.212335

C -0.264643 -2.889471 -0.128097

C -1.459098 -3.193250 0.516529

C -2.590605 -2.279568 0.459276

C -2.451833 -1.097854 -0.302111

C -3.088399 0.154177 -0.009991

C -4.139091 0.113315 0.891374

C -4.470831 -1.128748 1.501093

C -3.710990 -2.281909 1.338265

C 0.490816 2.224845 -0.702473

C -0.512586 3.033986 -0.124709

C -1.870314 2.512042 -0.069386

C -2.162622 1.231687 -0.530148

C -0.017184 4.127292 0.642055

C 1.344934 4.237361 0.899007

C 2.290140 3.249919 0.504066

C 1.864444 2.197002 -0.288890

H 4.037376 0.446950 0.750158

H -4.675036 1.009669 1.190998

H -5.307775 -1.151817 2.193204

H -3.939155 -3.162366 1.933245

H -2.589624 3.058895 0.536302

H -0.705809 4.840434 1.087739

H 1.694195 5.067576 1.506276

H 3.306500 3.309450 0.883858

H -1.505510 -4.003862 1.240062

H 1.380533 -4.871184 1.480216

C 4.097605 -4.428919 -0.049962

H 4.000264 -5.517072 0.009321

H 3.576206 -4.117401 -0.962636

C 5.278084 -2.108041 1.444584

H 5.536923 -1.061324 1.246155

H 5.589278 -2.288436 2.481978

C 6.070053 -3.000865 0.527241

H 7.131481 -2.780418 0.430380

C 5.547467 -4.036300 -0.132502

H 6.181103 -4.640785 -0.778487

C 3.749808 -4.626045 2.420041

O 3.886715 -5.829668 2.430422

O 3.850536 -3.890599 3.554332

H 4.047305 -4.527510 4.262625

H 3.316953 -1.955068 2.293269

Adduct of the reaction of butadiene with Fragment 1 substituted with one CF₃ groupMolecular formula: C₃₅H₁₇F₃

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.436399

Thermal correction to Enthalpy= 0.437344

Thermal correction to Gibbs Free Energy= 0.361208

Sum of electronic and zero-point Energies= -1643.038655

Sum of electronic and thermal Energies= -1643.014623

Sum of electronic and thermal Enthalpies= -1643.013679

Sum of electronic and thermal Free Energies= -1643.089815

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

273.845 105.985 160.242

Cartesian coordinates

Atom X Y Z

C	-1.323607	-0.879721	-1.143387	H	-5.368762	-1.133847	2.086267
C	-1.131126	0.530617	-1.283656	H	-4.000572	-3.147299	1.847539
C	0.154357	1.017065	-1.356158	H	-2.618859	3.068799	0.469351
C	1.291053	0.147343	-1.263647	H	-0.739854	4.845198	1.052464
C	1.076973	-1.218353	-1.131796	H	1.653275	5.064180	1.512855
C	-0.255218	-1.742820	-1.036950	H	3.269948	3.300473	0.917821
C	2.340379	0.792601	-0.547213	H	-1.558909	-3.993609	1.190693
C	3.235090	-0.026425	0.165580	H	1.300948	-4.838857	1.503710
C	3.030412	-1.438230	0.285133	C	4.056558	-4.472037	-0.005860
C	1.915632	-1.998127	-0.332136	H	4.044865	-5.561984	0.114435
C	3.708071	-2.300878	1.356113	H	3.471097	-4.273456	-0.910858
C	3.305452	-3.824227	1.201547	C	5.241698	-2.106591	1.413567
C	1.790133	-4.007570	1.008069	H	5.471343	-1.044756	1.273593
C	1.146520	-3.152096	0.198771	H	5.609590	-2.353207	2.417058
C	-0.296955	-2.883540	-0.161380	C	5.989157	-2.923140	0.395694
C	-1.500913	-3.184201	0.466671	H	7.016794	-2.633040	0.187417
C	-2.629432	-2.268344	0.392233	C	5.464245	-3.983443	-0.218218
C	-2.476757	-1.087401	-0.367685	H	6.057960	-4.540999	-0.940042
C	-3.114977	0.165975	-0.085354	C	3.666627	-4.583736	2.489477
C	-4.178777	0.127856	0.800549	F	3.090066	-4.018605	3.576690
C	-4.522040	-1.113096	1.406121	F	3.227733	-5.867451	2.438153
C	-3.762329	-2.267859	1.255082	F	4.992439	-4.647923	2.732408
C	0.478904	2.227244	-0.719225	H	3.295262	-1.966746	2.318010
C	-0.531565	3.039035	-0.157800				
C	-1.891257	2.520686	-0.125149				
C	-2.179150	1.241314	-0.591307				
C	-0.045936	4.130150	0.618249				
C	1.311857	4.235573	0.899029				
C	2.260212	3.244965	0.520208				
C	1.844586	2.194449	-0.281226				
H	3.987552	0.437894	0.798270				
H	-4.716961	1.025559	1.091956				

Adduct of the reaction of butadiene with Fragment 1 substituted with one CHO groupMolecular formula: C₃₅H₁₈O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.438953

Thermal correction to Enthalpy= 0.439898

Thermal correction to Gibbs Free Energy= 0.366550

Sum of electronic and zero-point Energies= -1419.313119

Sum of electronic and thermal Energies= -1419.290449

Sum of electronic and thermal Enthalpies= -1419.289505

Sum of electronic and thermal Free Energies= -1419.362852

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

275.447 100.286 154.372

Cartesian coordinates

Atom X Y Z

C -1.324291 -0.877365 -1.160579

C -1.134012 0.534697 -1.283545

C 0.150568 1.025928 -1.335101

C 1.288748 0.158837 -1.235573

C 1.077191 -1.209383 -1.120849

C -0.254804 -1.738583 -1.048509

C 2.327116 0.801666 -0.501640

C 3.214605 -0.021546 0.216338

C 3.011398 -1.434011 0.319893

C 1.906946 -1.995497 -0.318171

C 3.655137 -2.307284 1.403746

C 3.275159 -3.833183 1.197369

C 1.773014 -4.022823 0.997699

C 1.134308 -3.161511 0.188198

C -0.304721 -2.888760 -0.185667

C -1.516820 -3.199641 0.421724

C -2.646380 -2.285597 0.342269

C -2.487272 -1.096174 -0.403073

C -3.132974 0.152412 -0.116346

C -4.208401 0.102141 0.754724

C -4.556071 -1.146206 1.342440

C -3.790996 -2.297182 1.189514

C 0.462840 2.231448 -0.683570

C -0.557543 3.034612 -0.127580

C -1.915842 2.511484 -0.117079

C -2.193524 1.235565 -0.598546

C -0.085633 4.120231 0.664396

C 1.268217 4.227929 0.962945

C 2.224898 3.244311 0.586813

C 1.823180 2.199400 -0.229004

H 3.957182 0.439063 0.863670

H -4.752998 0.995240 1.048410

H -5.411734 -1.176571 2.010968

H -4.034463 -3.183423 1.769582

H -2.652827 3.051821 0.472989

H -0.787536 4.828693 1.096608

H 1.598926 5.052111 1.588525

H 3.229458 3.300087 0.997396

H -1.581982 -4.017254 1.135761

H 1.289294 -4.844897 1.514721

C 4.059839 -4.412648 -0.024782

H 3.998405 -5.509397 -0.003221

H 3.544443 -4.111008 -0.944313

C 5.181293 -2.119354 1.556410

H 5.432133 -1.060538 1.426308

H 5.482660 -2.352445 2.588570

C 5.996376 -2.950061 0.602699

H 7.049246 -2.693376 0.504777

C 5.499447 -3.977702 -0.089438

H 6.147366 -4.538754 -0.760204

C 3.727961 -4.597479 2.440365

H 4.826305 -4.731889 2.531931

O 2.980116 -5.052045 3.279016

H 3.187675 -1.998741 2.351517

Adduct of the reaction of butadiene with Fragment 1 substituted with one CN groupMolecular formula: C₃₅H₁₇N

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.428143

Thermal correction to Enthalpy= 0.429087

Thermal correction to Gibbs Free Energy= 0.355951

Sum of electronic and zero-point Energies= -1398.239555

Sum of electronic and thermal Energies= -1398.217054

Sum of electronic and thermal Enthalpies= -1398.216110

Sum of electronic and thermal Free Energies= -1398.289246

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

268.664 99.698 153.928

Cartesian coordinates

Atom X Y Z

C	-1.344559	-0.693373	-1.271416	H	-5.478790	-1.468339	1.755029
C	-1.199118	0.729530	-1.233821	H	-4.032195	-3.393097	1.324961
C	0.068496	1.263260	-1.204066	H	-2.830451	2.988597	0.755754
C	1.234575	0.428619	-1.177262	H	-1.035444	4.744911	1.607455
C	1.065303	-0.950471	-1.211122	H	1.333884	4.990222	2.164842
C	-0.248210	-1.527055	-1.228785	H	3.033102	3.369202	1.415777
C	2.242198	1.023812	-0.365926	H	-1.539413	-4.067497	0.669098
C	3.166482	0.155657	0.247936	H	1.204802	-4.691378	1.219537
C	3.007530	-1.262845	0.189555	C	4.057035	-4.823504	0.606608
C	1.913361	-1.790425	-0.488953	H	3.638156	-5.787169	0.907977
C	3.869809	-2.229853	0.982368	H	3.927947	-4.745197	-0.481135
C	3.188980	-3.670071	1.241026	C	5.260514	-2.371586	0.279739
C	1.737503	-3.853527	0.778000	H	5.082714	-2.538002	-0.792445
C	1.161450	-3.005389	-0.086267	H	5.779730	-1.411818	0.354997
C	-0.275279	-2.762260	-0.495611	C	6.086288	-3.499073	0.836144
C	-1.487950	-3.177178	0.046650	H	7.124580	-3.326378	1.105707
C	-2.646876	-2.299033	0.037859	C	5.507059	-4.692890	0.984184
C	-2.513592	-1.030393	-0.569532	H	6.037982	-5.550658	1.386063
C	-3.205276	0.158702	-0.160788	C	3.180214	-3.889371	2.703112
C	-4.294160	-0.021772	0.675216	N	3.163971	-4.076935	3.849391
C	-4.612266	-1.338221	1.113094	H	4.064782	-1.796927	1.968357
C	-3.807358	-2.440952	0.851751				
C	0.329675	2.400011	-0.420816				
C	-0.726176	3.104021	0.199287				
C	-2.065916	2.540078	0.125289				
C	-2.293300	1.317134	-0.499691				
C	-0.303536	4.111092	1.113629				
C	1.041215	4.229582	1.446808				
C	2.037407	3.325610	0.982982				
C	1.684153	2.363570	0.051112				
H	3.917080	0.553476	0.928187				
H	-4.872976	0.815611	1.054896				

Adduct of the reaction of butadiene with Fragment 1 substituted with one NO₂ groupMolecular formula: C₃₄H₁₇NO₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.433107

Thermal correction to Enthalpy= 0.434051

Thermal correction to Gibbs Free Energy= 0.359606

Sum of electronic and zero-point Energies= -1510.504663

Sum of electronic and thermal Energies= -1510.481532

Sum of electronic and thermal Enthalpies= -1510.480588

Sum of electronic and thermal Free Energies= -1510.555033

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

271.779 102.044 156.684

Cartesian coordinates

Atom X Y Z

C -1.231308 -0.657132 -1.213003

C -0.994926 0.747936 -1.340131

C 0.305130 1.198143 -1.374029

C 1.413334 0.296353 -1.252615

C 1.156432 -1.062567 -1.132136

C -0.191701 -1.550880 -1.080858

C 2.460835 0.909638 -0.505168

C 3.314676 0.063786 0.225974

C 3.065360 -1.341754 0.334711

C 1.949254 -1.867443 -0.311490

C 3.675996 -2.222017 1.430796

C 3.234152 -3.710946 1.235560

C 1.729844 -3.881851 1.010797

C 1.131941 -3.002729 0.190057

C -0.291830 -2.694556 -0.214281

C -1.520877 -2.963555 0.378451

C -2.620274 -2.015402 0.276490

C -2.411743 -0.835593 -0.471734

C -3.021808 0.434116 -0.201146

C -4.111654 0.421723 0.653337

C -4.507775 -0.811877 1.241479

C -3.777183 -1.987180 1.106310

C 0.645860 2.396388 -0.723203

C -0.357093 3.233799 -0.186415

C -1.731139 2.753631 -0.194037

C -2.041821 1.484846 -0.674470

C 0.136953 4.307943 0.607828

C 1.488832 4.374644 0.926477

C 2.419660 3.359568 0.569612

C 1.997499 2.324268 -0.248024

H 4.064649 0.502498 0.879500

H -4.632736 1.332773 0.934063

H -5.374217 -0.811588 1.896557

H -4.057439 -2.862355 1.686462

H -2.459552 3.319870 0.382122

H -0.548586 5.040370 1.026009

H 1.835726 5.190960 1.553447

H 3.418979 3.385469 0.995445

H -1.622740 -3.775034 1.095185

H 1.234279 -4.726340 1.477318

C 4.022627 -4.407855 0.100796

H 3.860626 -5.485974 0.186506

H 3.563009 -4.102310 -0.846898

C 5.209842 -2.090151 1.592686

H 5.508730 -1.060737 1.364349

H 5.469736 -2.245220 2.646617

C 6.012723 -3.040076 0.747807

H 7.085825 -2.864647 0.707900

C 5.489868 -4.077669 0.093105

H 6.131507 -4.730867 -0.493944

O 3.827116 -3.866413 3.560827

O 3.378477 -5.708881 2.503675

N 3.524727 -4.491499 2.550144

H 3.223184 -1.889495 2.373457

Adduct of the reaction of butadiene with Fragment 2Molecular formula: C₃₄H₁₆

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.403845

Thermal correction to Enthalpy= 0.404789

Thermal correction to Gibbs Free Energy= 0.337919

Sum of electronic and zero-point Energies= -1304.751498

Sum of electronic and thermal Energies= -1304.731604

Sum of electronic and thermal Enthalpies= -1304.730660

Sum of electronic and thermal Free Energies= -1304.797531

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

253.417 90.804 140.742

Cartesian coordinates

Atom X Y Z

C	-0.514143	-0.064126	1.765768	H	4.881329	-1.660039	-1.561603
C	0.312284	-1.234814	1.733002	H	4.921510	1.386237	-1.562595
C	1.680884	-0.810425	1.674338	H	3.416929	3.523274	-1.504256
C	1.699991	0.623533	1.674095	H	0.526764	4.501785	-1.393143
C	0.343111	1.084150	1.732516	H	-1.967175	3.732414	-1.281826
C	-0.082139	-2.313138	0.972734	H	-3.186514	-1.169978	-1.544900
C	0.861633	-3.127007	0.224131	H	-2.067795	-3.822349	-1.279711
C	2.197322	-2.715802	0.175120	H	-3.155014	1.109933	-1.546020
C	2.566086	-1.493690	0.869983	C	-4.710153	-1.411861	-0.047787
C	3.609487	-0.820033	0.123120	H	-4.748524	-2.478259	-0.291056
C	3.628031	0.581172	0.122749	C	-4.672182	1.394883	-0.050125
C	2.602948	1.282641	0.869334	H	-4.681511	2.461512	-0.295246
C	2.266847	2.513859	0.173980	C	-5.873240	-0.660969	-0.647022
C	0.942565	2.960493	0.222862	H	-6.711858	-1.217174	-1.058334
C	-0.022530	2.172276	0.971794	C	-5.855099	0.674766	-0.648252
C	-1.313169	2.258863	0.325468	H	-6.678382	1.252747	-1.060517
C	-2.149157	1.144812	0.361759	H	-4.722424	1.334163	1.046895
C	-1.698021	-0.048572	1.035929	H	-4.758415	-1.347835	1.049124
C	-1.374766	-2.365785	0.326670				
C	-2.180946	-1.229963	0.362584				
C	0.030552	-3.905699	-0.706959				
C	-1.262056	-3.466633	-0.648514				
C	3.251515	-2.908360	-0.831721				
C	4.067990	-1.812276	-0.862284				
C	4.112627	1.560364	-0.863212				
C	3.325651	2.677840	-0.833067				
C	0.132558	3.760418	-0.708791				
C	-1.171245	3.355855	-0.650268				
C	-3.330268	0.766460	-0.520700				
C	-3.351749	-0.820738	-0.519843				
H	0.404850	-4.657644	-1.390940				
H	3.320452	-3.756237	-1.502494				

Adduct of the reaction of butadiene with Fragment 2 substituted with one NH₂ groupMolecular formula: C₃₄H₁₇N

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.421883

Thermal correction to Enthalpy= 0.422827

Thermal correction to Gibbs Free Energy= 0.353785

Sum of electronic and zero-point Energies= -1360.084606

Sum of electronic and thermal Energies= -1360.063472

Sum of electronic and thermal Enthalpies= -1360.062528

Sum of electronic and thermal Free Energies= -1360.131570

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

264.736 96.290 145.312

Cartesian coordinates

Atom X Y Z

C	1.445527	-0.303058	2.628292	H	-3.820265	1.773236	-0.637185
C	0.729780	0.938001	2.602460	H	-4.143259	-1.258595	-0.622234
C	-0.672853	0.641725	2.563353	H	-2.844539	-3.526157	-0.569391
C	-0.824610	-0.783867	2.570294	H	-0.053113	-4.783104	-0.476543
C	0.485850	-1.366815	2.609466	H	2.510437	-4.221240	-0.414122
C	1.212068	1.975094	1.835881	H	3.303712	3.292127	-0.440307
C	0.338377	2.870232	1.095796	C	5.720955	0.705396	0.757897
C	-1.030085	2.583100	1.063578	H	5.845496	1.742704	0.431391
C	-1.501823	1.402164	1.767903	C	5.445180	-2.063640	0.970720
C	-2.611075	0.824807	1.036231	H	5.370683	-3.146735	0.846345
C	-2.758882	-0.569126	1.041980	C	6.829510	-0.177673	0.240390
C	-1.793708	-1.359767	1.779324	H	7.717305	0.276482	-0.192706
C	-1.582481	-2.621220	1.087589	C	6.702312	-1.503733	0.350058
C	-0.304545	-3.187121	1.119848	H	7.480887	-2.181347	0.009134
C	0.739851	-2.483668	1.847171	H	5.443537	-1.861203	2.050641
C	2.008146	-2.693408	1.182910	H	5.760824	0.727017	1.856933
C	2.947019	-1.663837	1.213503	N	4.003913	-2.011339	-0.986143
C	2.614914	-0.430492	1.886195	H	3.211346	-1.581822	-1.459084
C	2.496971	1.907445	1.176826	H	4.828547	-1.810112	-1.549001
C	3.197391	0.702965	1.208776	H	4.159545	0.509972	-0.712394
C	1.227267	3.567007	0.153047				
C	2.475335	3.012088	0.199772				
C	-2.074246	2.868901	0.068523				
C	-2.988037	1.852044	0.051998				
C	-3.345251	-1.503648	0.068345				
C	-2.665768	-2.689931	0.095715				
C	0.417146	-4.072427	0.192286				
C	1.753429	-3.790720	0.226589				
C	4.177872	-1.412189	0.343211				
C	4.319338	0.189440	0.324074				
H	0.916591	4.349046	-0.529113				
H	-2.073639	3.717747	-0.604555				

Adduct of the reaction of butadiene with Fragment 2 substituted with one OMe groupMolecular formula: C₃₅H₁₈O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.438373

Thermal correction to Enthalpy= 0.439317

Thermal correction to Gibbs Free Energy= 0.366714

Sum of electronic and zero-point Energies= -1419.229731

Sum of electronic and thermal Energies= -1419.207184

Sum of electronic and thermal Enthalpies= -1419.206240

Sum of electronic and thermal Free Energies= -1419.278843

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

275.083 100.368 152.805

Cartesian coordinates

Atom X Y Z

C	1.426438	-0.360263	2.648095	H	-3.842364	1.818359	-0.545765
C	0.686780	0.865500	2.691228	H	-4.102113	-1.212347	-0.731975
C	-0.709249	0.545122	2.615449	H	-2.756685	-3.451588	-0.810159
C	-0.831886	-0.880721	2.527761	H	0.061424	-4.655934	-0.758571
C	0.489456	-1.439111	2.547031	H	2.595345	-4.091975	-0.612674
C	1.157462	1.956897	1.995874	H	3.239929	3.438559	-0.185401
C	0.273847	2.880327	1.302823	C	5.664414	0.968049	0.767125
C	-1.088396	2.570979	1.238166	H	5.741202	1.948702	0.286626
C	-1.544588	1.338949	1.860565	C	5.516177	-1.819140	1.169550
C	-2.633865	0.788399	1.079013	H	5.530458	-2.911445	1.129710
C	-2.752682	-0.605372	0.992257	C	6.851727	0.103101	0.429870
C	-1.779703	-1.422429	1.688467	H	7.756201	0.574753	0.053974
C	-1.533280	-2.630330	0.918251	C	6.793587	-1.212795	0.644427
C	-0.243658	-3.169578	0.931169	H	7.644975	-1.859030	0.446559
C	0.777586	-2.495520	1.714761	H	5.384519	-1.561693	2.229345
C	2.064677	-2.645694	1.067134	H	5.672338	1.166265	1.848951
C	2.989626	-1.610153	1.191152	O	4.201442	-1.686338	-0.952337
C	2.608186	-0.421178	1.918835	C	4.927146	-2.817135	-1.396583
C	2.447491	1.951083	1.344079	H	4.645549	-2.953785	-2.443764
C	3.168046	0.758960	1.308245	H	6.012577	-2.664954	-1.346172
C	1.156895	3.647558	0.411108	H	4.679282	-3.738875	-0.852457
C	2.413026	3.110206	0.433127	H	4.065520	0.586539	-0.643666
C	-2.126587	2.899491	0.250225				
C	-3.020265	1.869015	0.158017				
C	-3.307674	-1.486038	-0.048099				
C	-2.603825	-2.657437	-0.089422				
C	0.506762	-3.981593	-0.037251				
C	1.836955	-3.683233	0.040183				
C	4.273498	-1.270825	0.417619				
C	4.297719	0.321741	0.392363				
H	0.837298	4.462806	-0.226501				
H	-2.134235	3.788748	-0.368405				

Adduct of the reaction of butadiene with Fragment 2 substituted with one OH groupMolecular formula: C₃₄H₁₆O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.408832

Thermal correction to Enthalpy= 0.409776

Thermal correction to Gibbs Free Energy= 0.340948

Sum of electronic and zero-point Energies= -1379.962860

Sum of electronic and thermal Energies= -1379.941862

Sum of electronic and thermal Enthalpies= -1379.940918

Sum of electronic and thermal Free Energies= -1380.009746

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

256.546 95.523 144.861

Cartesian coordinates

Atom X Y Z

C	1.426377	-0.318583	2.643866	H	-3.832316	1.775060	-0.624264
C	0.699759	0.915877	2.634129	H	-4.124351	-1.256472	-0.677380
C	-0.699878	0.607360	2.577833	H	-2.802930	-3.511388	-0.663821
C	-0.838334	-0.819543	2.554320	H	-0.000166	-4.730473	-0.584929
C	0.476979	-1.391659	2.594035	H	2.553243	-4.150376	-0.483015
C	1.179247	1.971858	1.891136	H	3.266617	3.337891	-0.361277
C	0.302002	2.872999	1.162058	C	5.683103	0.807055	0.644322
C	-1.063512	2.575255	1.115092	H	5.772762	1.810769	0.217574
C	-1.529987	1.376419	1.792064	C	5.471554	-1.954214	1.068217
C	-2.627812	0.804083	1.039492	H	5.413943	-3.045105	1.018729
C	-2.761542	-0.590853	1.013992	C	6.795010	-0.096329	0.168204
C	-1.794650	-1.387650	1.742246	H	7.664917	0.340474	-0.316207
C	-1.565164	-2.631378	1.024386	C	6.706068	-1.413408	0.385871
C	-0.282253	-3.185287	1.055702	H	7.498107	-2.094308	0.084654
C	0.747429	-2.490303	1.810791	H	5.477443	-1.680457	2.132553
C	2.024791	-2.676778	1.157562	H	5.771167	0.932753	1.733331
C	2.953228	-1.643163	1.226679	O	4.044802	-1.935523	-0.896694
C	2.602667	-0.421451	1.909635	H	4.892237	-1.815553	-1.350682
C	2.466403	1.924487	1.233309	H	4.030216	0.477703	-0.714407
C	3.174548	0.724581	1.244873				
C	1.188321	3.591831	0.233876				
C	2.439251	3.043785	0.273699				
C	-2.102108	2.871741	0.117392				
C	-3.006674	1.847676	0.073438				
C	-3.330319	-1.509242	0.014961				
C	-2.639041	-2.688803	0.021751				
C	0.457263	-4.038721	0.111919				
C	1.789968	-3.746124	0.167494				
C	4.198998	-1.364408	0.401007				
C	4.277293	0.226112	0.322997				
H	0.873571	4.382088	-0.436793				
H	-2.103229	3.733509	-0.539025				

Adduct of the reaction of butadiene with Fragment 2 substituted with one Me groupMolecular formula: C₃₅H₁₈

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.432974

Thermal correction to Enthalpy= 0.433918

Thermal correction to Gibbs Free Energy= 0.364303

Sum of electronic and zero-point Energies= -1344.037591

Sum of electronic and thermal Energies= -1344.016271

Sum of electronic and thermal Enthalpies= -1344.015327

Sum of electronic and thermal Free Energies= -1344.084942

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

271.695 96.834 146.517

Cartesian coordinates

Atom X Y Z

C	1.415542	-0.265370	2.625777	H	-3.896237	1.699367	-0.622200
C	0.685198	0.967913	2.597534	H	-4.185626	-1.340405	-0.556152
C	-0.713513	0.653380	2.572863	H	-2.863926	-3.593172	-0.471631
C	-0.847190	-0.773955	2.599222	H	-0.059338	-4.853306	-0.342658
C	0.470387	-1.339002	2.632238	H	2.483918	-4.301108	-0.310355
C	1.147736	2.001719	1.815839	H	3.216340	3.335847	-0.470326
C	0.258665	2.877101	1.071013	C	5.683401	0.697525	0.919799
C	-1.105775	2.569287	1.049182	H	5.826768	1.766411	0.733158
C	-1.556839	1.391219	1.771543	C	5.389667	-2.074224	0.798961
C	-2.664315	0.789374	1.055813	H	5.319825	-3.134478	0.534724
C	-2.796614	-0.605777	1.085119	C	6.804479	-0.126884	0.339196
C	-1.817094	-1.373293	1.827669	H	7.706983	0.367158	-0.011748
C	-1.597385	-2.644121	1.157692	C	6.662520	-1.453703	0.278583
C	-0.312867	-3.196498	1.191035	H	7.444666	-2.092225	-0.124154
C	0.733169	-2.463253	1.884842	H	5.390147	-2.033123	1.897527
C	1.997388	-2.668135	1.207976	H	5.667459	0.578395	2.013170
C	2.916200	-1.614840	1.189268	C	3.863738	-1.724322	-1.191970
C	2.576022	-0.386482	1.869754	H	3.723130	-2.802003	-1.303529
C	2.432970	1.948887	1.156995	H	2.971695	-1.226336	-1.584331
C	3.148295	0.753833	1.197322	H	4.718894	-1.433521	-1.810035
C	1.136034	3.580742	0.122360	H	4.233682	0.659379	-0.664967
C	2.393576	3.047537	0.173196				
C	-2.160422	2.827274	0.057547				
C	-3.060938	1.798342	0.060610				
C	-3.380117	-1.564352	0.132898				
C	-2.688651	-2.743314	0.176907				
C	0.406254	-4.104877	0.286934				
C	1.739179	-3.806980	0.299972				
C	4.119502	-1.329252	0.275429				
C	4.303697	0.257265	0.351438				
H	0.812440	4.351611	-0.566434				
H	-2.175383	3.666443	-0.627412				

Adduct of the reaction of butadiene with Fragment 2 substituted with one *i*-Pr groupMolecular formula: C₃₇H₂₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.493025

Thermal correction to Enthalpy= 0.493969

Thermal correction to Gibbs Free Energy= 0.419785

Sum of electronic and zero-point Energies= -1422.598654

Sum of electronic and thermal Energies= -1422.574883

Sum of electronic and thermal Enthalpies= -1422.573939

Sum of electronic and thermal Free Energies= -1422.648123

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

309.378 106.828 156.134

Cartesian coordinates

Atom X Y Z

C	1.571278	-0.583392	2.622508	H	-3.651275	2.292514	-0.043783
C	0.926179	0.674783	2.840720	H	-4.142617	-0.674302	-0.549180
C	-0.491249	0.458929	2.798994	H	-2.966658	-2.975886	-0.940194
C	-0.720748	-0.936477	2.559057	H	-0.242094	-4.384221	-1.145663
C	0.555342	-1.579605	2.449110	H	2.324773	-4.052367	-1.054232
C	1.447738	1.805853	2.251917	H	3.524499	3.373955	0.126718
C	0.602404	2.858087	1.709360	C	5.633185	0.905081	0.181342
C	-0.779996	2.649169	1.677451	H	5.880110	1.189777	-0.849894
C	-1.298388	1.387574	2.180156	C	5.460065	-1.864829	1.322606
C	-2.456317	1.004798	1.396097	H	5.670183	-2.933397	1.228875
C	-2.680637	-0.358531	1.161471	C	6.805605	0.168488	0.762865
C	-1.740739	-1.313102	1.713485	H	7.756072	0.699111	0.764387
C	-1.614255	-2.437877	0.804232	C	6.737594	-1.072922	1.242927
C	-0.365109	-3.057969	0.692224	H	7.630309	-1.541190	1.653745
C	0.735207	-2.543524	1.486841	H	5.056677	-1.747631	2.337126
C	1.989051	-2.720315	0.773127	H	5.508973	1.855037	0.717662
C	3.002454	-1.779874	0.976157	C	4.922655	-3.612509	-1.031009
C	2.710487	-0.643781	1.833266	H	4.738590	-4.100243	-1.994558
C	2.700734	1.782871	1.532897	H	5.990599	-3.726472	-0.816392
C	3.323971	0.550916	1.322506	H	4.372330	-4.164526	-0.264977
C	1.495497	3.657233	0.857831	C	4.528502	-2.123819	-1.109390
C	2.707197	3.034423	0.751725	H	3.539251	-2.064147	-1.581970
C	-1.830387	3.157265	0.783134	C	5.509462	-1.419989	-2.065479
C	-2.799732	2.206809	0.620533	H	6.518425	-1.374287	-1.646701
C	-3.341455	-1.076267	0.059328	H	5.563806	-1.977750	-3.006743
C	-2.726381	-2.280185	-0.145266	H	5.194213	-0.403678	-2.314925
C	0.280629	-3.819375	-0.383270	H	3.760388	0.373831	-0.728288
C	1.633604	-3.638816	-0.334492				
C	4.352122	-1.451527	0.294964				
C	4.284233	0.139964	0.208917				
H	1.207778	4.558976	0.331128				
H	-1.798481	4.109924	0.268334				

Adduct of the reaction of butadiene with Fragment 2 substituted with one F groupMolecular formula: C₃₄H₁₅F

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.396110

Thermal correction to Enthalpy= 0.397055

Thermal correction to Gibbs Free Energy= 0.328384

Sum of electronic and zero-point Energies= -1403.994056

Sum of electronic and thermal Energies= -1403.973274

Sum of electronic and thermal Enthalpies= -1403.972330

Sum of electronic and thermal Free Energies= -1404.041001

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

248.563 94.023 144.530

Cartesian coordinates

Atom X Y Z

C	1.406596	-0.280580	2.664810	H	-3.856360	1.735014	-0.649614
C	0.675774	0.951257	2.628903	H	-4.136912	-1.297024	-0.648264
C	-0.722802	0.637150	2.576548	H	-2.806209	-3.546026	-0.594798
C	-0.856265	-0.790586	2.578935	H	-0.000599	-4.736219	-0.507380
C	0.461189	-1.357570	2.631321	H	2.546812	-4.144987	-0.414070
C	1.152688	1.992926	1.864673	H	3.238730	3.322939	-0.411398
C	0.273779	2.877614	1.117768	C	5.676942	0.762757	0.733713
C	-1.090789	2.575622	1.075935	H	5.774827	1.800264	0.399616
C	-1.553891	1.388253	1.774937	C	5.438588	-2.034770	0.893391
C	-2.649392	0.798714	1.032045	H	5.346862	-3.106387	0.694058
C	-2.778370	-0.596620	1.032419	C	6.774104	-0.106297	0.169023
C	-1.809521	-1.376497	1.776105	H	7.642506	0.363678	-0.285097
C	-1.574205	-2.631488	1.079093	C	6.660719	-1.434396	0.242332
C	-0.289714	-3.179842	1.121930	H	7.429031	-2.094346	-0.150434
C	0.735838	-2.472061	1.870542	H	5.497519	-1.922134	1.985260
C	2.013339	-2.661351	1.220433	H	5.754881	0.789361	1.830579
C	2.937199	-1.623066	1.274710	F	3.918364	-1.822974	-0.898807
C	2.585762	-0.391799	1.935602	H	4.078267	0.497758	-0.696705
C	2.440995	1.937450	1.208306				
C	3.153932	0.742350	1.245998				
C	1.158992	3.581739	0.177276				
C	2.411544	3.038729	0.228123				
C	-2.129822	2.850447	0.072467				
C	-3.031226	1.823082	0.046832				
C	-3.342367	-1.534598	0.048818				
C	-2.646362	-2.710842	0.076257				
C	0.453779	-4.037119	0.184039				
C	1.784448	-3.735868	0.235556				
C	4.151570	-1.345467	0.405313				
C	4.270190	0.230483	0.347556				
H	0.842326	4.358185	-0.508386				
H	-2.133190	3.699935	-0.599702				

Adduct of the reaction of butadiene with Fragment 2 substituted with one COOH groupMolecular formula: C₃₅H₁₆O₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.421402

Thermal correction to Enthalpy= 0.422346

Thermal correction to Gibbs Free Energy= 0.349082

Sum of electronic and zero-point Energies= -1493.303727

Sum of electronic and thermal Energies= -1493.280956

Sum of electronic and thermal Enthalpies= -1493.280012

Sum of electronic and thermal Free Energies= -1493.353276

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

264.434 101.242 154.199

Cartesian coordinates

Atom X Y Z

C 1.428098 -0.266968 2.622311
C 0.693662 0.963108 2.579877
C -0.704032 0.643268 2.551389
C -0.832878 -0.784362 2.585138
C 0.486501 -1.345392 2.629144
C 1.156140 1.992717 1.792184
C 0.266311 2.861011 1.039655
C -1.096873 2.549587 1.015925
C -1.546582 1.373859 1.742976
C -2.648868 0.764711 1.025837
C -2.775344 -0.630688 1.060580
C -1.796179 -1.391024 1.810732
C -1.567895 -2.663256 1.144801
C -0.281890 -3.210431 1.186246
C 0.754929 -2.475416 1.891420
C 2.021682 -2.677010 1.221290
C 2.933515 -1.622032 1.212236
C 2.592382 -0.386346 1.871516
C 2.441288 1.937394 1.131885
C 3.158846 0.744959 1.181659
C 1.142464 3.559595 0.086367
C 2.400194 3.028140 0.139869
C -2.148794 2.799249 0.019341
C -3.045691 1.767326 0.024329
C -3.350130 -1.594567 0.108446
C -2.653388 -2.769930 0.158640
C 0.447500 -4.104850 0.274321
C 1.779300 -3.802144 0.294093
C 4.144168 -1.349053 0.303377
C 4.305567 0.244144 0.321829
H 0.817278 4.324754 -0.607949
H -2.164134 3.635095 -0.669605

H -3.878388 1.662059 -0.660674
H -4.153859 -1.376186 -0.584437
H -2.821973 -3.622867 -0.487573
H -0.013640 -4.843234 -0.370329
H 2.533234 -4.260403 -0.333020
H 3.222145 3.311739 -0.506589
C 5.697170 0.696592 0.848496
H 5.827541 1.762103 0.635699
C 5.421325 -2.074631 0.815321
H 5.344436 -3.136800 0.578383
C 6.804889 -0.133943 0.250888
H 7.686538 0.357771 -0.151690
C 6.670140 -1.462419 0.231922
H 7.432143 -2.111183 -0.190037
H 5.438636 -1.984989 1.909761
H 5.708844 0.599655 1.943772
O 4.362964 -2.796365 -1.657378
O 2.899926 -1.095692 -1.733217
C 3.849533 -1.838544 -1.119397
H 2.753499 -1.507945 -2.601194
H 4.203997 0.621158 -0.698406

Adduct of the reaction of butadiene with Fragment 2 substituted with one CF₃ groupMolecular formula: C₃₅H₁₅F₃

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.412011

Thermal correction to Enthalpy= 0.412955

Thermal correction to Gibbs Free Energy= 0.338274

Sum of electronic and zero-point Energies= -1641.778771

Sum of electronic and thermal Energies= -1641.755355

Sum of electronic and thermal Enthalpies= -1641.754411

Sum of electronic and thermal Free Energies= -1641.829091

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

258.541 103.759 157.178

Cartesian coordinates

Atom X Y Z

C 1.421767 -0.264588 2.553580
C 0.689283 0.967314 2.538963
C -0.709138 0.650870 2.560058
C -0.840091 -0.775782 2.602236
C 0.480041 -1.338473 2.594995
C 1.125885 1.995818 1.736787
C 0.214723 2.864786 1.012310
C -1.149009 2.554350 1.032746
C -1.576674 1.381216 1.777918
C -2.703575 0.772210 1.100153
C -2.833172 -0.622995 1.145257
C -1.830551 -1.382083 1.864423
C -1.629373 -2.659772 1.199990
C -0.344016 -3.208598 1.197847
C 0.722707 -2.465382 1.847637
C 1.966860 -2.678018 1.132781
C 2.886890 -1.625647 1.091076
C 2.558831 -0.389452 1.764974
C 2.392135 1.941116 1.042732
C 3.110032 0.748571 1.075883
C 1.064323 3.563404 0.034960
C 2.324512 3.034537 0.054653
C -2.233044 2.802918 0.070992
C -3.131023 1.772522 0.108943
C -3.444322 -1.591857 0.221144
C -2.751026 -2.770080 0.255553
C 0.348547 -4.128316 0.285714
C 1.680315 -3.832617 0.251452
C 4.114508 -1.332050 0.199957
C 4.265608 0.260663 0.228806
H 0.719936 4.327945 -0.650699
H -2.269228 3.635971 -0.620508

H -3.985312 1.666237 -0.548747
H -4.270040 -1.375260 -0.445927
H -2.944734 -3.625799 -0.379742
H -0.135341 -4.882558 -0.322695
H 2.401844 -4.316939 -0.388028
H 3.127722 3.320045 -0.614167
C 5.633917 0.736161 0.804009
H 5.763477 1.796827 0.568208
C 5.386778 -2.050185 0.756397
H 5.336183 -3.112729 0.508926
C 6.789065 -0.090491 0.302523
H 7.697362 0.406904 -0.026782
C 6.670144 -1.418957 0.276485
H 7.473485 -2.059339 -0.076619
H 5.332615 -1.986519 1.851111
H 5.587359 0.673369 1.900954
C 3.900790 -1.748841 -1.263265
F 3.959398 -3.094453 -1.438660
F 2.704885 -1.334879 -1.729452
F 4.844514 -1.231614 -2.082553
H 4.191867 0.643433 -0.791928

Adduct of the reaction of butadiene with Fragment 2 substituted with one CHO groupMolecular formula: C₃₅H₁₆O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.414639

Thermal correction to Enthalpy= 0.415584

Thermal correction to Gibbs Free Energy= 0.343974

Sum of electronic and zero-point Energies= -1418.057272

Sum of electronic and thermal Energies= -1418.035275

Sum of electronic and thermal Enthalpies= -1418.034331

Sum of electronic and thermal Free Energies= -1418.105941

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

260.190 97.944 150.716

Cartesian coordinates

Atom X Y Z

C	1.434229	-0.251972	2.631832	H	-3.843999	1.699879	-0.685222
C	0.695621	0.976062	2.595536	H	-4.108446	-1.339502	-0.651043
C	-0.700354	0.651515	2.547708	H	-2.768795	-3.582105	-0.569289
C	-0.824369	-0.777061	2.562540	H	0.040486	-4.788476	-0.443140
C	0.496506	-1.333981	2.613648	H	2.582116	-4.195330	-0.374405
C	1.162660	2.017148	1.825630	H	3.251114	3.376400	-0.430021
C	0.278209	2.891347	1.074117	C	5.725230	0.714186	0.937262
C	-1.083446	2.575438	1.031429	H	5.862680	1.788597	0.780576
C	-1.536633	1.389209	1.739196	C	5.440678	-2.073192	0.713401
C	-2.629003	0.785446	1.002780	H	5.354007	-3.098992	0.348586
C	-2.750631	-0.610608	1.018369	C	6.832629	-0.089549	0.302785
C	-1.776706	-1.376996	1.769463	H	7.724485	0.420231	-0.051967
C	-1.536815	-2.639610	1.089485	C	6.691448	-1.412327	0.189270
C	-0.249386	-3.182790	1.137612	H	7.461349	-2.029830	-0.264695
C	0.777127	-2.453810	1.864407	H	5.479473	-2.121571	1.809815
C	2.050695	-2.639556	1.202518	H	5.724379	0.560547	2.025995
C	2.963062	-1.583422	1.221014	O	4.294549	-2.502505	-1.807792
C	2.606711	-0.357688	1.892365	C	3.775864	-1.641005	-1.134508
C	2.455685	1.975077	1.179239	H	2.940497	-1.026536	-1.537298
C	3.177690	0.784895	1.224503	H	4.267827	0.707769	-0.637580
C	1.162490	3.604977	0.139243				
C	2.422091	3.078771	0.200968				
C	-2.125807	2.834274	0.027076				
C	-3.018904	1.799326	0.009717				
C	-3.311709	-1.564112	0.047814				
C	-2.611027	-2.737339	0.090145				
C	0.492219	-4.060106	0.219095				
C	1.822187	-3.751264	0.255403				
C	4.162869	-1.292645	0.306050				
C	4.338516	0.294590	0.376603				
H	0.842535	4.378527	-0.548159				
H	-2.137059	3.678836	-0.651176				

Adduct of the reaction of butadiene with Fragment 2 substituted with one CN groupMolecular formula: C₃₅H₁₅N

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.403830

Thermal correction to Enthalpy= 0.404774

Thermal correction to Gibbs Free Energy= 0.333950

Sum of electronic and zero-point Energies= -1396.986376

Sum of electronic and thermal Energies= -1396.964620

Sum of electronic and thermal Enthalpies= -1396.963675

Sum of electronic and thermal Free Energies= -1397.034500

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

253.407 97.266 149.062

Cartesian coordinates

Atom X Y Z

C	1.430462	-0.287821	2.607471	H	-3.887340	1.746533	-0.594195
C	0.700589	0.945163	2.598476	H	-4.174565	-1.289732	-0.595908
C	-0.698844	0.632069	2.571246	H	-2.850147	-3.542078	-0.568798
C	-0.833566	-0.795276	2.569213	H	-0.046469	-4.765765	-0.510981
C	0.484544	-1.362626	2.589644	H	2.496191	-4.193669	-0.477078
C	1.162590	1.992936	1.834770	H	3.218715	3.357186	-0.448112
C	0.272161	2.883369	1.109749	C	5.688423	0.759559	0.783397
C	-1.092348	2.578884	1.086967	H	5.808340	1.812898	0.513345
C	-1.543062	1.387066	1.787542	C	5.444144	-2.017205	0.872840
C	-2.652164	0.801485	1.061798	H	5.382149	-3.095115	0.703990
C	-2.783713	-0.593739	1.060187	C	6.807582	-0.088115	0.234201
C	-1.802727	-1.377091	1.783753	H	7.686807	0.393531	-0.184675
C	-1.583501	-2.632145	1.081719	C	6.694330	-1.417667	0.282074
C	-0.299910	-3.184262	1.100124	H	7.471077	-2.074287	-0.098510
C	0.743280	-2.472711	1.819584	H	5.424113	-1.866404	1.960587
C	2.006104	-2.662942	1.137503	H	5.706046	0.722772	1.882166
C	2.926575	-1.618067	1.167045	C	3.974859	-1.792800	-1.089559
C	2.592485	-0.393561	1.851114	N	3.844422	-2.165563	-2.182045
C	2.442536	1.947560	1.163325	H	4.156939	0.628559	-0.728239
C	3.156365	0.752120	1.182714				
C	1.144803	3.599472	0.166133				
C	2.400431	3.061696	0.197628				
C	-2.149301	2.858898	0.104016				
C	-3.050627	1.831151	0.088676				
C	-3.368312	-1.529855	0.086633				
C	-2.675628	-2.708404	0.100343				
C	0.421299	-4.054715	0.158750				
C	1.754002	-3.759249	0.179221				
C	4.158561	-1.329073	0.294553				
C	4.293058	0.272876	0.297232				
H	0.818282	4.381726	-0.508135				
H	-2.164613	3.711535	-0.563896				

Adduct of the reaction of butadiene with Fragment 2 substituted with one NO₂ groupMolecular formula: C₃₄H₁₅NO₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.408692

Thermal correction to Enthalpy= 0.409636

Thermal correction to Gibbs Free Energy= 0.336815

Sum of electronic and zero-point Energies= -1509.245304

Sum of electronic and thermal Energies= -1509.222822

Sum of electronic and thermal Enthalpies= -1509.221878

Sum of electronic and thermal Free Energies= -1509.294699

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

256.458 99.758 153.265

Cartesian coordinates

Atom X Y Z

C	1.422412	-0.278881	2.625581	H	-3.868924	1.717452	-0.639612
C	0.688051	0.951286	2.605542	H	-4.142771	-1.320647	-0.630937
C	-0.709744	0.631448	2.564977	H	-2.810137	-3.567543	-0.578436
C	-0.838253	-0.796535	2.566922	H	-0.003387	-4.782030	-0.482345
C	0.482167	-1.357817	2.601871	H	2.539698	-4.204015	-0.420965
C	1.153674	1.997555	1.842074	H	3.224854	3.359885	-0.428487
C	0.266483	2.881107	1.104390	C	5.696540	0.751500	0.807708
C	-1.096233	2.570033	1.068517	H	5.809124	1.811650	0.562328
C	-1.548722	1.378898	1.768757	C	5.438928	-2.023088	0.817822
C	-2.647389	0.785035	1.033388	H	5.356232	-3.090389	0.613625
C	-2.772878	-0.610689	1.036694	C	6.797375	-0.082421	0.199851
C	-1.796357	-1.386183	1.774096	H	7.667227	0.408950	-0.227427
C	-1.564509	-2.644080	1.080498	C	6.673061	-1.411898	0.200905
C	-0.279391	-3.191383	1.116023	H	7.428940	-2.062904	-0.227311
C	0.753490	-2.472050	1.841975	H	5.466104	-1.904932	1.909770
C	2.023766	-2.661393	1.173866	H	5.741513	0.685067	1.904456
C	2.935642	-1.607581	1.202996	N	3.851062	-1.768373	-1.114446
C	2.589478	-0.381468	1.877382	O	4.403477	-2.781398	-1.533998
C	2.440465	1.955154	1.182284	O	3.033851	-1.108500	-1.744387
C	3.157438	0.762561	1.210682	H	4.153317	0.617081	-0.694970
C	1.145112	3.597768	0.167072				
C	2.402446	3.065323	0.212285				
C	-2.143813	2.840770	0.073041				
C	-3.040274	1.808866	0.052125				
C	-3.343035	-1.554160	0.061495				
C	-2.646088	-2.729920	0.088386				
C	0.454878	-4.064291	0.186900				
C	1.786475	-3.765342	0.220275				
C	4.160594	-1.307517	0.338962				
C	4.296473	0.274347	0.331711				
H	0.821354	4.375007	-0.514250				
H	-2.155585	3.690259	-0.598932				

Adduct of the reaction of butadiene with Fragment 1 substituted with two NH₂ groupsMolecular formula: C₃₄H₂₀N₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.464215

Thermal correction to Enthalpy= 0.465159

Thermal correction to Gibbs Free Energy= 0.392126

Sum of electronic and zero-point Energies= -1416.665882

Sum of electronic and thermal Energies= -1416.642886

Sum of electronic and thermal Enthalpies= -1416.641941

Sum of electronic and thermal Free Energies= -1416.714974

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

291.299 104.091 153.711

Cartesian coordinates

Atom X Y Z

C -1.339367 -0.701972 -1.274459

C -1.200297 0.721406 -1.262924

C 0.065509 1.258802 -1.218500

C 1.233597 0.428616 -1.154723

C 1.072470 -0.951534 -1.168576

C -0.239744 -1.529478 -1.194295

C 2.225033 1.040989 -0.337186

C 3.137613 0.190289 0.314826

C 2.989889 -1.231720 0.276972

C 1.912623 -1.777531 -0.416896

C 3.870267 -2.176623 1.097160

C 3.174856 -3.665829 1.323256

C 1.727809 -3.813882 0.876443

C 1.155743 -2.985363 -0.008365

C -0.275737 -2.749779 -0.436660

C -1.497064 -3.159935 0.089176

C -2.659090 -2.286591 0.043240

C -2.519527 -1.029779 -0.586885

C -3.223151 0.164465 -0.214224

C -4.327228 -0.003612 0.604374

C -4.648497 -1.312379 1.062265

C -3.834398 -2.416652 0.837528

C 0.308808 2.411170 -0.452325

C -0.760309 3.124103 0.134240

C -2.096907 2.554556 0.046178

C -2.309357 1.319498 -0.559853

C -0.357675 4.149481 1.037290

C 0.980329 4.276771 1.393473

C 1.987375 3.366923 0.965279

C 1.654704 2.386420 0.045225

H 3.863651 0.583537 1.019180

H -4.916119 0.839032 0.956157

H -5.526874 -1.433734 1.689899

H -4.065055 -3.360475 1.324851

H -2.874048 3.011917 0.654719

H -1.100402 4.790515 1.505206

H 1.257849 5.051298 2.102911

H 2.974342 3.419248 1.416599

H -1.557234 -4.039143 0.726823

H 1.170373 -4.631309 1.332761

C 4.007714 -4.762338 0.563516

H 3.587379 -5.745625 0.801903

H 3.872229 -4.619643 -0.517978

C 5.215366 -2.337835 0.303230

H 4.971451 -2.503040 -0.754098

H 5.741332 -1.381351 0.359689

C 6.056088 -3.481320 0.804107

H 7.105353 -3.326277 1.043032

C 5.468520 -4.677656 0.915797

H 6.005731 -5.558852 1.257664

N 4.215985 -1.512051 2.356563

H 3.452702 -1.646833 3.016331

H 5.021619 -1.973141 2.774700

N 3.170370 -3.928178 2.778426

H 2.651804 -4.786464 2.956836

H 4.124725 -4.109381 3.085971

Adduct of the reaction of butadiene with Fragment 1 substituted with two OMe groupMolecular formula: C₃₆H₂₂O₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.496968

Thermal correction to Enthalpy= 0.497913

Thermal correction to Gibbs Free Energy= 0.418842

Sum of electronic and zero-point Energies= -1534.964934

Sum of electronic and thermal Energies= -1534.939206

Sum of electronic and thermal Enthalpies= -1534.938262

Sum of electronic and thermal Free Energies= -1535.017332

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

311.852 112.341 166.417

Cartesian coordinates

Atom X Y Z

C	-1.364813	-0.736475	-1.254560	H	-5.474157	-1.382537	1.836573
C	-1.218789	0.685672	-1.277415	H	-4.029679	-3.323336	1.476724
C	0.050562	1.217060	-1.277921	H	-2.830941	3.023879	0.635582
C	1.215343	0.381353	-1.228389	H	-1.028336	4.808048	1.404639
C	1.048331	-0.997968	-1.215058	H	1.345293	5.067009	1.939147
C	-0.267446	-1.568061	-1.188000	H	3.034982	3.411811	1.243020
C	2.228828	1.004689	-0.444504	H	-1.541298	-4.026950	0.826476
C	3.144814	0.161355	0.208393	H	1.226550	-4.636556	1.352798
C	2.992651	-1.260486	0.193558	C	4.048727	-4.666191	0.272729
C	1.905016	-1.816970	-0.471917	H	3.629945	-5.673583	0.346143
C	3.861365	-2.177993	1.055673	H	3.877400	-4.345070	-0.763804
C	3.236944	-3.692158	1.188151	C	5.273011	-2.233591	0.362446
C	1.760958	-3.836702	0.847640	H	5.093563	-2.224364	-0.720269
C	1.153806	-3.012566	-0.018500	H	5.787809	-1.294902	0.583913
C	-0.288053	-2.770069	-0.400723	C	6.102757	-3.442295	0.695749
C	-1.495715	-3.162603	0.167779	H	7.149546	-3.325080	0.963640
C	-2.654760	-2.284966	0.133917	C	5.514251	-4.637117	0.611009
C	-2.527113	-1.043292	-0.527832	H	6.045281	-5.563673	0.812565
C	-3.215745	0.161896	-0.163478	O	3.915524	-1.533658	2.321984
C	-4.298287	0.017463	0.687696	O	3.397614	-4.021002	2.575145
C	-4.612365	-1.279200	1.183284	C	5.016942	-1.759497	3.191986
C	-3.808731	-2.391806	0.962090	H	4.762706	-1.241997	4.120606
C	0.318987	2.382925	-0.540408	H	5.168946	-2.819643	3.400014
C	-0.731041	3.113761	0.058618	H	5.948483	-1.324848	2.803052
C	-2.072298	2.550251	0.016277	C	3.330624	-5.381528	2.956145
C	-2.306214	1.304291	-0.558122	H	4.202952	-5.956224	2.616944
C	-0.300702	4.154107	0.930948	H	3.316661	-5.386301	4.048729
C	1.046276	4.280688	1.251820	H	2.421519	-5.886841	2.601487
C	2.036963	3.356541	0.817027				
C	1.675840	2.360492	-0.075152				
H	3.872017	0.574195	0.900465				
H	-4.874147	0.870500	1.035910				

Adduct of the reaction of butadiene with Fragment 1 substituted with two OH groupMolecular formula: C₃₄H₁₈O₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.438395

Thermal correction to Enthalpy= 0.439339

Thermal correction to Gibbs Free Energy= 0.366811

Sum of electronic and zero-point Energies= -1456.432357

Sum of electronic and thermal Energies= -1456.409608

Sum of electronic and thermal Enthalpies= -1456.408664

Sum of electronic and thermal Free Energies= -1456.481192

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

275.097 102.363 152.648

Cartesian coordinates

Atom X Y Z

C	-1.348980	-0.694954	-1.277519	H	-5.509932	-1.434329	1.721893
C	-1.201247	0.727380	-1.251800	H	-4.062133	-3.365059	1.322950
C	0.067887	1.257529	-1.214797	H	-2.843721	3.006959	0.705428
C	1.231560	0.420106	-1.172050	H	-1.051908	4.766619	1.557267
C	1.062226	-0.959236	-1.203278	H	1.313316	5.009018	2.134513
C	-0.253734	-1.529816	-1.218956	H	3.014328	3.375633	1.414197
C	2.233887	1.019633	-0.356164	H	-1.563370	-4.050482	0.692867
C	3.147840	0.156284	0.275580	H	1.178915	-4.648963	1.311524
C	2.993404	-1.263040	0.213875	C	4.006894	-4.794276	0.531976
C	1.906874	-1.799174	-0.472570	H	3.567034	-5.765912	0.773618
C	3.851896	-2.218062	1.037005	H	3.909164	-4.656572	-0.553591
C	3.163491	-3.692810	1.245341	C	5.244511	-2.353720	0.351665
C	1.715024	-3.839042	0.823950	H	5.089463	-2.481968	-0.727874
C	1.144796	-3.005045	-0.058539	H	5.762326	-1.400393	0.486151
C	-0.288530	-2.756742	-0.472222	C	6.043731	-3.511062	0.888141
C	-1.506165	-3.165300	0.063507	H	7.074525	-3.359155	1.196537
C	-2.663709	-2.285589	0.037826	C	5.451133	-4.707717	0.953531
C	-2.523736	-1.023235	-0.581013	H	5.967056	-5.591960	1.318171
C	-3.216989	0.170781	-0.189247	O	4.138292	-1.660501	2.317380
C	-4.313502	0.000292	0.638873	H	3.406438	-1.923121	2.897144
C	-4.637280	-1.311386	1.086728	O	3.147473	-3.974482	2.650941
C	-3.831513	-2.417619	0.842886	H	4.077670	-4.012890	2.925879
C	0.324839	2.400088	-0.438249				
C	-0.734464	3.112779	0.166069				
C	-2.074960	2.551623	0.084921				
C	-2.300081	1.324146	-0.531704				
C	-0.317330	4.126375	1.075700				
C	1.024725	4.243160	1.420216				
C	2.022399	3.332422	0.972868				
C	1.674826	2.363542	0.045991				
H	3.878141	0.542909	0.980600				
H	-4.894329	0.842350	1.005065				

Adduct of the reaction of butadiene with Fragment 1 substituted with two Me groupMolecular formula: C₃₆H₂₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.486508

Thermal correction to Enthalpy= 0.487452

Thermal correction to Gibbs Free Energy= 0.414303

Sum of electronic and zero-point Energies= -1384.581305

Sum of electronic and thermal Energies= -1384.557986

Sum of electronic and thermal Enthalpies= -1384.557042

Sum of electronic and thermal Free Energies= -1384.630191

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

305.288 105.148 153.955

Cartesian coordinates

Atom X Y Z

C -1.338688 -0.872218 -1.158337

C -1.140184 0.535161 -1.315373

C 0.147378 1.018903 -1.361909

C 1.279719 0.149883 -1.222716

C 1.059687 -1.212510 -1.070175

C -0.274912 -1.734701 -1.007892

C 2.312912 0.806883 -0.495543

C 3.185984 -0.001238 0.256598

C 2.971865 -1.409503 0.409900

C 1.871099 -1.978164 -0.229151

C 3.591765 -2.256739 1.544605

C 3.241627 -3.797336 1.303280

C 1.735960 -3.997643 1.082744

C 1.090255 -3.137860 0.275830

C -0.343196 -2.865887 -0.120537

C -1.566371 -3.155422 0.475219

C -2.689610 -2.236512 0.359046

C -2.513624 -1.066445 -0.412545

C -3.156409 0.192319 -0.166127

C -4.244604 0.169009 0.690328

C -4.607079 -1.062613 1.303625

C -3.846136 -2.221061 1.189775

C 0.457351 2.240468 -0.740300

C -0.566477 3.062729 -0.219619

C -1.927389 2.545682 -0.212210

C -2.205182 1.258636 -0.663286

C -0.099549 4.168162 0.547671

C 1.251150 4.278456 0.859169

C 2.208337 3.280987 0.522155

C 1.812496 2.214807 -0.268607

H 3.928752 0.476055 0.891252

H -4.788850 1.071758 0.953696

H -5.472557 -1.072314 1.960143

H -4.103370 -3.091654 1.787551

H -2.669219 3.105110 0.353581

H -0.803442 4.891333 0.951431

H 1.578066 5.118537 1.465419

H 3.208136 3.344598 0.943151

H -1.648170 -3.956757 1.206079

H 1.244224 -4.840551 1.563360

C 3.982567 -4.300469 0.020175

H 3.918917 -5.396347 -0.009728

H 3.451060 -3.953727 -0.874065

C 5.128165 -2.077038 1.643516

H 5.371562 -1.010917 1.557292

H 5.457307 -2.353677 2.656290

C 5.926973 -2.859963 0.639303

H 6.975121 -2.589091 0.525632

C 5.419348 -3.867977 -0.071495

H 6.050768 -4.402852 -0.778972

C 2.962451 -1.737584 2.863931

H 3.187066 -0.674464 2.991953

H 1.874950 -1.850260 2.857458

H 3.359222 -2.264002 3.736554

C 3.691288 -4.668655 2.494611

H 3.178132 -4.398533 3.421182

H 3.458422 -5.718773 2.287468

H 4.768945 -4.600326 2.662892

Adduct of the reaction of butadiene with Fragment 1 substituted with two *i*-Pr group

Molecular formula: C40H30

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.605927

Thermal correction to Enthalpy= 0.606871

Thermal correction to Gibbs Free Energy= 0.523284

Sum of electronic and zero-point Energies= -1541.701974

Sum of electronic and thermal Energies= -1541.673540

Sum of electronic and thermal Enthalpies= -1541.672596

Sum of electronic and thermal Free Energies= -1541.756183

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

380.225 125.646 175.925

Cartesian coordinates			
Atom	X	Y	Z
C	-1.358883	-0.831449	-1.074314
C	-1.106228	0.547651	-1.356259
C	0.196295	0.962430	-1.511778
C	1.294013	0.053583	-1.355224
C	1.022036	-1.276177	-1.066929
C	-0.328654	-1.730226	-0.905022
C	2.400257	0.714635	-0.756574
C	3.287853	-0.073218	0.005348
C	3.005026	-1.441845	0.328303
C	1.836847	-2.000578	-0.194963
C	3.683749	-2.235111	1.471933
C	3.214025	-3.795979	1.363357
C	1.690640	-3.936725	1.233514
C	1.038817	-3.094063	0.414436
C	-0.400457	-2.786576	0.069838
C	-1.603401	-2.968398	0.744687
C	-2.687187	-2.004551	0.612355
C	-2.500019	-0.907792	-0.258123
C	-3.069024	0.397568	-0.081014
C	-4.108765	0.495250	0.828944
C	-4.493781	-0.665566	1.556005
C	-3.794864	-1.866500	1.496503
C	0.598148	2.214440	-1.017722
C	-0.355987	3.124593	-0.510779
C	-1.736105	2.676943	-0.384737
C	-2.098575	1.373012	-0.711370
C	0.204556	4.264818	0.133309
C	1.575370	4.334653	0.355838
C	2.467058	3.268721	0.048571
C	1.978611	2.161255	-0.625226
H	4.119313	0.412819	0.504529
H	-4.595746	1.441739	1.046988
H	-5.321827	-0.580889	2.254117
H	-4.059302	-2.674069	2.174288
H	-2.417577	3.316717	0.171774
H	-0.440981	5.051509	0.515262
H	1.974741	5.204276	0.870071
H	3.492581	3.319393	0.404517
H	-1.684910	-3.707098	1.538847
H	1.183471	-4.739286	1.759792
C	3.776265	-4.356279	0.005227
H	3.549317	-5.423685	-0.059111
H	3.220980	-3.900989	-0.820800
C	5.237886	-2.173796	1.355654
H	5.531033	-1.151948	1.091984
H	5.684694	-2.338499	2.347419
C	5.886518	-3.116054	0.382898
H	6.946714	-2.957365	0.192484
C	5.238555	-4.113436	-0.215984
H	5.758955	-4.762496	-0.918231
C	4.002105	-0.226488	3.180579
H	3.816107	0.029800	4.229035
H	5.085374	-0.247963	3.045035
H	3.594126	0.590646	2.579514
C	4.180418	-6.095573	2.231498
H	4.993465	-6.135807	1.504128
H	4.527784	-6.601465	3.138736
H	3.337149	-6.678818	1.842873
C	3.306638	-1.571871	2.873887
H	3.689833	-2.271660	3.624109
C	3.767065	-4.651874	2.583281
H	4.681544	-4.154120	2.922070
C	2.825152	-4.747145	3.805678
H	2.007085	-5.453508	3.626355
H	3.385848	-5.130787	4.664722
H	2.379270	-3.797884	4.102182
C	1.804162	-1.366215	3.139623
H	1.367602	-0.670015	2.417157
H	1.225247	-2.288030	3.096578
H	1.667691	-0.930654	4.135744

Adduct of the reaction of butadiene with Fragment 1 substituted with two F groupMolecular formula: C₃₄H₁₆F₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.412725

Thermal correction to Enthalpy= 0.413669

Thermal correction to Gibbs Free Energy= 0.341323

Sum of electronic and zero-point Energies= -1504.485415

Sum of electronic and thermal Energies= -1504.463146

Sum of electronic and thermal Enthalpies= -1504.462202

Sum of electronic and thermal Free Energies= -1504.534548

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

258.989 99.496 152.266

Cartesian coordinates

Atom X Y Z

C	-1.363077	-0.687245	-1.285144	H	-5.523205	-1.433331	1.713516
C	-1.215221	0.735173	-1.255774	H	-4.075218	-3.363082	1.310780
C	0.053671	1.266050	-1.217392	H	-2.859037	3.009958	0.705271
C	1.216791	0.428477	-1.174837	H	-1.068848	4.768102	1.562016
C	1.047499	-0.950715	-1.212723	H	1.295596	5.009733	2.142254
C	-0.268331	-1.522498	-1.229570	H	2.997239	3.378365	1.420345
C	2.218452	1.026937	-0.356292	H	-1.576735	-4.045868	0.679782
C	3.132981	0.162904	0.272601	H	1.178735	-4.644456	1.301358
C	2.976169	-1.254897	0.202318	C	4.017529	-4.783652	0.599260
C	1.890681	-1.791854	-0.483345	H	3.578485	-5.744824	0.880879
C	3.823287	-2.212527	1.017240	H	3.936626	-4.703467	-0.493955
C	3.150521	-3.666864	1.232677	C	5.235632	-2.333363	0.385269
C	1.705017	-3.828360	0.813614	H	5.110554	-2.470402	-0.697657
C	1.129406	-2.998301	-0.069191	H	5.729251	-1.367151	0.521107
C	-0.303037	-2.750569	-0.48484	C	6.036730	-3.471160	0.959258
C	-1.520044	-3.159991	0.051473	H	7.056921	-3.298555	1.289087
C	-2.677740	-2.280746	0.026995	C	5.451104	-4.666245	1.047260
C	-2.537767	-1.017167	-0.589248	H	5.958418	-5.533458	1.459070
C	-3.231201	0.175825	-0.195277	F	3.173916	-3.911944	2.611198
C	-4.327449	0.003364	0.632711	F	4.013264	-1.657029	2.286118
C	-4.650969	-1.309223	1.078124				
C	-3.845169	-2.414839	0.832204				
C	0.310118	2.406677	-0.437783				
C	-0.749790	3.117722	0.167301				
C	-2.089846	2.556236	0.084208				
C	-2.314505	1.330016	-0.535160				
C	-0.333683	4.129323	1.079533				
C	1.007954	4.245830	1.425645				
C	2.006045	3.336197	0.977413				
C	1.659268	2.369823	0.047694				
H	3.864084	0.551608	0.975622				
H	-4.908320	0.844485	1.000837				

Adduct of the reaction of butadiene with Fragment 1 substituted with two COOH groupMolecular formula: C₃₆H₁₈O₄

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.463094

Thermal correction to Enthalpy= 0.464039

Thermal correction to Gibbs Free Energy= 0.383038

Sum of electronic and zero-point Energies= -1683.108559

Sum of electronic and thermal Energies= -1683.082236

Sum of electronic and thermal Enthalpies= -1683.081292

Sum of electronic and thermal Free Energies= -1683.162293

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

290.596 114.144 170.481

Cartesian coordinates

Atom X Y Z

C -1.287226 -0.886653 -1.110150

C -1.100904 0.523613 -1.256040

C 0.182216 1.018204 -1.317397

C 1.322598 0.156380 -1.203016

C 1.114962 -1.209922 -1.063490

C -0.215010 -1.742310 -0.983170

C 2.361564 0.815186 -0.484383

C 3.256796 0.008688 0.240886

C 3.057781 -1.404075 0.364585

C 1.945654 -1.979399 -0.244890

C 3.778700 -2.263806 1.436453

C 3.334059 -3.786041 1.287227

C 1.820994 -3.982138 1.094004

C 1.177376 -3.140147 0.272925

C -0.261785 -2.879254 -0.103150

C -1.473342 -3.184542 0.508202

C -2.605336 -2.274914 0.414298

C -2.449673 -1.096842 -0.349627

C -3.098489 0.154587 -0.082523

C -4.173787 0.115183 0.789262

C -4.518150 -1.124864 1.396368

C -3.750246 -2.276206 1.261362

C 0.491952 2.235111 -0.685932

C -0.530578 3.043934 -0.142070

C -1.887059 2.516786 -0.121908

C -2.162104 1.232447 -0.582614

C -0.061453 4.142983 0.633003

C 1.292082 4.258456 0.929848

C 2.251641 3.272000 0.568634

C 1.852658 2.214618 -0.232186

H 3.991101 0.474558 0.891773

H -4.720893 1.011273 1.068833

H -5.374156 -1.147149 2.064833

H -3.992138 -3.154246 1.854500

H -2.625243 3.064655 0.459726

H -0.765279 4.855909 1.054632

H 1.620570 5.092065 1.543932

H 3.255051 3.334279 0.980507

H -1.536743 -3.991805 1.234042

H 1.359282 -4.824470 1.595996

C 4.018141 -4.429451 0.025471

H 3.860258 -5.511460 0.084867

H 3.471263 -4.092846 -0.862427

C 5.328700 -2.089706 1.360690

H 5.544404 -1.064058 1.046577

H 5.748573 -2.173657 2.366805

C 6.043071 -3.047722 0.454372

H 7.103114 -2.853198 0.302618

C 5.474411 -4.103680 -0.125592

H 6.061974 -4.757969 -0.766092

C 3.742317 -4.660546 2.483498

C 3.338112 -1.642657 2.778261

O 3.345919 -5.794323 2.644081

O 3.882412 -0.693150 3.298548

O 4.607802 -4.082988 3.345486

H 4.784045 -4.747245 4.033704

O 2.232878 -2.213362 3.309123

H 2.032498 -1.705181 4.114203

Adduct of the reaction of butadiene with Fragment 1 substituted with two CF₃ groupMolecular formula: C₃₆H₁₆F₆

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.444354

Thermal correction to Enthalpy= 0.445299

Thermal correction to Gibbs Free Energy= 0.362355

Sum of electronic and zero-point Energies= -1980.055966

Sum of electronic and thermal Energies= -1980.028506

Sum of electronic and thermal Enthalpies= -1980.027562

Sum of electronic and thermal Free Energies= -1980.110505

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

278.837 119.014 174.569

Cartesian coordinates

Atom X Y Z

C -1.312662 -0.918111 -1.110270

C -1.112274 0.486723 -1.288294

C 0.175173 0.967853 -1.362529

C 1.305059 0.097563 -1.220791

C 1.084446 -1.260607 -1.045000

C -0.250145 -1.781701 -0.963233

C 2.352363 0.762438 -0.523120

C 3.237564 -0.032864 0.227018

C 3.012451 -1.436534 0.414260

C 1.900288 -2.011611 -0.196556

C 3.703054 -2.288842 1.515068

C 3.304661 -3.832747 1.261330

C 1.788254 -4.042346 1.088523

C 1.127794 -3.172759 0.312389

C -0.310015 -2.902895 -0.064179

C -1.522833 -3.179819 0.556910

C -2.644501 -2.258297 0.445510

C -2.476941 -1.099227 -0.344293

C -3.111439 0.164818 -0.104557

C -4.184542 0.156530 0.771022

C -4.540489 -1.065164 1.407332

C -3.785774 -2.227817 1.296364

C 0.498898 2.197250 -0.764040

C -0.515378 3.028869 -0.239399

C -1.876529 2.514419 -0.202840

C -2.165360 1.221632 -0.631047

C -0.034566 4.143964 0.504983

C 1.320836 4.255735 0.794454

C 2.270728 3.251371 0.457808

C 1.860746 2.175932 -0.312724

H 3.991915 0.454230 0.834106

H -4.720864 1.064599 1.032047

H -5.393701 -1.062333 2.079569

H -4.034536 -3.088778 1.911115

H -2.608044 3.083719 0.366398

H -0.730745 4.873831 0.909801

H 1.658314 5.102617 1.384946

H 3.275803 3.317186 0.865187

H -1.594586 -3.969901 1.300565

H 1.322077 -4.893022 1.572338

C 4.001805 -4.299191 -0.067882

H 3.942253 -5.389593 -0.115762

H 3.398857 -3.936213 -0.905865

C 5.246909 -2.088555 1.507456

H 5.452226 -1.018198 1.410441

H 5.657762 -2.379815 2.479173

C 5.965857 -2.839837 0.426759

H 6.997081 -2.549106 0.240068

C 5.419276 -3.842839 -0.256433

H 5.995095 -4.360067 -1.020845

C 3.732312 -4.799973 2.391365

C 3.208062 -1.747125 2.888122

F 2.967872 -4.668523 3.496080

F 3.567178 -6.087253 1.988126

F 5.020267 -4.674327 2.763339

F 3.832083 -2.329500 3.935688

F 3.476695 -0.421833 3.001457

F 1.884494 -1.897415 3.069950

Adduct of the reaction of butadiene with Fragment 1 substituted with two CHO groupMolecular formula: C₃₆H₁₈O₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.449710

Thermal correction to Enthalpy= 0.450654

Thermal correction to Gibbs Free Energy= 0.372121

Sum of electronic and zero-point Energies= -1532.616393

Sum of electronic and thermal Energies= -1532.591482

Sum of electronic and thermal Enthalpies= -1532.590538

Sum of electronic and thermal Free Energies= -1532.669072

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

282.197 107.666 165.287

Cartesian coordinates

Atom X Y Z

C -1.318227 -0.879295 -1.158213

C -1.128390 0.532778 -1.283667

C 0.155698 1.026218 -1.330918

C 1.293523 0.160952 -1.220056

C 1.082620 -1.207412 -1.102251

C -0.249086 -1.739401 -1.038058

C 2.327895 0.809069 -0.484646

C 3.214893 -0.009579 0.238221

C 3.016203 -1.424837 0.337799

C 1.907205 -1.989544 -0.291603

C 3.678081 -2.289547 1.431739

C 3.273078 -3.823218 1.224908

C 1.771638 -4.016986 1.021873

C 1.133360 -3.158541 0.208766

C -0.303355 -2.888152 -0.174317

C -1.518582 -3.198401 0.427764

C -2.648161 -2.285477 0.339591

C -2.485412 -1.097445 -0.407256

C -3.133631 0.151376 -0.127510

C -4.213651 0.102125 0.737762

C -4.563805 -1.145243 1.326392

C -3.797525 -2.296169 1.180553

C 0.463296 2.234456 -0.681976

C -0.561398 3.037614 -0.134009

C -1.918582 2.512134 -0.128571

C -2.192551 1.234202 -0.607460

C -0.095558 4.126170 0.657593

C 1.256318 4.236770 0.963779

C 2.216614 3.253638 0.596131

C 1.820836 2.206761 -0.220055

H 3.955182 0.450231 0.888195

H -4.760507 0.995341 1.026624

H -5.422982 -1.174372 1.990326

H -4.043873 -3.181227 1.761061

H -2.659497 3.053620 0.455401

H -0.800962 4.834431 1.084210

H 1.581989 5.062217 1.590070

H 3.217944 3.310763 1.013897

H -1.587433 -4.015320 1.142198

H 1.296472 -4.847973 1.532171

C 4.037267 -4.405654 -0.014394

H 3.947237 -5.500138 0.006901

H 3.512044 -4.088151 -0.922868

C 5.208908 -2.116165 1.527219

H 5.458346 -1.062740 1.360677

H 5.526320 -2.304214 2.561063

C 5.996836 -2.972877 0.578169

H 7.052151 -2.730663 0.470925

C 5.482859 -4.001962 -0.097006

H 6.114800 -4.583516 -0.764981

C 3.741888 -4.626927 2.442071

H 4.837809 -4.628126 2.607907

C 3.024970 -1.778065 2.734429

H 1.919207 -1.845082 2.751631

O 3.006491 -5.257929 3.169612

O 3.638975 -1.302254 3.663873

Adduct of the reaction of butadiene with Fragment 1 substituted with two CN groupMolecular formula: C₃₆H₁₆N₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.427747

Thermal correction to Enthalpy= 0.428691

Thermal correction to Gibbs Free Energy= 0.351452

Sum of electronic and zero-point Energies= -1490.466136

Sum of electronic and thermal Energies= -1490.441767

Sum of electronic and thermal Enthalpies= -1490.440823

Sum of electronic and thermal Free Energies= -1490.518061

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

268.415 106.284 162.562

Cartesian coordinates

Atom X Y Z

C	-1.330166	-0.727734	-1.247177	H	-5.506034	-1.409028	1.743846
C	-1.182837	0.695290	-1.249428	H	-4.057538	-3.347703	1.389745
C	0.085455	1.227933	-1.218630	H	-2.835280	3.011848	0.653188
C	1.247548	0.391024	-1.148938	H	-1.050562	4.785467	1.482517
C	1.078113	-0.987667	-1.147954	H	1.310159	5.038889	2.071514
C	-0.236775	-1.561792	-1.166561	H	3.015214	3.393630	1.392515
C	2.244431	1.008105	-0.339796	H	-1.557370	-4.044826	0.786774
C	3.156327	0.160300	0.315234	H	1.208611	-4.700284	1.335714
C	2.991993	-1.259071	0.291437	C	4.054883	-4.748144	0.433290
C	1.913870	-1.811627	-0.390779	H	3.627360	-5.742476	0.581581
C	3.856956	-2.218752	1.125499	H	3.907741	-4.489701	-0.623547
C	3.208046	-3.715807	1.276720	C	5.270849	-2.308547	0.412275
C	1.734881	-3.866219	0.881638	H	5.063144	-2.372603	-0.663400
C	1.154153	-3.016439	0.023783	H	5.788952	-1.360942	0.573526
C	-0.276957	-2.774991	-0.399262	C	6.091499	-3.491251	0.840986
C	-1.496402	-3.172685	0.140111	H	7.122354	-3.349839	1.150618
C	-2.653308	-2.293333	0.090104	C	5.506679	-4.690952	0.819642
C	-2.509059	-1.042961	-0.551601	H	6.023457	-5.597682	1.117807
C	-3.204107	0.158375	-0.187541	C	3.299870	-4.167102	2.681082
C	-4.304411	0.003653	0.638534	C	4.078818	-1.618753	2.454690
C	-4.630819	-1.299033	1.110144	N	3.321199	-4.604964	3.755994
C	-3.824638	-2.410136	0.892186	N	4.288235	-1.074502	3.458860
C	0.338998	2.385850	-0.463680				
C	-0.724101	3.108340	0.122099				
C	-2.063458	2.544692	0.045632				
C	-2.285685	1.305180	-0.547980				
C	-0.312679	4.138104	1.016061				
C	1.026904	4.262118	1.367359				
C	2.027467	3.344051	0.943048				
C	1.685456	2.360642	0.029538				
H	3.884609	0.576781	1.005995				
H	-4.886876	0.852422	0.985775				

Adduct of the reaction of butadiene with Fragment 1 substituted with two NO₂ groupMolecular formula: C₃₄H₁₆N₂O₄

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.437682

Thermal correction to Enthalpy= 0.438627

Thermal correction to Gibbs Free Energy= 0.359034

Sum of electronic and zero-point Energies= -1714.990855

Sum of electronic and thermal Energies= -1714.965173

Sum of electronic and thermal Enthalpies= -1714.964229

Sum of electronic and thermal Free Energies= -1715.043821

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

274.650 111.215 167.516

Cartesian coordinates

Atom X Y Z

C	-1.207257	-0.672351	-1.211975	H	-5.410435	-0.801416	1.815086
C	-0.968068	0.731575	-1.344869	H	-4.089183	-2.853020	1.649691
C	0.331801	1.184411	-1.359230	H	-2.467962	3.318201	0.321272
C	1.435638	0.284649	-1.202524	H	-0.574154	5.045447	0.989354
C	1.178472	-1.074913	-1.080855	H	1.798105	5.202681	1.566132
C	-0.170727	-1.564760	-1.051322	H	3.393521	3.394058	1.057297
C	2.469957	0.908683	-0.445527	H	-1.643425	-3.768656	1.115937
C	3.315150	0.073226	0.304834	H	1.222196	-4.692440	1.594343
C	3.060815	-1.331535	0.413480	C	3.960489	-4.371498	0.115191
C	1.951676	-1.871364	-0.234768	H	3.777350	-5.447904	0.189197
C	3.710002	-2.217802	1.492725	H	3.459298	-4.040860	-0.800914
C	3.217460	-3.702357	1.313970	C	5.249936	-2.074888	1.552345
C	1.714203	-3.868196	1.094384	H	5.514162	-1.049051	1.283821
C	1.126798	-3.008456	0.250491	H	5.584120	-2.212631	2.583235
C	-0.287836	-2.700540	-0.177441	C	5.989026	-3.031890	0.662015
C	-1.528513	-2.964899	0.392837	H	7.057569	-2.855044	0.565329
C	-2.625417	-2.018375	0.259916	C	5.427694	-4.066734	0.039360
C	-2.402807	-0.845019	-0.494447	H	6.030900	-4.726973	-0.578787
C	-3.018385	0.426714	-0.247247	O	2.165473	-2.178744	3.334704
C	-4.124638	0.421412	0.585618	O	3.715678	-0.654428	3.285807
C	-4.531884	-0.807403	1.176476	O	4.342142	-4.078022	3.401213
C	-3.798615	-1.983421	1.066450	O	3.144988	-5.691463	2.579450
C	0.659391	2.389285	-0.713654	N	3.153053	-1.648517	2.842535
C	-0.355304	3.230060	-0.204828	N	3.598225	-4.553056	2.553657
C	-1.727788	2.747321	-0.234918				
C	-2.029026	1.473631	-0.709252				
C	0.120920	4.311398	0.590406				
C	1.465744	4.382395	0.936738				
C	2.404881	3.365827	0.607916				
C	2.000760	2.324406	-0.211078				
H	4.045307	0.513162	0.976659				
H	-4.650872	1.334601	0.849011				

Adduct of the reaction of butadiene with Fragment 2 substituted with two NH₂ groupMolecular formula: C₃₄H₁₈N₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.439875

Thermal correction to Enthalpy= 0.440819

Thermal correction to Gibbs Free Energy= 0.369099

Sum of electronic and zero-point Energies= -1415.414059

Sum of electronic and thermal Energies= -1415.391539

Sum of electronic and thermal Enthalpies= -1415.390595

Sum of electronic and thermal Free Energies= -1415.462315

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

276.026 102.010 150.948

Cartesian coordinates

Atom X Y Z

C 1.472356 -0.282358 2.585647
C 0.750886 0.954251 2.562158
C -0.651120 0.654106 2.548570
C -0.797151 -0.771595 2.568040
C 0.515912 -1.349210 2.593430
C 1.217501 1.987071 1.782395
C 0.328701 2.881587 1.060998
C -1.038673 2.587704 1.047448
C -1.494514 1.406541 1.761482
C -2.611322 0.820944 1.048614
C -2.752730 -0.573732 1.064287
C -1.774539 -1.356242 1.794015
C -1.568587 -2.622225 1.109037
C -0.288721 -3.185051 1.130187
C 0.762177 -2.471823 1.838305
C 2.023266 -2.684448 1.163812
C 2.958799 -1.651143 1.169346
C 2.631889 -0.408616 1.827703
C 2.497111 1.926741 1.110019
C 3.204905 0.722644 1.137394
C 1.203980 3.596836 0.120911
C 2.456658 3.051860 0.151088
C -2.099075 2.865751 0.067318
C -3.007009 1.843282 0.066305
C -3.348712 -1.517269 0.105561
C -2.664843 -2.701247 0.132424
C 0.425620 -4.078172 0.204466
C 1.762097 -3.793842 0.223104
C 4.183869 -1.424150 0.295363
C 4.352851 0.213126 0.257757
H 0.885749 4.391893 -0.542483
H -2.113037 3.712532 -0.608214

H -3.848189 1.758020 -0.611147
H -4.156771 -1.280103 -0.576007
H -2.849917 -3.542742 -0.524246
H -0.049336 -4.797684 -0.451445
H 2.514711 -4.231014 -0.418862
H 3.276943 3.367892 -0.480764
C 5.726277 0.645352 0.852479
H 5.883196 1.711576 0.651864
C 5.437995 -2.086522 0.948227
H 5.355219 -3.165929 0.803128
C 6.856459 -0.203049 0.326716
H 7.746789 0.271331 -0.076634
C 6.717872 -1.529925 0.378401
H 7.490303 -2.204844 0.019782
H 5.408310 -1.901658 2.031497
H 5.670920 0.550410 1.945335
N 4.010877 -2.039712 -1.019758
H 3.132808 -1.730097 -1.431162
H 4.739997 -1.673925 -1.630880
N 4.325956 0.662914 -1.139220
H 3.371440 0.678226 -1.489752
H 4.670259 1.616414 -1.205021

Adduct of the reaction of butadiene with Fragment 2 substituted with two OMe groupMolecular formula: C₃₆H₂₀O₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.472928

Thermal correction to Enthalpy= 0.473872

Thermal correction to Gibbs Free Energy= 0.397105

Sum of electronic and zero-point Energies= -1533.708002

Sum of electronic and thermal Energies= -1533.683034

Sum of electronic and thermal Enthalpies= -1533.682090

Sum of electronic and thermal Free Energies= -1533.758858

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

296.767 109.839 161.571

Cartesian coordinates

Atom X Y Z

C	1.458905	-0.340166	2.605334	H	-3.881814	1.804705	-0.494214
C	0.716127	0.882895	2.651761	H	-4.135626	-1.227478	-0.658411
C	-0.681545	0.558833	2.609507	H	-2.784791	-3.462948	-0.752175
C	-0.801197	-0.867143	2.532257	H	0.039260	-4.654255	-0.753700
C	0.522167	-1.421296	2.527895	H	2.573649	-4.081183	-0.659950
C	1.168450	1.968682	1.937347	H	3.197682	3.430973	-0.301815
C	0.267956	2.888036	1.259917	C	5.672407	0.916995	0.890221
C	-1.093723	2.576310	1.227561	H	5.768162	1.958331	0.569071
C	-1.533085	1.345303	1.865887	C	5.502002	-1.833780	1.141673
C	-2.636851	0.787634	1.110710	H	5.505855	-2.925813	1.100990
C	-2.753660	-0.607330	1.035157	C	6.877297	0.088920	0.528230
C	-1.764602	-1.417211	1.715791	H	7.784742	0.581380	0.188370
C	-1.529703	-2.628435	0.946956	C	6.802527	-1.236707	0.666966
C	-0.238094	-3.162938	0.936341	H	7.645526	-1.887319	0.449597
C	0.795844	-2.481606	1.696092	H	5.340886	-1.578732	2.197758
C	2.070596	-2.631862	1.025662	H	5.581569	0.947673	1.984593
C	2.995989	-1.595237	1.130392	O	4.202900	-1.739202	-0.991390
C	2.627903	-0.402174	1.855245	O	4.030950	0.882384	-0.958334
C	2.444276	1.962929	1.258109	C	4.954159	-2.864738	-1.408727
C	3.172408	0.775825	1.232715	H	4.682934	-3.025092	-2.455235
C	1.132386	3.656353	0.350613	H	6.036801	-2.694025	-1.352684
C	2.388527	3.121518	0.345129	H	4.715692	-3.779543	-0.849466
C	-2.153902	2.896033	0.260538	C	5.048358	0.905044	-1.949275
C	-3.045846	1.862098	0.192514	H	5.453088	-0.088168	-2.153080
C	-3.326842	-1.495261	0.010851	H	4.566337	1.286862	-2.852757
C	-2.620218	-2.664597	-0.038706	H	5.871828	1.583181	-1.685372
C	0.496418	-3.976763	-0.042771				
C	1.827170	-3.674474	0.007745				
C	4.278306	-1.280692	0.355717				
C	4.326766	0.359044	0.326145				
H	0.796530	4.466151	-0.285545				
H	-2.176926	3.781225	-0.363509				

Adduct of the reaction of butadiene with Fragment 2 substituted with two OH groupMolecular formula: C₃₄H₁₆O₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.414155

Thermal correction to Enthalpy= 0.415099

Thermal correction to Gibbs Free Energy= 0.344447

Sum of electronic and zero-point Energies= -1455.178554

Sum of electronic and thermal Energies= -1455.156474

Sum of electronic and thermal Enthalpies= -1455.155530

Sum of electronic and thermal Free Energies= -1455.226182

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

259.886 99.997 148.699

Cartesian coordinates

Atom X Y Z

C	1.441573	-0.283962	2.630156	H	-3.853898	1.742062	-0.626858
C	0.708363	0.947109	2.606546	H	-4.133363	-1.291681	-0.635244
C	-0.691215	0.632182	2.566292	H	-2.802043	-3.540820	-0.601520
C	-0.823069	-0.794895	2.562440	H	0.007535	-4.740556	-0.533754
C	0.495616	-1.360013	2.598702	H	2.556850	-4.146828	-0.462960
C	1.175869	1.993308	1.843711	H	3.244304	3.318441	-0.447943
C	0.290424	2.881323	1.107990	C	5.710726	0.751696	0.826425
C	-1.073498	2.578464	1.077132	H	5.821889	1.801597	0.541907
C	-1.528984	1.386006	1.774348	C	5.460095	-2.019625	0.954287
C	-2.630734	0.799134	1.039146	H	5.380628	-3.098453	0.791386
C	-2.759547	-0.596768	1.035453	C	6.821349	-0.104756	0.269411
C	-1.783800	-1.378814	1.766713	H	7.694461	0.371859	-0.167747
C	-1.554171	-2.631217	1.063534	C	6.708683	-1.435047	0.337768
C	-0.268415	-3.178085	1.091741	H	7.486635	-2.095905	-0.035382
C	0.764196	-2.469109	1.829444	H	5.469187	-1.864396	2.042079
C	2.035848	-2.654958	1.166121	H	5.728940	0.715446	1.924342
C	2.961052	-1.616704	1.215570	O	3.963223	-1.831264	-0.956392
C	2.615973	-0.389354	1.891712	H	4.786279	-1.670049	-1.444885
C	2.460210	1.945607	1.181444	O	4.219983	0.738984	-1.003829
C	3.182613	0.756162	1.223062	H	3.545506	0.186775	-1.430256
C	1.170558	3.592930	0.167166				
C	2.424220	3.052410	0.205356				
C	-2.122202	2.856336	0.084801				
C	-3.022517	1.827760	0.062465				
C	-3.332260	-1.531409	0.053591				
C	-2.635936	-2.707799	0.070747				
C	0.467198	-4.037517	0.150215				
C	1.798544	-3.736581	0.190070				
C	4.190999	-1.348808	0.367646				
C	4.325728	0.272095	0.333428				
H	0.846784	4.369211	-0.515431				
H	-2.132890	3.708990	-0.583302				

Adduct of the reaction of butadiene with Fragment 2 substituted with two Me groupMolecular formula: C₃₆H₂₀

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.462351

Thermal correction to Enthalpy= 0.463295

Thermal correction to Gibbs Free Energy= 0.390888

Sum of electronic and zero-point Energies= -1383.317396

Sum of electronic and thermal Energies= -1383.294803

Sum of electronic and thermal Enthalpies= -1383.293859

Sum of electronic and thermal Free Energies= -1383.366266

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

290.129 102.714 152.393

Cartesian coordinates

Atom X Y Z

C	1.453900	-0.280343	2.526161	H	-3.981801	1.754884	-0.458193
C	0.723946	0.949435	2.549085	H	-4.264703	-1.293802	-0.451393
C	-0.675039	0.637312	2.580942	H	-2.941198	-3.546521	-0.463779
C	-0.807675	-0.789766	2.584551	H	-0.125099	-4.816835	-0.455557
C	0.509865	-1.354788	2.555509	H	2.415337	-4.283968	-0.488370
C	1.157011	1.992268	1.766291	H	3.131993	3.463048	-0.509994
C	0.236615	2.894837	1.095852	C	5.643643	0.719413	0.865716
C	-1.127969	2.587918	1.122582	H	5.790530	1.788241	0.682401
C	-1.549800	1.391483	1.831666	C	5.400785	-2.001235	0.939816
C	-2.684402	0.805004	1.146974	H	5.358279	-3.088279	0.821797
C	-2.813949	-0.591219	1.150089	C	6.820672	-0.099557	0.403948
C	-1.806202	-1.373351	1.837605	H	7.726435	0.392384	0.059185
C	-1.612064	-2.630184	1.134223	C	6.703154	-1.429519	0.443319
C	-0.327262	-3.183239	1.110002	H	7.506637	-2.091735	0.131601
C	0.743285	-2.463191	1.777953	H	5.306082	-1.805572	2.017235
C	1.989655	-2.666543	1.069024	H	5.532293	0.608318	1.953529
C	2.917589	-1.619533	1.051740	C	4.084981	-1.986533	-1.197260
C	2.584558	-0.387564	1.727189	H	4.036713	-3.074748	-1.117113
C	2.417153	1.957559	1.053691	H	3.204112	-1.654267	-1.751232
C	3.134376	0.756088	1.038728	H	4.975869	-1.749839	-1.783981
C	1.077206	3.645713	0.153927	C	4.287050	0.844552	-1.245913
C	2.336128	3.115458	0.134628	H	3.348559	0.640214	-1.766719
C	-2.222913	2.869940	0.182324	H	4.419123	1.928016	-1.213366
C	-3.120843	1.838319	0.194176	H	5.110482	0.441274	-1.840498
C	-3.433333	-1.530837	0.201640				
C	-2.740684	-2.710159	0.194909				
C	0.361388	-4.081254	0.173435				
C	1.697000	-3.794209	0.154972				
C	4.168067	-1.361011	0.206639				
C	4.305096	0.265371	0.180865				
H	0.733725	4.456313	-0.477156				
H	-2.266165	3.725637	-0.480663				

Adduct of the reaction of butadiene with Fragment 2 substituted with two *i*-Pr groupMolecular formula: C₄₀H₂₈

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.581838

Thermal correction to Enthalpy= 0.582783

Thermal correction to Gibbs Free Energy= 0.501076

Sum of electronic and zero-point Energies= -1540.436881

Sum of electronic and thermal Energies= -1540.409009

Sum of electronic and thermal Enthalpies= -1540.408065

Sum of electronic and thermal Free Energies= -1540.489772

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

365.109 123.461 171.965

Cartesian coordinates

	H	-4.203009	-0.600590	-0.411007
	H	-3.050254	-2.882404	-0.951004
	H	-0.337992	-4.316913	-1.309133
Atom X Y Z	H	2.236383	-4.020126	-1.291304
C 1.631862 -0.634525 2.477295	H	3.499108	3.578108	0.273343
C 0.998997 0.602552 2.793519	C	5.507651	0.941557	-0.149446
C -0.416967 0.383354 2.827301	H	5.926273	0.947322	-1.164501
C -0.654489 -1.000587 2.535532	C	5.394885	-1.717719	1.242665
C 0.613893 -1.636552 2.338708	H	5.810809	-2.720321	1.106720
C 1.488609 1.759768 2.237894	C	6.565107	0.448665	0.790855
C 0.618109 2.855225 1.841447	H	7.414994	1.108266	0.955798
C -0.764128 2.634562 1.855375	C	6.521777	-0.739629	1.386879
C -1.252966 1.338845 2.297845	H	7.325141	-1.037912	2.058919
C -2.442888 0.991487 1.545841	H	4.881279	-1.769906	2.210252
C -2.672264 -0.360380 1.251581	H	5.300877	1.994232	0.075617
C -1.710852 -1.339983 1.718609	C	4.861716	-3.808276	-0.851542
C -1.625603 -2.425361 0.758828	H	4.717346	-4.391083	-1.767898
C -0.385991 -3.051791 0.575603	H	5.871027	-4.036515	-0.494583
C 0.747158 -2.571807 1.343108	H	4.158431	-4.176080	-0.102881
C 1.975352 -2.741228 0.585155	C	3.479363	1.894162	-2.056008
C 2.985351 -1.789913 0.753485	H	4.469438	2.352205	-2.002356
C 2.705048 -0.647255 1.602730	H	3.190208	1.883226	-3.112451
C 2.696660 1.789090 1.438362	H	2.770148	2.543256	-1.539650
C 3.276577 0.564393 1.071881	C	4.700141	-2.299329	-1.164086
C 1.484168 3.751177 1.063142	H	3.860193	-2.207712	-1.861866
C 2.687363 3.142451 0.839906	C	3.424192	0.444912	-1.526152
C -1.859515 3.186657 1.044256	H	3.988838	-0.143716	-2.254432
C -2.826554 2.236152 0.861583	C	1.956794	-0.011945	-1.614535
C -3.378678 -1.028862 0.146504	H	1.823366	-1.084504	-1.480932
C -2.775316 -2.223264 -0.136375	H	1.332956	0.499784	-0.875393
C 0.215870 -3.784859 -0.545015	H	1.562697	0.243723	-2.604266
C 1.573992 -3.627179 -0.532820	C	5.977481	-1.855929	-1.905109
C 4.338621 -1.447171 0.096260	H	6.840950	-1.848208	-1.233202
C 4.163742 0.167852 -0.137840	H	6.193775	-2.561962	-2.714143
H 1.195971 4.723387 0.682435	H	5.897885	-0.864828	-2.355499
H -1.858584 4.169287 0.588081				
H -3.705075 2.354986 0.238785				

Adduct of the reaction of butadiene with Fragment 2 substituted with two F groupMolecular formula: C₃₄H₁₄F₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.388544

Thermal correction to Enthalpy= 0.389488

Thermal correction to Gibbs Free Energy= 0.319310

Sum of electronic and zero-point Energies= -1503.230641

Sum of electronic and thermal Energies= -1503.209050

Sum of electronic and thermal Enthalpies= -1503.208106

Sum of electronic and thermal Free Energies= -1503.278283

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

243.815 97.100 147.701

Cartesian coordinates

Atom X Y Z

C 1.418114 -0.267713 2.657290
C 0.684827 0.963101 2.613693
C -0.714672 0.647177 2.572348
C -0.845840 -0.780190 2.583034
C 0.473032 -1.344919 2.630504
C 1.154169 2.001449 1.840669
C 0.271367 2.878603 1.089630
C -1.092146 2.576308 1.058959
C -1.549541 1.391922 1.769139
C -2.649196 0.797434 1.037061
C -2.777262 -0.598040 1.047330
C -1.803257 -1.372120 1.789476
C -1.570196 -2.630297 1.097236
C -0.284310 -3.175045 1.133792
C 0.744650 -2.462260 1.872920
C 2.017434 -2.650073 1.212896
C 2.941134 -1.612124 1.259170
C 2.595336 -0.381001 1.924507
C 2.439479 1.945290 1.180704
C 3.158901 0.757404 1.243167
C 1.152881 3.573650 0.137286
C 2.405334 3.032549 0.184421
C -2.138198 2.843677 0.061115
C -3.038458 1.815246 0.048057
C -3.346147 -1.542037 0.072231
C -2.648490 -2.717076 0.101678
C 0.454382 -4.032412 0.192350
C 1.784451 -3.727548 0.232645
C 4.146422 -1.340776 0.377776
C 4.293444 0.259386 0.366796
H 0.829495 4.336341 -0.560472
H -2.146459 3.688476 -0.616784

H -3.867729 1.721605 -0.642670
H -4.145015 -1.309023 -0.621387
H -2.810888 -3.555976 -0.564030
H -0.003366 -4.733955 -0.494303
H 2.542355 -4.136275 -0.422518
H 3.224456 3.286787 -0.475163
C 5.686635 0.730630 0.824650
H 5.780352 1.789212 0.565725
C 5.431226 -2.052033 0.843250
H 5.330312 -3.113108 0.597612
C 6.782186 -0.107139 0.211253
H 7.644275 0.385558 -0.228643
C 6.660338 -1.435848 0.220462
H 7.417847 -2.083069 -0.211684
H 5.487372 -1.987878 1.939103
H 5.731833 0.671114 1.921284
F 4.125069 0.708668 -0.942407
F 3.897416 -1.768869 -0.925735

Adduct of the reaction of butadiene with Fragment 2 substituted with two COOH groupMolecular formula: C₃₆H₁₆O₄

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.438343

Thermal correction to Enthalpy= 0.439287

Thermal correction to Gibbs Free Energy= 0.360161

Sum of electronic and zero-point Energies= -1681.841789

Sum of electronic and thermal Energies= -1681.816208

Sum of electronic and thermal Enthalpies= -1681.815264

Sum of electronic and thermal Free Energies= -1681.894390

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

275.064 111.933 166.534

Cartesian coordinates

Atom X Y Z

C	1.470931	-0.213559	2.541837	H	-3.914728	1.641534	-0.626643
C	0.730456	1.011947	2.509319	H	-4.174034	-1.410088	-0.489213
C	-0.665570	0.686169	2.527248	H	-2.839635	-3.652629	-0.367962
C	-0.785305	-0.740278	2.588937	H	-0.022694	-4.907103	-0.244641
C	0.538504	-1.294122	2.603795	H	2.513977	-4.313513	-0.301624
C	1.165756	2.034005	1.701904	H	3.199684	3.445043	-0.566346
C	0.254683	2.899426	0.974869	C	5.673923	0.574856	1.086456
C	-1.105570	2.572730	0.979417	H	5.848204	1.651416	1.101740
C	-1.529537	1.399604	1.726973	C	5.380371	-2.120626	0.658625
C	-2.642767	0.772950	1.043911	H	5.309488	-3.147561	0.292339
C	-2.761181	-0.623179	1.106440	C	6.839876	-0.176551	0.501655
C	-1.763094	-1.365419	1.849945	H	7.745691	0.360087	0.239400
C	-1.547621	-2.654521	1.211132	C	6.686349	-1.480892	0.270133
C	-0.261081	-3.201344	1.237997	H	7.461941	-2.087655	-0.186035
C	0.793281	-2.437678	1.885507	H	5.310980	-2.173984	1.752835
C	2.039388	-2.648269	1.180543	H	5.486550	0.258400	2.120848
C	2.931583	-1.576885	1.093348	O	4.778001	-1.987584	-2.082445
C	2.603062	-0.337783	1.746616	O	5.445838	1.764649	-1.357697
C	2.442323	1.993785	1.020334	O	2.585221	-1.810833	-1.641404
C	3.157579	0.798144	1.053892	O	3.474751	0.852949	-1.903009
C	1.114688	3.628565	0.029131	C	3.885811	-1.737078	-1.300419
C	2.381448	3.118309	0.062390	C	4.525195	1.031799	-1.071749
C	-2.182989	2.802609	0.005001	H	2.569611	-2.034926	-2.587225
C	-3.068965	1.761425	0.039715	H	3.675876	1.371320	-2.700753
C	-3.355118	-1.610742	0.191148				
C	-2.656681	-2.784987	0.254318				
C	0.449155	-4.134335	0.349844				
C	1.777398	-3.820896	0.320251				
C	4.123108	-1.321324	0.160604				
C	4.370959	0.295794	0.268629				
H	0.777455	4.411760	-0.638886				
H	-2.221893	3.630608	-0.692424				

Adduct of the reaction of butadiene with Fragment 2 substituted with two CF₃ groupMolecular formula: C₃₆H₁₄F₆

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.419958

Thermal correction to Enthalpy= 0.420903

Thermal correction to Gibbs Free Energy= 0.339406

Sum of electronic and zero-point Energies= -1978.791172

Sum of electronic and thermal Energies= -1978.764311

Sum of electronic and thermal Enthalpies= -1978.763367

Sum of electronic and thermal Free Energies= -1978.844863

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

263.528 116.719 171.524

Cartesian coordinates

	H	-4.120018	-1.660247	-0.239351
	H	-2.696533	-3.838329	-0.015419
Atom	X	Y	Z	
C	1.581608	-0.043972	2.455205	H 0.166056 -4.997117 0.101444
C	0.792177	1.151315	2.382710	H 2.660827 -4.310416 -0.137719
C	-0.586712	0.773336	2.481403	H 3.053584 3.515335 -0.901063
C	-0.645440	-0.649302	2.640562	C 5.567925 0.438651 1.334611
C	0.699608	-1.150132	2.626389	H 6.099047 1.391225 1.264088
C	1.153429	2.130260	1.493652	C 5.235887 -2.111040 -0.232608
C	0.182392	2.912023	0.753157	H 5.610287 -2.113351 -1.263017
C	-1.162530	2.532818	0.832250	C 6.547087 -0.696285 1.350175
C	-1.508636	1.396521	1.670169	H 7.416658 -0.558849 1.989327
C	-2.620892	0.682541	1.076556	C 6.386229 -1.836746 0.686145
C	-2.680735	-0.709706	1.238789	H 7.136214 -2.620590 0.761763
C	-1.625753	-1.360056	1.989318	H 4.853240 -3.121369 -0.053409
C	-1.384219	-2.683534	1.434827	H 5.064307 0.468292 2.306968
C	-0.077438	-3.180389	1.444887	C 4.983018 1.259188 -0.956277
C	0.974488	-2.329326	1.978154	C 3.290918 -1.224702 -1.482939
C	2.190574	-2.534295	1.214746	F 2.871831 -2.493144 -1.702997
C	3.029595	-1.428692	1.009746	F 2.209081 -0.431196 -1.541798
C	2.674337	-0.171627	1.614766	F 4.083670 -0.929046 -2.538483
C	2.418335	2.115125	0.780656	F 4.070141 1.500682 -1.916377
C	3.189853	0.961619	0.876067	F 5.368499 2.486522 -0.511327
C	0.982394	3.628555	-0.252120	F 6.062231 0.694920 -1.535258
C	2.276231	3.191340	-0.225141	
C	-2.285601	2.655088	-0.109731	
C	-3.125599	1.584545	0.028414	
C	-3.269659	-1.781866	0.420786	
C	-2.524478	-2.923065	0.537781	
C	0.628667	-4.155224	0.601538	
C	1.937786	-3.792486	0.475893	
C	4.046947	-1.120527	-0.126864	
C	4.458597	0.412397	0.212127	
H	0.589866	4.351906	-0.956402	
H	-2.384698	3.431713	-0.858362	
H	-3.989426	1.387692	-0.594989	

Adduct of the reaction of butadiene with Fragment 2 substituted with two CHO groupMolecular formula: C₃₆H₁₆O₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.425388

Thermal correction to Enthalpy= 0.426332

Thermal correction to Gibbs Free Energy= 0.350176

Sum of electronic and zero-point Energies= -1531.354139

Sum of electronic and thermal Energies= -1531.330142

Sum of electronic and thermal Enthalpies= -1531.329198

Sum of electronic and thermal Free Energies= -1531.405354

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

266.935 105.118 160.284

Cartesian coordinates

Atom X Y Z

C	1.445267	-0.270968	2.592653	H	-3.867405	1.742611	-0.623668
C	0.709229	0.957331	2.583878	H	-4.136194	-1.303477	-0.632477
C	-0.688360	0.637573	2.554074	H	-2.803682	-3.550886	-0.593359
C	-0.814777	-0.790566	2.550418	H	0.010537	-4.786951	-0.493447
C	0.505192	-1.350848	2.577562	H	2.555916	-4.220558	-0.429174
C	1.168061	2.009068	1.825929	H	3.234263	3.442764	-0.404005
C	0.275275	2.903180	1.108762	C	5.707145	0.738607	0.864909
C	-1.086748	2.587643	1.075676	H	5.838493	1.805569	0.674291
C	-1.532064	1.388411	1.766856	C	5.460478	-2.015821	0.828629
C	-2.633776	0.797604	1.033657	H	5.400115	-3.083172	0.606823
C	-2.757161	-0.598542	1.029887	C	6.831570	-0.072775	0.275594
C	-1.776548	-1.377442	1.759342	H	7.697770	0.437291	-0.134029
C	-1.548295	-2.632516	1.061448	C	6.711576	-1.401466	0.256622
C	-0.262603	-3.182029	1.091722	H	7.473951	-2.046512	-0.168811
C	0.772959	-2.462507	1.813449	H	5.453769	-1.911232	1.921667
C	2.041688	-2.650204	1.143290	H	5.673595	0.605208	1.954239
C	2.956102	-1.595587	1.160993	O	4.618052	-2.623733	-1.733406
C	2.604362	-0.371007	1.832635	O	5.012722	1.551742	-1.682994
C	2.451178	1.976103	1.157594	C	3.898813	-1.855439	-1.135702
C	3.166534	0.777451	1.169318	C	4.167588	0.896539	-1.116275
C	1.150485	3.645346	0.188607	H	2.940207	-1.517824	-1.581534
C	2.410686	3.118627	0.219382	H	3.177747	0.725709	-1.588122
C	-2.141646	2.864585	0.089413				
C	-3.034605	1.829410	0.063667				
C	-3.332021	-1.538622	0.054221				
C	-2.634837	-2.714699	0.074135				
C	0.469021	-4.060306	0.166004				
C	1.801887	-3.761956	0.197914				
C	4.177875	-1.326691	0.277648				
C	4.327481	0.303800	0.290044				
H	0.827042	4.444964	-0.466424				
H	-2.161034	3.720905	-0.573644				

Adduct of the reaction of butadiene with Fragment 2 substituted with two CN groupMolecular formula: C₃₆H₁₄N₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.403522

Thermal correction to Enthalpy= 0.404466

Thermal correction to Gibbs Free Energy= 0.329720

Sum of electronic and zero-point Energies= -1489.213912

Sum of electronic and thermal Energies= -1489.190306

Sum of electronic and thermal Enthalpies= -1489.189362

Sum of electronic and thermal Free Energies= -1489.264109

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

253.214 103.830 157.318

Cartesian coordinates

Atom X Y Z

C	1.458585	-0.273307	2.553518	H	-3.927030	1.747401	-0.535248
C	0.725460	0.956068	2.557385	H	-4.202761	-1.294938	-0.534042
C	-0.674471	0.639775	2.565092	H	-2.873211	-3.543842	-0.529476
C	-0.804018	-0.787351	2.565866	H	-0.061471	-4.770792	-0.513299
C	0.516281	-1.350554	2.558462	H	2.479992	-4.200308	-0.522708
C	1.167024	2.003667	1.784613	H	3.168683	3.402897	-0.526826
C	0.258934	2.898485	1.088062	C	5.694316	0.721842	0.870276
C	-1.103560	2.588554	1.092151	H	5.827597	1.793520	0.707065
C	-1.535176	1.391458	1.798039	C	5.446789	-2.015513	0.867224
C	-2.656134	0.803143	1.093749	H	5.386114	-3.093365	0.701670
C	-2.782705	-0.592893	1.094380	C	6.838636	-0.090626	0.324766
C	-1.785659	-1.372589	1.799048	H	7.718063	0.412656	-0.064592
C	-1.576491	-2.628493	1.094314	C	6.718234	-1.420133	0.323019
C	-0.291900	-3.178356	1.090491	H	7.493137	-2.072161	-0.067721
C	0.762379	-2.461007	1.786484	H	5.384663	-1.857186	1.951953
C	2.014135	-2.653301	1.084647	H	5.603264	0.574792	1.954517
C	2.933092	-1.606435	1.098444	C	4.272151	0.839978	-1.125265
C	2.604485	-0.377379	1.773852	C	4.022483	-1.874002	-1.125733
C	2.432941	1.967262	1.082940	N	3.920018	-2.360829	-2.174777
C	3.148626	0.772235	1.097836	N	4.261096	1.336932	-2.174508
C	1.112146	3.631656	0.140307				
C	2.370645	3.102351	0.138141				
C	-2.182229	2.866912	0.132857				
C	-3.078214	1.834257	0.132135				
C	-3.383269	-1.532097	0.133520				
C	-2.687827	-2.709172	0.135346				
C	0.415621	-4.054360	0.143951				
C	1.748825	-3.760124	0.141394				
C	4.173416	-1.340722	0.235889				
C	4.321512	0.287719	0.236349				
H	0.771036	4.420863	-0.518193				
H	-2.214410	3.720471	-0.533089				

Adduct of the reaction of butadiene with Fragment 2 substituted with two NO₂ groupMolecular formula: C₃₄H₁₄N₂O₄

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.412789

Thermal correction to Enthalpy= 0.413733

Thermal correction to Gibbs Free Energy= 0.335727

Sum of electronic and zero-point Energies= -1713.719419

Sum of electronic and thermal Energies= -1713.694383

Sum of electronic and thermal Enthalpies= -1713.693439

Sum of electronic and thermal Free Energies= -1713.771445

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

259.029 109.048 164.178

Cartesian coordinates

Atom X Y Z

C	1.462663	-0.226965	2.548985	H	-3.910504	1.689075	-0.602987
C	0.725624	1.000604	2.532356	H	-4.177196	-1.360915	-0.516207
C	-0.672331	0.676978	2.543988	H	-2.847832	-3.607176	-0.431754
C	-0.795409	-0.749750	2.580945	H	-0.036660	-4.862926	-0.331994
C	0.528440	-1.306263	2.584155	H	2.496409	-4.277076	-0.379561
C	1.163781	2.036937	1.744322	H	3.190271	3.443667	-0.541361
C	0.255803	2.912301	1.025360	C	5.683364	0.637825	1.032825
C	-1.103986	2.588910	1.022937	H	5.840687	1.716124	0.996281
C	-1.532070	1.404648	1.752783	C	5.392464	-2.089227	0.647012
C	-2.645059	0.792188	1.057081	H	5.311044	-3.109778	0.264220
C	-2.766649	-0.604284	1.095822	C	6.842408	-0.131130	0.454869
C	-1.771171	-1.359974	1.828072	H	7.747530	0.400035	0.181211
C	-1.557426	-2.639352	1.166673	C	6.694093	-1.439923	0.253511
C	-0.273002	-3.188126	1.185569	H	7.473535	-2.050765	-0.189477
C	0.781803	-2.437711	1.847185	H	5.330227	-2.165558	1.740154
C	2.027838	-2.640960	1.137749	H	5.529214	0.372200	2.087347
C	2.924451	-1.571743	1.082764	N	3.884474	-1.687088	-1.288408
C	2.595167	-0.340890	1.753403	N	4.380453	0.995035	-1.082814
C	2.439545	2.003901	1.060613	O	4.880331	-1.721051	-2.005071
C	3.151733	0.808153	1.089226	O	5.355643	1.676371	-1.375987
C	1.116373	3.643621	0.081490	O	2.748541	-1.950349	-1.646244
C	2.381710	3.131173	0.106681	O	3.377112	0.864593	-1.771868
C	-2.178756	2.836710	0.050543				
C	-3.067071	1.797568	0.068037				
C	-3.361332	-1.575378	0.163387				
C	-2.665868	-2.751888	0.207312				
C	0.436647	-4.107594	0.282928				
C	1.765659	-3.800471	0.259528				
C	4.132672	-1.291252	0.196098				
C	4.356959	0.310703	0.307141				
H	0.777472	4.422255	-0.590600				
H	-2.212709	3.673962	-0.635684				

Aromatized adduct for the reaction of butadiene with Fragment 1Molecular formula: C₃₄H₁₄

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.381663

Thermal correction to Enthalpy= 0.382608

Thermal correction to Gibbs Free Energy= 0.316562

Sum of electronic and zero-point Energies= -1303.689500

Sum of electronic and thermal Energies= -1303.670057

Sum of electronic and thermal Enthalpies= -1303.669113

Sum of electronic and thermal Free Energies= -1303.735159

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 239.497 89.001 139.005

Cartesian coordinates

Atom X Y Z

C -1.354713 -0.424365 -1.380729
C -1.142959 0.983749 -1.258970
C 0.147518 1.464526 -1.303205
C 1.267961 0.584483 -1.431071
C 1.031662 -0.773437 -1.537878
C -0.296782 -1.300840 -1.494399
C 2.380771 1.087751 -0.677956
C 3.312975 0.160604 -0.203920
C 3.081792 -1.264306 -0.314597
C 1.888450 -1.692462 -0.917198
C 3.817547 -2.305916 0.387151
C 3.175657 -3.580476 0.595216
C 1.810585 -3.824283 0.184953
C 1.147498 -2.890316 -0.561627
C -0.306309 -2.585958 -0.842790
C -1.484476 -2.988396 -0.220406
C -2.601622 -2.067909 -0.064621
C -2.470876 -0.765867 -0.597591
C -3.068464 0.416094 -0.046216
C -4.083689 0.218870 0.874932
C -4.417327 -1.111862 1.252526
C -3.686834 -2.222494 0.844542
C 0.528245 2.532857 -0.472690
C -0.438389 3.233441 0.282666
C -1.803142 2.725464 0.293262
C -2.139491 1.560119 -0.389182
C 0.105748 4.166158 1.211118
C 1.479246 4.217978 1.422310
C 2.392507 3.311591 0.814951
C 1.917627 2.420558 -0.133260

H 4.119288 0.492971 0.444177
H -4.587632 1.049033 1.362118
H -5.226451 -1.254758 1.963112
H -3.907607 -3.196216 1.274015
H -2.488507 3.157147 1.019390
H -0.551998 4.793360 1.807237
H 1.866497 4.922953 2.152420
H 3.425056 3.295757 1.152884
H -1.519381 -3.914892 0.348422
H 1.328607 -4.733773 0.534939
C 3.886299 -4.586408 1.291469
H 3.400009 -5.544774 1.454401
C 5.124637 -2.120544 0.883478
H 5.624584 -1.172392 0.710406
C 5.793048 -3.131250 1.552965
H 6.803945 -2.964815 1.913112
C 5.169163 -4.374355 1.760210
H 5.694866 -5.165900 2.285654

Aromatized adduct for the reaction of butadiene with Fragment 2Molecular formula: C₃₄H₁₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.356921

Thermal correction to Enthalpy= 0.357865

Thermal correction to Gibbs Free Energy= 0.293496

Sum of electronic and zero-point Energies= -1302.409936

Sum of electronic and thermal Energies= -1302.391102

Sum of electronic and thermal Enthalpies= -1302.390158

Sum of electronic and thermal Free Energies= -1302.454527

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 223.971 86.938 135.476

Cartesian coordinates

Atom X Y Z

C -0.375285 -0.065864 2.016806
C 0.440528 -1.237453 1.886994
C 1.793873 -0.812059 1.672021
C 1.812927 0.622392 1.671661
C 0.471353 1.083588 1.886281
C -0.043076 -2.317656 1.184816
C 0.808237 -3.130050 0.332534
C 2.128344 -2.715878 0.123499
C 2.577838 -1.494511 0.769657
C 3.525379 -0.818671 -0.096433
C 3.544045 0.581966 -0.096769
C 2.614876 1.283292 0.769038
C 2.197984 2.515782 0.122155
C 0.889333 2.965005 0.330917
C 0.016721 2.175990 1.183626
C -1.344208 2.267094 0.691600
C -2.175777 1.150197 0.829398
C -1.627874 -0.049279 1.437557
C -1.405974 -2.372687 0.692767
C -2.207514 -1.233992 0.829866
C -0.124606 -3.907020 -0.495428
C -1.403711 -3.470591 -0.287599
C 3.054838 -2.906640 -1.001416
C 3.861769 -1.809614 -1.129184
C 3.906557 1.562990 -1.130141
C 3.129121 2.681172 -1.002945
C -0.022454 3.765875 -0.497699
C -1.312728 3.363809 -0.289584
C -3.366271 0.689832 0.087456
C -3.385333 -0.742423 0.087703
H 0.167245 -4.655052 -1.222561

H 3.043105 -3.753086 -1.677386
H 4.584262 -1.657190 -1.921899
H 4.624665 1.390853 -1.922801
H 3.139825 3.527175 -1.679493
H 0.289366 4.505107 -1.225546
H -2.172193 3.737232 -0.831899
H -2.272830 -3.821652 -0.829467
C -4.400238 -1.426186 -0.577818
H -4.430745 -2.511557 -0.572742
C -4.362468 1.400217 -0.578401
H -4.363843 2.486020 -0.573827
C -5.396963 -0.698595 -1.236556
H -6.197508 -1.225777 -1.746860
C -5.378306 0.699253 -1.236840
H -6.164480 1.247406 -1.747389

NH₂-HMolecular formula: NH₃

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.037302

Thermal correction to Enthalpy= 0.038246

Thermal correction to Gibbs Free Energy= 0.015363

Sum of electronic and zero-point Energies= -56.523329

Sum of electronic and thermal Energies= -56.520467

Sum of electronic and thermal Enthalpies= -56.519522

Sum of electronic and thermal Free Energies= -56.542406

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin
23.407 6.325 48.162

Cartesian coordinates

Atom X Y Z

N 1.738631 0.297904 0.000000
H 2.135986 -0.639399 0.000000
H 2.136359 0.766353 0.811607
H 2.136359 0.766353 -0.811607

OMe-HMolecular formula: CH₄O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.054706

Thermal correction to Enthalpy= 0.055650

Thermal correction to Gibbs Free Energy= 0.028675

Sum of electronic and zero-point Energies= -115.672560

Sum of electronic and thermal Energies= -115.669258

Sum of electronic and thermal Enthalpies= -115.668314

Sum of electronic and thermal Free Energies= -115.695289

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin
34.328 8.709 56.774

Cartesian coordinates

Atom X Y Z

C -0.661664 -0.019442 0.000000
H -1.082201 0.989439 -0.000001
H -1.038268 -0.542915 -0.891823
H -1.038268 -0.542914 0.891823
O 0.749367 0.122045 0.000000
H 1.133788 -0.763319 0.000000

OH-H

Molecular formula: H2O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.024204

Thermal correction to Enthalpy= 0.025148

Thermal correction to Gibbs Free Energy= 0.003058

Sum of electronic and zero-point Energies= -76.398368

Sum of electronic and thermal Energies= -76.395533

Sum of electronic and thermal Enthalpies= -76.394589

Sum of electronic and thermal Free Energies= -76.416679

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

15.188 6.003 46.493

Cartesian coordinates

Atom X Y Z

O -0.022803 0.000000 -0.016114

H 0.025652 0.000000 0.947893

H 0.902087 0.000000 -0.292233

Me-H

Molecular formula: CH4

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.047885

Thermal correction to Enthalpy= 0.048829

Thermal correction to Gibbs Free Energy= 0.025352

Sum of electronic and zero-point Energies= -40.478995

Sum of electronic and thermal Energies= -40.476129

Sum of electronic and thermal Enthalpies= -40.475185

Sum of electronic and thermal Free Energies= -40.498662

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

30.048 6.444 49.411

Cartesian coordinates

Atom X Y Z

C -1.849376 0.360502 -0.024210

H -1.485388 -0.669029 -0.024210

H -1.485370 0.875259 0.867385

H -1.485370 0.875259 -0.915804

H -2.941352 0.360515 -0.024210

***i*-Pr-H**

Molecular formula: C3H8

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.108198

Thermal correction to Enthalpy= 0.109142

Thermal correction to Gibbs Free Energy= 0.078019

Sum of electronic and zero-point Energies= -119.051677

Sum of electronic and thermal Energies= -119.047155

Sum of electronic and thermal Enthalpies= -119.046211

Sum of electronic and thermal Free Energies= -119.077334

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

67.895 14.756 65.504

Cartesian coordinates

Atom X Y Z

C -1.052150 -0.567362 0.021602

H -0.670815 -1.596369 -0.007419

H -0.670610 -0.077848 -0.883883

C -0.497238 0.146176 1.258108

H 0.597913 0.150175 1.263954

H -0.834021 1.188658 1.297235

H -0.833195 -0.342209 2.180229

C -2.583118 -0.590875 -0.019382

H -2.993978 0.425395 -0.027542

H -2.954739 -1.106904 -0.911022

H -2.993991 -1.104246 0.857739

F-H

Molecular formula: HF

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.011666

Thermal correction to Enthalpy= 0.012611

Thermal correction to Gibbs Free Energy= -0.007107

Sum of electronic and zero-point Energies= -100.418156

Sum of electronic and thermal Energies= -100.415795

Sum of electronic and thermal Enthalpies= -100.414851

Sum of electronic and thermal Free Energies= -100.434569

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

7.321 4.968 41.499

Cartesian coordinates

Atom X Y Z

F 0.000000 0.000000 0.092540

H 0.000000 0.000000 -0.832859

COOH-H

Molecular formula: CH2O2

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.036839

Thermal correction to Enthalpy= 0.037784

Thermal correction to Gibbs Free Energy= 0.009512

Sum of electronic and zero-point Energies= -189.720503

Sum of electronic and thermal Energies= -189.717263

Sum of electronic and thermal Enthalpies= -189.716319

Sum of electronic and thermal Free Energies= -189.744591

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

23.117 8.911 59.502

Cartesian coordinates

Atom X Y Z

C -0.130515 0.361852 -0.000032

H -0.034904 1.465190 0.000011

O -1.178538 -0.219002 0.000019

O 1.058604 -0.281510 0.000003

H 1.777465 0.367795 0.000009

CF₃-H

Molecular formula: CHF3

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.028929

Thermal correction to Enthalpy= 0.029873

Thermal correction to Gibbs Free Energy= 0.000362

Sum of electronic and zero-point Energies= -338.201920

Sum of electronic and thermal Energies= -338.198450

Sum of electronic and thermal Enthalpies= -338.197506

Sum of electronic and thermal Free Energies= -338.227017

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

18.153 10.185 62.111

Cartesian coordinates

Atom X Y Z

C 0.000000 0.000000 0.339252

H 0.000000 0.000000 1.433090

F 0.000000 1.258016 -0.128467

F 1.089474 -0.629008 -0.128467

F -1.089474 -0.629008 -0.128467

CHO-HMolecular formula: CH₂O

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.029586

Thermal correction to Enthalpy= 0.030530

Thermal correction to Gibbs Free Energy= 0.005055

Sum of electronic and zero-point Energies= -114.476480

Sum of electronic and thermal Energies= -114.473614

Sum of electronic and thermal Enthalpies= -114.472669

Sum of electronic and thermal Free Energies= -114.498144

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

18.565 6.411 53.616

Cartesian coordinates

Atom X Y Z

C 0.000006 0.529016 0.000000

H -0.937820 1.123848 0.000000

H 0.937738 1.124007 0.000000

O 0.000006 -0.677744 0.000000

CN-H

Molecular formula: CHN

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.019005

Thermal correction to Enthalpy= 0.019949

Thermal correction to Gibbs Free Energy= -0.002906

Sum of electronic and zero-point Energies= -93.408114

Sum of electronic and thermal Energies= -93.405576

Sum of electronic and thermal Enthalpies= -93.404632

Sum of electronic and thermal Free Energies= -93.427487

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin

11.926 6.388 48.103

Cartesian coordinates

Atom X Y Z

C 0.000000 0.000000 -0.502180

H 0.000000 0.000000 -1.570809

N 0.000000 0.000000 0.654841

NO₂-HMolecular formula: HNO₂

Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.024930
Thermal correction to Enthalpy= 0.025874
Thermal correction to Gibbs Free Energy= -0.001180
Sum of electronic and zero-point Energies= -205.667710
Sum of electronic and thermal Energies= -205.664750
Sum of electronic and thermal Enthalpies= -205.663806
Sum of electronic and thermal Free Energies= -205.690860

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin
15.644 7.173 56.941
Cartesian coordinates

Atom X Y Z
O 0.000000 1.100354 -0.220639
O 0.000000 -1.100354 -0.220639
N 0.000000 0.000000 0.310793
H 0.000000 0.000000 1.354666

H₂

Molecular formula: H2
Charge = 0 Multiplicity = 1

Hartree/particle

Thermal correction to Energy= 0.012534
Thermal correction to Enthalpy= 0.013478
Thermal correction to Gibbs Free Energy= -0.001314
Sum of electronic and zero-point Energies= -1.168366
Sum of electronic and thermal Energies= -1.166005
Sum of electronic and thermal Enthalpies= -1.165061
Sum of electronic and thermal Free Energies= -1.179853

E (Thermal) KCal/Mol CV Cal/Mol-Kelvin S Cal/Mol-Kelvin
7.865 4.968 31.132
Cartesian coordinates

Atom X Y Z
H 0.000000 0.000000 0.371396
H 0.000000 0.000000 -0.371396