Supplementary Materials

Reaction of Triazolic Aldehydes with Diisopropyl Zinc: Chirality Dissipation versus Amplification

Oleg A. Mikhaylov [1], Elena Sh. Saigitbatalova [2], Liliya Z. Latypova [2], Almira R. Kurbangalieva [2,*] and Ilya D. Gridnev [1,*]

[1] N. D. Zelinsky Institute of Organic Chemistry, Leninsky prosp. 47, Moscow 119991 Russia
[2] Biofunctional Chemistry Laboratory, A. Butlerov Institute of Chemistry, Kazan Federal University, 18 Kremlyovskaya Street, Kazan 420008, Russia
* Correspondence: akurbang@kpfu.ru (A.R.K); ilyaiochem@gmail.com (I.D.G.)

Content

1. Materials and Methods

1.1. General Information

Di*iso*propylzinc 1M solution in toluene (Sigma-Aldrich) was used as received without further purification. All solvents were purified and distilled using standard procedures. Analytical thin layer chromatography (TLC) was carried out on Sorbfil PTLC-AF-A-UF plates using acetone-chloroform (1:4) as the eluent and UV light (254 nm) as the visualizing agent. Silica gel 60A (Acros Organics, 400–230 mesh, 0.040–0.063 mm) was used for open-column chromatography. Melting points were recorded with a Boëtius melting point instrument and are uncorrected. NMR spectra were measured on a Bruker Avance 300 spectrometer at 300.13 MHz (^{1}H) and 75.47 MHz (^{13}C), Bruker Avance 600 spectrometer at 600.13 MHz (^{1}H) and 150.90 MHz (^{13}C) at 20 °C in the deuterated chloroform. The chemical shifts (δ) are expressed in parts per million (ppm) and are calibrated using residual undeuterated solvent peak as an internal reference ($CDCl_3$: δ_H 7.26, δ_C 77.16). All coupling constants (J) are reported in Hertz (Hz), and multiplicities are indicated as follows: s (singlet), d (doublet) and m (multiplet). High-resolution mass spectra (HRMS) were obtained through electrospray ionization (ESI) with positive (+) ion detection on a Bruker micrOTOF–QIII quadrupole time-of-flight mass spectrometer. The *ee* measurements were performed via HPLC analysis. HPLC analysis was performed on an HPLC system equipped with chiral stationary phase columns (AD-H, AS-H, OD-H, OJ-H), detection at 220 or 254 nm.

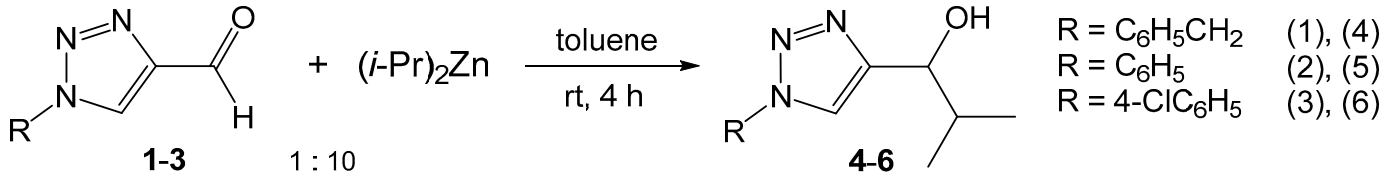
1.2. Chemical Synthesis.

1-Benzyl-1*H*-1,2,3-triazole-4-carbaldehyde (**1**) [1], 1-phenyl-1*H*-1,2,3-triazole-4-carboxaldehyde (**2**) and 1-(4-chlorophenyl)-1*H*-1,2,3-triazole-4-carboxaldehyde (**3**) [2] were synthesized according to the known methods.
All reactions were carried out using standard Schlenk techniques under argon atmosphere.

1. Song, H.; Rogers, N.J.; Brabec, V.; Clarkson, G.J.; Coverdale, J.P.C.; Kostrhunova, H.; Phillips, R.M.; Postings, M.; Shepherd, S.L.; Scott P. Triazole-based, optically-pure metallosupramolecules; highly potent and selective anticancer compounds. *Chem. Commun.* **2020**, *56*, 6392–6395.
2. Dai, Z.C.; Chen, Y.F.; Zhang, M.; Li, S.K. Yang, T.-T.; Shen, L.; Wang, J.X.; Qian, S.S.; Zhu, H.L.; Ye, Y.H. Synthesis and antifungal activity of 1,2,3-triazole phenylhydrazone derivatives. *Org. Biomol. Chem.* **2015**, *13*, 477–486.

2. Experimental section

General procedure for the alkylation reaction of triazolyl carbaldehydes using diisopropylzinc



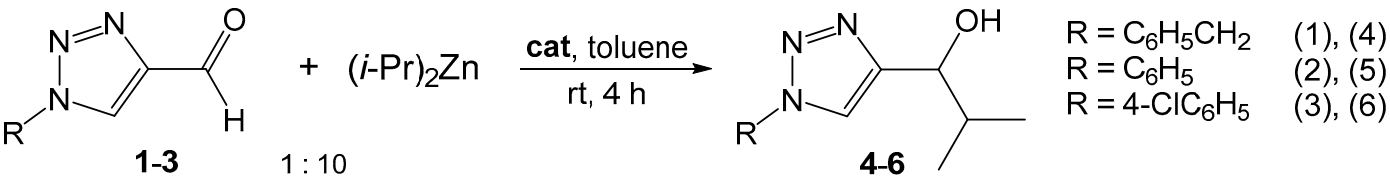
To the solution of aldehyde (0.50 mmol) in dry toluene (5 mL) with intense stirring was added dropwise the solution of (iPr)$_2$Zn (1M, 5 mL) *via* syringe under argon atmosphere. The reaction mixture was stirred for 4 hours at room temperature and was then quenched with aqueous HCl solution (0.1 M, 10 mL). After stirring for 15 minutes the reaction mixture was neutralized with saturated solution of $NaHCO_3$ (15 mL). The organic phase was separated and the colorless aqueous layer was extracted with $CHCl_3$ (3 × 10 mL). The solvent from the combined organic layers was removed *in vacuo*. The remaining yellow solid was purified by column chromatography (eluent acetone – chloroform, 1 : 4) to yield the corresponding alcohol. Samples were analyzed by chiral HPLC in order to determine *ee*.

1-(1-Benzyl-1*H*-1,2,3-triazol-4-yl)-2-methylpropan-1-ol (4): colorless crystals, 0.049 g (42% yield); mp 84 °C; R_f 0.26 (acetone – $CHCl_3$, 1:4); ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) δ 7.42–7.23 (m, 6H, Ar-H, H$_{triaz}$), 5.51 (s, 2H), 4.63 (d, ^3J = 5.9 Hz, 1H, CH–OH), 2.20–1.97 (m, 1H, CH(iPr)), 0.95 (d, 3H, ^3J = 6.8 Hz, CH_3), 0.91 (d, 3H, ^3J = 6.8 Hz, CH_3); ^{13}C {^{1}H} NMR ($CDCl_3$, 125 MHz, ppm) δ 150.79 (C$_{triaz}$), 134.80, 129.28, 128.90, 128.15 (C$_{Ar}$), 120.81 (C–H$_{triaz}$), 72.63 (C–OH), 54.32 (CH_2), 34.35 (CH(iPr)), 18.70, 17.47 (CH_3); HRMS (ESI) m/z 232.1444 (calcd for $C_{13}H_{18}N_3O$, 232.1444).

2-Methyl-1-(1-phenyl-1*H*-1,2,3-triazol-4-yl)propan-1-ol (5): colorless crystals, 0.052 g (48% yield); mp 107 °C; R_f = 0.38 (acetone – $CHCl_3$, 1:4); ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) δ 7.91 (s, 1H, H$_{triaz}$), 7.79–7.70 (m, 2H, Ar-H), 7.58–7.39 (m, 3H, Ar-H), 4.77 (d, ^3J = 5.8 Hz, 1H, CH–OH), 2.34–2.11 (m, 1H, CH(iPr)), 1.02 (d, 3H, ^3J = 6.8 Hz, CH_3), 0.99 (d, 3H, ^3J = 6.8 Hz, CH_3); ^{13}C {^{1}H} NMR ($CDCl_3$, 125 MHz, ppm) δ 151.10 (C$_{triaz}$), 137.27, 129.91, 128.87, 120.65 (C$_{Ar}$), 119.20 (CH$_{triaz}$), 72.63 (C–OH), 34.38 (CH(iPr)), 18.72, 17.48 (2CH_3); HRMS (ESI) m/z 218.1287 (calcd for $C_{12}H_{16}N_3O$, 218.1288).

1-(1-(4-Chlorophenyl)-1*H*-1,2,3-triazol-4-yl)-2-methylpropan-1-ol (6): colorless crystals, 0.06 g (48% yield); mp 143 °C; R_f = 0.38 (acetone – $CHCl_3$, 1:4); ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) δ 7.88 (s, 1H, H$_{triaz}$), 7.70, 7.51 (4H, AA'BB', ^3JAB = ^3JA'B' = 8.6 Hz, ^4JAA' = ^4JBB' = 2.5 Hz, ^5JAB' = ^5JA'B = 0.3 Hz, Ar-H), 4.77 (d, ^3J = 5.7 Hz, 1H, CH–OH), 2.28–2.11 (m, 1H, CH(iPr)), 1.01 (d, 3H, ^3J = 7.1 Hz, CH_3), 0.99 (d, 3H, ^3J = 7.1 Hz, CH_3); ^{13}C {^{1}H} NMR ($CDCl_3$, 125 MHz, ppm) δ 151.43 (C$_{triaz}$), 135.72, 134.63, 130.07, 121.75 (C$_{Ar}$), 119.15 (CH$_{triaz}$), 72.55 (C–OH), 34.33 (CH(iPr)), 18.70, 17.43 (CH_3); HRMS (ESI) m/z 252.0898 (calcd for $C_{12}H_{15}ClN_3O$ 252.0898).

General procedure for the alkylation reaction of triazolyl carbaldehydes using diisopropylzinc in the presence of chiral catalysts



To the solution of chiral catalyst **cat** (0.05 or 0.10 mmol) in dry toluene (5 mL) with intense stirring was added dropwise a solution of (iPr)$_2$Zn (1M, 5 mL) *via* syringe under argon atmosphere. Obtained mixture was stirred for 15 minutes at room temperature. The aldehyde (0.50 mmol) was dissolved in 5 mL of dry toluene and then was added dropwise to the reaction mixture under argon atmosphere. Reaction times, conditions and yields are given in a Table 1. Work up of the reaction mixture was carried out similarly to the general procedure described above.

General procedure for the alkylation reaction of triazolyl carbaldehydes using diisopropylzinc in the presence of autocatalyst

To the solution of alcohol (0.09 mmol) in dry toluene (5 mL) with intense stirring was added dropwise the solution of (iPr)$_2$Zn (1M, 4.5 mL) *via* syringe under argon atmosphere. Obtained mixture was stirred for 15 minutes at the room temperature. The aldehyde (0.45 mmol) was dissolved in 5 mL of dry toluene and then was added dropwise to the reaction mixture under a nitrogen atmosphere. The reaction mixture was stirred overnight at room temperature. Work up of the reaction mixture was carried out similarly to the general procedure described above.

3. NMR Spectra of alcohols 4-6

a)

b)

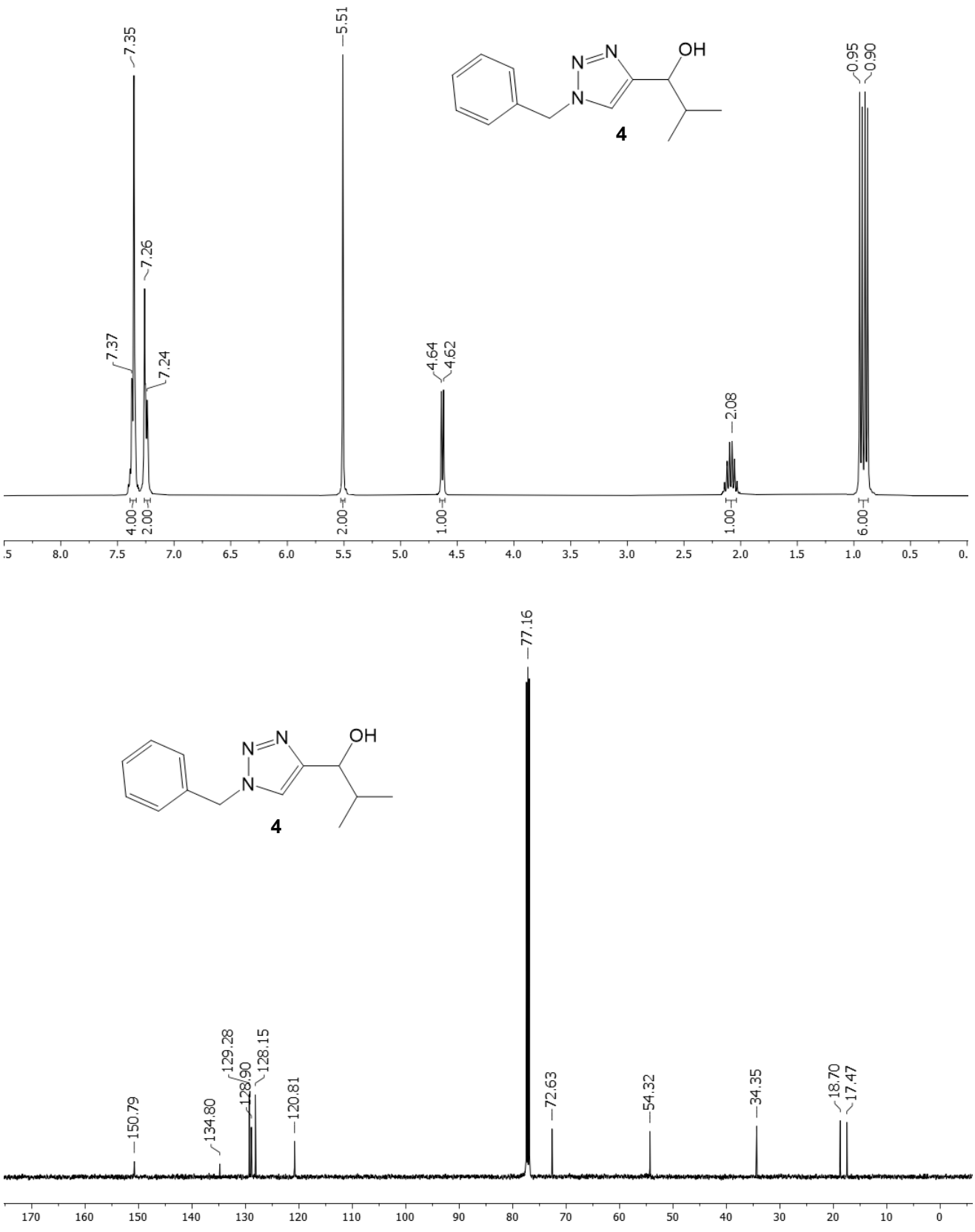
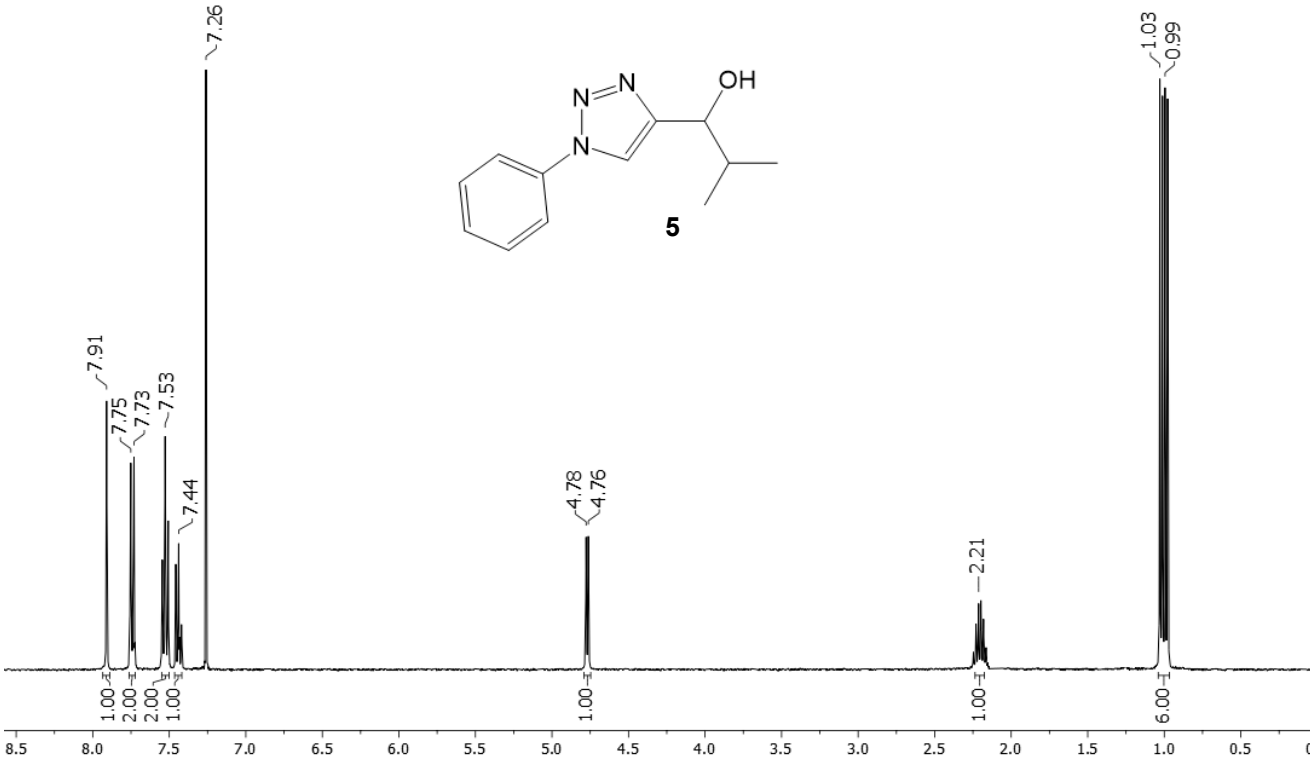


Figure S1. ^{1}H (a) and $^{13}C\{^{1}H\}$ (b) NMR spectra of compound **4** ($CDCl_3$).

a)



b)

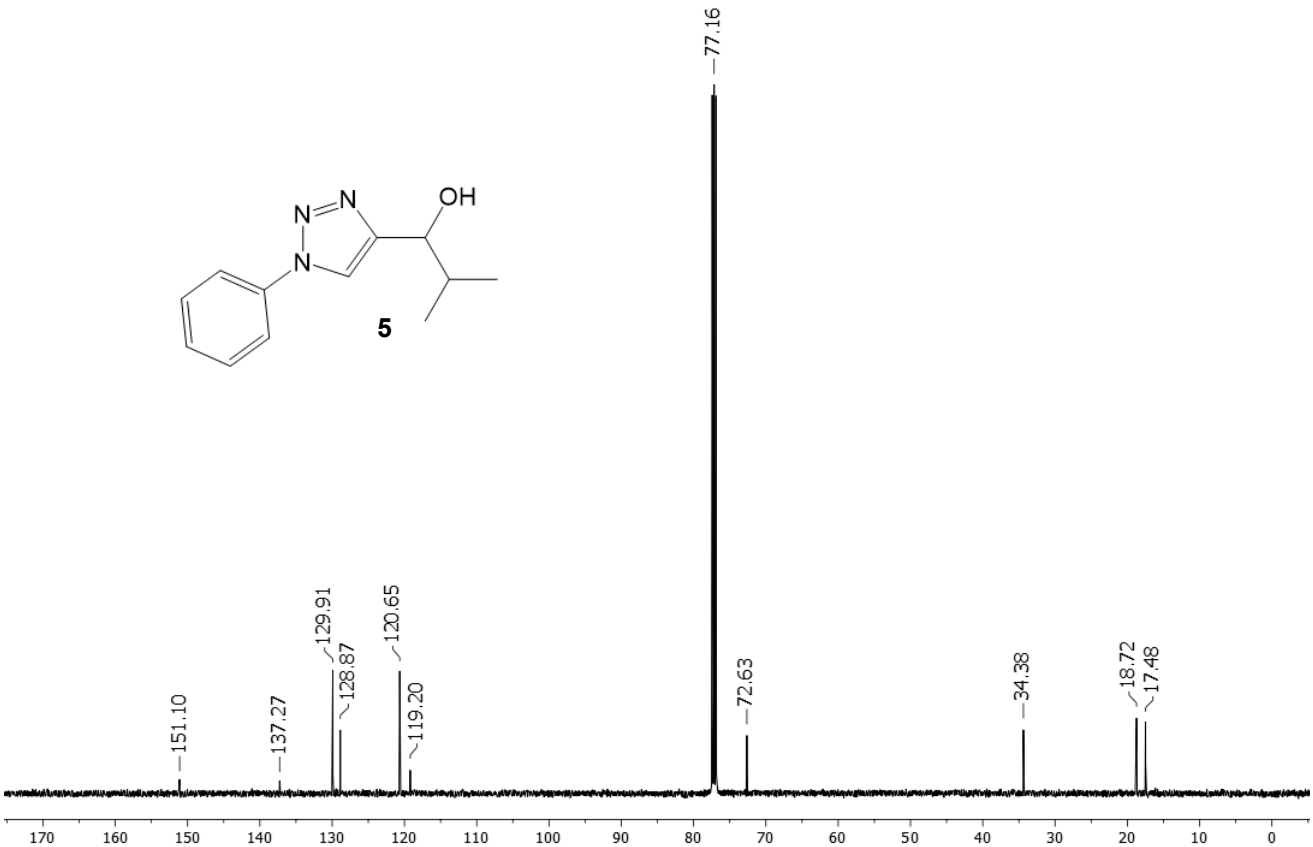
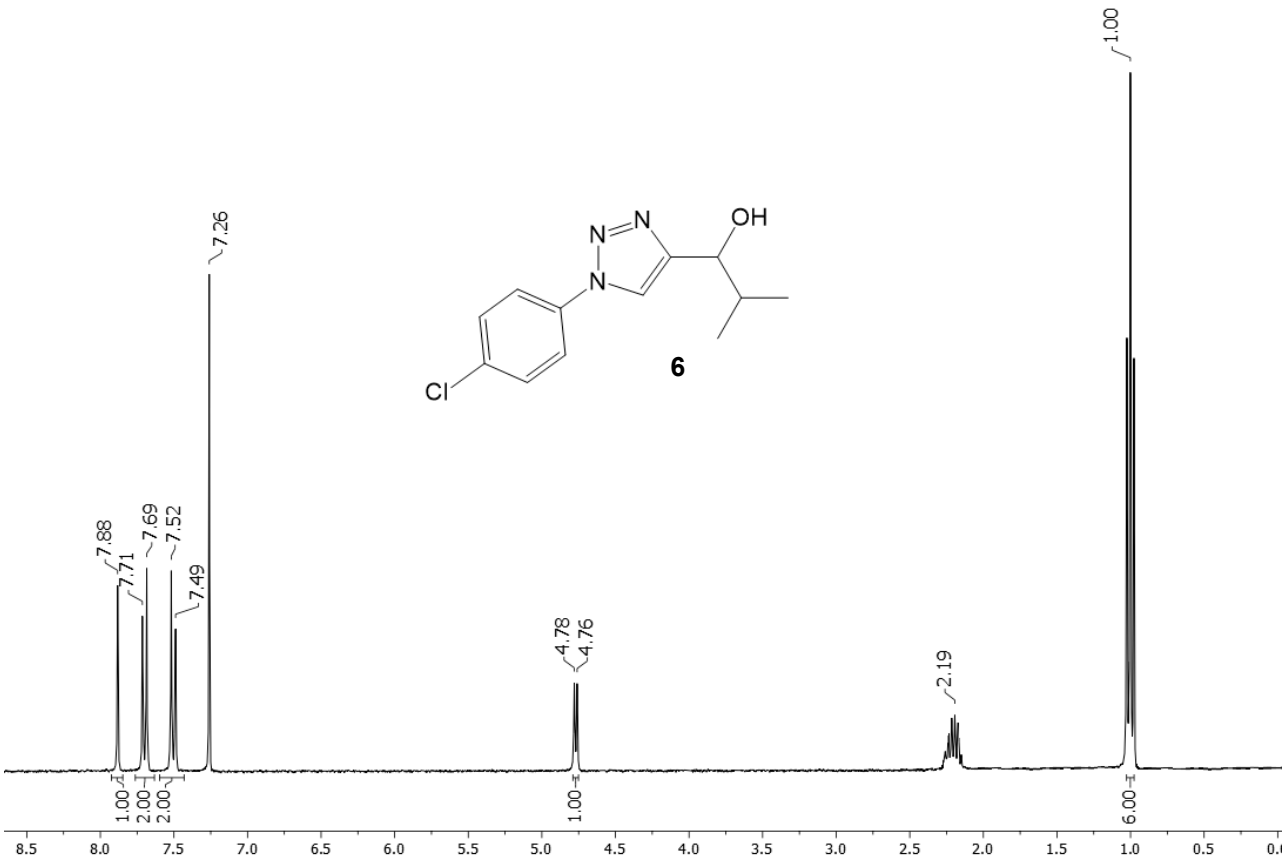


Figure S2. ^{1}H (a) and $^{13}C\{^{1}H\}$ (b) NMR spectra of compound **5** ($CDCl_3$).

a)



b)

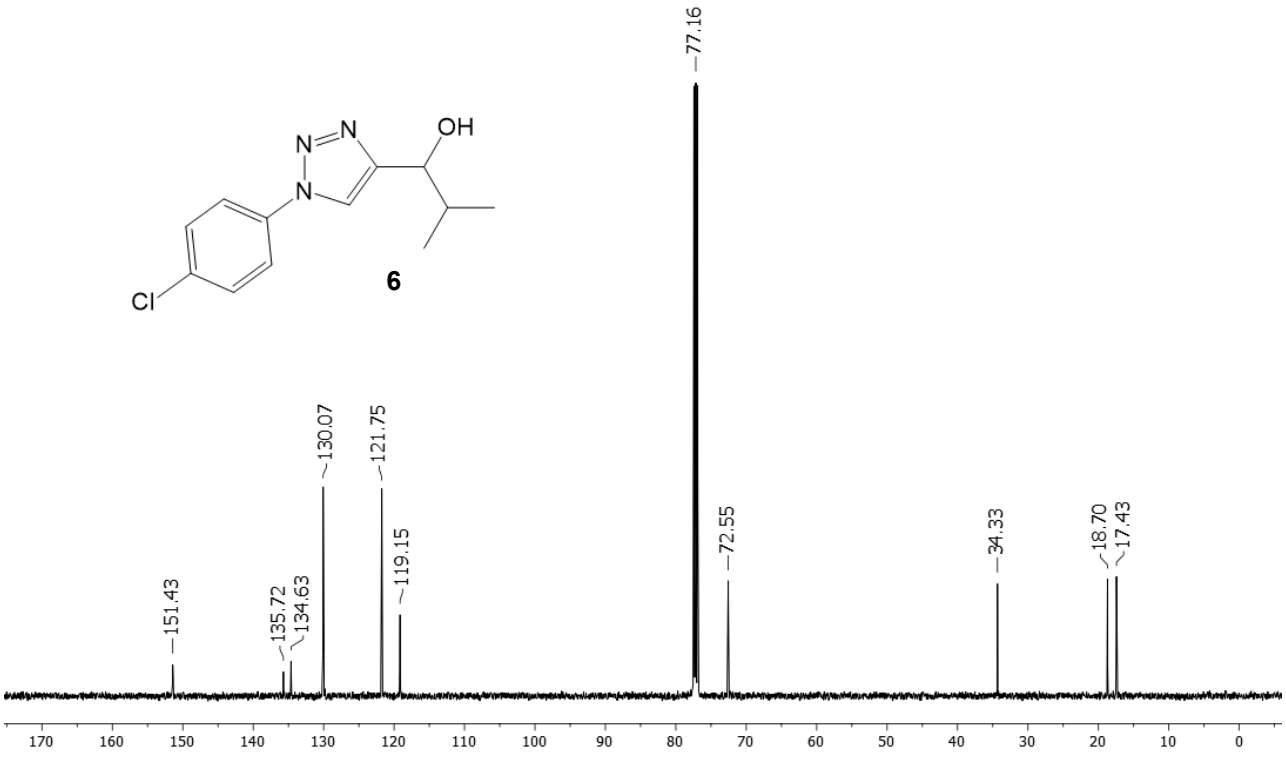


Figure S3. ^{1}H (a) and $^{13}C\{^{1}H\}$ (b) NMR spectra of compound **6** ($CDCl_3$).

4. HRMS data of alcohols 4-6

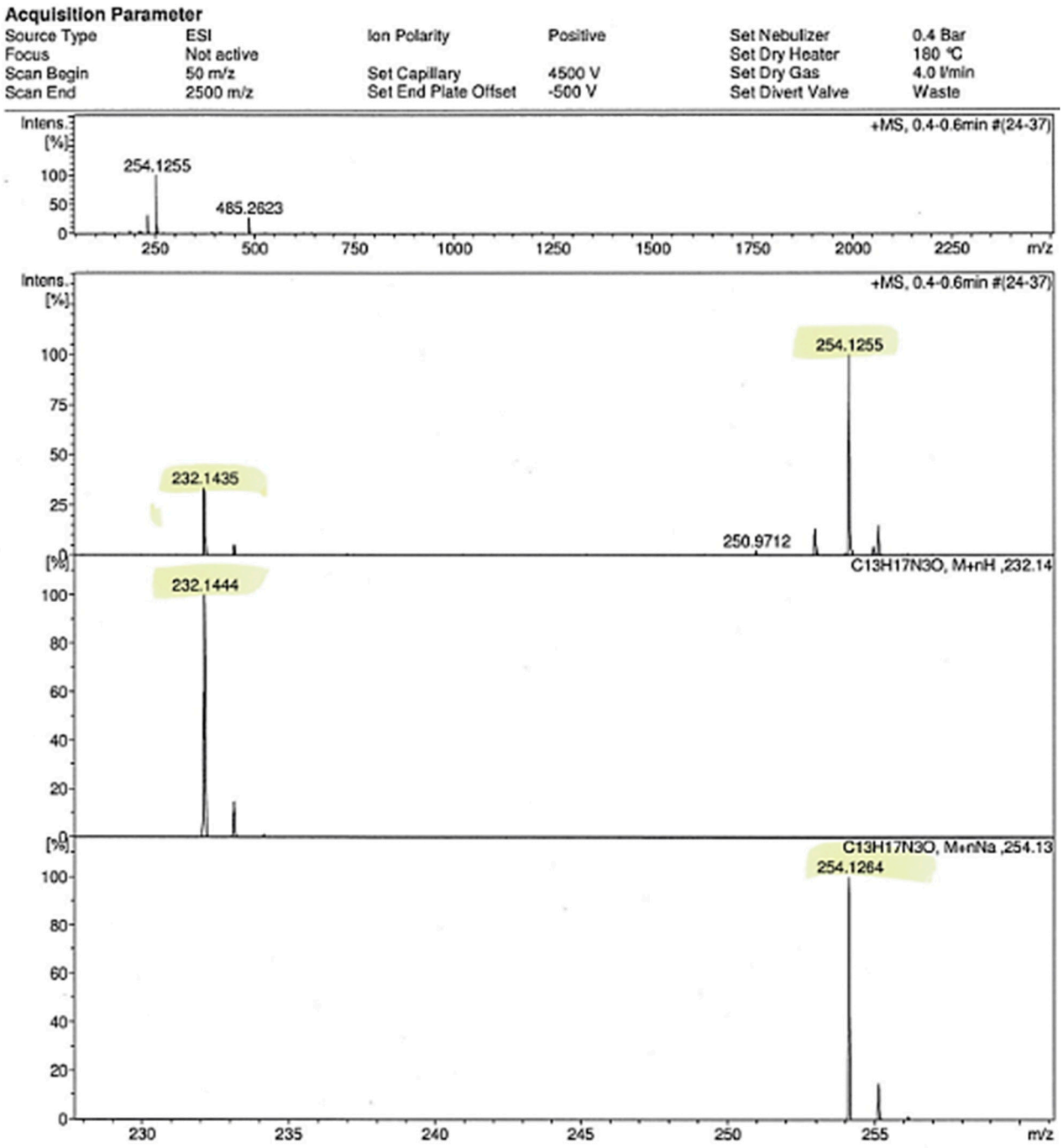


Figure S4. HRMS data of compound **4**.

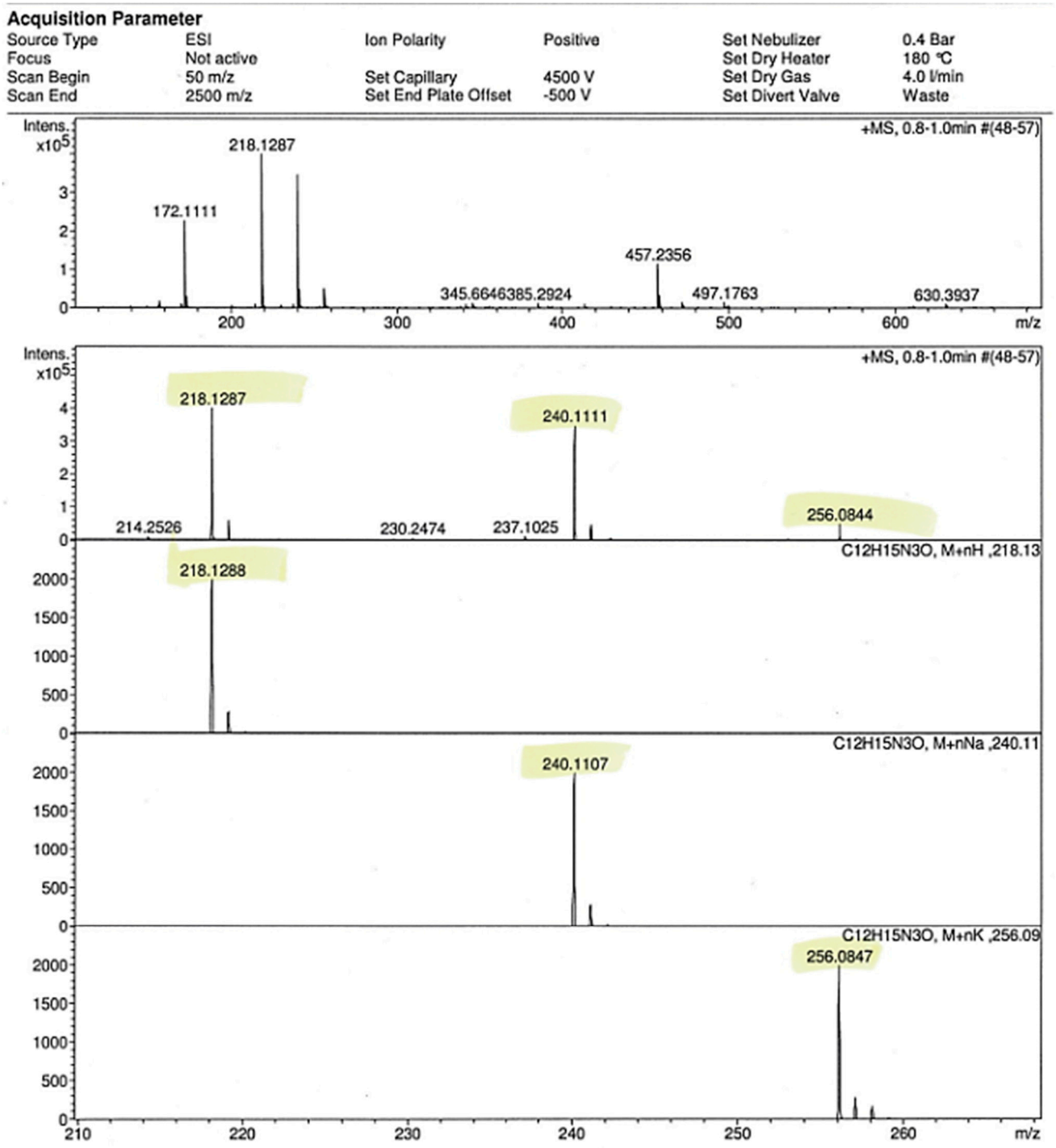


Figure S5. HRMS data of compound **5**.

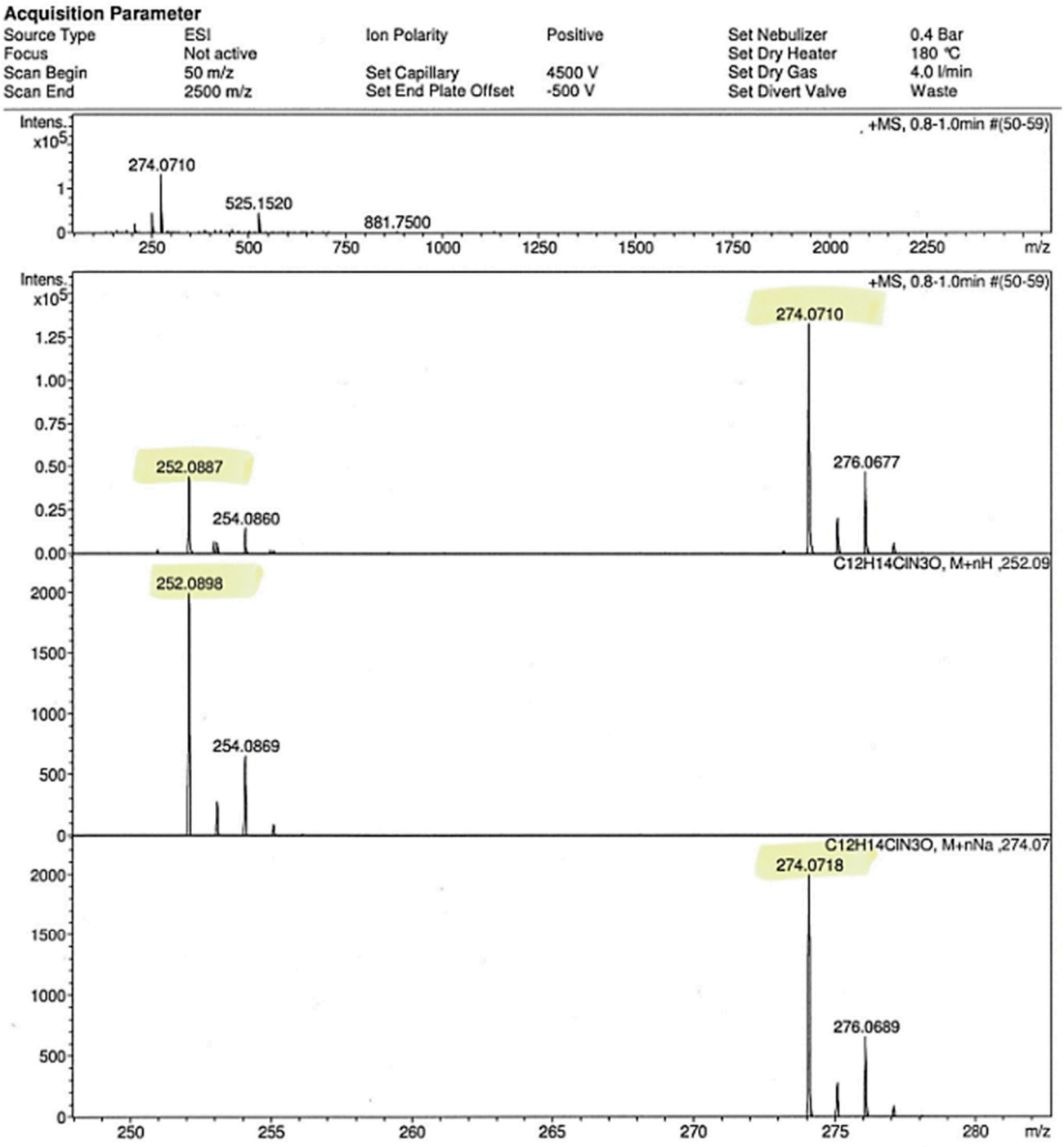


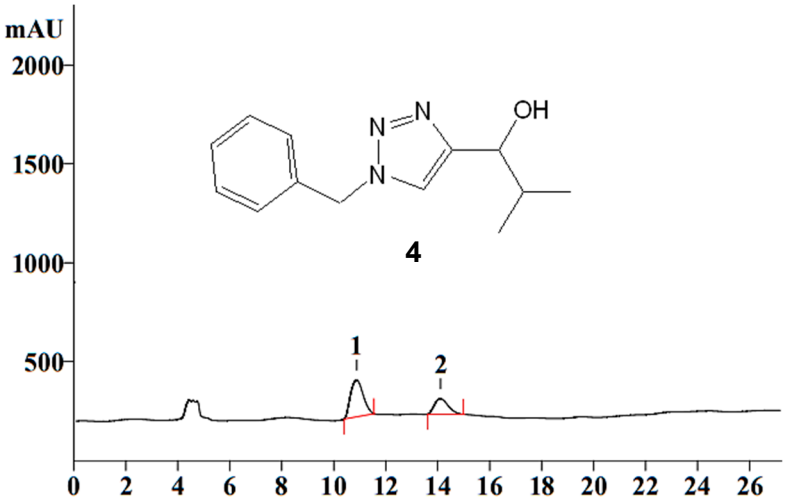
Figure S6. HRMS data of compound **6**.

5. HPLS data for alcohols 4-6

Conditions: hexane : 2-propanol = 90:10,
Flow rate = 1.0 mL/min, λ = 220 nm, Chiralpak AD.

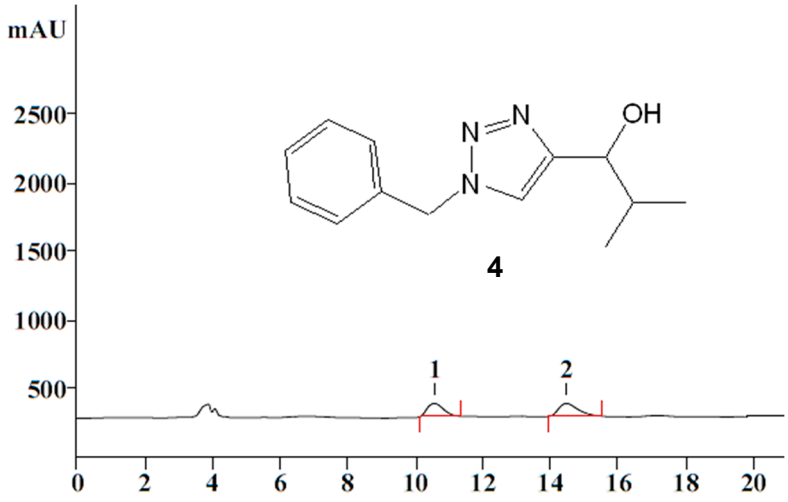
	Peak 1	Peak 2
Retention Time (min)	10.96	14.89
Relative Area (%)	48.68	51.32

Figure S7. HPLC chromatogram for compound **4**, obtained in the experiment without catalyst.



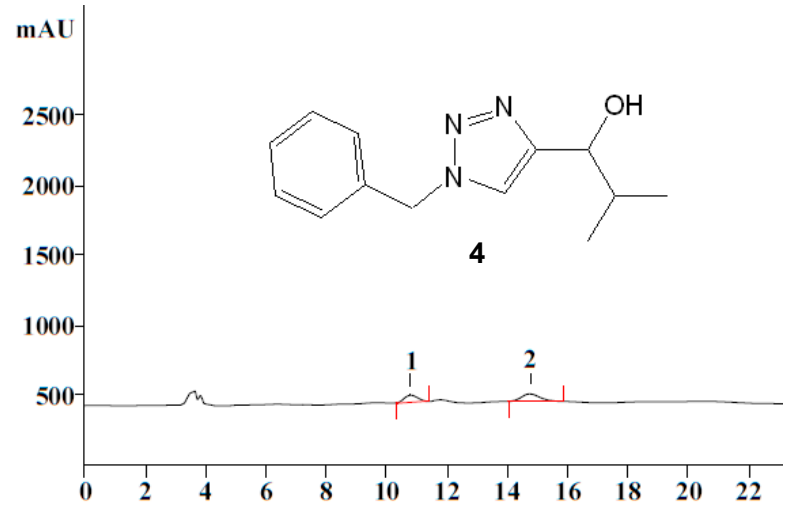
	Peak 1	Peak 2
Retention Time (min)	10.87	14.11
Relative Area (%)	68.38	31.62

Figure S8. HPLC chromatogram for compound **4**, obtained in the experiment with Ephedrine. Yield 33%.



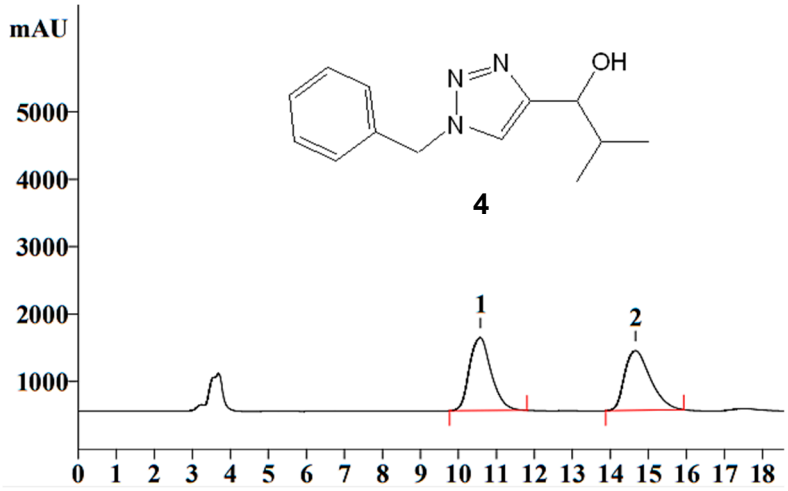
	Peak 1	Peak 2
Retention Time (min)	10.56	14.47
Relative Area (%)	46.74	53.26

Figure S9. HPLC chromatogram for compound **4**, obtained in the experiment with (*R*,*R*)-QiunoxP*. Yield 25%.



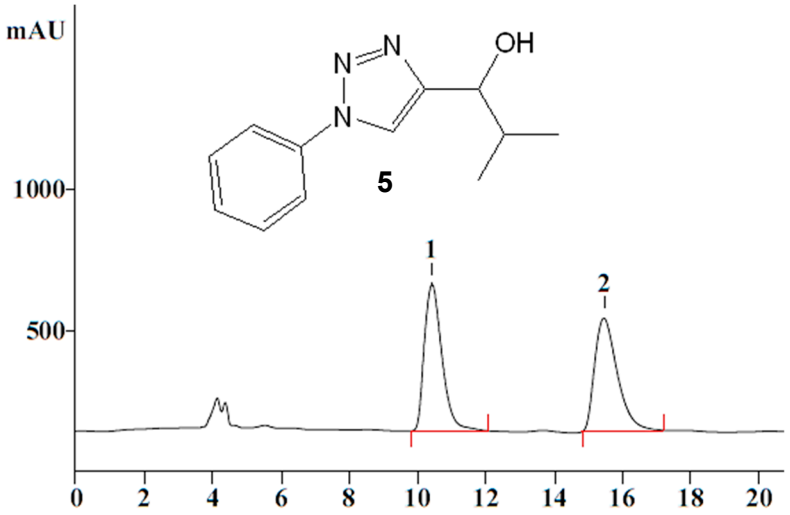
	Peak 1	Peak 2
Retention Time (min)	10.79	14.74
Relative Area (%)	39.39	60.61

Figure S10. HPLC chromatogram for compound **4**, obtained in the experiment with (*R*,*R*)-BenzP*. Yield 30%.



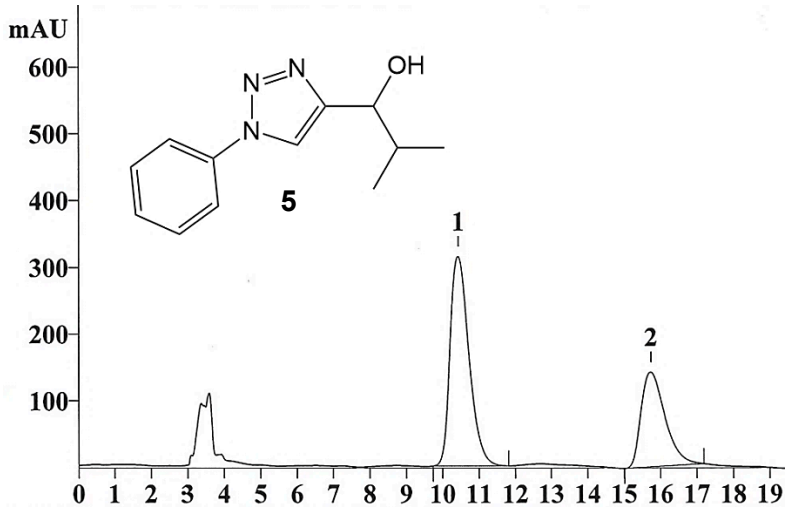
	Peak 1	Peak 2
Retention Time (min)	10.57	14.66
Relative Area (%)	50.77	49.23

Figure S11. HPLC chromatogram for compound **4**, obtained in the autocatalysis experiment. Yield 30%.



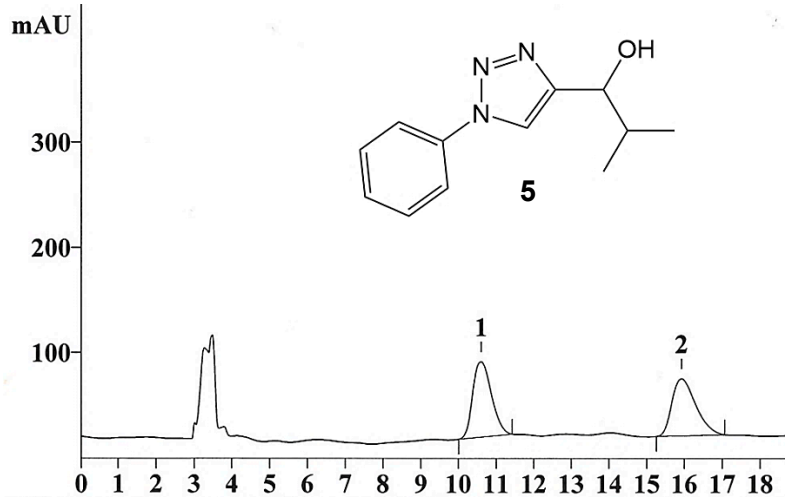
	Peak 1	Peak 2
Retention Time (min)	10.43	15.46
Relative Area (%)	50.35	49.65

Figure S12. HPLC chromatogram for compound **5**, obtained in the experiment without catalyst.



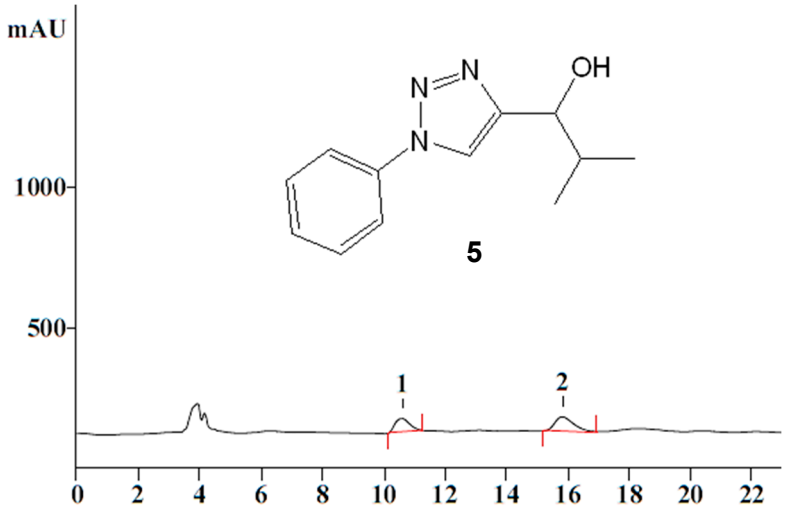
	Peak 1	Peak 2
Retention Time (min)	10.43	15.73
Relative Area (%)	63.52	36.48

Figure S13. HPLC chromatogram for compound **5**, obtained in the experiment with Ephedrine. Yield 40%.



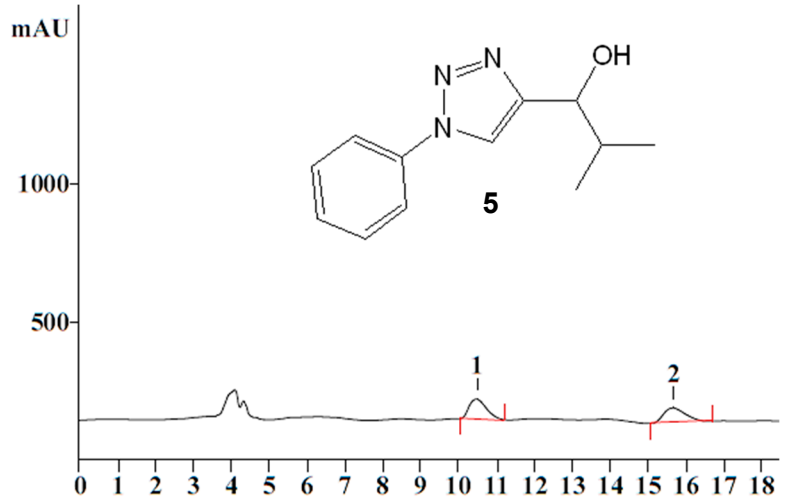
	Peak 1	Peak 2
Retention Time (min)	10.60	15.93
Relative Area (%)	51.03	48.97

Figure S14. HPLC chromatogram for compound **5**, obtained in the experiment with (*R*,*R*)-QiunoxP*. Yield 75%.



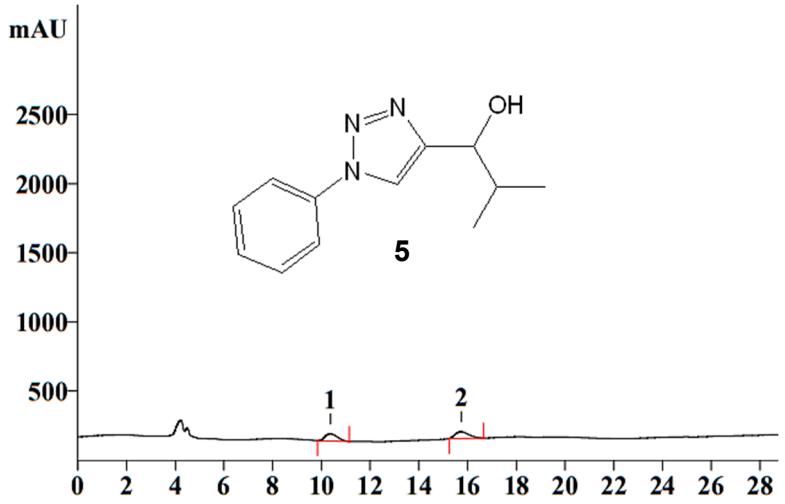
	Peak 1	Peak 2
Retention Time (min)	10.58	15.83
Relative Area (%)	43.42	56.58

Figure S15. HPLC chromatogram for compound **5**, obtained in the experiment with (*R*,*R*)-BenzP*. Yield 24%.



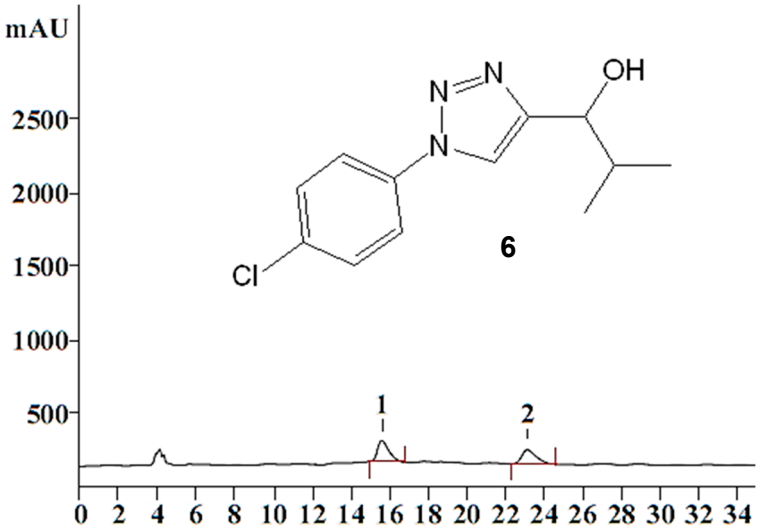
	Peak 1	Peak 2
Retention Time (min)	10.48	15.65
Relative Area (%)	51.35	48.65

Figure S16. HPLC chromatogram for compound **5**, obtained in the experiment with Sparteine. Yield 13%.



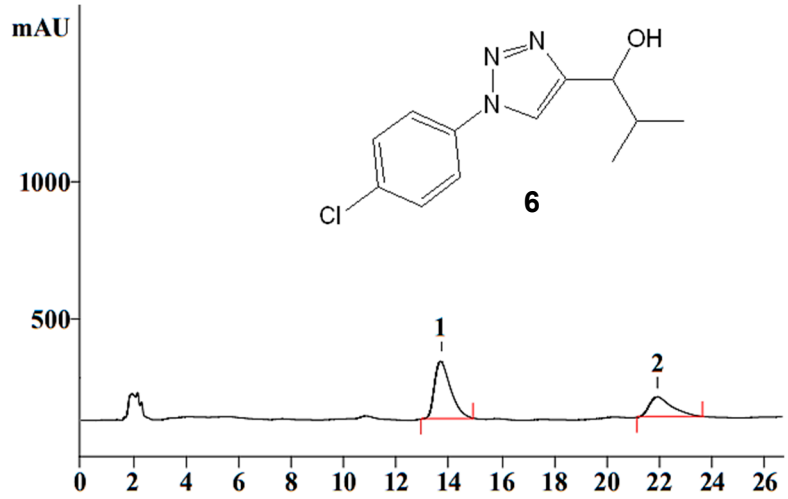
	Peak 1	Peak 2
Retention Time (min)	10.38	15.73
Relative Area (%)	49.41	50.59

Figure S17. HPLC chromatogram for compound **5**, obtained in the autocatalysis experiment. Yield 48%.



	Peak 1	Peak 2
Retention Time (min)	15.61	23.14
Relative Area (%)	54.88	45.12

Figure S18. HPLC chromatogram for compound **6**, obtained in the experiment without catalyst.



	Peak 1	Peak 2
Retention Time (min)	13.68	21.91
Relative Area (%)	66.49	33.51

Figure S19. HPLC chromatogram for compound **6**, obtained in the experiment with Ephedrine. Yield 31%.

	Peak 1	Peak 2
Retention Time (min)	10.64	15.36
Relative Area (%)	42.20	57.80

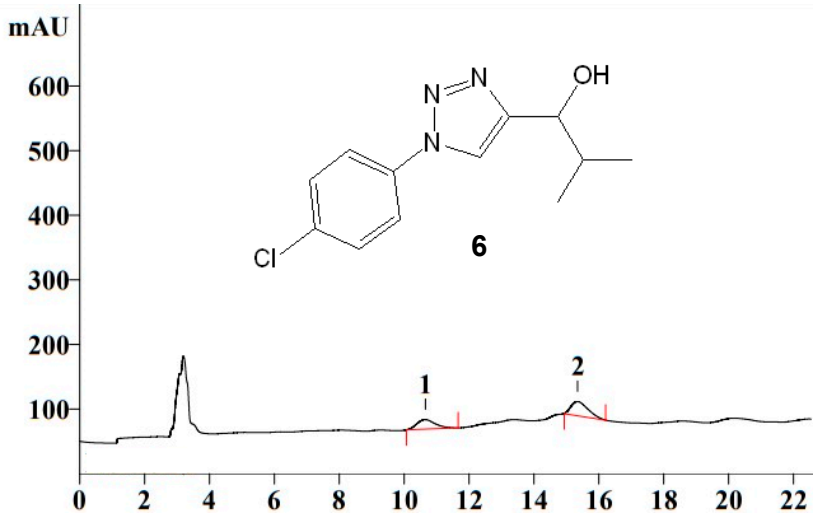


Figure S20. HPLC chromatogram for compound **6**, obtained in the experiment with (*R*,*R*)-QiunoxP*. Yield 25%.

	Peak 1	Peak 2
Retention Time (min)	15.12	22.91
Relative Area (%)	54.28	45.72

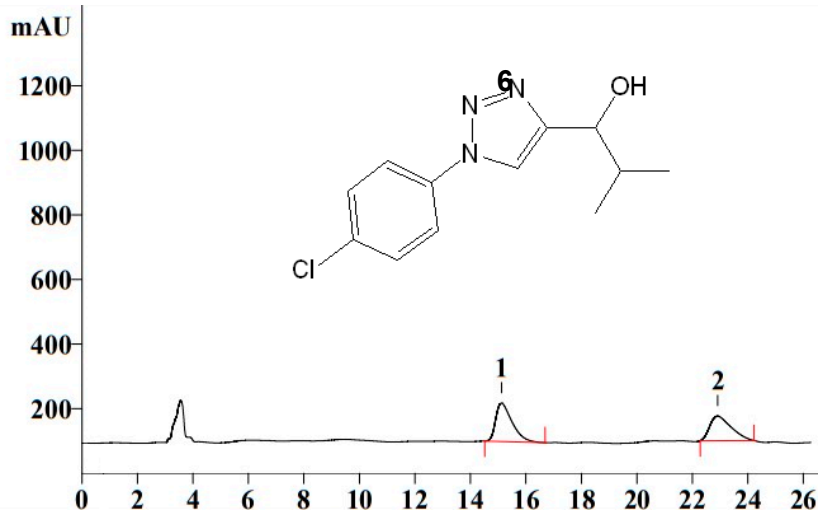
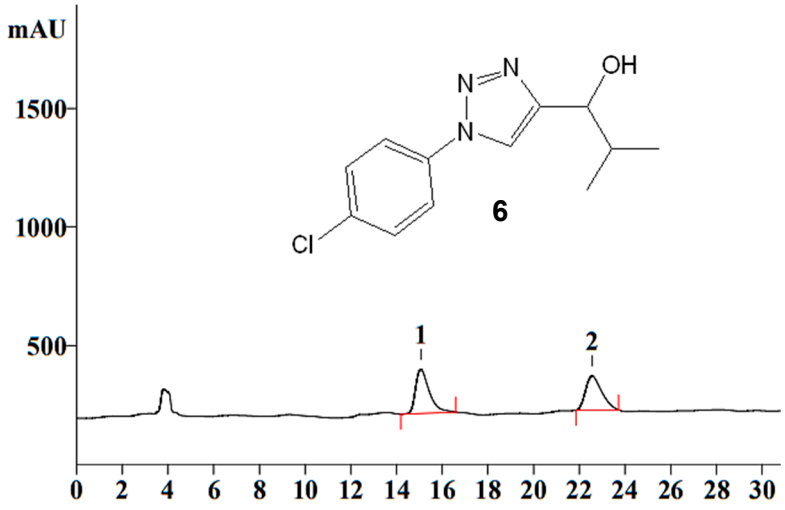


Figure S21. HPLC chromatogram for compound **6**, obtained in the experiment with (*R*,*R*)-BenzP*. Yield 20%.



	Peak 1	Peak 2
Retention Time (min)	15.06	22.55
Relative Area (%)	52.47	47.53

Figure S22. HPLC chromatogram for compound **6**, obtained in the autocatalysis experiment. Yield 53%.

6. Computational details

Geometry optimizations were performed without any symmetry constraints (C1 symmetry) using the ωB97XD functional [1] as implemented in the Gaussian09 software package [2]. Frequency calculations were undertaken to confirm the nature of the stationary points, yielding one imaginary frequency for all transition states (TSs) and zero for all minima. Constrained energy hypersurface scans were conducted to investigate the molecular reactivity and to locate viable reaction channels. Where low-lying barriers were estimated, frequency calculations were performed at the crude saddle points, and the obtained force constants were used to optimize the transition-state structures employing the Berny algorithm [3]. All atoms were described with 6–31G** basis set in the geometry optimization and frequency calculation [4–9]. Non-specific solvation was introduced by using the SMD continuum model [10] (acetonitrile).

1 Chai, J.-D.; Head-Gordon, M. Long-Range Corrected Hybrid Density Functionals with Damped Atom–Atom Dispersion Corrections. *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615–6620.

2 Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Rev. D.01*; Gaussian, Inc.: 2013.

3 Becke, A. D. Density-functional exchange-energy approximation with correct asymptotic behavior. *Phys. Rev. A* **1988**, *38*, 3098– 3100.

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Table S1. Changes of the thermodynamic parameters within three computed catalytic cycles.

Process	DH	DS	DG_{298}
7(*S*) -> **9**(*S*)	-15.1	-49.4	0.4
9(*S*) -> **10**	-16.3	-41.8	-3.8
10 -> **TS1**(*S*)	20.3	-15.8	25.1
TS1(*S*) -> 7(S).7(S)	-54.0	5.1	-56.0
10 -> **TS1**(R)	28.3	-13.2	32.2
TS1(*R*) -> 7(S).7(*R*)	-51.3	4.7	-52.7
8(*SS*) -> **11**	-11.4	-53.4	4.5
11 -> **12**	-16.6	61.7	-3.1
12 -> **TS2**(*S*)	14.9	-6.4	16.8
TS2(*S*) -> **8**(*SS*).**7**(*S*)	-62.9	-7.9	-60.6
12 -> **TS2**(*R*)	16.0	-18.2	18.0
TS2(*R*) -> 8(SS).7(R)	-55.4	-116.0	-54.9
13(*SSSS*) -> **14**(*SSSS*)	-16.5	-48.7	-2.02
14(*SSSS*) -> **15**(*SSSS*)s	-9.8	-52.2	5.8
15(*SSSS*)s -> **TS3**(S)	22.8	-3.7	23.9
TS3(*S*) -> **13**(SSSS).**7**(S)	-58.7	-0.3	-58.6
14(*SSSS*) -> **15**(*SSSS*)r	-6.8	-37.3	4.3
15(*SSSS*)r -> **TS3**(*R*)	15.1	-17.5	20.4
TS3(*R*) -> 13(*SSSS*)**.7**(*R*)	-61.8	-8.4	-59.3

3

Sum of electronic and zero-point Energies = -1045.865202

Sum of electronic and thermal Energies = -1045.854121

Sum of electronic and thermal Enthalpies = -1045.853177

Sum of electronic and thermal Free Energies = -1045.904010

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.088255	-0.586477	-0.146254
2	6	0	3.262954	0.113749	0.019795
3	7	0	1.126595	0.324910	0.089629
4	1	0	1.889054	-1.609495	-0.421346
5	7	0	1.672092	1.532901	0.384996
6	7	0	2.953516	1.402817	0.340273
7	6	0	4.648236	-0.345412	-0.113765
8	8	0	4.948072	-1.486221	-0.396496
9	6	0	-0.286742	0.166174	0.058439
10	6	0	-0.851568	-1.062266	0.385505
11	6	0	-1.081888	1.249674	-0.303700
12	6	0	-2.230852	-1.217783	0.333669
13	1	0	-0.227760	-1.893085	0.696017
14	6	0	-2.461425	1.099294	-0.340814
15	1	0	-0.622472	2.198781	-0.551531
16	6	0	-3.022875	-0.134206	-0.028168
17	1	0	-2.683450	-2.169720	0.584598
18	1	0	-3.093557	1.933665	-0.621143
19	17	0	-4.759109	-0.325276	-0.086518
20	1	0	5.408471	0.438434	0.063654

Zn(*i*-Pr)$_2$

Sum of electronic and zero-point Energies = -2015.961290

Sum of electronic and thermal Energies = -2015.950366

Sum of electronic and thermal Enthalpies = -2015.949422

Sum of electronic and thermal Free Energies = -2015.998456

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	-0.000002	-0.000030	0.326530
2	6	0	1.921276	-0.262576	0.242273
3	1	0	2.234812	-0.851544	1.117703
4	6	0	2.698334	1.058027	0.285270
5	1	0	3.785227	0.895960	0.218104
6	1	0	2.431217	1.720018	-0.549039
7	1	0	2.514712	1.617324	1.210475
8	6	0	2.304848	-1.068695	-1.005610
9	1	0	3.390422	-1.241006	-1.066299
10	1	0	1.822159	-2.053062	-1.029714
11	1	0	2.020532	-0.550061	-1.930747
12	6	0	-1.921269	0.262578	0.242277
13	1	0	-2.234791	0.851515	1.117733
14	6	0	-2.698365	-1.058002	0.285221
15	1	0	-2.514783	-1.617331	1.210415
16	1	0	-3.785251	-0.895906	0.218029
17	1	0	-2.431238	-1.719976	-0.549098
18	6	0	-2.304818	1.068764	-1.005574
19	1	0	-3.390386	1.241119	-1.066245
20	1	0	-1.822093	2.053114	-1.029637
21	1	0	-2.020529	0.550158	-1.930735

7

Sum of electronic and zero-point Energies = -3061.899889

Sum of electronic and thermal Energies = -3061.878054

Sum of electronic and thermal Enthalpies = -3061.877110

Sum of electronic and thermal Free Energies = -3061.953001

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.455754	-1.507521	-0.527699
2	6	0	0.858819	-1.113966	-0.533672
3	7	0	-1.152245	-0.378697	-0.225987
4	1	0	-0.934823	-2.450291	-0.733858
5	7	0	-0.336332	0.660094	-0.050675
6	7	0	0.869786	0.208649	-0.235559
7	6	0	2.186983	-1.808520	-0.766698
8	8	0	3.207965	-0.885754	-0.868942
9	1	0	2.088440	-2.378184	-1.708682
10	6	0	2.449396	-2.847961	0.355711
11	6	0	2.594518	-2.174507	1.719551
12	1	0	1.580114	-3.521471	0.385047
13	1	0	1.694056	-1.616717	2.000764
14	1	0	2.783230	-2.913828	2.504097
15	30	0	2.902403	0.860572	-0.377800
16	6	0	3.309315	2.712730	0.028270
17	1	0	4.002223	3.112729	-0.724666
18	6	0	3.969341	2.884075	1.400716
19	6	0	2.016665	3.534314	-0.048303
20	1	0	4.927783	2.356872	1.469124
21	1	0	4.163141	3.943416	1.630609
22	1	0	3.331286	2.500470	2.207794
23	1	0	2.192442	4.599980	0.165701
24	1	0	1.546240	3.475608	-1.037036
25	1	0	1.271157	3.182713	0.676578
26	1	0	3.436611	-1.475370	1.708027
27	6	0	3.691448	-3.668026	0.012014

28	1	0	4.562344	-3.011302	-0.068657
29	1	0	3.895226	-4.421481	0.779930
30	1	0	3.572702	-4.186464	-0.945856
31	6	0	-2.561104	-0.205965	-0.109665
32	6	0	-3.356662	-1.276054	0.286145
33	6	0	-3.118559	1.036878	-0.395991
34	6	0	-4.732019	-1.107110	0.382867
35	1	0	-2.914437	-2.233888	0.535538
36	6	0	-4.491080	1.210796	-0.283584
37	1	0	-2.481484	1.857581	-0.702624
38	6	0	-5.286240	0.135396	0.098595
39	1	0	-5.363618	-1.932748	0.688739
40	1	0	-4.938763	2.173282	-0.500925
41	17	0	-7.015797	0.350017	0.225405

9

Sum of electronic and zero-point Energies = -5077.885364

Sum of electronic and thermal Energies = -5077.851559

Sum of electronic and thermal Enthalpies = -5077.850615

Sum of electronic and thermal Free Energies = -5077.952078

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.823406	-1.225562	-0.403781
2	6	0	-0.573449	-0.685511	-0.239930
3	7	0	-2.675693	-0.226278	-0.060022
4	1	0	-2.166732	-2.187110	-0.748392
5	7	0	-2.004992	0.872707	0.297509
6	7	0	-0.744286	0.591210	0.186031
7	6	0	0.815510	-1.211962	-0.498386
8	8	0	1.708629	-0.393561	0.198992
9	1	0	0.985068	-1.128023	-1.587764
10	6	0	0.940696	-2.704318	-0.126162
11	6	0	0.783284	-2.932903	1.376379
12	1	0	0.130334	-3.225961	-0.654097
13	1	0	-0.174653	-2.557962	1.748902
14	1	0	0.843916	-3.999727	1.613171
15	30	0	3.507700	-0.464232	-0.034822
16	6	0	5.411074	-0.537504	-0.276270
17	1	0	5.812550	0.392469	0.149927
18	6	0	5.783155	-0.567010	-1.762729
19	6	0	6.059109	-1.704913	0.473933
20	1	0	5.388657	0.298428	-2.306381
21	1	0	6.873925	-0.569127	-1.900198
22	1	0	5.400666	-1.467653	-2.260312
23	1	0	7.150620	-1.703925	0.342223
24	1	0	5.863686	-1.666878	1.551668
25	1	0	5.700639	-2.676627	0.110597
26	1	0	1.574850	-2.416992	1.928488
27	6	0	2.261579	-3.284465	-0.631034

28	1	0	3.115022	-2.864058	-0.084616
29	1	0	2.302344	-4.366024	-0.475064
30	1	0	2.411867	-3.092011	-1.699496
31	6	0	-4.097383	-0.236144	-0.059396
32	6	0	-4.776709	-1.416795	0.222181
33	6	0	-4.785140	0.938228	-0.349598
34	6	0	-6.165639	-1.429931	0.197080
35	1	0	-4.233820	-2.320721	0.475890
36	6	0	-6.173362	0.929929	-0.358370
37	1	0	-4.237571	1.847539	-0.566490
38	6	0	-6.850439	-0.255387	-0.091844
39	1	0	-6.707367	-2.343426	0.412665
40	1	0	-6.722023	1.837645	-0.580910
41	17	0	-8.598226	-0.269090	-0.119062
42	30	0	1.082071	1.790886	0.274363
43	6	0	1.360276	2.321779	-1.630259
44	1	0	1.468802	3.416666	-1.667320
45	6	0	2.661536	1.740906	-2.191444
46	1	0	2.665016	0.639363	-2.139006
47	1	0	2.834204	1.988800	-3.252013
48	1	0	3.543242	2.093609	-1.638100
49	6	0	0.192488	1.962744	-2.552610
50	1	0	0.030892	0.876143	-2.599439
51	1	0	-0.751970	2.401964	-2.208612
52	1	0	0.347561	2.297734	-3.592228
53	6	0	1.618841	2.079087	2.161271
54	1	0	1.443118	3.122307	2.464011
55	6	0	0.821067	1.179729	3.107628
56	1	0	-0.253075	1.399279	3.071387
57	1	0	0.935117	0.123020	2.830693
58	1	0	1.137250	1.272552	4.161125
59	6	0	3.118208	1.815447	2.337708
60	1	0	3.738027	2.479034	1.720349
61	1	0	3.463283	1.925025	3.379516
62	1	0	3.381244	0.781928	2.054878

10

Sum of electronic and zero-point Energies = -6123.777553

Sum of electronic and thermal Energies = -6123.730666

Sum of electronic and thermal Enthalpies = -6123.729722

Sum of electronic and thermal Free Energies = -6123.862177

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.778966	1.547672	2.649061
2	6	0	0.225839	0.610102	2.652857
3	7	0	-1.534132	1.238157	1.563701
4	1	0	-1.013829	2.383623	3.287689
5	7	0	-1.046419	0.180571	0.925983
6	7	0	0.008640	-0.189866	1.585197
7	6	0	1.461527	0.322663	3.483003
8	8	0	1.895802	-0.963924	3.250129
9	1	0	1.186109	0.460450	4.543924
10	6	0	2.554650	1.384281	3.166417
11	6	0	3.024908	1.301666	1.713137
12	1	0	2.102765	2.373703	3.330988
13	1	0	2.198700	1.414514	1.002628
14	1	0	3.757639	2.085028	1.494771
15	30	0	1.374851	-1.791434	1.656521
16	6	0	1.842782	-3.220416	0.419509
17	1	0	1.087703	-3.207515	-0.376977
18	6	0	1.769773	-4.605543	1.069258
19	6	0	3.216929	-2.994602	-0.219052
20	1	0	0.777540	-4.804650	1.489324
21	1	0	1.982215	-5.409072	0.346384
22	1	0	2.495613	-4.712471	1.885640
23	1	0	3.453196	-3.753118	-0.983186
24	1	0	3.296415	-2.010824	-0.699159
25	1	0	4.017533	-3.039869	0.530047
26	1	0	3.507232	0.336903	1.522831
27	6	0	3.727388	1.214563	4.128828

28	1	0	4.160103	0.216124	4.017195
29	1	0	4.510486	1.955114	3.934616
30	1	0	3.408099	1.328300	5.170644
31	6	0	-2.705017	1.895236	1.079607
32	6	0	-2.678880	2.462164	-0.187626
33	6	0	-3.843747	1.935712	1.875056
34	6	0	-3.821388	3.079815	-0.677825
35	1	0	-1.776026	2.404665	-0.784513
36	6	0	-4.985512	2.561794	1.391203
37	1	0	-3.844241	1.464391	2.851747
38	6	0	-4.960853	3.123320	0.118600
39	1	0	-3.827316	3.516096	-1.669312
40	1	0	-5.888382	2.596595	1.988989
41	17	0	-6.400769	3.897063	-0.497656
42	30	0	-1.929769	-1.480685	-0.664456
43	6	0	-1.833715	-2.841360	0.772124
44	1	0	-0.861981	-2.761760	1.280806
45	6	0	-2.898700	-2.524895	1.828854
46	1	0	-3.912185	-2.559953	1.406603
47	1	0	-2.884830	-3.236884	2.671019
48	1	0	-2.768616	-1.521772	2.258173
49	6	0	-1.971507	-4.288261	0.299067
50	1	0	-2.911779	-4.445894	-0.246331
51	1	0	-1.164194	-4.572074	-0.383868
52	1	0	-1.968533	-5.008905	1.134901
53	6	0	-3.132016	-0.511777	-1.908424
54	1	0	-2.737937	0.508744	-2.040095
55	6	0	-3.195705	-1.131536	-3.307184
56	1	0	-2.208435	-1.175282	-3.783859
57	1	0	-3.576845	-2.160221	-3.280842
58	1	0	-3.856676	-0.567078	-3.987475
59	6	0	-4.547101	-0.377401	-1.334714
60	1	0	-4.553435	0.104774	-0.349377
61	1	0	-5.219724	0.209582	-1.983780
62	1	0	-5.019029	-1.361048	-1.206291
63	8	0	-0.888271	-3.520837	-2.757374
64	6	0	0.160325	-3.047079	-3.131423
65	1	0	0.788158	-3.551522	-3.889000
66	6	0	0.698306	-1.781320	-2.619419

67	6	0	1.873655	-1.141756	-2.938452
68	7	0	0.070068	-1.045243	-1.659726
69	1	0	2.660246	-1.368324	-3.640459
70	7	0	0.777946	-0.004409	-1.380796
71	7	0	1.882154	-0.049991	-2.149044
72	6	0	2.879935	0.954834	-2.001223
73	6	0	2.485062	2.277237	-1.830750
74	6	0	4.220829	0.589512	-1.985325
75	6	0	3.452198	3.254011	-1.639772
76	1	0	1.432548	2.534935	-1.842995
77	6	0	5.190238	1.568410	-1.807132
78	1	0	4.510348	-0.450934	-2.086282
79	6	0	4.795401	2.890109	-1.632332
80	1	0	3.164523	4.289514	-1.501594
81	1	0	6.240009	1.301132	-1.786499
82	17	0	6.011150	4.119946	-1.389625

TS1(*S*)

Sum of electronic and zero-point Energies = -6123.743006

Sum of electronic and thermal Energies = -6123.698264

Sum of electronic and thermal Enthalpies = -6123.697319

Sum of electronic and thermal Free Energies = -6123.822245

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.228026	2.645144	-0.515747
2	6	0	0.080806	2.207512	0.107884
3	7	0	2.168551	1.736531	-0.188802
4	1	0	1.446460	3.495499	-1.141025
5	7	0	1.659083	0.784011	0.585201
6	7	0	0.401129	1.075192	0.770691
7	6	0	-1.346332	2.704304	0.173229
8	8	0	-2.153596	1.713288	0.692073
9	1	0	-1.643058	2.947877	-0.863882
10	6	0	-1.429427	4.023687	0.983421
11	6	0	-1.054532	3.808987	2.449134
12	1	0	-0.710747	4.726115	0.536370
13	1	0	-0.054194	3.374332	2.561701
14	1	0	-1.062795	4.757803	2.993862
15	30	0	-1.383360	0.305606	1.669397
16	6	0	-2.052360	-0.973070	2.976223
17	1	0	-1.211010	-1.432345	3.511272
18	6	0	-2.846934	-2.102821	2.310679
19	6	0	-2.918532	-0.249514	4.014345
20	1	0	-2.238908	-2.696956	1.619702
21	1	0	-3.251453	-2.801852	3.058288
22	1	0	-3.705243	-1.720249	1.743442
23	1	0	-3.321545	-0.949619	4.762055
24	1	0	-2.358408	0.518469	4.561514
25	1	0	-3.779533	0.248878	3.550940
26	1	0	-1.772892	3.141061	2.934875
27	6	0	-2.833005	4.612098	0.854960

28	1	0	-3.572933	3.905976	1.243341
29	1	0	-2.922559	5.548317	1.414813
30	1	0	-3.081149	4.821463	-0.191510
31	6	0	3.529959	1.659488	-0.633377
32	6	0	4.540533	2.111438	0.204076
33	6	0	3.794408	1.094520	-1.874536
34	6	0	5.860788	1.998712	-0.212788
35	1	0	4.299201	2.537616	1.171571
36	6	0	5.114040	0.981814	-2.292108
37	1	0	2.980678	0.713813	-2.481578
38	6	0	6.130094	1.435334	-1.456584
39	1	0	6.669369	2.337645	0.423696
40	1	0	5.349320	0.530066	-3.248196
41	17	0	7.788433	1.285618	-1.978233
42	30	0	2.462567	-1.238606	0.263946
43	6	0	0.792394	-2.330739	1.241256
44	1	0	-0.219031	-1.930865	1.284231
45	6	0	0.771447	-3.849887	1.281293
46	1	0	1.781325	-4.262025	1.156649
47	1	0	0.390268	-4.212880	2.245561
48	1	0	0.132984	-4.281002	0.505921
49	6	0	1.481532	-1.814869	2.536177
50	1	0	2.499083	-2.198788	2.664895
51	1	0	1.512621	-0.723310	2.629786
52	1	0	0.905076	-2.176637	3.398447
53	6	0	4.370567	-1.715433	0.222949
54	1	0	4.941231	-0.781630	0.125775
55	6	0	4.909248	-2.443046	1.456223
56	1	0	4.811509	-1.842661	2.368658
57	1	0	4.384337	-3.390412	1.637209
58	1	0	5.976631	-2.692314	1.348749
59	6	0	4.641511	-2.538782	-1.042291
60	1	0	4.286506	-2.035786	-1.949065
61	1	0	5.714662	-2.742949	-1.181139
62	1	0	4.138178	-3.514033	-1.002615
63	8	0	1.346794	-1.043808	-1.430432
64	6	0	0.726255	-2.065968	-0.923284
65	1	0	1.154442	-3.067832	-1.075877
66	6	0	-0.751186	-2.076877	-1.031890

67	6	0	-1.619613	-1.021168	-1.196542
68	7	0	-1.482246	-3.225817	-1.017348
69	1	0	-1.468845	0.039998	-1.300264
70	7	0	-2.737292	-2.939935	-1.159451
71	7	0	-2.840422	-1.602043	-1.267966
72	6	0	-4.112618	-0.992626	-1.460192
73	6	0	-5.113453	-1.707202	-2.113549
74	6	0	-4.333168	0.297870	-0.989003
75	6	0	-6.357678	-1.120157	-2.300945
76	1	0	-4.919899	-2.712360	-2.467925
77	6	0	-5.576654	0.886411	-1.189091
78	1	0	-3.558173	0.844974	-0.448791
79	6	0	-6.575481	0.173972	-1.840767
80	1	0	-7.147588	-1.662653	-2.807233
81	1	0	-5.763896	1.889589	-0.823694
82	17	0	-8.142388	0.917527	-2.083834

7(*S*)·7(*S*)

Sum of electronic and zero-point Energies = -6123.829391

Sum of electronic and thermal Energies = -6123.784352

Sum of electronic and thermal Enthalpies = -6123.783408

Sum of electronic and thermal Free Energies = -6123.911536

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.215904	-2.131266	0.838844
2	6	0	-1.008089	-1.519777	0.731973
3	7	0	1.019158	-1.191635	1.400624
4	1	0	0.569192	-3.112283	0.567299
5	7	0	0.350948	-0.066630	1.644459
6	7	0	-0.870462	-0.268806	1.243417
7	6	0	-2.317658	-1.891426	0.076356
8	8	0	-3.020186	-0.722865	-0.243896
9	1	0	-2.904209	-2.473548	0.802771
10	6	0	-2.112431	-2.772556	-1.173188
11	6	0	-1.353529	-2.031221	-2.273674
12	1	0	-1.531823	-3.652741	-0.860357
13	1	0	-0.365225	-1.692081	-1.948053
14	1	0	-1.219261	-2.674588	-3.148894
15	30	0	-5.122985	-0.717754	-0.157995
16	6	0	-5.598866	-1.644346	1.521935
17	1	0	-6.638027	-1.345110	1.731797
18	6	0	-4.744772	-1.074114	2.661895
19	6	0	-5.592826	-3.176255	1.558573
20	1	0	-4.867441	0.011556	2.761543
21	1	0	-4.999236	-1.514446	3.640574
22	1	0	-3.671771	-1.249659	2.506826
23	1	0	-5.958792	-3.570963	2.521311
24	1	0	-6.225679	-3.610432	0.774506
25	1	0	-4.587367	-3.596709	1.422049
26	1	0	-1.921233	-1.150660	-2.591016
27	6	0	-3.469650	-3.250644	-1.687361

28	1	0	-4.061311	-2.401007	-2.044071
29	1	0	-3.351152	-3.943467	-2.526246
30	1	0	-4.040683	-3.762205	-0.906034
31	6	0	2.428291	-1.225669	1.600349
32	6	0	3.232330	-1.899948	0.686652
33	6	0	2.979840	-0.536802	2.674959
34	6	0	4.609469	-1.910415	0.864931
35	1	0	2.798296	-2.387523	-0.178743
36	6	0	4.358313	-0.530815	2.842833
37	1	0	2.335527	-0.007432	3.366963
38	6	0	5.159579	-1.222654	1.940338
39	1	0	5.247769	-2.430802	0.160844
40	1	0	4.803261	-0.002017	3.677573
41	17	0	6.893946	-1.217580	2.154290
42	30	0	-2.040012	0.872167	-0.177963
43	6	0	-0.449937	3.560998	1.692487
44	1	0	-0.471222	2.523878	2.040677
45	6	0	0.913188	4.182200	1.873396
46	1	0	0.987687	5.155956	1.373820
47	1	0	1.121644	4.352403	2.938104
48	1	0	1.708943	3.532043	1.495604
49	6	0	-1.604089	4.355090	2.252688
50	1	0	-1.605514	5.381761	1.866782
51	1	0	-2.551886	3.885387	1.974613
52	1	0	-1.556238	4.412663	3.348267
53	6	0	-5.534999	0.606869	-1.562810
54	1	0	-6.528467	0.390390	-1.985218
55	6	0	-5.617530	2.008740	-0.938890
56	1	0	-6.374687	2.064610	-0.146708
57	1	0	-4.662616	2.322089	-0.495638
58	1	0	-5.873521	2.781236	-1.682597
59	6	0	-4.552770	0.617171	-2.736335
60	1	0	-4.527081	-0.343768	-3.265748
61	1	0	-4.792097	1.392915	-3.481885
62	1	0	-3.524994	0.817497	-2.404773
63	8	0	-2.140758	2.718843	-0.283649
64	6	0	-0.927995	3.312000	-0.213214
65	1	0	-0.914529	4.343911	-0.585907
66	6	0	0.177777	2.477036	-0.773776

67	6	0	1.537611	2.613306	-0.940531
68	7	0	-0.116768	1.189625	-1.090191
69	1	0	2.206580	3.452484	-0.850875
70	7	0	0.952256	0.517974	-1.402091
71	7	0	1.963590	1.379304	-1.318660
72	6	0	3.292726	0.917885	-1.535027
73	6	0	4.326282	1.403460	-0.740848
74	6	0	3.522094	-0.049596	-2.508091
75	6	0	5.615778	0.922219	-0.929620
76	1	0	4.127641	2.130461	0.038620
77	6	0	4.807869	-0.540693	-2.687981
78	1	0	2.699965	-0.411891	-3.114254
79	6	0	5.842535	-0.049130	-1.898137
80	1	0	6.430236	1.284135	-0.313347
81	1	0	5.004414	-1.293815	-3.441989
82	17	0	7.456917	-0.679195	-2.118665

TS1(*R*)

Sum of electronic and zero-point Energies = -6123.730920

Sum of electronic and thermal Energies = -6123.685577

Sum of electronic and thermal Enthalpies = -6123.684633

Sum of electronic and thermal Free Energies = -6123.810825

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.092436	-1.759622	1.423346
2	6	0	1.140141	-0.894402	1.195758
3	7	0	-1.017855	-1.041031	1.156049
4	1	0	0.045263	-2.780069	1.766393
5	7	0	-0.708306	0.196393	0.771787
6	7	0	0.598853	0.281300	0.812231
7	6	0	2.647509	-0.997081	1.327298
8	8	0	3.235497	0.204346	1.003473
9	1	0	2.966991	-1.787882	0.623933
10	6	0	3.030480	-1.482014	2.748623
11	6	0	2.600749	-0.480600	3.819848
12	1	0	2.502572	-2.431718	2.922042
13	1	0	1.520246	-0.294486	3.798591
14	1	0	2.850992	-0.843912	4.821128
15	30	0	2.185532	1.732797	1.062213
16	6	0	2.338443	3.582881	1.662174
17	1	0	1.380016	3.871191	2.113240
18	6	0	2.644020	4.592882	0.554148
19	6	0	3.400657	3.659884	2.767058
20	1	0	1.875236	4.597619	-0.225243
21	1	0	2.713574	5.617911	0.949472
22	1	0	3.603265	4.381878	0.063364
23	1	0	3.506992	4.683458	3.158738
24	1	0	3.157162	3.015828	3.620788
25	1	0	4.390711	3.352653	2.407079
26	1	0	3.114555	0.475238	3.674720
27	6	0	4.533251	-1.744612	2.809585

28	1	0	5.083118	-0.819064	2.617630
29	1	0	4.828414	-2.125418	3.792742
30	1	0	4.839639	-2.478517	2.056075
31	6	0	-2.374703	-1.439096	1.334365
32	6	0	-3.236264	-0.588958	2.017438
33	6	0	-2.793069	-2.671988	0.850057
34	6	0	-4.553391	-0.979277	2.217990
35	1	0	-2.876904	0.360683	2.397883
36	6	0	-4.106696	-3.068463	1.062525
37	1	0	-2.112691	-3.295634	0.281891
38	6	0	-4.972543	-2.217121	1.741410
39	1	0	-5.242342	-0.330540	2.745524
40	1	0	-4.459069	-4.019961	0.682853
41	17	0	-6.629153	-2.708891	1.990375
42	30	0	-1.695413	1.604417	-0.878878
43	6	0	-0.561919	3.173807	-0.605799
44	1	0	0.465302	2.825690	-0.423877
45	6	0	-0.532990	4.128637	-1.799540
46	1	0	-1.534945	4.502018	-2.041003
47	1	0	0.095260	5.011241	-1.600157
48	1	0	-0.159109	3.645039	-2.706367
49	6	0	-1.017007	3.907590	0.660225
50	1	0	-2.050172	4.268716	0.565394
51	1	0	-0.980091	3.262850	1.548098
52	1	0	-0.395604	4.789984	0.874128
53	6	0	-3.692490	1.187203	-1.124808
54	1	0	-3.556856	1.366355	-0.029555
55	6	0	-4.409473	2.425850	-1.654759
56	1	0	-3.831162	3.342610	-1.492609
57	1	0	-4.578432	2.353248	-2.734222
58	1	0	-5.386315	2.562629	-1.171259
59	6	0	-4.580032	-0.053409	-1.160531
60	1	0	-4.022577	-0.971061	-0.959147
61	1	0	-5.396340	0.018933	-0.431233
62	1	0	-5.056829	-0.174140	-2.141092
63	8	0	-2.111401	1.788403	-3.461688
64	6	0	-2.520568	0.749281	-2.906183
65	1	0	-3.472937	0.281570	-3.185568
66	6	0	-1.470239	-0.256483	-2.507797

67	6	0	-0.110737	-0.117717	-2.685244
68	7	0	-1.700047	-1.478514	-1.948913
69	1	0	0.475277	0.667658	-3.133245
70	7	0	-0.570178	-2.078936	-1.755863
71	7	0	0.410544	-1.264714	-2.196802
72	6	0	1.771895	-1.656817	-2.087429
73	6	0	2.088618	-3.013038	-2.058915
74	6	0	2.760039	-0.686305	-1.978508
75	6	0	3.413324	-3.398217	-1.912055
76	1	0	1.304515	-3.755017	-2.147361
77	6	0	4.088044	-1.070277	-1.844252
78	1	0	2.504237	0.366267	-1.959487
79	6	0	4.400999	-2.422301	-1.806553
80	1	0	3.675761	-4.449436	-1.884585
81	1	0	4.860647	-0.320486	-1.730570
82	17	0	6.067642	-2.912587	-1.610712

7(S).7(R)

Sum of electronic and zero-point Energies= -6123.812489

Sum of electronic and thermal Energies= -6123.767385

Sum of electronic and thermal Enthalpies= -6123.766440

Sum of electronic and thermal Free Energies= -6123.894865

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.278978	-1.081912	1.735384
2	6	0	0.643826	-0.103591	1.468849
3	7	0	-1.478201	-0.503781	1.477037
4	1	0	-0.179875	-2.098440	2.076109
5	7	0	-1.331862	0.757963	1.073844
6	7	0	-0.048604	0.993313	1.073413
7	6	0	2.148239	-0.004184	1.571136
8	8	0	2.592529	1.090201	0.849767
9	1	0	2.559172	-0.935779	1.152373
10	6	0	2.598005	0.023755	3.056942
11	6	0	2.098970	1.264689	3.796088
12	1	0	2.163106	-0.865058	3.536493
13	1	0	1.009078	1.370785	3.739235
14	1	0	2.364542	1.218866	4.856621
15	30	0	1.421115	2.547190	0.866157
16	6	0	1.250434	4.478738	1.074533
17	1	0	0.186617	4.731675	0.960088
18	6	0	2.025174	5.272670	0.018248
19	6	0	1.672139	4.913489	2.483635
20	1	0	1.716986	5.020868	-1.003045
21	1	0	1.883033	6.357674	0.138840
22	1	0	3.104665	5.085794	0.084529
23	1	0	1.535007	5.995569	2.632495
24	1	0	1.095992	4.406976	3.267286
25	1	0	2.732386	4.701618	2.673662
26	1	0	2.556428	2.172547	3.388055
27	6	0	4.120011	-0.079932	3.127201

28	1	0	4.578336	0.770846	2.614495
29	1	0	4.469885	-0.086526	4.164608
30	1	0	4.478632	-0.995893	2.644913
31	6	0	-2.775459	-1.076835	1.609725
32	6	0	-3.860380	-0.249079	1.880616
33	6	0	-2.931922	-2.450725	1.466409
34	6	0	-5.123754	-0.808633	2.015046
35	1	0	-3.716290	0.818942	1.989891
36	6	0	-4.192724	-3.012169	1.620598
37	1	0	-2.092636	-3.075918	1.184882
38	6	0	-5.276562	-2.186085	1.892667
39	1	0	-5.979243	-0.178467	2.227276
40	1	0	-4.331179	-4.080049	1.501987
41	17	0	-6.866905	-2.889336	2.073707
42	30	0	-1.055504	1.774081	-2.460225
43	6	0	-0.970968	3.462543	-1.569704
44	1	0	-0.122557	3.410014	-0.878446
45	6	0	-0.723162	4.632973	-2.524271
46	1	0	-1.532905	4.740090	-3.256892
47	1	0	-0.660936	5.584303	-1.976294
48	1	0	0.210418	4.523116	-3.087730
49	6	0	-2.220122	3.701461	-0.717064
50	1	0	-3.131135	3.754734	-1.327015
51	1	0	-2.367812	2.910999	0.026400
52	1	0	-2.148448	4.655230	-0.174075
53	6	0	-3.027136	-0.499061	-1.966851
54	1	0	-2.652719	-0.131077	-1.000331
55	6	0	-3.898842	0.596473	-2.585975
56	1	0	-3.401392	1.570736	-2.628360
57	1	0	-4.194985	0.338175	-3.608242
58	1	0	-4.806723	0.732632	-1.990504
59	6	0	-3.882052	-1.744361	-1.723252
60	1	0	-3.283168	-2.583749	-1.368071
61	1	0	-4.661165	-1.540248	-0.981960
62	1	0	-4.377764	-2.047504	-2.653434
63	8	0	-1.200821	0.281014	-3.443982
64	6	0	-1.793886	-0.832679	-2.847958
65	1	0	-2.151930	-1.496373	-3.653240
66	6	0	-0.713981	-1.578173	-2.085390

67	6	0	0.638805	-1.350969	-2.193141
68	7	0	-0.889837	-2.602145	-1.204494
69	1	0	1.213464	-0.676822	-2.805137
70	7	0	0.267415	-3.015307	-0.775074
71	7	0	1.207531	-2.263346	-1.370955
72	6	0	2.588742	-2.512177	-1.150939
73	6	0	3.028542	-3.826322	-1.024114
74	6	0	3.474949	-1.442882	-1.057373
75	6	0	4.375839	-4.076406	-0.799864
76	1	0	2.318234	-4.641108	-1.100313
77	6	0	4.825184	-1.693122	-0.845733
78	1	0	3.114970	-0.417865	-1.075996
79	6	0	5.261450	-3.006993	-0.719112
80	1	0	4.734966	-5.093683	-0.697145
81	1	0	5.522930	-0.869182	-0.754015
82	17	0	6.959532	-3.323380	-0.439509

8(*SS*)

Sum of electronic and zero-point Energies = -6123.864057

Sum of electronic and thermal Energies = -6123.818808

Sum of electronic and thermal Enthalpies = -6123.817864

Sum of electronic and thermal Free Energies = -6123.947982

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.747414	1.342104	0.910051
2	6	0	-2.461685	1.485768	0.458563
3	7	0	-4.381385	0.644489	-0.070386
4	1	0	-4.233219	1.633462	1.826454
5	7	0	-3.552106	0.362768	-1.074812
6	7	0	-2.402246	0.870686	-0.751193
7	6	0	-1.187316	2.095223	1.000206
8	8	0	-0.115253	1.372698	0.479450
9	30	0	0.301282	-0.374246	1.314306
10	6	0	-0.321292	-0.982504	3.077884
11	1	0	-1.397771	-0.768362	3.167752
12	6	0	0.383668	-0.240657	4.218883
13	1	0	0.224577	0.843796	4.166078
14	1	0	0.041316	-0.571390	5.213680
15	1	0	1.470223	-0.399952	4.192126
16	6	0	-0.149570	-2.495865	3.245181
17	1	0	-0.492366	-2.855636	4.229878
18	1	0	-0.706495	-3.057920	2.485179
19	1	0	0.904706	-2.792670	3.154007
20	8	0	-0.053657	-1.134015	-0.554519
21	6	0	0.961691	-1.951408	-1.046554
22	30	0	-0.413299	0.621210	-1.409874
23	6	0	2.278846	-1.410515	-0.533744
24	6	0	0.368583	1.338218	-3.066057
25	6	0	3.575819	-1.408322	-0.975554
26	7	0	2.265810	-0.725659	0.639045
27	1	0	-0.115940	0.871094	-3.936494

28	6	0	1.870410	1.053328	-3.178695
29	6	0	0.114297	2.846604	-3.166427
30	7	0	4.261259	-0.713398	-0.029266
31	1	0	4.050727	-1.836102	-1.843060
32	7	0	3.453848	-0.302129	0.948513
33	1	0	2.080089	-0.021999	-3.233066
34	1	0	2.316290	1.514332	-4.076001
35	1	0	2.423848	1.445519	-2.314722
36	1	0	0.536514	3.284424	-4.086242
37	1	0	-0.957112	3.083209	-3.159156
38	1	0	0.568487	3.387996	-2.325387
39	6	0	-5.725602	0.178756	-0.102920
40	6	0	-6.721060	0.898374	0.549142
41	6	0	-6.017524	-0.999520	-0.783656
42	6	0	-8.027880	0.427092	0.532660
43	1	0	-6.491629	1.828469	1.057189
44	6	0	-7.325594	-1.462667	-0.813181
45	1	0	-5.226257	-1.547331	-1.280993
46	6	0	-8.317976	-0.748373	-0.150107
47	1	0	-8.813349	0.977506	1.036909
48	1	0	-7.566630	-2.379188	-1.338737
49	17	0	-9.962843	-1.339386	-0.175615
50	6	0	5.647979	-0.396033	0.004992
51	6	0	6.310795	-0.382716	1.227799
52	6	0	6.314416	-0.106501	-1.180798
53	6	0	7.664206	-0.075272	1.264594
54	1	0	5.771053	-0.609739	2.139565
55	6	0	7.672220	0.185340	-1.146657
56	1	0	5.780046	-0.085428	-2.124284
57	6	0	8.333233	0.198619	0.076227
58	1	0	8.194153	-0.058758	2.209622
59	1	0	8.204535	0.412984	-2.062650
60	17	0	10.040695	0.570695	0.121074
61	6	0	-1.071437	3.591354	0.637658
62	1	0	-1.086318	3.650037	-0.459981
63	6	0	0.269216	4.129345	1.133361
64	1	0	0.411562	5.170646	0.826951
65	1	0	0.320364	4.093365	2.229032
66	1	0	1.093403	3.532535	0.738062

67	6	0	-2.236681	4.412158	1.189971
68	1	0	-2.092383	5.475862	0.977747
69	1	0	-3.194676	4.117407	0.750468
70	1	0	-2.314337	4.301765	2.278951
71	1	0	-1.217971	2.018595	2.100832
72	1	0	0.988437	-1.925236	-2.149426
73	6	0	0.745348	-3.419251	-0.616495
74	1	0	0.792700	-3.435175	0.481793
75	6	0	-0.646257	-3.878740	-1.046197
76	1	0	-0.845972	-4.895506	-0.692782
77	1	0	-1.412812	-3.211498	-0.647428
78	1	0	-0.734620	-3.881240	-2.139988
79	6	0	1.827984	-4.346646	-1.168280
80	1	0	1.873168	-4.290043	-2.263201
81	1	0	2.820265	-4.104441	-0.775155
82	1	0	1.616883	-5.387097	-0.903156

8(*RS*)

Sum of electronic and zero-point Energies = -6123.868490

Sum of electronic and thermal Energies = -6123.822956

Sum of electronic and thermal Enthalpies = -6123.822012

Sum of electronic and thermal Free Energies = -6123.952680

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.747414	1.342104	0.910051
2	6	0	-2.461685	1.485768	0.458563
3	7	0	-4.381385	0.644489	-0.070386
4	1	0	-4.233219	1.633462	1.826454
5	7	0	-3.552106	0.362768	-1.074812
6	7	0	-2.402246	0.870686	-0.751193
7	6	0	-1.187316	2.095223	1.000206
8	8	0	-0.115253	1.372698	0.479450
9	30	0	0.301282	-0.374246	1.314306
10	6	0	-0.321292	-0.982504	3.077884
11	1	0	-1.397771	-0.768362	3.167752
12	6	0	0.383668	-0.240657	4.218883
13	1	0	0.224577	0.843796	4.166078
14	1	0	0.041316	-0.571390	5.213680
15	1	0	1.470223	-0.399952	4.192126
16	6	0	-0.149570	-2.495865	3.245181
17	1	0	-0.492366	-2.855636	4.229878
18	1	0	-0.706495	-3.057920	2.485179
19	1	0	0.904706	-2.792670	3.154007
20	8	0	-0.053657	-1.134015	-0.554519
21	6	0	0.961691	-1.951408	-1.046554
22	30	0	-0.413299	0.621210	-1.409874
23	6	0	2.278846	-1.410515	-0.533744
24	6	0	0.368583	1.338218	-3.066057
25	6	0	3.575819	-1.408322	-0.975554
26	7	0	2.265810	-0.725659	0.639045
27	1	0	-0.115940	0.871094	-3.936494

28	6	0	1.870410	1.053328	-3.178695
29	6	0	0.114297	2.846604	-3.166427
30	7	0	4.261259	-0.713398	-0.029266
31	1	0	4.050727	-1.836102	-1.843060
32	7	0	3.453848	-0.302129	0.948513
33	1	0	2.080089	-0.021999	-3.233066
34	1	0	2.316290	1.514332	-4.076001
35	1	0	2.423848	1.445519	-2.314722
36	1	0	0.536514	3.284424	-4.086242
37	1	0	-0.957112	3.083209	-3.159156
38	1	0	0.568487	3.387996	-2.325387
39	6	0	-5.725602	0.178756	-0.102920
40	6	0	-6.721060	0.898374	0.549142
41	6	0	-6.017524	-0.999520	-0.783656
42	6	0	-8.027880	0.427092	0.532660
43	1	0	-6.491629	1.828469	1.057189
44	6	0	-7.325594	-1.462667	-0.813181
45	1	0	-5.226257	-1.547331	-1.280993
46	6	0	-8.317976	-0.748373	-0.150107
47	1	0	-8.813349	0.977506	1.036909
48	1	0	-7.566630	-2.379188	-1.338737
49	17	0	-9.962843	-1.339386	-0.175615
50	6	0	5.647979	-0.396033	0.004992
51	6	0	6.310795	-0.382716	1.227799
52	6	0	6.314416	-0.106501	-1.180798
53	6	0	7.664206	-0.075272	1.264594
54	1	0	5.771053	-0.609739	2.139565
55	6	0	7.672220	0.185340	-1.146657
56	1	0	5.780046	-0.085428	-2.124284
57	6	0	8.333233	0.198619	0.076227
58	1	0	8.194153	-0.058758	2.209622
59	1	0	8.204535	0.412984	-2.062650
60	17	0	10.040695	0.570695	0.121074
61	6	0	-1.071437	3.591354	0.637658
62	1	0	-1.086318	3.650037	-0.459981
63	6	0	0.269216	4.129345	1.133361
64	1	0	0.411562	5.170646	0.826951
65	1	0	0.320364	4.093365	2.229032
66	1	0	1.093403	3.532535	0.738062

67	6	0	-2.236681	4.412158	1.189971
68	1	0	-2.092383	5.475862	0.977747
69	1	0	-3.194676	4.117407	0.750468
70	1	0	-2.314337	4.301765	2.278951
71	1	0	-1.217971	2.018595	2.100832
72	1	0	0.988437	-1.925236	-2.149426
73	6	0	0.745348	-3.419251	-0.616495
74	1	0	0.792700	-3.435175	0.481793
75	6	0	-0.646257	-3.878740	-1.046197
76	1	0	-0.845972	-4.895506	-0.692782
77	1	0	-1.412812	-3.211498	-0.647428
78	1	0	-0.734620	-3.881240	-2.139988
79	6	0	1.827984	-4.346646	-1.168280
80	1	0	1.873168	-4.290043	-2.263201
81	1	0	2.820265	-4.104441	-0.775155
82	1	0	1.616883	-5.387097	-0.903156

11

Sum of electronic and zero-point Energies = -8139.843464

Sum of electronic and thermal Energies = -8139.786398

Sum of electronic and thermal Enthalpies = -8139.785453

Sum of electronic and thermal Free Energies = -8139.939256

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.558419	1.043631	1.110164
2	6	0	-3.215725	0.826289	0.929161
3	7	0	-5.149609	0.467691	0.030602
4	1	0	-5.120109	1.513058	1.900453
5	7	0	-4.241902	-0.082375	-0.778074
6	7	0	-3.084765	0.133935	-0.231797
7	6	0	-1.964069	1.160554	1.714314
8	8	0	-0.925741	0.375350	1.216065
9	30	0	-0.461608	-1.326407	2.024989
10	6	0	-0.106211	-1.808992	3.876808
11	1	0	0.577754	-2.669702	3.901432
12	6	0	-1.383817	-2.222756	4.615642
13	1	0	-1.862599	-3.097420	4.159812
14	1	0	-1.182426	-2.474207	5.668585
15	1	0	-2.130373	-1.417481	4.626148
16	6	0	0.592550	-0.657409	4.608541
17	1	0	0.781836	-0.896925	5.666956
18	1	0	1.557910	-0.408813	4.154705
19	1	0	-0.006096	0.262708	4.595099
20	1	0	-2.166167	0.919928	2.771412
21	6	0	-1.583804	2.657579	1.668164
22	6	0	-2.696754	3.557737	2.203076
23	1	0	-0.722577	2.737615	2.343004
24	1	0	-2.328409	4.578612	2.340978
25	1	0	-3.540838	3.608011	1.505834
26	8	0	-0.704736	-2.096389	0.260852
27	6	0	0.313035	-2.943812	-0.183800

28 30 0 -1.005032 -0.313500 -0.710675

29 6 0 1.607775 -2.157566 -0.207382

30 1 0 0.442406 -3.780765 0.524690

31 6 0 -0.037190 -3.563854 -1.552490

32 6 0 -0.510321 0.152392 -2.557388

33 6 0 2.937299 -2.511709 -0.168888

34 7 0 1.549469 -0.802245 -0.253507

35 6 0 1.037455 -4.537950 -2.034353

36 1 0 0.149221 -0.654937 -2.912998

37 6 0 0.306067 1.442283 -2.662368

38 6 0 -1.715804 0.203028 -3.499092

39 7 0 3.607651 -1.336228 -0.203073

40 1 0 3.442829 -3.460468 -0.091065

41 7 0 2.747116 -0.316086 -0.257828

42 1 0 0.730971 -5.011552 -2.971664

43 1 0 1.994098 -4.040508 -2.220069

44 1 0 1.148555 1.447192 -1.959259

45 1 0 0.730486 1.591641 -3.667916

46 1 0 -0.300630 2.330076 -2.441829

47 1 0 -1.434228 0.435766 -4.539375

48 1 0 -2.260496 -0.749365 -3.518083

49 1 0 -2.438164 0.970214 -3.189321

50 1 0 1.203635 -5.337248 -1.300791

51 1 0 -0.110981 -2.738120 -2.271233

52 6 0 -1.399721 -4.249835 -1.464180

53 1 0 -1.379338 -5.063577 -0.728437

54 1 0 -2.173931 -3.542162 -1.160853

55 1 0 -1.680394 -4.678670 -2.431330

56 1 0 -3.072420 3.209585 3.172832

57 6 0 -1.125820 3.082678 0.276365

58 1 0 -1.909754 2.921016 -0.474479

59 1 0 -0.868388 4.146544 0.262609

60 1 0 -0.239994 2.519920 -0.026524

61 6 0 -6.534670 0.378886 -0.282038

62 6 0 -7.401306 1.382044 0.138600

63 6 0 -6.997762 -0.717555 -1.003159

64 6 0 -8.756618 1.279561 -0.148848

65 1 0 -7.027565 2.249339 0.671521

66 6 0 -8.349351 -0.812329 -1.304646

67 1 0 -6.304644 -1.485750 -1.323953

68 6 0 -9.217281 0.183225 -0.868569

69 1 0 -9.444268 2.052264 0.173969

70 1 0 -8.724488 -1.660378 -1.865327

71 17 0 -10.921561 0.055303 -1.235013

72 6 0 5.007703 -1.092376 -0.158630

73 6 0 5.490639 -0.096418 0.684583

74 6 0 5.859667 -1.830590 -0.970811

75 6 0 6.851575 0.176930 0.705092

76 1 0 4.811480 0.455622 1.325563

77 6 0 7.224340 -1.572268 -0.936144

78 1 0 5.460935 -2.582577 -1.642831

79 6 0 7.704714 -0.567385 -0.102928

80 1 0 7.242993 0.954035 1.350776

81 1 0 7.903080 -2.134786 -1.566038

82 17 0 9.418221 -0.230701 -0.073392

83 30 0 3.220870 1.901746 -0.585687

84 6 0 4.003709 1.956117 -2.387672

85 1 0 3.603468 1.102640 -2.957065

86 6 0 2.728810 2.662989 1.164542

87 1 0 1.945903 3.416663 0.984997

88 6 0 5.532033 1.845655 -2.417498

89 1 0 5.892029 0.891537 -2.017309

90 1 0 5.933452 1.934112 -3.440546

91 1 0 6.011865 2.639392 -1.828456

92 6 0 3.567854 3.230324 -3.121756

93 1 0 2.477290 3.330132 -3.176385

94 1 0 3.946335 4.132555 -2.621753

95 1 0 3.946194 3.265951 -4.156567

96 6 0 3.922581 3.409853 1.776005

97 1 0 4.315625 4.184962 1.106641

98 1 0 3.667814 3.902396 2.728472

99 1 0 4.760599 2.732907 1.998564

100 6 0 2.152649 1.663163 2.170786

101 1 0 2.854829 0.841908 2.382031

102 1 0 1.932784 2.132297 3.144260

103 1 0 1.226010 1.204189 1.809373

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Sum of electronic and zero-point Energies = -9185.735773

Sum of electronic and thermal Energies = -9185.666053

Sum of electronic and thermal Enthalpies = -9185.665109

Sum of electronic and thermal Free Energies = -9185.848242

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.306984	-0.707596	1.450933
2	6	0	-2.974984	-0.696473	1.119130
3	7	0	-4.946282	-1.073880	0.308988
4	1	0	-4.825626	-0.533912	2.378903
5	7	0	-4.079712	-1.287808	-0.680376
6	7	0	-2.900166	-1.061335	-0.186056
7	6	0	-1.692343	-0.401397	1.868765
8	8	0	-0.612582	-0.787692	1.075110
9	30	0	0.195073	-2.537092	1.584516
10	6	0	-0.183967	-3.449497	3.294063
11	1	0	0.446991	-4.351481	3.328847
12	6	0	-1.637745	-3.931940	3.372241
13	1	0	-1.898206	-4.590883	2.535364
14	1	0	-1.842623	-4.487914	4.302308
15	1	0	-2.352406	-3.097394	3.347089
16	6	0	0.171881	-2.620463	4.532082
17	1	0	-0.060026	-3.152392	5.470013
18	1	0	1.237232	-2.364349	4.560620
19	1	0	-0.378549	-1.670143	4.567015
20	1	0	-1.719972	-0.998165	2.795077
21	6	0	-1.572110	1.073666	2.308689
22	6	0	-2.645726	1.465395	3.323125
23	1	0	-0.596740	1.120596	2.806989
24	1	0	-2.415388	2.437213	3.770604
25	1	0	-3.631151	1.556212	2.851088
26	8	0	-0.423433	-3.111957	-0.287472
27	6	0	0.520413	-3.876066	-0.968588

28 30 0 -0.927242 -1.274572 -0.877483

29 6 0 1.890968 -3.288863 -0.656827

30 1 0 0.519880 -4.899684 -0.548363

31 6 0 0.215323 -4.017199 -2.472307

32 6 0 -0.536015 -0.342075 -2.568727

33 6 0 3.140915 -3.263336 -1.224232

34 7 0 1.996905 -2.613918 0.520321

35 6 0 1.066676 -5.106981 -3.129135

36 1 0 0.507848 -0.522675 -2.866322

37 6 0 -0.709078 1.168805 -2.392096

38 6 0 -1.433671 -0.823723 -3.713015

39 7 0 3.911721 -2.568892 -0.345098

40 1 0 3.545229 -3.674829 -2.132340

41 7 0 3.203496 -2.179470 0.710121

42 1 0 0.818396 -5.199516 -4.190869

43 1 0 2.140648 -4.915230 -3.068630

44 1 0 -0.008592 1.581415 -1.658014

45 1 0 -0.553638 1.717878 -3.338124

46 1 0 -1.721606 1.416416 -2.043412

47 1 0 -1.260639 -0.257828 -4.643768

48 1 0 -1.279757 -1.881903 -3.951537

49 1 0 -2.498443 -0.705752 -3.468306

50 1 0 0.879832 -6.079621 -2.658760

51 1 0 0.430330 -3.053646 -2.953008

52 6 0 -1.266516 -4.342761 -2.667542

53 1 0 -1.526591 -5.275605 -2.153069

54 1 0 -1.914406 -3.557466 -2.272753

55 1 0 -1.492763 -4.471721 -3.730835

56 1 0 -2.720348 0.735729 4.137920

57 6 0 -1.543326 2.028071 1.121000

58 1 0 -2.495846 2.020901 0.576662

59 1 0 -1.364383 3.054965 1.456405

60 1 0 -0.746296 1.759016 0.426855

61 6 0 -6.340752 -1.250374 0.089344

62 6 0 -7.251342 -0.476240 0.800532

63 6 0 -6.768885 -2.196238 -0.837111

64 6 0 -8.612792 -0.658688 0.594342

65 1 0 -6.908597 0.277306 1.500661

66 6 0 -8.129014 -2.368159 -1.055240

67 1 0 -6.043047 -2.790109 -1.379459

68 6 0 -9.038175 -1.601786 -0.333683

69 1 0 -9.333132 -0.062527 1.142118

70 1 0 -8.477923 -3.100024 -1.774237

71 17 0 -10.750669 -1.827182 -0.600444

72 6 0 5.287974 -2.218672 -0.438818

73 6 0 5.997898 -1.959547 0.729569

74 6 0 5.889782 -2.105545 -1.686644

75 6 0 7.330760 -1.580923 0.646348

76 1 0 5.509564 -2.045569 1.692346

77 6 0 7.227789 -1.741871 -1.769410

78 1 0 5.321440 -2.261477 -2.596361

79 6 0 7.934554 -1.479626 -0.602111

80 1 0 7.893212 -1.370100 1.548164

81 1 0 7.706743 -1.640761 -2.735959

82 17 0 9.614240 -1.006452 -0.705256

83 30 0 2.861642 1.214955 0.395840

84 6 0 3.648361 0.833061 -1.362161

85 1 0 3.591601 -0.246936 -1.561769

86 6 0 2.421761 1.365553 2.302855

87 1 0 1.529303 2.012125 2.354058

88 6 0 5.131079 1.224369 -1.289322

89 1 0 5.673590 0.690937 -0.499260

90 1 0 5.662682 1.027297 -2.234862

91 1 0 5.246663 2.295852 -1.080060

92 6 0 2.998321 1.537413 -2.553827

93 1 0 1.966190 1.214155 -2.718611

94 1 0 2.977772 2.626553 -2.418301

95 1 0 3.549038 1.350459 -3.491226

96 6 0 3.549714 2.103126 3.035432

97 1 0 3.792346 3.065827 2.572136

98 1 0 3.303786 2.300638 4.092046

99 1 0 4.479354 1.517591 3.038867

100 6 0 2.081154 0.072759 3.043384

101 1 0 2.914390 -0.641235 3.027157

102 1 0 1.837191 0.252127 4.103988

103 1 0 1.218870 -0.424123 2.589514

104 8 0 5.149331 4.398292 0.713851

105 6 0 4.241441 5.193442 0.623016

106 1 0 4.404627 6.275143 0.794910

107 6 0 2.859412 4.835209 0.281372

108 6 0 1.774461 5.670948 0.127684

109 1 0 1.657684 6.740393 0.205869

110 7 0 2.439584 3.560818 0.043202

111 7 0 1.186045 3.568621 -0.247105

112 7 0 0.762006 4.845962 -0.200776

113 6 0 -0.604432 5.144567 -0.469056

114 6 0 -1.289589 6.036698 0.347602

115 6 0 -1.233102 4.496250 -1.525667

116 6 0 -2.632121 6.292241 0.097131

117 1 0 -0.792537 6.507953 1.188623

118 6 0 -2.578246 4.738388 -1.766852

119 1 0 -0.677744 3.803567 -2.146390

120 6 0 -3.263150 5.636071 -0.954513

121 1 0 -3.185316 6.979457 0.726328

122 1 0 -3.083290 4.234907 -2.582705

123 17 0 -4.956641 5.943856 -1.257972

TS2(*S*)

Sum of electronic and zero-point Energies = -9185.710883

Sum of electronic and thermal Energies = -9185.642323

Sum of electronic and thermal Enthalpies = -9185.641379

Sum of electronic and thermal Free Energies = -9185.821473

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.836707	-2.821872	-1.410550
2	6	0	2.055330	-1.804715	-0.926279
3	7	0	3.322662	-3.437683	-0.302126
4	1	0	3.035569	-3.178907	-2.407197
5	7	0	2.884654	-2.850518	0.811090
6	7	0	2.126701	-1.868500	0.426556
7	6	0	1.264800	-0.688497	-1.559222
8	8	0	0.338241	-0.218070	-0.589987
9	30	0	-1.052848	-1.774816	-0.512234
10	6	0	-1.340655	-3.188393	-1.860038
11	1	0	-1.949626	-3.920253	-1.302296
12	6	0	-0.154443	-3.963581	-2.431540
13	1	0	0.467039	-4.413262	-1.648842
14	1	0	-0.482405	-4.778577	-3.096669
15	1	0	0.497059	-3.318877	-3.036809
16	6	0	-2.227713	-2.675246	-3.002301
17	1	0	-2.536108	-3.487786	-3.680112
18	1	0	-3.142174	-2.196230	-2.633482
19	1	0	-1.708666	-1.930324	-3.618599
20	1	0	0.707778	-1.096619	-2.412847
21	6	0	2.200798	0.406761	-2.112072
22	6	0	2.776088	-0.005775	-3.465707
23	1	0	1.557314	1.275801	-2.278475
24	1	0	3.361202	0.812979	-3.894851
25	1	0	3.447729	-0.868405	-3.373992
26	8	0	-0.670130	-1.707954	1.463813
27	6	0	-1.756190	-1.754649	2.344626

28	30	0	0.899516	-0.473347	1.421681
29	6	0	-3.015267	-1.390497	1.576357
30	1	0	-1.907219	-2.794836	2.685887
31	6	0	-1.482447	-0.903982	3.601794
32	6	0	1.764846	0.658406	2.788014
33	6	0	-4.353639	-1.305078	1.878461
34	7	0	-2.918121	-1.207545	0.235461
35	6	0	-2.709313	-0.624268	4.467865
36	1	0	1.010557	0.867754	3.560893
37	6	0	2.332517	2.009486	2.342440
38	6	0	2.885840	-0.151145	3.456075
39	7	0	-4.963976	-1.066196	0.689119
40	1	0	-4.908248	-1.423487	2.793816
41	7	0	-4.082714	-1.012566	-0.303801
42	1	0	-2.403560	-0.129638	5.394702
43	1	0	-3.425105	0.036605	3.971562
44	1	0	1.611189	2.620861	1.789845
45	1	0	2.685709	2.608874	3.196334
46	1	0	3.199874	1.868830	1.686103
47	1	0	3.372137	0.407333	4.271880
48	1	0	2.529468	-1.095566	3.883199
49	1	0	3.673727	-0.409672	2.736048
50	1	0	-3.224404	-1.551135	4.750451
51	1	0	-1.096685	0.053402	3.235169
52	6	0	-0.394930	-1.587709	4.432256
53	1	0	-0.793713	-2.484199	4.922393
54	1	0	0.448450	-1.896554	3.810243
55	1	0	-0.013429	-0.918961	5.209484
56	1	0	1.985165	-0.261351	-4.178506
57	6	0	3.304482	0.797065	-1.133158
58	1	0	4.046630	-0.002903	-1.028090
59	1	0	3.819291	1.696039	-1.479985
60	1	0	2.890912	1.014453	-0.146313
61	6	0	4.177277	-4.573223	-0.232770
62	6	0	5.162581	-4.740571	-1.199421
63	6	0	4.005827	-5.497884	0.792243
64	6	0	5.985240	-5.858437	-1.151240
65	1	0	5.301799	-3.998225	-1.977458
66	6	0	4.837547	-6.608326	0.849532

67	1	0	3.229555	-5.349943	1.533633
68	6	0	5.814174	-6.781611	-0.125982
69	1	0	6.757475	-6.001814	-1.897676
70	1	0	4.718139	-7.339867	1.639990
71	17	0	6.848510	-8.188797	-0.062115
72	6	0	-6.346335	-0.856651	0.425511
73	6	0	-6.891264	-1.346888	-0.756488
74	6	0	-7.120710	-0.159315	1.345538
75	6	0	-8.238487	-1.140242	-1.018711
76	1	0	-6.265662	-1.881084	-1.461861
77	6	0	-8.472060	0.036257	1.090006
78	1	0	-6.672513	0.249915	2.244310
79	6	0	-9.016999	-0.457333	-0.089856
80	1	0	-8.679677	-1.515550	-1.934432
81	1	0	-9.088942	0.581555	1.794368
82	17	0	-10.716346	-0.209369	-0.415018
83	30	0	-0.831054	1.543590	-1.155504
84	6	0	-1.997610	2.050271	0.604721
85	1	0	-1.713099	0.974702	0.545574
86	6	0	-1.373157	1.101345	-3.005820
87	1	0	-0.955727	0.113285	-3.258375
88	6	0	-3.518252	2.047623	0.510520
89	1	0	-3.867239	1.706369	-0.468298
90	1	0	-3.977290	1.406040	1.279128
91	1	0	-3.936237	3.050621	0.661479
92	6	0	-1.498958	2.473213	1.979899
93	1	0	-0.441039	2.235838	2.124014
94	1	0	-1.609015	3.553575	2.154629
95	1	0	-2.056640	1.984714	2.793608
96	6	0	-0.783408	2.110095	-3.996729
97	1	0	0.313012	2.157516	-3.943499
98	1	0	-1.043338	1.874931	-5.042653
99	1	0	-1.157150	3.119186	-3.787661
100	6	0	-2.891613	1.017519	-3.182091
101	1	0	-3.359752	1.982026	-2.951222
102	1	0	-3.179650	0.755812	-4.214533
103	1	0	-3.345552	0.270710	-2.520031
104	8	0	-2.269320	4.105781	-1.544810
105	6	0	-1.754469	4.011175	-0.423813

106	1	0	-2.289835	4.354191	0.477528
107	6	0	-0.255851	4.148825	-0.325006
108	6	0	0.581138	5.174409	0.023826
109	1	0	0.407845	6.148690	0.450048
110	7	0	0.522532	3.138378	-0.777223
111	7	0	1.776893	3.466635	-0.746411
112	7	0	1.827579	4.704113	-0.254945
113	6	0	3.084561	5.342221	-0.065823
114	6	0	3.195807	6.715724	-0.253460
115	6	0	4.185143	4.573991	0.301180
116	6	0	4.423979	7.335142	-0.057780
117	1	0	2.339163	7.301544	-0.568448
118	6	0	5.415799	5.189592	0.482393
119	1	0	4.072049	3.507110	0.450056
120	6	0	5.522956	6.565014	0.305221
121	1	0	4.526143	8.403991	-0.203141
122	1	0	6.281290	4.604134	0.769528
123	17	0	7.072905	7.340019	0.539501

8(*SS*)·**7**(*S*)

Sum of electronic and zero-point Energies = -9185.810473

Sum of electronic and thermal Energies = -9185.742634

Sum of electronic and thermal Enthalpies = -9185.741689

Sum of electronic and thermal Free Energies = -9185.918038

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.324451	0.200958	-1.429270
2	6	0	3.040249	0.203059	-0.948585
3	7	0	5.096266	-0.046545	-0.339428
4	1	0	4.732931	0.300801	-2.421013
5	7	0	4.351872	-0.188508	0.758177
6	7	0	3.118985	-0.035091	0.384748
7	6	0	1.680457	0.417737	-1.561585
8	8	0	0.732045	-0.162137	-0.684319
9	30	0	0.937159	-2.211885	-0.884362
10	6	0	1.790192	-3.135951	-2.402662
11	1	0	1.915740	-4.172489	-2.049469
12	6	0	3.168269	-2.675026	-2.878231
13	1	0	3.904298	-2.652100	-2.066042
14	1	0	3.570436	-3.333928	-3.664851
15	1	0	3.131969	-1.667093	-3.312448
16	6	0	0.815295	-3.191347	-3.586600
17	1	0	1.219216	-3.771210	-4.432633
18	1	0	-0.140815	-3.651036	-3.308792
19	1	0	0.582850	-2.189210	-3.971957
20	1	0	1.645420	-0.104899	-2.527939
21	6	0	1.403659	1.909210	-1.837455
22	6	0	2.269679	2.431905	-2.981714
23	1	0	0.359561	1.950671	-2.167351
24	1	0	1.971450	3.450296	-3.247982
25	1	0	3.329997	2.467696	-2.704736
26	8	0	1.196887	-2.194491	1.116082
27	6	0	0.406859	-3.106697	1.825992
28	30	0	1.228686	-0.216606	1.373730
29	6	0	-0.883411	-3.321763	1.048305
30	1	0	0.925581	-4.082600	1.851655

31 6 0 0.213240 -2.668606 3.290414

32 6 0 1.106667 0.933760 2.978199

33 6 0 -2.134922 -3.828679 1.293613

34 7 0 -0.875012 -2.970238 -0.263093

35 6 0 -0.638863 -3.638162 4.112913

36 1 0 0.517283 0.377712 3.722751

37 6 0 0.462930 2.317467 2.841570

38 6 0 2.515900 1.102844 3.564058

39 7 0 -2.798160 -3.708257 0.113509

40 1 0 -2.599177 -4.269870 2.157948

41 7 0 -2.018535 -3.193699 -0.827874

42 1 0 -0.526713 -3.421721 5.179854

43 1 0 -1.704236 -3.557188 3.889190

44 1 0 -0.511708 2.289166 2.344097

45 1 0 0.318069 2.800953 3.821078

46 1 0 1.098029 2.993896 2.256408

47 1 0 2.504735 1.664572 4.511946

48 1 0 3.011293 0.145981 3.764269

49 1 0 3.168664 1.656907 2.876612

50 1 0 -0.326888 -4.678086 3.956763

51 1 0 -0.286251 -1.692087 3.268357

52 6 0 1.585019 -2.507275 3.948094

53 1 0 2.063718 -3.485047 4.083606

54 1 0 2.252049 -1.893800 3.340917

55 1 0 1.489959 -2.038320 4.931997

56 1 0 2.169485 1.811526 -3.879113

57 6 0 1.541216 2.763044 -0.583259

58 1 0 2.573405 2.780671 -0.214158

59 1 0 1.238131 3.794068 -0.786158

60 1 0 0.899139 2.381817 0.211420

61 6 0 6.509863 -0.187638 -0.265923

62 6 0 7.321094 0.581061 -1.093109

63 6 0 7.052980 -1.094590 0.638364

64 6 0 8.700743 0.431857 -1.026561

65 1 0 6.888038 1.305325 -1.774159

66 6 0 8.432095 -1.233177 0.716296

67 1 0 6.401053 -1.684711 1.271324

68 6 0 9.242417 -0.472815 -0.120508

69 1 0 9.345003 1.025222 -1.664446

70 1 0 8.870056 -1.935113 1.416021

71 17 0 10.978658 -0.657497 -0.029945

72 6 0 -4.157130 -4.005592 -0.175499

73 6 0 -4.500484 -4.435503 -1.453265

74 6 0 -5.119286 -3.845676 0.815288

75 6 0 -5.828626 -4.717525 -1.740779

76 1 0 -3.735537 -4.539642 -2.213381

77 6 0 -6.446769 -4.142634 0.532741

78 1 0 -4.844576 -3.466233 1.793318

79 6 0 -6.787546 -4.576157 -0.743152

80 1 0 -6.112953 -5.050494 -2.731977

81 1 0 -7.207924 -4.022470 1.294553

82 17 0 -8.458855 -4.946020 -1.104014

83 30 0 -1.300017 0.189463 -1.107643

84 6 0 -2.625014 0.355621 2.758497

85 1 0 -1.535534 0.354885 2.871662

86 6 0 -1.595848 0.084624 -3.060026

87 1 0 -0.618240 -0.018433 -3.560869

88 6 0 -3.150513 -1.013699 3.183499

89 1 0 -2.783486 -1.773112 2.492471

90 1 0 -2.827189 -1.266593 4.199245

91 1 0 -4.248822 -1.028119 3.168367

92 6 0 -3.210852 1.447029 3.653169

93 1 0 -2.704793 2.407560 3.523481

94 1 0 -4.283250 1.589557 3.464557

95 1 0 -3.102700 1.170213 4.707046

96 6 0 -2.219302 1.390468 -3.567798

97 1 0 -1.606146 2.270525 -3.335915

98 1 0 -2.377298 1.383588 -4.659311

99 1 0 -3.202777 1.569702 -3.111255

100 6 0 -2.450799 -1.105122 -3.503209

101 1 0 -3.428131 -1.110827 -3.001926

102 1 0 -2.648497 -1.095618 -4.588991

103 1 0 -1.975511 -2.061045 -3.264245

104 8 0 -2.146779 -0.377332 0.514686

105 6 0 -2.887423 0.529809 1.239738

106 1 0 -3.978490 0.368928 1.096422

107 6 0 -2.627816 1.945091 0.741675

108 6 0 -3.131237 3.192335 1.026028

109 1 0 -3.840474 3.547697 1.754256

110 7 0 -1.745445 2.113751 -0.275879

111 7 0 -1.664815 3.360514 -0.631988

112 7 0 -2.502207 4.029106 0.160783

113 6 0 -2.635163 5.438752 0.035896

114 6 0 -3.871206 6.036769 0.256988

115 6 0 -1.519711 6.197140 -0.305158

116 6 0 -3.994214 7.416106 0.144868

117 1 0 -4.740863 5.434681 0.497002

118 6 0 -1.644535 7.573799 -0.432672

119 1 0 -0.564699 5.711102 -0.463766

120 6 0 -2.879441 8.170650 -0.201987

121 1 0 -4.951734 7.894973 0.311514

122 1 0 -0.784687 8.177446 -0.698490

123 17 0 -3.033282 9.906192 -0.352273

TS2(*R*) one small imaginary frequency was neglected

Sum of electronic and zero-point Energies = -9185.707882

Sum of electronic and thermal Energies = -9185.640516

Sum of electronic and thermal Enthalpies = -9185.639572

Sum of electronic and thermal Free Energies = -9185.814069

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.068527	-2.486287	-1.501156
2	6	0	2.225576	-1.577336	-0.913905
3	7	0	3.538564	-3.235097	-0.470106
4	1	0	3.319285	-2.686715	-2.529112
5	7	0	3.031770	-2.827117	0.692956
6	7	0	2.248559	-1.829683	0.418628
7	6	0	1.387657	-0.426212	-1.414862
8	8	0	0.389223	-0.175515	-0.437587
9	30	0	-0.841718	-1.857358	-0.580578
10	6	0	-1.002886	-2.970758	-2.201494
11	1	0	-1.665381	-3.789277	-1.875216
12	6	0	0.221431	-3.627158	-2.836233
13	1	0	0.792937	-4.231436	-2.121968
14	1	0	-0.056114	-4.287763	-3.673383
15	1	0	0.908960	-2.878234	-3.251882
16	6	0	-1.779588	-2.181970	-3.265001
17	1	0	-2.035323	-2.800878	-4.140308
18	1	0	-2.718327	-1.772879	-2.872144
19	1	0	-1.196567	-1.330894	-3.642206
20	1	0	0.901813	-0.732411	-2.352906
21	6	0	2.266305	0.798940	-1.737021
22	6	0	3.046073	0.589441	-3.033973
23	1	0	1.558728	1.616345	-1.901046
24	1	0	3.567468	1.509256	-3.315453
25	1	0	3.808021	-0.191768	-2.927767
26	8	0	-0.544497	-2.031298	1.394128
27	6	0	-1.677972	-2.249525	2.189819

28	30	0	0.917285	-0.700019	1.602419
29	6	0	-2.909516	-1.797918	1.417090
30	1	0	-1.809793	-3.336647	2.336887
31	6	0	-1.498130	-1.636236	3.594581
32	6	0	1.716743	0.249235	3.140868
33	6	0	-4.261080	-1.749309	1.662294
34	7	0	-2.752231	-1.460013	0.112813
35	6	0	-2.779250	-1.558662	4.422517
36	1	0	0.914718	0.403220	3.877853
37	6	0	2.368015	1.615400	2.892872
38	6	0	2.762805	-0.671427	3.788497
39	7	0	-4.816882	-1.372265	0.481869
40	1	0	-4.858344	-1.971482	2.529836
41	7	0	-3.890074	-1.201299	-0.455716
42	1	0	-2.539626	-1.263487	5.448508
43	1	0	-3.479313	-0.816595	4.029831
44	1	0	1.737160	2.301671	2.318295
45	1	0	2.625451	2.116914	3.839130
46	1	0	3.307479	1.508487	2.336121
47	1	0	3.217408	-0.213697	4.681647
48	1	0	2.349425	-1.636579	4.100649
49	1	0	3.584942	-0.889477	3.093621
50	1	0	-3.284738	-2.531308	4.476446
51	1	0	-1.126970	-0.616237	3.446739
52	6	0	-0.433625	-2.440551	4.343018
53	1	0	-0.835919	-3.411845	4.656393
54	1	0	0.438628	-2.630154	3.713303
55	1	0	-0.098133	-1.910354	5.238919
56	1	0	2.386965	0.310979	-3.863902
57	6	0	3.181330	1.185140	-0.582050
58	1	0	3.961582	0.432683	-0.417813
59	1	0	3.673668	2.142191	-0.776731
60	1	0	2.613451	1.299140	0.341335
61	6	0	4.411033	-4.358962	-0.511938
62	6	0	5.382029	-4.443248	-1.503465
63	6	0	4.264589	-5.362137	0.441134
64	6	0	6.216810	-5.552925	-1.549234
65	1	0	5.503410	-3.646459	-2.228974
66	6	0	5.108580	-6.463245	0.405270

67	1	0	3.496872	-5.280418	1.200885
68	6	0	6.072966	-6.551658	-0.593115
69	1	0	6.978428	-5.631610	-2.315907
70	1	0	5.008178	-7.250609	1.143000
71	17	0	7.125624	-7.945498	-0.646485
72	6	0	-6.185490	-1.127973	0.180229
73	6	0	-6.653481	-1.398189	-1.101575
74	6	0	-7.023293	-0.611526	1.162264
75	6	0	-7.985680	-1.152787	-1.403172
76	1	0	-5.978611	-1.789949	-1.853242
77	6	0	-8.360534	-0.380976	0.865232
78	1	0	-6.635446	-0.364061	2.144281
79	6	0	-8.828128	-0.654246	-0.414878
80	1	0	-8.366377	-1.353426	-2.397699
81	1	0	-9.026649	0.023050	1.618251
82	17	0	-10.508819	-0.356512	-0.792763
83	30	0	-0.940435	1.517898	-0.277766
84	6	0	-1.938832	1.475648	1.429399
85	1	0	-1.835501	0.474836	1.862249
86	6	0	-1.692984	1.596229	-2.362501
87	1	0	-1.443136	0.606918	-1.912165
88	6	0	-3.434038	1.759512	1.264735
89	1	0	-3.919336	1.054159	0.583599
90	1	0	-3.971963	1.714724	2.227781
91	1	0	-3.595584	2.756101	0.841000
92	6	0	-1.340877	2.460475	2.438571
93	1	0	-0.297810	2.228797	2.674421
94	1	0	-1.364083	3.491289	2.061776
95	1	0	-1.894498	2.461060	3.392414
96	6	0	-0.869020	1.626338	-3.643899
97	1	0	0.203353	1.513749	-3.454036
98	1	0	-1.161063	0.834189	-4.348741
99	1	0	-0.996303	2.574243	-4.186046
100	6	0	-3.190040	1.514927	-2.626249
101	1	0	-3.525867	2.349093	-3.254857
102	1	0	-3.474212	0.585707	-3.140034
103	1	0	-3.760990	1.575739	-1.694900
104	8	0	-2.668574	4.031697	-1.077358
105	6	0	-1.744683	3.718234	-1.847792

106	1	0	-1.865372	3.832536	-2.940728
107	6	0	-0.338526	4.018936	-1.369725
108	6	0	0.449878	5.140371	-1.434462
109	1	0	0.339661	6.077886	-1.954210
110	7	0	0.270618	3.171737	-0.509693
111	7	0	1.365952	3.677448	-0.036152
112	7	0	1.491553	4.878078	-0.598433
113	6	0	2.622743	5.680111	-0.280139
114	6	0	3.100022	6.603779	-1.203617
115	6	0	3.242005	5.510584	0.955339
116	6	0	4.206626	7.381187	-0.883721
117	1	0	2.629897	6.710523	-2.174802
118	6	0	4.356596	6.275758	1.268299
119	1	0	2.856893	4.784902	1.661766
120	6	0	4.826336	7.206883	0.347942
121	1	0	4.588097	8.105732	-1.593484
122	1	0	4.849226	6.151956	2.225444
123	17	0	6.227615	8.173533	0.746993

8(*SS*).**7**(*R*)

Sum of electronic and zero-point Energies= -9185.796028
Sum of electronic and thermal Energies= -9185.728878
Sum of electronic and thermal Enthalpies= -9185.727934
Sum of electronic and thermal Free Energies= -9185.901538

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.843286	-1.467169	-1.354193
2	6	0	2.781411	-0.805438	-0.794505
3	7	0	4.292398	-2.289156	-0.368872
4	1	0	4.271631	-1.460284	-2.342793
5	7	0	3.564329	-2.154388	0.741355
6	7	0	2.663146	-1.260071	0.478866
7	6	0	1.813297	0.259103	-1.258632
8	8	0	0.641348	0.159250	-0.497251
9	30	0	-0.455428	-1.395373	-1.118758
10	6	0	-0.282450	-2.246931	-2.894569
11	1	0	-1.001052	-3.082519	-2.879066
12	6	0	1.089646	-2.853852	-3.198532
13	1	0	1.428056	-3.537960	-2.411082
14	1	0	1.094269	-3.417755	-4.146057
15	1	0	1.858445	-2.076455	-3.299278
16	6	0	-0.711751	-1.327357	-4.042071
17	1	0	-0.674990	-1.831705	-5.022114
18	1	0	-1.734047	-0.955354	-3.906637
19	1	0	-0.061438	-0.444729	-4.119646
20	1	0	1.589625	0.076043	-2.321381
21	6	0	2.449787	1.664078	-1.159188
22	6	0	3.482587	1.894739	-2.260748
23	1	0	1.609602	2.348030	-1.322470
24	1	0	3.893629	2.907539	-2.197351
25	1	0	4.326003	1.200315	-2.166293
26	8	0	-0.141374	-2.128568	0.742610
27	6	0	-1.203444	-2.788116	1.355733
28	30	0	0.876668	-0.546762	1.416376
29	6	0	-2.495565	-2.285078	0.729538
30	1	0	-1.152226	-3.868244	1.122941
31	6	0	-1.127990	-2.659310	2.890530
32	6	0	1.139248	0.192060	3.228180
33	6	0	-3.834587	-2.538903	0.897213
34	7	0	-2.398597	-1.446755	-0.337845
35	6	0	-2.328736	-3.257509	3.621677
36	1	0	0.429903	-0.322777	3.892575
37	6	0	0.941281	1.693800	3.445538
38	6	0	2.544549	-0.211368	3.695727
39	7	0	-4.450363	-1.822080	-0.079635
40	1	0	-4.382341	-3.168138	1.577349
41	7	0	-3.568353	-1.168475	-0.827415
42	1	0	-2.136557	-3.288218	4.698397
43	1	0	-3.235781	-2.663373	3.479173
44	1	0	-0.037997	2.046387	3.105723
45	1	0	1.035813	1.966088	4.509494
46	1	0	1.686403	2.286668	2.903015
47	1	0	2.746038	0.112151	4.729647
48	1	0	2.701648	-1.296416	3.660657

49 1 0 3.323279 0.238916 3.065508
50 1 0 -2.526679 -4.286669 3.296111
51 1 0 -1.087634 -1.587045 3.109380
52 6 0 0.172698 -3.296633 3.381248
53 1 0 0.145704 -4.385041 3.245443
54 1 0 1.038102 -2.915161 2.833789
55 1 0 0.327593 -3.093074 4.445231
56 1 0 3.047299 1.765355 -3.258135
57 6 0 3.043982 1.933895 0.220943
58 1 0 3.942880 1.330784 0.391271
59 1 0 3.329593 2.984046 0.328036
60 1 0 2.321893 1.703175 1.006388
61 6 0 5.358456 -3.228714 -0.422082
62 6 0 6.502772 -2.923221 -1.150880
63 6 0 5.233428 -4.440506 0.249816
64 6 0 7.534106 -3.850622 -1.225891
65 1 0 6.600718 -1.963324 -1.645634
66 6 0 6.270163 -5.361991 0.188459
67 1 0 4.331256 -4.658571 0.808871
68 6 0 7.407000 -5.061263 -0.554581
69 1 0 8.431975 -3.626208 -1.789562
70 1 0 6.187041 -6.311502 0.703855
71 17 0 8.703170 -6.231147 -0.647601
72 6 0 -5.839926 -1.713507 -0.366429
73 6 0 -6.242371 -1.514567 -1.683491
74 6 0 -6.766970 -1.799132 0.666332
75 6 0 -7.595214 -1.401472 -1.970804
76 1 0 -5.501425 -1.446302 -2.470855
77 6 0 -8.122411 -1.702368 0.376732
78 1 0 -6.441170 -1.916327 1.694057
79 6 0 -8.522621 -1.504207 -0.939458
80 1 0 -7.924357 -1.244039 -2.991076
81 1 0 -8.857053 -1.764427 1.170766
82 17 0 -10.227504 -1.376544 -1.306089
83 30 0 -2.266949 1.615313 1.170103
84 6 0 -2.978566 0.618084 2.690939
85 1 0 -2.694650 -0.431894 2.569242
86 6 0 -2.237214 1.781042 -2.536952
87 1 0 -1.731659 0.915223 -2.087336
88 6 0 -4.506125 0.678964 2.539470
89 1 0 -4.842091 0.352523 1.549292
90 1 0 -5.016985 0.054530 3.291344
91 1 0 -4.887627 1.699427 2.672462
92 6 0 -2.573031 1.035520 4.104245
93 1 0 -1.511927 0.856401 4.299836
94 1 0 -2.760173 2.100903 4.290661
95 1 0 -3.141495 0.477726 4.866229
96 6 0 -1.343755 2.358340 -3.633555
97 1 0 -0.318238 2.523336 -3.287355
98 1 0 -1.294139 1.672681 -4.485079
99 1 0 -1.739307 3.312384 -4.006872
100 6 0 -3.579775 1.327334 -3.106348
101 1 0 -4.085223 2.164275 -3.606457
102 1 0 -3.450374 0.530175 -3.846361
103 1 0 -4.220617 0.962635 -2.302745
104 8 0 -3.220490 2.150315 -0.359191
105 6 0 -2.516983 2.763664 -1.369383
106 1 0 -3.089723 3.607837 -1.802606
107 6 0 -1.244715 3.356993 -0.799466
108 6 0 -0.333253 4.295258 -1.208271
109 1 0 -0.264466 4.905224 -2.093467
110 7 0 -0.846589 2.944797 0.432620
111 7 0 0.239465 3.553390 0.806617

112 7 0 0.560104 4.377758 -0.186816
113 6 0 1.746741 5.156003 -0.115167
114 6 0 2.457470 5.416655 -1.282020
115 6 0 2.199748 5.604606 1.120994
116 6 0 3.633716 6.152403 -1.216869
117 1 0 2.115542 5.027173 -2.234646
118 6 0 3.383603 6.327060 1.188902
119 1 0 1.636543 5.379336 2.018861
120 6 0 4.086165 6.599240 0.019328
121 1 0 4.196915 6.362602 -2.118540
122 1 0 3.752461 6.681623 2.144230
123 17 0 5.570457 7.518628 0.103288

13(SSSS) one small imaginary frequency was neglected

Sum of electronic and zero-point Energies = -12247.727919

Sum of electronic and thermal Energies = -12247.637296

Sum of electronic and thermal Enthalpies = -12247.636352

Sum of electronic and thermal Free Energies = -12247.863322

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	3.536268	1.065253	0.720390
2	6	0	4.809485	2.543176	0.447542
3	6	0	5.023019	2.811905	-1.047482
4	6	0	-1.605435	-0.476596	2.049076
5	8	0	-2.085704	-0.658420	0.738529
6	30	0	-3.531454	0.525108	0.051825
7	6	0	-4.647725	1.340401	1.427286
8	6	0	-5.542017	2.521467	1.064206
9	8	0	2.907653	-0.296281	-0.625822
10	30	0	3.146272	-1.893633	0.432667
11	8	0	3.765863	-0.607549	1.757055
12	6	0	4.690366	-0.851593	2.778133
13	6	0	2.426186	-0.095651	-1.924586
14	6	0	1.844320	-1.396343	-2.519776
15	6	0	0.725491	-1.996303	-1.670420
16	6	0	1.391909	-1.206931	-3.966401
17	6	0	3.387985	-3.833169	0.311431
18	6	0	2.342829	-4.654266	1.070098
19	6	0	4.250297	-2.070010	3.617546
20	6	0	5.264529	-2.444393	4.696857
21	6	0	2.877220	-1.787443	4.226709
22	6	0	6.162027	2.285898	1.121447
23	6	0	-1.301376	-1.803687	2.759414
24	6	0	-0.933914	-1.564948	4.224027
25	6	0	-0.254851	-2.668245	2.059455
26	30	0	-2.522604	-2.178915	-0.379861
27	8	0	-3.293717	-0.690021	-1.452951

28	6	0	-4.232409	-0.828324	-2.503722
29	6	0	-2.711042	-4.117788	-0.249715
30	6	0	-2.035728	-4.925725	-1.359327
31	6	0	-4.181655	-4.528939	-0.110383
32	6	0	-5.469847	0.181204	2.012299
33	6	0	-4.000757	-2.121759	-3.297453
34	6	0	-2.562394	-2.181173	-3.811469
35	6	0	-4.993455	-2.250190	-4.453187
36	1	0	3.254657	0.208587	-2.583155
37	1	0	2.680770	-2.106884	-2.516063
38	1	0	1.102966	-2.164703	-4.410434
39	1	0	2.188000	-0.775680	-4.581900
40	1	0	0.526402	-0.538078	-4.027164
41	1	0	-0.180511	-1.382614	-1.726432
42	1	0	0.472037	-3.001279	-2.021837
43	1	0	1.019234	-2.069928	-0.620856
44	1	0	4.355911	-4.012662	0.807012
45	1	0	2.265947	-4.364427	2.124360
46	1	0	2.574967	-5.730138	1.044892
47	1	0	1.344616	-4.538062	0.629061
48	1	0	4.726662	0.014070	3.459679
49	1	0	4.157065	-2.911360	2.916157
50	1	0	2.439895	-2.689664	4.666672
51	1	0	2.194630	-1.398836	3.467762
52	1	0	2.956218	-1.033176	5.019934
53	1	0	6.218120	-2.767580	4.271775
54	1	0	4.876691	-3.259533	5.316402
55	1	0	5.470909	-1.592455	5.354785
56	1	0	4.401612	3.462015	0.892540
57	1	0	6.855028	3.131514	0.984924
58	1	0	6.662740	1.403963	0.702965
59	1	0	6.070331	2.113781	2.199767
60	1	0	4.094651	3.043816	-1.583211
61	1	0	5.721455	3.646071	-1.223624
62	1	0	5.454285	1.934726	-1.548625
63	1	0	-0.441113	-2.727114	0.984597
64	1	0	0.749731	-2.267484	2.200894
65	1	0	-0.275188	-3.685981	2.458478
66	1	0	-2.256611	-2.348108	2.731483

67	1	0	0.001094	-1.001092	4.309761
68	1	0	-0.792349	-2.516675	4.744670
69	1	0	-1.716891	-1.008745	4.750979
70	1	0	-2.389210	0.017034	2.645337
71	1	0	-4.282002	-5.603425	0.102489
72	1	0	-4.742575	-4.348469	-1.037109
73	1	0	-4.693884	-3.992188	0.698060
74	1	0	-2.159592	-6.007259	-1.200434
75	1	0	-2.459132	-4.701298	-2.346499
76	1	0	-0.958633	-4.732039	-1.416550
77	1	0	-2.214826	-4.388253	0.693055
78	1	0	-3.970783	1.683150	2.225700
79	1	0	-6.173352	-0.223008	1.275626
80	1	0	-6.067703	0.496846	2.880397
81	1	0	-4.838459	-0.654120	2.343139
82	1	0	-4.954449	3.399592	0.777768
83	1	0	-6.176679	2.821897	1.912751
84	1	0	-6.211375	2.292869	0.227945
85	1	0	-4.106380	0.014982	-3.202197
86	1	0	-4.154912	-2.963890	-2.607441
87	1	0	-4.874328	-1.425677	-5.165493
88	1	0	-6.031028	-2.244148	-4.107697
89	1	0	-4.826709	-3.184715	-4.996881
90	1	0	-2.393831	-3.091934	-4.393180
91	1	0	-2.344767	-1.323365	-4.458577
92	1	0	-1.839319	-2.171003	-2.993432
93	6	0	3.517861	-4.363874	-1.119849
94	1	0	4.294454	-3.844132	-1.694895
95	1	0	3.767874	-5.436116	-1.135270
96	1	0	2.577662	-4.254200	-1.674759
97	6	0	6.072281	-0.990695	2.197344
98	6	0	6.449165	-1.377521	0.934513
99	1	0	5.897814	-1.674190	0.057018
100	7	0	7.197516	-0.640605	2.880293
101	7	0	8.234723	-0.788069	2.116067
102	7	0	7.797986	-1.235126	0.925139
103	6	0	8.707603	-1.423492	-0.145850
104	6	0	8.468957	-2.407119	-1.100987
105	6	0	9.831653	-0.605696	-0.225789

106	6	0	9.358476	-2.567862	-2.156797
107	1	0	7.604673	-3.057435	-1.017566
108	6	0	10.729960	-0.776817	-1.269643
109	1	0	9.993926	0.157385	0.525687
110	6	0	10.481828	-1.752645	-2.228839
111	1	0	9.184390	-3.329689	-2.907607
112	1	0	11.609201	-0.147529	-1.341774
113	17	0	11.608133	-1.958510	-3.552789
114	6	0	-5.615257	-0.695212	-1.936793
115	6	0	-6.419362	-1.592467	-1.273846
116	1	0	-6.311500	-2.639495	-1.039212
117	7	0	-6.231272	0.518089	-1.903304
118	7	0	-7.357498	0.420250	-1.267086
119	7	0	-7.487497	-0.858172	-0.878637
120	6	0	-8.611782	-1.258733	-0.106655
121	6	0	-9.165427	-2.521402	-0.287733
122	6	0	-9.129889	-0.371487	0.832517
123	6	0	-10.250512	-2.909144	0.489081
124	1	0	-8.768618	-3.195266	-1.039340
125	6	0	-10.222171	-0.752830	1.599513
126	1	0	-8.676360	0.604209	0.961171
127	6	0	-10.769292	-2.019351	1.422989
128	1	0	-10.695756	-3.888245	0.357925
129	1	0	-10.635983	-0.073173	2.335155
130	17	0	-12.140425	-2.501190	2.394795
131	6	0	-0.470604	0.509151	1.963589
132	6	0	-0.565079	1.882567	2.000498
133	1	0	-1.388733	2.551531	2.195452
134	7	0	0.797338	0.193116	1.610195
135	7	0	1.475852	1.286077	1.437889
136	7	0	0.663506	2.327611	1.663485
137	6	0	1.066254	3.679039	1.463941
138	6	0	0.657270	4.649861	2.371964
139	6	0	1.802245	4.011108	0.334237
140	6	0	0.980342	5.979599	2.136230
141	1	0	0.099410	4.372089	3.259733
142	6	0	2.141183	5.337629	0.103536
143	1	0	2.113450	3.245486	-0.363998
144	6	0	1.718283	6.309943	1.003322

145	1	0	0.669143	6.748928	2.832747
146	1	0	2.716913	5.602482	-0.775452
147	17	0	2.117916	7.983795	0.705491
148	6	0	1.454894	1.056290	-1.987955
149	6	0	0.181172	1.225034	-1.490312
150	1	0	-0.460363	0.609485	-0.876011
151	7	0	1.785046	2.194035	-2.664863
152	7	0	0.802520	3.040010	-2.617630
153	7	0	-0.180937	2.463759	-1.902000
154	6	0	-1.431404	3.120327	-1.763684
155	6	0	-2.602422	2.418312	-2.038967
156	6	0	-1.462858	4.464883	-1.411616
157	6	0	-3.830409	3.069556	-1.967269
158	1	0	-2.541845	1.381166	-2.355151
159	6	0	-2.685853	5.121469	-1.351066
160	1	0	-0.537791	4.991945	-1.206881
161	6	0	-3.854294	4.420434	-1.633452
162	1	0	-4.751262	2.531147	-2.175779
163	1	0	-2.728748	6.173203	-1.092594
164	17	0	-5.383589	5.262546	-1.583394

14(SSSS)

Sum of electronic and zero-point Energies = -14263.727930

Sum of electronic and thermal Energies = -14263.624817

Sum of electronic and thermal Enthalpies = -14263.623873

Sum of electronic and thermal Free Energies = -14263.874871

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	-3.042973	0.167826	-1.140958
2	6	0	-4.502161	1.490764	-1.304268
3	6	0	-5.813582	1.167469	-0.574288
4	6	0	2.314261	-0.521805	-2.245179
5	8	0	2.733878	-0.644515	-0.915856
6	30	0	3.724231	0.816926	0.012978
7	6	0	4.768198	1.891077	-1.231162
8	6	0	5.462062	3.166019	-0.764680
9	8	0	-2.410435	-1.175452	0.237730
10	30	0	-2.289503	-2.751933	-0.910455
11	8	0	-2.925349	-1.497116	-2.257560
12	6	0	-3.981682	-1.850187	-3.112494
13	6	0	-1.914660	-0.952914	1.533442
14	6	0	-1.136561	-2.161034	2.082985
15	6	0	0.036059	-2.606052	1.209037
16	6	0	-0.722188	-1.948410	3.539659
17	6	0	-2.230461	-4.710540	-0.830197
18	6	0	-1.098571	-5.328723	-1.655438
19	6	0	-3.627099	-3.109167	-3.932657
20	6	0	-4.720159	-3.474655	-4.936215
21	6	0	-2.286856	-2.906577	-4.640570
22	6	0	-4.827564	1.791023	-2.773611
23	6	0	2.248212	-1.877341	-2.973942
24	6	0	1.951978	-1.686453	-4.460864
25	6	0	1.269711	-2.865207	-2.344631
26	30	0	3.336944	-2.085871	0.199537
27	8	0	3.563730	-0.520742	1.433497

28	6	0	4.436188	-0.548093	2.549735
29	6	0	3.833644	-3.970340	0.058584
30	6	0	3.009692	-4.916724	0.934969
31	6	0	5.331037	-4.227881	0.259241
32	6	0	5.791848	0.893782	-1.797635
33	6	0	4.340201	-1.886592	3.296227
34	6	0	2.889488	-2.176290	3.674498
35	6	0	5.236508	-1.901129	4.534108
36	1	0	-2.763049	-0.803973	2.213918
37	1	0	-1.864878	-2.981829	2.072820
38	1	0	-0.297256	-2.866925	3.955985
39	1	0	-1.582360	-1.669028	4.157134
40	1	0	0.030293	-1.160800	3.642245
41	1	0	0.783892	-1.823255	1.058621
42	1	0	0.529290	-3.473038	1.656382
43	1	0	-0.306343	-2.900974	0.216507
44	1	0	-3.177513	-5.020680	-1.297523
45	1	0	-1.091766	-4.973130	-2.692700
46	1	0	-1.171699	-6.426349	-1.688121
47	1	0	-0.117041	-5.091235	-1.225797
48	1	0	-4.152965	-1.033299	-3.832101
49	1	0	-3.517964	-3.937254	-3.219482
50	1	0	-1.988839	-3.814180	-5.175513
51	1	0	-1.497771	-2.647167	-3.931059
52	1	0	-2.355442	-2.094068	-5.374933
53	1	0	-5.677480	-3.674769	-4.449972
54	1	0	-4.432391	-4.366018	-5.503158
55	1	0	-4.880925	-2.660430	-5.652922
56	1	0	-4.119996	2.426268	-0.874358
57	1	0	-5.545074	2.620293	-2.875519
58	1	0	-5.289302	0.921074	-3.258781
59	1	0	-3.942958	2.057255	-3.362740
60	1	0	-5.669719	0.754986	0.429912
61	1	0	-6.452954	2.057765	-0.470259
62	1	0	-6.402543	0.434825	-1.136681
63	1	0	1.434997	-2.958040	-1.268366
64	1	0	0.233712	-2.548024	-2.498806
65	1	0	1.390340	-3.856526	-2.789756
66	1	0	3.260937	-2.294970	-2.876885

67	1	0	0.941495	-1.291164	-4.614654
68	1	0	2.016104	-2.641009	-4.991176
69	1	0	2.661609	-0.995230	-4.928616
70	1	0	3.039516	0.093603	-2.802506
71	1	0	5.588030	-5.275582	0.044577
72	1	0	5.643501	-4.043407	1.296111
73	1	0	5.955495	-3.605404	-0.394139
74	1	0	3.328505	-5.961629	0.804851
75	1	0	3.110010	-4.686711	2.003763
76	1	0	1.942335	-4.879449	0.691258
77	1	0	3.608463	-4.229803	-0.986749
78	1	0	4.095462	2.165980	-2.057890
79	1	0	6.520007	0.594544	-1.034331
80	1	0	6.368511	1.325320	-2.629176
81	1	0	5.323694	-0.025818	-2.172512
82	1	0	4.740167	3.950241	-0.520423
83	1	0	6.126518	3.570013	-1.544802
84	1	0	6.077678	2.999078	0.125914
85	1	0	4.139304	0.243131	3.255945
86	1	0	4.677706	-2.672179	2.604976
87	1	0	4.934330	-1.121126	5.242379
88	1	0	6.288661	-1.735895	4.286400
89	1	0	5.159320	-2.863109	5.049150
90	1	0	2.801940	-3.138813	4.186935
91	1	0	2.504295	-1.403360	4.350733
92	1	0	2.243529	-2.203156	2.795499
93	6	0	-2.223637	-5.303351	0.581548
94	1	0	-3.061987	-4.945047	1.191399
95	1	0	-2.290315	-6.401893	0.559525
96	1	0	-1.299920	-5.057173	1.120214
97	6	0	-5.242552	-1.989729	-2.292026
98	6	0	-5.342103	-2.080540	-0.923296
99	1	0	-4.612853	-2.029146	-0.130307
100	7	0	-6.506932	-1.943569	-2.796718
101	7	0	-7.366539	-2.004537	-1.824095
102	7	0	-6.672033	-2.089197	-0.676701
103	6	0	-7.321588	-2.046811	0.582828
104	6	0	-6.706443	-2.616617	1.694067
105	6	0	-8.549314	-1.401271	0.698933

106	6	0	-7.318437	-2.531150	2.937678
107	1	0	-5.757185	-3.131827	1.596756
108	6	0	-9.170860	-1.331251	1.938560
109	1	0	-9.005687	-0.952705	-0.174900
110	6	0	-8.547085	-1.891668	3.047159
111	1	0	-6.844446	-2.963008	3.811038
112	1	0	-10.125177	-0.828583	2.042590
113	17	0	-9.316775	-1.778035	4.614453
114	6	0	5.825598	-0.210855	2.094688
115	6	0	6.768764	-0.985027	1.462066
116	1	0	6.797281	-2.028431	1.190657
117	7	0	6.300988	1.063657	2.149828
118	7	0	7.473274	1.116790	1.595537
119	7	0	7.771640	-0.122534	1.171658
120	6	0	8.988594	-0.380983	0.484470
121	6	0	9.640002	-1.594951	0.674786
122	6	0	9.498922	0.583766	-0.379089
123	6	0	10.813772	-1.857763	-0.019844
124	1	0	9.248792	-2.327774	1.372030
125	6	0	10.680301	0.327849	-1.062709
126	1	0	8.973831	1.522275	-0.513636
127	6	0	11.322433	-0.892709	-0.881612
128	1	0	11.331389	-2.799602	0.118576
129	1	0	11.089882	1.067611	-1.740496
130	17	0	12.800225	-1.221534	-1.755588
131	6	0	1.019597	0.241775	-2.255234
132	6	0	0.714466	1.440720	-2.858898
133	1	0	1.283716	2.110690	-3.483553
134	7	0	-0.061922	-0.151305	-1.541623
135	7	0	-1.001982	0.730831	-1.679238
136	7	0	-0.551333	1.708940	-2.478433
137	6	0	-1.346634	2.844754	-2.803781
138	6	0	-1.519081	3.190732	-4.139615
139	6	0	-1.933033	3.576178	-1.779875
140	6	0	-2.298114	4.295018	-4.458461
141	1	0	-1.069273	2.590859	-4.923292
142	6	0	-2.726676	4.670662	-2.097358
143	1	0	-1.785315	3.285852	-0.745007
144	6	0	-2.900281	5.017270	-3.432329

145	1	0	-2.454393	4.575250	-5.493287
146	1	0	-3.209169	5.238059	-1.309799
147	17	0	-3.901875	6.390354	-3.833429
148	6	0	-1.149190	0.346368	1.566106
149	6	0	0.189320	0.656539	1.584937
150	1	0	1.091086	0.064200	1.613242
151	7	0	-1.827636	1.526479	1.507334
152	7	0	-0.996594	2.526440	1.480426
153	7	0	0.231363	2.009392	1.528721
154	6	0	1.361920	2.868024	1.597685
155	6	0	2.512205	2.432147	2.249727
156	6	0	1.290071	4.139903	1.038591
157	6	0	3.605936	3.284969	2.361592
158	1	0	2.542784	1.452853	2.711584
159	6	0	2.373780	4.998404	1.166651
160	1	0	0.387972	4.462471	0.532925
161	6	0	3.517669	4.567428	1.832505
162	1	0	4.515428	2.944139	2.844141
163	1	0	2.326424	5.997319	0.749279
164	17	0	4.865061	5.661623	2.009462
165	30	0	-3.996802	2.170400	1.927966
166	6	0	-3.896777	4.077366	1.446934
167	1	0	-3.066945	4.215921	0.739450
168	6	0	-3.536009	4.889416	2.697570
169	1	0	-3.421628	5.965247	2.483887
170	1	0	-4.309451	4.809488	3.473903
171	1	0	-2.593628	4.550508	3.146729
172	6	0	-5.156231	4.643336	0.787298
173	1	0	-6.045507	4.505760	1.416610
174	1	0	-5.078598	5.726691	0.591342
175	1	0	-5.369314	4.157951	-0.172724
176	6	0	-4.769483	0.719580	3.011330
177	1	0	-4.732763	-0.240337	2.471841
178	6	0	-3.981711	0.552694	4.316222
179	1	0	-2.913452	0.368648	4.142468
180	1	0	-4.042743	1.458048	4.935697
181	1	0	-4.358713	-0.274688	4.939753
182	6	0	-6.246266	0.985034	3.325315
183	1	0	-6.862295	1.010896	2.418244

184	1	0	-6.679893	0.219637	3.988514
185	1	0	-6.386019	1.950166	3.831665

15(SSSS)s

Sum of electronic and zero-point Energies = -15309.608762

Sum of electronic and thermal Energies = -15309.493634

Sum of electronic and thermal Enthalpies = -15309.492689

Sum of electronic and thermal Free Energies = -15309.769716

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	2.885450	-1.361656	1.229470
2	6	0	3.978059	-0.792348	2.770331
3	6	0	4.063046	0.721294	2.978096
4	6	0	-2.312748	-3.366130	0.464094
5	8	0	-2.867795	-2.310732	-0.270243
6	30	0	-3.691453	-0.757476	0.641505
7	6	0	-4.641375	-1.253992	2.267186
8	6	0	-5.225584	-0.193268	3.194455
9	8	0	2.410342	-0.895814	-0.663501
10	30	0	2.551932	-2.646249	-1.464223
11	8	0	2.979689	-3.171003	0.360986
12	6	0	3.922895	-4.166334	0.655805
13	6	0	2.035676	0.348296	-1.193839
14	6	0	1.344658	0.219017	-2.563854
15	6	0	0.163610	-0.750742	-2.584219
16	6	0	0.961961	1.589572	-3.124610
17	6	0	2.871852	-3.494199	-3.198510
18	6	0	1.827323	-4.536406	-3.605637
19	6	0	3.504173	-5.505460	0.013157
20	6	0	4.520982	-6.621291	0.248123
21	6	0	2.123422	-5.901881	0.534357
22	6	0	5.388332	-1.394084	2.734034
23	6	0	-2.004195	-4.593660	-0.411168
24	6	0	-1.667443	-5.805581	0.458229
25	6	0	-0.918447	-4.354774	-1.459820
26	30	0	-2.864410	-1.647831	-2.077238
27	8	0	-3.291164	0.051652	-1.093982

28	6	0	-4.188330	1.034903	-1.594484
29	6	0	-3.255899	-2.498982	-3.796150
30	6	0	-2.674368	-1.871407	-5.062142
31	6	0	-4.775310	-2.671612	-3.932765
32	6	0	-5.733214	-2.231935	1.805502
33	6	0	-4.112237	1.134602	-3.124048
34	6	0	-2.693943	1.510605	-3.548292
35	6	0	-5.127765	2.131922	-3.679236
36	1	0	2.934344	0.953045	-1.369673
37	1	0	2.115235	-0.200558	-3.221825
38	1	0	0.609367	1.499034	-4.157101
39	1	0	1.820947	2.269348	-3.118497
40	1	0	0.164302	2.054242	-2.535978
41	1	0	-0.661765	-0.379741	-1.968789
42	1	0	-0.203356	-0.882452	-3.606465
43	1	0	0.445117	-1.731625	-2.198150
44	1	0	3.823307	-4.030781	-3.054797
45	1	0	1.694114	-5.313851	-2.843742
46	1	0	2.099889	-5.044807	-4.543272
47	1	0	0.845034	-4.074829	-3.771664
48	1	0	3.960256	-4.324516	1.746414
49	1	0	3.430220	-5.322735	-1.068498
50	1	0	1.708273	-6.743693	-0.029013
51	1	0	1.433446	-5.058254	0.464303
52	1	0	2.181401	-6.200594	1.588861
53	1	0	5.487632	-6.403272	-0.212279
54	1	0	4.152541	-7.563741	-0.170466
55	1	0	4.694572	-6.775982	1.319134
56	1	0	3.493167	-1.205530	3.667321
57	1	0	5.991667	-1.052363	3.590226
58	1	0	5.939142	-1.112247	1.828431
59	1	0	5.375572	-2.488398	2.768565
60	1	0	3.080092	1.187980	3.090880
61	1	0	4.651436	0.980562	3.873180
62	1	0	4.543735	1.220311	2.130002
63	1	0	-1.084895	-3.428391	-2.015744
64	1	0	0.070724	-4.291188	-0.998752
65	1	0	-0.901096	-5.174206	-2.183527
66	1	0	-2.946880	-4.796846	-0.937461

67	1	0	-0.762331	-5.627977	1.048735
68	1	0	-1.486500	-6.689308	-0.160670
69	1	0	-2.481568	-6.043482	1.151368
70	1	0	-3.051385	-3.696877	1.212202
71	1	0	-5.035762	-3.285973	-4.807279
72	1	0	-5.283200	-1.707794	-4.076308
73	1	0	-5.222434	-3.156729	-3.055578
74	1	0	-2.982445	-2.423537	-5.962951
75	1	0	-3.003210	-0.833939	-5.202056
76	1	0	-1.578702	-1.866894	-5.052557
77	1	0	-2.830946	-3.509904	-3.715930
78	1	0	-3.918970	-1.839338	2.857227
79	1	0	-6.517421	-1.715520	1.239944
80	1	0	-6.231143	-2.719676	2.656510
81	1	0	-5.342272	-3.025896	1.156918
82	1	0	-4.449024	0.445924	3.625902
83	1	0	-5.769679	-0.652393	4.034316
84	1	0	-5.934903	0.460648	2.674273
85	1	0	-3.910204	2.019910	-1.186622
86	1	0	-4.342046	0.138273	-3.526097
87	1	0	-4.975863	3.124919	-3.244502
88	1	0	-6.159123	1.836893	-3.468873
89	1	0	-5.018227	2.221125	-4.764102
90	1	0	-2.623275	1.624620	-4.634080
91	1	0	-2.397093	2.460808	-3.089567
92	1	0	-1.970019	0.754199	-3.245288
93	6	0	3.086379	-2.501201	-4.345023
94	1	0	3.844315	-1.743222	-4.111381
95	1	0	3.407929	-3.006161	-5.268976
96	1	0	2.159163	-1.966463	-4.588561
97	6	0	5.297373	-3.705479	0.245863
98	6	0	5.640054	-2.752432	-0.681142
99	1	0	5.069660	-2.108549	-1.329949
100	7	0	6.440887	-4.123842	0.855635
101	7	0	7.457939	-3.484408	0.362037
102	7	0	6.986055	-2.646178	-0.576040
103	6	0	7.841081	-1.748165	-1.264013
104	6	0	7.653436	-1.535348	-2.625577
105	6	0	8.814190	-1.053329	-0.553985

106	6	0	8.434295	-0.595681	-3.286437
107	1	0	6.901170	-2.099038	-3.167178
108	6	0	9.606274	-0.124348	-1.215023
109	1	0	8.931460	-1.226866	0.509178
110	6	0	9.401916	0.101449	-2.572079
111	1	0	8.293002	-0.412261	-4.344955
112	1	0	10.360622	0.434494	-0.674078
113	17	0	10.382052	1.292732	-3.398557
114	6	0	-5.564444	0.741311	-1.074794
115	6	0	-6.465281	-0.233413	-1.435435
116	1	0	-6.440416	-1.010377	-2.183163
117	7	0	-6.093639	1.430801	-0.027127
118	7	0	-7.259290	0.944791	0.270312
119	7	0	-7.500623	-0.067295	-0.578617
120	6	0	-8.712749	-0.805596	-0.495032
121	6	0	-9.272785	-1.342802	-1.649425
122	6	0	-9.314049	-0.983131	0.747643
123	6	0	-10.445121	-2.082409	-1.560256
124	1	0	-8.813028	-1.176380	-2.617483
125	6	0	-10.494151	-1.709127	0.835130
126	1	0	-8.860039	-0.556122	1.633998
127	6	0	-11.045221	-2.256878	-0.318457
128	1	0	-10.892560	-2.507793	-2.450726
129	1	0	-10.974696	-1.854940	1.795292
130	17	0	-12.523436	-3.182977	-0.207026
131	6	0	-1.141138	-2.834381	1.248508
132	6	0	-0.993496	-2.730307	2.613508
133	1	0	-1.609055	-3.041116	3.442697
134	7	0	-0.076933	-2.223097	0.668493
135	7	0	0.702383	-1.759721	1.595836
136	7	0	0.162053	-2.056404	2.785343
137	6	0	0.748905	-1.595761	3.999412
138	6	0	1.136956	-2.515941	4.964817
139	6	0	0.927851	-0.230450	4.179760
140	6	0	1.714913	-2.058201	6.141884
141	1	0	1.006353	-3.578254	4.790158
142	6	0	1.514559	0.229612	5.350163
143	1	0	0.635420	0.465044	3.401151
144	6	0	1.899120	-0.690409	6.319528

145	1	0	2.033521	-2.758312	6.904741
146	1	0	1.685265	1.289103	5.498621
147	17	0	2.634618	-0.115896	7.795219
148	6	0	1.256471	1.107865	-0.156037
149	6	0	-0.070904	1.120780	0.190470
150	1	0	-0.938242	0.629576	-0.220929
151	7	0	1.908759	1.923457	0.719186
152	7	0	1.072410	2.420596	1.577133
153	7	0	-0.136266	1.945366	1.264732
154	6	0	-1.279615	2.358240	1.998195
155	6	0	-2.541784	2.194756	1.436367
156	6	0	-1.125681	2.951535	3.248094
157	6	0	-3.671075	2.615190	2.127791
158	1	0	-2.648928	1.777909	0.442389
159	6	0	-2.252865	3.376389	3.940719
160	1	0	-0.136589	3.094866	3.665918
161	6	0	-3.513680	3.202169	3.377993
162	1	0	-4.651908	2.488255	1.678571
163	1	0	-2.146765	3.841869	4.913693
164	17	0	-4.927378	3.730150	4.258092
165	30	0	3.864064	3.136674	0.504856
166	6	0	3.720304	4.293780	2.107168
167	1	0	3.326241	3.657691	2.916251
168	6	0	5.100053	2.207551	-0.742081
169	1	0	4.639440	2.215823	-1.745362
170	6	0	5.413215	0.746926	-0.397944
171	1	0	5.949142	0.240053	-1.216701
172	1	0	6.072376	0.690109	0.477668
173	1	0	4.529132	0.146864	-0.158068
174	6	0	6.431583	2.959519	-0.872840
175	1	0	7.127792	2.457820	-1.567828
176	1	0	6.293687	3.984406	-1.228019
177	1	0	6.950746	3.020959	0.093463
178	6	0	2.771892	5.486966	1.983689
179	1	0	2.714642	6.081859	2.912520
180	1	0	3.091320	6.179637	1.192540
181	1	0	1.750339	5.169878	1.738475
182	6	0	5.109973	4.766416	2.549209
183	1	0	5.595864	5.377921	1.776617

184	1	0	5.082585	5.380914	3.466645
185	1	0	5.781749	3.922580	2.751741
186	8	0	4.808800	5.700563	-1.927911
187	6	0	3.752161	5.859442	-2.491753
188	1	0	3.676623	6.483720	-3.404196
189	6	0	2.468310	5.301008	-2.045307
190	6	0	1.220198	5.685608	-2.480539
191	7	0	2.303782	4.369055	-1.060228
192	1	0	0.894932	6.412248	-3.208012
193	7	0	1.043813	4.174751	-0.869752
194	7	0	0.368690	4.970894	-1.720639
195	6	0	-1.051527	5.030668	-1.671823
196	6	0	-1.776320	5.191512	-2.847706
197	6	0	-1.685495	4.956680	-0.435937
198	6	0	-3.160106	5.304540	-2.785859
199	1	0	-1.271727	5.216342	-3.807411
200	6	0	-3.069302	5.053518	-0.375336
201	1	0	-1.101446	4.839222	0.469394
202	6	0	-3.793459	5.234862	-1.549063
203	1	0	-3.737412	5.435946	-3.693473
204	1	0	-3.576753	5.003163	0.580335
205	17	0	-5.530525	5.378416	-1.463010

TS3(S)

Sum of electronic and zero-point Energies = -15309.571699

Sum of electronic and thermal Energies = -15309.457234

Sum of electronic and thermal Enthalpies = -15309.456290

Sum of electronic and thermal Free Energies = -15309.731573

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	2.892399	-2.413358	0.521498
2	6	0	4.253058	-2.379603	1.946215
3	6	0	4.828314	-0.984011	2.205533
4	6	0	-2.528017	-3.162296	-0.275960
5	8	0	-2.890811	-1.827259	-0.533676
6	30	0	-3.937196	-0.835642	0.834150
7	6	0	-5.003165	-1.949897	2.020882
8	6	0	-5.582022	-1.354465	3.299873
9	8	0	2.266719	-1.103533	-0.896589
10	30	0	2.178637	-2.327229	-2.404070
11	8	0	2.774881	-3.602524	-1.061488
12	6	0	3.701650	-4.615105	-1.342030
13	6	0	1.950691	0.255647	-0.821614
14	6	0	1.198194	0.757652	-2.073767
15	6	0	-0.056687	-0.047613	-2.399716
16	6	0	0.877520	2.248022	-1.974399
17	6	0	2.212451	-2.363857	-4.362622
18	6	0	1.058068	-3.148551	-4.992429
19	6	0	3.213278	-5.493895	-2.513092
20	6	0	4.146041	-6.675806	-2.774967
21	6	0	1.789436	-5.978846	-2.234135
22	6	0	5.405001	-3.367849	1.731733
23	6	0	-2.448167	-4.017615	-1.550506
24	6	0	-2.100161	-5.467929	-1.214814
25	6	0	-1.514828	-3.461096	-2.623290
26	30	0	-3.480641	-0.779031	-2.039056
27	8	0	-3.737368	0.518411	-0.539534

28	6	0	-4.513841	1.699630	-0.601552
29	6	0	-3.977997	-0.944295	-3.918624
30	6	0	-3.145420	-0.083385	-4.871474
31	6	0	-5.474312	-0.723629	-4.168410
32	6	0	-6.115091	-2.502266	1.115126
33	6	0	-4.328484	2.413278	-1.947094
34	6	0	-2.840295	2.646156	-2.204148
35	6	0	-5.103987	3.729961	-1.986007
36	1	0	2.874412	0.844257	-0.773135
37	1	0	1.907139	0.619870	-2.899204
38	1	0	0.473512	2.622393	-2.920112
39	1	0	1.767498	2.836810	-1.731977
40	1	0	0.134481	2.436013	-1.192807
41	1	0	-0.818494	0.057105	-1.620662
42	1	0	-0.490432	0.295190	-3.344026
43	1	0	0.163700	-1.110313	-2.503771
44	1	0	3.138958	-2.912813	-4.592413
45	1	0	0.954632	-4.155376	-4.570250
46	1	0	1.187935	-3.263961	-6.079156
47	1	0	0.099406	-2.635668	-4.841520
48	1	0	3.796798	-5.273851	-0.463000
49	1	0	3.194059	-4.858744	-3.409713
50	1	0	1.397057	-6.546608	-3.084008
51	1	0	1.116502	-5.142379	-2.031517
52	1	0	1.771463	-6.636598	-1.355932
53	1	0	5.160978	-6.356585	-3.022565
54	1	0	3.766612	-7.283144	-3.603021
55	1	0	4.211884	-7.321046	-1.890822
56	1	0	3.748562	-2.695731	2.869911
57	1	0	6.061051	-3.416431	2.615028
58	1	0	6.045110	-3.076359	0.891497
59	1	0	5.060644	-4.388813	1.530503
60	1	0	4.059528	-0.244092	2.459824
61	1	0	5.555716	-0.982706	3.032302
62	1	0	5.360249	-0.600877	1.325125
63	1	0	-1.699007	-2.397423	-2.792315
64	1	0	-0.467762	-3.582074	-2.337257
65	1	0	-1.672720	-3.981978	-3.571723
66	1	0	-3.469840	-3.995489	-1.956550

67	1	0	-1.080985	-5.547839	-0.821279
68	1	0	-2.157092	-6.093521	-2.110375
69	1	0	-2.786478	-5.886356	-0.470292
70	1	0	-3.303519	-3.624887	0.355302
71	1	0	-5.742839	-0.954007	-5.209844
72	1	0	-5.766217	0.322144	-4.002183
73	1	0	-6.105232	-1.351520	-3.527195
74	1	0	-3.452438	-0.230672	-5.917499
75	1	0	-3.249610	0.988663	-4.659490
76	1	0	-2.077537	-0.323501	-4.818264
77	1	0	-3.767532	-1.994225	-4.169842
78	1	0	-4.377944	-2.808272	2.311748
79	1	0	-6.788803	-1.705988	0.775093
80	1	0	-6.740541	-3.241916	1.636431
81	1	0	-5.716269	-2.992682	0.217038
82	1	0	-4.796334	-1.062440	4.004311
83	1	0	-6.231564	-2.074285	3.821032
84	1	0	-6.187020	-0.463140	3.100407
85	1	0	-4.167082	2.390983	0.183544
86	1	0	-4.713783	1.750334	-2.734941
87	1	0	-4.761419	4.408551	-1.195513
88	1	0	-6.178094	3.579666	-1.846342
89	1	0	-4.960499	4.233889	-2.946551
90	1	0	-2.678447	3.196058	-3.135576
91	1	0	-2.397444	3.222681	-1.383070
92	1	0	-2.293878	1.703773	-2.270337
93	6	0	2.335363	-0.995267	-5.038293
94	1	0	3.184381	-0.413557	-4.658606
95	1	0	2.473294	-1.091076	-6.126184
96	1	0	1.432231	-0.389916	-4.889774
97	6	0	5.055033	-3.985371	-1.564088
98	6	0	5.338828	-2.651756	-1.745205
99	1	0	4.728992	-1.762363	-1.778098
100	7	0	6.237388	-4.654084	-1.474191
101	7	0	7.222852	-3.815750	-1.588958
102	7	0	6.691830	-2.591906	-1.754042
103	6	0	7.518522	-1.441406	-1.836705
104	6	0	7.217724	-0.441480	-2.755319
105	6	0	8.609758	-1.325983	-0.981109

106	6	0	8.007530	0.700767	-2.808741
107	1	0	6.379184	-0.557400	-3.434025
108	6	0	9.409016	-0.192097	-1.042589
109	1	0	8.821441	-2.113927	-0.268186
110	6	0	9.095413	0.812557	-1.951654
111	1	0	7.779532	1.490518	-3.514487
112	1	0	10.255357	-0.083603	-0.374841
113	17	0	10.083763	2.254543	-2.009323
114	6	0	-5.933474	1.355678	-0.262838
115	6	0	-6.943916	0.819708	-1.024231
116	1	0	-7.023666	0.588399	-2.074458
117	7	0	-6.358560	1.387878	1.030002
118	7	0	-7.563123	0.912557	1.106486
119	7	0	-7.934277	0.562499	-0.135515
120	6	0	-9.201859	-0.037963	-0.365689
121	6	0	-9.871342	0.199373	-1.561421
122	6	0	-9.743468	-0.868831	0.610993
123	6	0	-11.094660	-0.416483	-1.793926
124	1	0	-9.456952	0.872679	-2.303773
125	6	0	-10.973176	-1.472787	0.385342
126	1	0	-9.205378	-1.038930	1.536151
127	6	0	-11.633646	-1.246732	-0.817874
128	1	0	-11.625910	-0.241008	-2.721854
129	1	0	-11.407405	-2.123499	1.135239
130	17	0	-13.174439	-2.019978	-1.107402
131	6	0	-1.281774	-3.110615	0.566892
132	6	0	-1.208385	-2.993185	1.938050
133	1	0	-1.958781	-3.017049	2.713077
134	7	0	-0.032203	-2.951423	0.072706
135	7	0	0.791634	-2.754726	1.056031
136	7	0	0.095679	-2.767713	2.201267
137	6	0	0.688900	-2.511920	3.471715
138	6	0	0.318230	-3.295256	4.559661
139	6	0	1.587980	-1.462376	3.613922
140	6	0	0.851359	-3.019298	5.811608
141	1	0	-0.371950	-4.122078	4.431812
142	6	0	2.139323	-1.196198	4.860013
143	1	0	1.877683	-0.863102	2.760407
144	6	0	1.759013	-1.973207	5.948627

145	1	0	0.573904	-3.621246	6.668873
146	1	0	2.856834	-0.390870	4.972036
147	17	0	2.437874	-1.634008	7.520186
148	6	0	1.222048	0.593971	0.451720
149	6	0	-0.050434	0.319618	0.899030
150	1	0	-0.857512	-0.273727	0.495258
151	7	0	1.817324	1.359264	1.408064
152	7	0	0.997198	1.580007	2.393771
153	7	0	-0.138148	0.953381	2.093733
154	6	0	-1.264509	1.076383	2.954787
155	6	0	-2.507841	1.352743	2.395570
156	6	0	-1.096114	0.961633	4.328915
157	6	0	-3.614486	1.513332	3.222374
158	1	0	-2.594293	1.488339	1.321895
159	6	0	-2.197844	1.130824	5.158595
160	1	0	-0.116356	0.755337	4.744100
161	6	0	-3.442685	1.403184	4.598833
162	1	0	-4.592135	1.719507	2.794501
163	1	0	-2.085683	1.050078	6.233361
164	17	0	-4.818789	1.621906	5.649496
165	30	0	3.699507	2.532634	1.757415
166	6	0	3.980053	2.380796	3.703173
167	1	0	3.457393	1.472075	4.042787
168	6	0	5.093512	2.191307	0.073921
169	1	0	4.498663	1.303094	0.388317
170	6	0	6.527202	1.863631	0.466438
171	1	0	6.874021	0.908437	0.046122
172	1	0	7.223341	2.636274	0.116151
173	1	0	6.642896	1.808556	1.553103
174	6	0	4.901539	2.255942	-1.436243
175	1	0	5.079906	1.288779	-1.928210
176	1	0	3.894462	2.583784	-1.719405
177	1	0	5.603851	2.964921	-1.895178
178	6	0	3.312254	3.570684	4.401844
179	1	0	3.416323	3.523031	5.498831
180	1	0	3.761381	4.518323	4.080460
181	1	0	2.239860	3.627711	4.176877
182	6	0	5.444533	2.263300	4.127485
183	1	0	6.031835	3.109161	3.752504

184	1	0	5.561075	2.244497	5.224297
185	1	0	5.909242	1.348344	3.739938
186	8	0	5.555413	4.700999	1.583193
187	6	0	5.175063	4.372693	0.448026
188	1	0	5.877608	4.356233	-0.403755
189	6	0	3.758974	4.731948	0.062227
190	6	0	3.169057	5.610504	-0.805189
191	7	0	2.761334	4.136730	0.755901
192	1	0	3.569360	6.272627	-1.554783
193	7	0	1.600125	4.575658	0.388420
194	7	0	1.831928	5.482056	-0.566099
195	6	0	0.745507	6.131818	-1.214344
196	6	0	-0.499956	5.510772	-1.242343
197	6	0	0.937180	7.371122	-1.816719
198	6	0	-1.561245	6.129277	-1.887197
199	1	0	-0.632729	4.550893	-0.760389
200	6	0	-0.121541	7.986181	-2.473822
201	1	0	1.897189	7.871965	-1.765674
202	6	0	-1.361219	7.359075	-2.504372
203	1	0	-2.533122	5.650261	-1.918255
204	1	0	0.018143	8.950399	-2.948123
205	17	0	-2.694683	8.129914	-3.331124

13(SSSS)-7(S)

Sum of electronic and zero-point Energies = -15309.664604

Sum of electronic and thermal Energies = -15309.550827

Sum of electronic and thermal Enthalpies = -15309.549883

Sum of electronic and thermal Free Energies = -15309.825010

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	2.821614	-0.183764	1.743477
2	6	0	4.137597	1.268409	1.921234
3	6	0	4.073266	2.288304	0.779082
4	6	0	-2.375270	-2.020681	2.201501
5	8	0	-2.693481	-1.657276	0.879897
6	30	0	-4.108808	-0.282036	0.591349
7	6	0	-5.335747	-0.041850	2.086791
8	6	0	-6.171973	1.229350	2.195395
9	8	0	2.226933	-1.007719	0.014189
10	30	0	2.431741	-2.865864	0.484766
11	8	0	3.033114	-2.105123	2.169182
12	6	0	3.894719	-2.711620	3.088811
13	6	0	1.794063	-0.364935	-1.146687
14	6	0	1.204055	-1.362484	-2.166153
15	6	0	0.053261	-2.188851	-1.595529
16	6	0	0.790241	-0.668575	-3.462127
17	6	0	2.685048	-4.644084	-0.299615
18	6	0	1.573138	-5.656177	-0.014997
19	6	0	3.317807	-4.071302	3.536731
20	6	0	4.248750	-4.818309	4.490333
21	6	0	1.939591	-3.856506	4.163648
22	6	0	5.546765	0.662116	1.982218
23	6	0	-2.188039	-3.534977	2.381021
24	6	0	-1.993835	-3.887253	3.854938
25	6	0	-1.079139	-4.128406	1.516678
26	30	0	-3.046395	-2.602159	-0.780212
27	8	0	-3.701031	-0.777223	-1.237642

28	6	0	-4.516668	-0.409374	-2.337570
29	6	0	-3.346681	-4.439964	-1.369779
30	6	0	-2.569899	-4.876588	-2.613301
31	6	0	-4.844377	-4.718618	-1.548626
32	6	0	-6.231079	-1.290238	2.051692
33	6	0	-4.245004	-1.284574	-3.569592
34	6	0	-2.755673	-1.286766	-3.905160
35	6	0	-5.066149	-0.815329	-4.771544
36	1	0	2.650314	0.119103	-1.640788
37	1	0	2.026334	-2.052179	-2.395724
38	1	0	0.468120	-1.402099	-4.207644
39	1	0	1.616125	-0.096291	-3.896270
40	1	0	-0.038450	0.025530	-3.295556
41	1	0	-0.786843	-1.539577	-1.325987
42	1	0	-0.292355	-2.918957	-2.333020
43	1	0	0.354957	-2.733871	-0.699994
44	1	0	3.591975	-5.027828	0.194935
45	1	0	1.393769	-5.788395	1.058128
46	1	0	1.811884	-6.648002	-0.428468
47	1	0	0.621357	-5.348985	-0.466879
48	1	0	3.984707	-2.081151	3.988287
49	1	0	3.196865	-4.671702	2.622675
50	1	0	1.427836	-4.809909	4.330782
51	1	0	1.317304	-3.230229	3.519318
52	1	0	2.033195	-3.352411	5.133921
53	1	0	5.201590	-5.073676	4.019322
54	1	0	3.781509	-5.747766	4.831267
55	1	0	4.472242	-4.211950	5.375805
56	1	0	3.978838	1.814238	2.862164
57	1	0	6.324413	1.439343	2.059112
58	1	0	5.777496	0.079376	1.079855
59	1	0	5.679071	-0.010403	2.836401
60	1	0	3.118884	2.825246	0.723787
61	1	0	4.867920	3.048967	0.869353
62	1	0	4.208418	1.807690	-0.198417
63	1	0	-1.126532	-3.727248	0.502279
64	1	0	-0.091395	-3.900946	1.924655
65	1	0	-1.178595	-5.215504	1.455232
66	1	0	-3.141852	-3.968206	2.046531

67	1	0	-1.064782	-3.455111	4.242941
68	1	0	-1.931822	-4.971326	3.987914
69	1	0	-2.821749	-3.521684	4.472169
70	1	0	-3.210200	-1.738902	2.861717
71	1	0	-5.036328	-5.785576	-1.735490
72	1	0	-5.256281	-4.177013	-2.410476
73	1	0	-5.434353	-4.434828	-0.667997
74	1	0	-2.799549	-5.917494	-2.886446
75	1	0	-2.809497	-4.258690	-3.488230
76	1	0	-1.486135	-4.820361	-2.462440
77	1	0	-3.002280	-5.069570	-0.536946
78	1	0	-4.736443	-0.107914	3.008132
79	1	0	-6.852153	-1.316577	1.147872
80	1	0	-6.920775	-1.326209	2.908338
81	1	0	-5.649801	-2.222162	2.067119
82	1	0	-5.547627	2.112557	2.363289
83	1	0	-6.880059	1.171700	3.036868
84	1	0	-6.764174	1.416240	1.293653
85	1	0	-4.281673	0.631754	-2.612173
86	1	0	-4.540616	-2.314281	-3.318686
87	1	0	-4.819759	0.221657	-5.027091
88	1	0	-6.142639	-0.865592	-4.585697
89	1	0	-4.848395	-1.433057	-5.647711
90	1	0	-2.551057	-1.915248	-4.776844
91	1	0	-2.403577	-0.273624	-4.127790
92	1	0	-2.161832	-1.664353	-3.072375
93	6	0	2.975322	-4.611345	-1.804669
94	1	0	3.777139	-3.910282	-2.070789
95	1	0	3.271461	-5.600626	-2.186206
96	1	0	2.086656	-4.310785	-2.374349
97	6	0	5.275707	-2.822138	2.500856
98	6	0	5.638561	-3.003360	1.189839
99	1	0	5.069435	-3.107549	0.281292
100	7	0	6.414525	-2.686089	3.234635
101	7	0	7.448122	-2.775845	2.454422
102	7	0	6.992869	-2.967934	1.203393
103	6	0	7.895660	-3.089387	0.116443
104	6	0	7.551104	-3.863523	-0.987937
105	6	0	9.120792	-2.430884	0.174127

106	6	0	8.437559	-3.974213	-2.052199
107	1	0	6.606291	-4.395456	-1.016779
108	6	0	10.014587	-2.554395	-0.880529
109	1	0	9.367172	-1.830860	1.041621
110	6	0	9.662945	-3.321888	-1.985771
111	1	0	8.179850	-4.572614	-2.918205
112	1	0	10.972336	-2.048696	-0.846277
113	17	0	10.786438	-3.468775	-3.320183
114	6	0	-5.950186	-0.423613	-1.894716
115	6	0	-6.865644	-1.446393	-1.831335
116	1	0	-6.831695	-2.480772	-2.134356
117	7	0	-6.515457	0.676224	-1.324133
118	7	0	-7.716714	0.392811	-0.923496
119	7	0	-7.945074	-0.895080	-1.226197
120	6	0	-9.183226	-1.510284	-0.899027
121	6	0	-9.731125	-2.444621	-1.771266
122	6	0	-9.819289	-1.176309	0.292758
123	6	0	-10.926394	-3.070507	-1.442698
124	1	0	-9.239616	-2.671258	-2.710938
125	6	0	-11.022552	-1.790340	0.615189
126	1	0	-9.373948	-0.446809	0.959345
127	6	0	-11.560815	-2.735741	-0.251868
128	1	0	-11.364490	-3.800113	-2.113307
129	1	0	-11.530958	-1.543004	1.539618
130	17	0	-13.068005	-3.518687	0.162598
131	6	0	-1.213303	-1.158878	2.615563
132	6	0	-1.250422	0.023162	3.321867
133	1	0	-2.043864	0.539637	3.839186
134	7	0	0.042542	-1.311530	2.130624
135	7	0	0.766023	-0.301514	2.502429
136	7	0	-0.002165	0.525420	3.224318
137	6	0	0.513186	1.732216	3.774870
138	6	0	0.314071	2.002414	5.124127
139	6	0	1.205938	2.611252	2.952185
140	6	0	0.818588	3.178184	5.664220
141	1	0	-0.216926	1.294341	5.751087
142	6	0	1.741523	3.769212	3.498705
143	1	0	1.337149	2.392870	1.897981
144	6	0	1.534761	4.044980	4.845498

145	1	0	0.672164	3.406617	6.713178
146	1	0	2.316462	4.445019	2.880081
147	17	0	2.189771	5.514863	5.521918
148	6	0	0.857946	0.775017	-0.828431
149	6	0	-0.386976	0.826893	-0.229606
150	1	0	-1.035319	0.071450	0.191855
151	7	0	1.202362	2.042788	-1.167799
152	7	0	0.253641	2.857980	-0.825114
153	7	0	-0.715604	2.136856	-0.239549
154	6	0	-1.909175	2.787775	0.180879
155	6	0	-3.127111	2.393664	-0.362749
156	6	0	-1.824058	3.857099	1.063912
157	6	0	-4.288710	3.075142	-0.020143
158	1	0	-3.146728	1.598202	-1.100449
159	6	0	-2.981361	4.546917	1.404851
160	1	0	-0.863213	4.159693	1.465587
161	6	0	-4.198889	4.147921	0.861527
162	1	0	-5.239313	2.769682	-0.445873
163	1	0	-2.933103	5.390018	2.083929
164	17	0	-5.648127	5.019865	1.292147
165	30	0	-0.351952	4.690429	-2.158689
166	6	0	-1.754336	3.924830	-3.290922
167	1	0	-2.727516	3.960641	-2.781439
168	6	0	-1.876924	4.745931	-4.579422
169	1	0	-2.631593	4.334557	-5.269935
170	1	0	-2.154687	5.786836	-4.377322
171	1	0	-0.926619	4.771162	-5.129225
172	6	0	-1.466393	2.460724	-3.636461
173	1	0	-2.204724	2.052737	-4.347460
174	1	0	-0.478922	2.341096	-4.101928
175	1	0	-1.476230	1.808680	-2.753857
176	6	0	1.707156	5.962840	0.688045
177	1	0	1.454640	4.901874	0.832288
178	6	0	3.131859	6.218600	1.195020
179	1	0	3.546982	7.132977	0.753319
180	1	0	3.145957	6.365056	2.280633
181	1	0	3.815428	5.393555	0.978240
182	6	0	0.703981	6.807136	1.471136
183	1	0	0.712033	6.540624	2.534600

184	1	0	0.951691	7.873178	1.395588
185	1	0	-0.301336	6.671752	1.068844
186	8	0	0.221249	6.195591	-1.212765
187	6	0	1.541212	6.244265	-0.830263
188	1	0	1.956806	7.257014	-1.005670
189	6	0	2.363076	5.266100	-1.668567
190	6	0	3.629516	4.738203	-1.621576
191	1	0	4.474066	4.909827	-0.977654
192	7	0	1.722547	4.626989	-2.685615
193	7	0	2.492376	3.749083	-3.250018
194	7	0	3.656752	3.802918	-2.608835
195	6	0	4.653083	2.821769	-2.859879
196	6	0	5.982525	3.070068	-2.539103
197	6	0	4.256792	1.585423	-3.361749
198	6	0	6.924537	2.060300	-2.695339
199	1	0	6.292341	4.039086	-2.164194
200	6	0	5.197937	0.580364	-3.530891
201	1	0	3.212460	1.417649	-3.592168
202	6	0	6.522814	0.822638	-3.183833
203	1	0	7.962276	2.237901	-2.439312
204	1	0	4.897120	-0.388607	-3.912554
205	17	0	7.701226	-0.456809	-3.354960

15(SSSS)r

Sum of electronic and zero-point Energies = -15309.601767

Sum of electronic and thermal Energies = -15309.486700

Sum of electronic and thermal Enthalpies = -15309.485756

Sum of electronic and thermal Free Energies = -15309.764728

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	2.791179	-0.109432	1.875882
2	6	0	4.043940	1.338563	2.314990
3	6	0	4.029689	2.420362	1.232825
4	6	0	-2.269776	-2.299552	1.913654
5	8	0	-2.613559	-1.810220	0.641060
6	30	0	-4.109823	-0.489499	0.490042
7	6	0	-5.271674	-0.486398	2.059446
8	6	0	-6.247604	0.664893	2.280975
9	8	0	2.286086	-0.661389	0.007000
10	30	0	2.538754	-2.572762	0.194884
11	8	0	3.162190	-2.045100	1.959189
12	6	0	3.982793	-2.745215	2.848546
13	6	0	1.855741	0.149942	-1.044053
14	6	0	1.372175	-0.685708	-2.245836
15	6	0	0.252093	-1.649944	-1.860889
16	6	0	0.957113	0.188813	-3.428275
17	6	0	2.890567	-4.171084	-0.884685
18	6	0	1.730276	-5.149969	-1.072631
19	6	0	3.333112	-4.098360	3.218609
20	6	0	4.217342	-4.965189	4.114752
21	6	0	1.977944	-3.846960	3.879400
22	6	0	5.452082	0.739264	2.427211
23	6	0	-1.974379	-3.806565	1.916352
24	6	0	-1.838290	-4.328493	3.346447
25	6	0	-0.779632	-4.219017	1.058954
26	30	0	-2.780256	-2.508516	-1.163534
27	8	0	-3.637659	-0.727949	-1.368916

28	6	0	-4.512054	-0.316637	-2.407022
29	6	0	-2.822727	-4.246553	-2.047153
30	6	0	-2.166941	-4.343113	-3.424924
31	6	0	-4.272902	-4.745199	-2.116611
32	6	0	-6.010539	-1.832714	2.008221
33	6	0	-4.178479	-1.002246	-3.738627
34	6	0	-2.712260	-0.770632	-4.103652
35	6	0	-5.095162	-0.503475	-4.856113
36	1	0	2.690449	0.769245	-1.400195
37	1	0	2.246934	-1.280372	-2.540409
38	1	0	0.813611	-0.417535	-4.327960
39	1	0	1.698263	0.962056	-3.655772
40	1	0	0.013300	0.703945	-3.224569
41	1	0	-0.681524	-1.098206	-1.700709
42	1	0	0.080795	-2.386035	-2.651398
43	1	0	0.492087	-2.185660	-0.939436
44	1	0	3.666161	-4.713255	-0.320488
45	1	0	1.378626	-5.556662	-0.119046
46	1	0	2.019731	-6.006714	-1.700740
47	1	0	0.867197	-4.679247	-1.561345
48	1	0	4.095878	-2.171002	3.782786
49	1	0	3.167140	-4.628220	2.268266
50	1	0	1.438575	-4.786956	4.035634
51	1	0	1.362700	-3.186161	3.265056
52	1	0	2.111536	-3.371997	4.859813
53	1	0	5.146198	-5.261943	3.622382
54	1	0	3.684136	-5.876299	4.405086
55	1	0	4.489119	-4.430255	5.031863
56	1	0	3.804601	1.814839	3.276250
57	1	0	6.214833	1.506695	2.637059
58	1	0	5.755609	0.245624	1.494479
59	1	0	5.526834	-0.014198	3.219627
60	1	0	3.069557	2.945036	1.158317
61	1	0	4.805239	3.187211	1.397099
62	1	0	4.218837	1.986060	0.244400
63	1	0	-0.792127	-3.712590	0.091182
64	1	0	0.166724	-3.985612	1.552988
65	1	0	-0.805373	-5.296032	0.870599
66	1	0	-2.875189	-4.254801	1.472617

67	1	0	-0.985407	-3.865044	3.854125
68	1	0	-1.674325	-5.410196	3.349015
69	1	0	-2.737809	-4.124251	3.937166
70	1	0	-3.125609	-2.159397	2.591714
71	1	0	-4.328410	-5.780693	-2.483359
72	1	0	-4.873454	-4.141962	-2.811359
73	1	0	-4.776031	-4.721602	-1.141563
74	1	0	-2.269046	-5.354011	-3.847324
75	1	0	-2.617638	-3.652678	-4.148553
76	1	0	-1.094666	-4.120305	-3.391887
77	1	0	-2.280586	-4.934508	-1.383949
78	1	0	-4.609702	-0.520186	2.938983
79	1	0	-6.725437	-1.866067	1.176837
80	1	0	-6.586044	-2.022088	2.926299
81	1	0	-5.326948	-2.681906	1.874177
82	1	0	-5.723773	1.604439	2.480521
83	1	0	-6.904633	0.473742	3.143832
84	1	0	-6.894791	0.835114	1.414001
85	1	0	-4.392729	0.768003	-2.558667
86	1	0	-4.338941	-2.082805	-3.605386
87	1	0	-4.968329	0.574148	-5.009380
88	1	0	-6.151151	-0.689134	-4.640475
89	1	0	-4.853583	-1.002620	-5.799005
90	1	0	-2.473312	-1.232219	-5.065913
91	1	0	-2.495046	0.301165	-4.181436
92	1	0	-2.036849	-1.192126	-3.357377
93	6	0	3.496318	-3.818494	-2.249323
94	1	0	4.314225	-3.088024	-2.183162
95	1	0	3.895179	-4.706826	-2.762601
96	1	0	2.743383	-3.384999	-2.919348
97	6	0	5.362516	-2.908570	2.269079
98	6	0	5.750218	-2.975863	0.954757
99	1	0	5.216314	-2.875822	0.025095
100	7	0	6.478038	-3.042101	3.040244
101	7	0	7.516930	-3.200843	2.279769
102	7	0	7.091833	-3.164761	1.004584
103	6	0	8.003324	-3.327213	-0.067999
104	6	0	7.553823	-3.821980	-1.289026
105	6	0	9.338594	-2.975025	0.111342

106	6	0	8.443234	-3.946358	-2.349340
107	1	0	6.520249	-4.124845	-1.418751
108	6	0	10.231666	-3.114985	-0.942315
109	1	0	9.669169	-2.588808	1.067787
110	6	0	9.774044	-3.592406	-2.165935
111	1	0	8.102299	-4.328581	-3.304409
112	1	0	11.273069	-2.844048	-0.813458
113	17	0	10.896683	-3.753464	-3.498809
114	6	0	-5.923402	-0.531796	-1.944817
115	6	0	-6.678820	-1.678175	-1.868926
116	1	0	-6.497995	-2.696798	-2.173122
117	7	0	-6.632913	0.472530	-1.359771
118	7	0	-7.771421	0.015326	-0.937129
119	7	0	-7.814086	-1.292124	-1.239258
120	6	0	-8.940024	-2.079996	-0.877038
121	6	0	-9.360440	-3.107228	-1.715286
122	6	0	-9.596417	-1.811754	0.320527
123	6	0	-10.446658	-3.890315	-1.345363
124	1	0	-8.859475	-3.287775	-2.660264
125	6	0	-10.691295	-2.584483	0.683851
126	1	0	-9.249610	-1.008232	0.959669
127	6	0	-11.101843	-3.619877	-0.149383
128	1	0	-10.787189	-4.692304	-1.989628
129	1	0	-11.212418	-2.389045	1.613522
130	17	0	-12.472363	-4.600889	0.315472
131	6	0	-1.180080	-1.405645	2.443737
132	6	0	-1.314647	-0.300593	3.257157
133	1	0	-2.154183	0.114333	3.792942
134	7	0	0.094652	-1.426677	1.987118
135	7	0	0.736183	-0.410163	2.473634
136	7	0	-0.102397	0.292765	3.243511
137	6	0	0.292292	1.515605	3.858966
138	6	0	0.037106	1.713551	5.210511
139	6	0	0.900866	2.496679	3.084275
140	6	0	0.391152	2.920997	5.799349
141	1	0	-0.421809	0.928444	5.801559
142	6	0	1.272445	3.696728	3.674517
143	1	0	1.084852	2.331757	2.029484
144	6	0	1.007975	3.898626	5.025040

145	1	0	0.201448	3.093417	6.852005
146	1	0	1.755117	4.466273	3.084441
147	17	0	1.461260	5.413647	5.763136
148	6	0	0.822237	1.147206	-0.592742
149	6	0	-0.447435	0.989726	-0.072953
150	1	0	-1.040973	0.120578	0.173949
151	7	0	1.065550	2.480057	-0.693540
152	7	0	0.030154	3.137025	-0.270775
153	7	0	-0.894250	2.248350	0.122562
154	6	0	-2.179787	2.712083	0.520707
155	6	0	-3.290397	2.328711	-0.222664
156	6	0	-2.288543	3.606986	1.577942
157	6	0	-4.540985	2.851338	0.087122
158	1	0	-3.159442	1.666201	-1.071431
159	6	0	-3.532965	4.148230	1.879316
160	1	0	-1.406532	3.895526	2.139017
161	6	0	-4.642429	3.769283	1.128720
162	1	0	-5.415036	2.546515	-0.480536
163	1	0	-3.635481	4.864554	2.686013
164	17	0	-6.197234	4.466809	1.501690
165	30	0	-0.636178	5.156855	-1.060985
166	6	0	-1.811855	4.518130	-2.507852
167	1	0	-2.782591	4.339880	-2.014764
168	6	0	-2.061971	5.558413	-3.604202
169	1	0	-2.816593	5.214792	-4.330756
170	1	0	-2.418298	6.512772	-3.197478
171	1	0	-1.147819	5.772493	-4.167301
172	6	0	-1.385686	3.193610	-3.150058
173	1	0	-2.103929	2.863101	-3.919152
174	1	0	-0.410207	3.279423	-3.644571
175	1	0	-1.301444	2.377046	-2.423029
176	6	0	0.045851	6.303822	0.384190
177	1	0	-0.555352	5.968031	1.247614
178	6	0	1.507259	6.070141	0.776437
179	1	0	2.198521	6.500245	0.039467
180	1	0	1.766063	6.544802	1.737031
181	1	0	1.750531	5.002526	0.852610
182	6	0	-0.232412	7.800241	0.218506
183	1	0	0.071508	8.386683	1.101019

184	1	0	0.303443	8.225827	-0.640226
185	1	0	-1.296962	8.000598	0.049113
186	8	0	0.844489	7.032486	-3.776576
187	6	0	1.581971	6.584295	-2.926616
188	1	0	1.828887	7.165701	-2.017265
189	6	0	2.266624	5.287316	-3.008325
190	6	0	3.279388	4.837518	-2.189341
191	1	0	3.721178	5.247536	-1.295768
192	7	0	2.066433	4.355778	-3.988861
193	7	0	2.896091	3.385897	-3.821659
194	7	0	3.657945	3.668497	-2.734062
195	6	0	4.730176	2.817117	-2.353754
196	6	0	5.778150	3.330224	-1.596097
197	6	0	4.720661	1.480264	-2.742180
198	6	0	6.803976	2.492048	-1.181610
199	1	0	5.806875	4.378476	-1.322395
200	6	0	5.750829	0.642697	-2.335751
201	1	0	3.916709	1.100040	-3.359768
202	6	0	6.778571	1.152982	-1.549857
203	1	0	7.615346	2.880884	-0.578148
204	1	0	5.753048	-0.400320	-2.630051
205	17	0	8.068838	0.096812	-1.035018

TS3(R)

Sum of electronic and zero-point Energies = -15309.579221

Sum of electronic and thermal Energies = -15309.464715

Sum of electronic and thermal Enthalpies = -15309.463771

Sum of electronic and thermal Free Energies = -15309.739560

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	2.974960	-0.826881	1.225090
2	6	0	4.185337	0.272897	2.330526
3	6	0	5.542798	0.592702	1.698459
4	6	0	-2.243163	-2.842806	1.415750
5	8	0	-2.839485	-2.131374	0.366300
6	30	0	-3.704722	-0.377996	0.725313
7	6	0	-4.565279	-0.286720	2.463899
8	6	0	-5.106100	1.043418	2.976996
9	8	0	2.431343	-1.084372	-0.702266
10	30	0	2.677582	-2.985930	-0.827559
11	8	0	3.100843	-2.821309	1.059753
12	6	0	4.065569	-3.585009	1.735322
13	6	0	1.885419	-0.156438	-1.596751
14	6	0	1.186628	-0.805859	-2.796599
15	6	0	0.106739	-1.811157	-2.408811
16	6	0	0.674967	0.253433	-3.772700
17	6	0	2.899847	-4.416885	-2.137847
18	6	0	1.836862	-5.513904	-2.022918
19	6	0	3.816222	-5.094858	1.546367
20	6	0	4.840992	-5.930661	2.312703
21	6	0	2.392564	-5.450972	1.972206
22	6	0	4.426465	-0.375904	3.700293
23	6	0	-1.935441	-4.305877	1.050312
24	6	0	-1.466630	-5.082720	2.280653
25	6	0	-0.950317	-4.455907	-0.105393
26	30	0	-3.092412	-2.223882	-1.533768
27	8	0	-3.483511	-0.273850	-1.210198

28	6	0	-4.445994	0.446800	-1.964456
29	6	0	-3.520509	-3.589942	-2.866661
30	6	0	-2.990274	-3.385777	-4.286383
31	6	0	-5.032464	-3.852854	-2.906789
32	6	0	-5.677845	-1.344124	2.411741
33	6	0	-4.377550	0.081013	-3.452369
34	6	0	-2.952467	0.279283	-3.966608
35	6	0	-5.378156	0.900504	-4.266084
36	1	0	2.688487	0.463956	-2.024035
37	1	0	1.981770	-1.366083	-3.304592
38	1	0	0.302464	-0.213755	-4.689532
39	1	0	1.470337	0.953865	-4.047544
40	1	0	-0.140659	0.840196	-3.339214
41	1	0	-0.750224	-1.323585	-1.930280
42	1	0	-0.253715	-2.347639	-3.290900
43	1	0	0.489704	-2.548757	-1.702118
44	1	0	3.866488	-4.881900	-1.886739
45	1	0	1.771930	-5.932856	-1.011769
46	1	0	2.039593	-6.350401	-2.709083
47	1	0	0.840554	-5.132202	-2.280242
48	1	0	4.004412	-3.376534	2.815150
49	1	0	3.923516	-5.306907	0.472450
50	1	0	2.177430	-6.507779	1.783288
51	1	0	1.657816	-4.845869	1.437452
52	1	0	2.256136	-5.268183	3.045637
53	1	0	5.865730	-5.718491	1.995696
54	1	0	4.656114	-6.999019	2.162829
55	1	0	4.781540	-5.728075	3.388437
56	1	0	3.685248	1.235126	2.516477
57	1	0	5.002103	0.284598	4.367548
58	1	0	5.009759	-1.299446	3.603379
59	1	0	3.498581	-0.631474	4.223245
60	1	0	5.452917	1.139362	0.756370
61	1	0	6.168100	1.203634	2.368436
62	1	0	6.110935	-0.320128	1.489154
63	1	0	-1.257094	-3.859538	-0.967485
64	1	0	0.053398	-4.132109	0.181859
65	1	0	-0.892947	-5.499301	-0.427251
66	1	0	-2.900745	-4.720568	0.727464

67	1	0	-0.520261	-4.684492	2.662785
68	1	0	-1.303672	-6.136404	2.035890
69	1	0	-2.204368	-5.038174	3.089294
70	1	0	-2.954032	-2.879359	2.257575
71	1	0	-5.272200	-4.734947	-3.518319
72	1	0	-5.575968	-3.012669	-3.361031
73	1	0	-5.458585	-4.029562	-1.910929
74	1	0	-3.269393	-4.224366	-4.941423
75	1	0	-3.392827	-2.477388	-4.750928
76	1	0	-1.898679	-3.307600	-4.318083
77	1	0	-3.053524	-4.507038	-2.479018
78	1	0	-3.818462	-0.640462	3.191524
79	1	0	-6.485773	-1.033784	1.739128
80	1	0	-6.137597	-1.504400	3.398198
81	1	0	-5.316745	-2.317902	2.056698
82	1	0	-4.304692	1.770606	3.140555
83	1	0	-5.634250	0.920195	3.935064
84	1	0	-5.817689	1.493073	2.274806
85	1	0	-4.231874	1.524755	-1.892980
86	1	0	-4.634641	-0.983363	-3.546437
87	1	0	-5.195141	1.974743	-4.145650
88	1	0	-6.410823	0.708469	-3.961959
89	1	0	-5.292642	0.664684	-5.330726
90	1	0	-2.882252	0.065786	-5.036809
91	1	0	-2.626639	1.314698	-3.807687
92	1	0	-2.243819	-0.370453	-3.449344
93	6	0	2.999854	-3.940092	-3.589814
94	1	0	3.769668	-3.171109	-3.728268
95	1	0	3.241756	-4.766826	-4.275300
96	1	0	2.050614	-3.514038	-3.938934
97	6	0	5.442093	-3.165285	1.292910
98	6	0	5.875563	-2.852919	0.027253
99	1	0	5.395827	-2.835327	-0.937923
100	7	0	6.474083	-2.945909	2.152455
101	7	0	7.504618	-2.503904	1.494008
102	7	0	7.152982	-2.440138	0.199021
103	6	0	8.016906	-1.876463	-0.775974
104	6	0	8.114537	-2.473101	-2.027772
105	6	0	8.698975	-0.700412	-0.482644

106	6	0	8.899507	-1.881486	-3.009392
107	1	0	7.584425	-3.396695	-2.234606
108	6	0	9.491476	-0.111300	-1.459121
109	1	0	8.588681	-0.241313	0.492828
110	6	0	9.579954	-0.705727	-2.713493
111	1	0	8.984858	-2.334201	-3.990134
112	1	0	10.015351	0.814386	-1.252490
113	17	0	10.563518	0.045695	-3.950492
114	6	0	-5.799469	0.255519	-1.346811
115	6	0	-6.634468	-0.836446	-1.347888
116	1	0	-6.566125	-1.806354	-1.813633
117	7	0	-6.363228	1.210255	-0.556719
118	7	0	-7.489983	0.775136	-0.083224
119	7	0	-7.671286	-0.468259	-0.559464
120	6	0	-8.822449	-1.222232	-0.203901
121	6	0	-9.319031	-2.173289	-1.089554
122	6	0	-9.427202	-1.002698	1.030187
123	6	0	-10.428274	-2.928906	-0.732265
124	1	0	-8.858832	-2.318868	-2.060662
125	6	0	-10.545708	-1.746849	1.381195
126	1	0	-9.025081	-0.257418	1.705991
127	6	0	-11.032241	-2.706485	0.499609
128	1	0	-10.824118	-3.673414	-1.412875
129	1	0	-11.028530	-1.586600	2.337930
130	17	0	-12.433395	-3.650906	0.947620
131	6	0	-1.058944	-2.058904	1.923196
132	6	0	-0.913679	-1.438140	3.143255
133	1	0	-1.545735	-1.386463	4.015734
134	7	0	0.031730	-1.757949	1.174903
135	7	0	0.825853	-0.998260	1.865606
136	7	0	0.268018	-0.792758	3.068954
137	6	0	0.874941	0.026751	4.063367
138	6	0	1.014230	-0.473781	5.353645
139	6	0	1.305718	1.303887	3.729556
140	6	0	1.597327	0.319944	6.332001
141	1	0	0.693587	-1.483841	5.585357
142	6	0	1.902937	2.093372	4.702972
143	1	0	1.195947	1.675864	2.717023
144	6	0	2.041262	1.594157	5.993045

145	1	0	1.724888	-0.056842	7.339689
146	1	0	2.261266	3.085432	4.454094
147	17	0	2.794105	2.587126	7.216145
148	6	0	1.060329	0.816393	-0.807670
149	6	0	-0.277324	1.004913	-0.574017
150	1	0	-1.161974	0.503352	-0.936809
151	7	0	1.728980	1.747586	-0.079014
152	7	0	0.894147	2.491598	0.583172
153	7	0	-0.328169	2.051381	0.288934
154	6	0	-1.467508	2.721513	0.810817
155	6	0	-2.691729	2.554921	0.174833
156	6	0	-1.342120	3.557880	1.915345
157	6	0	-3.816479	3.219208	0.645114
158	1	0	-2.759375	1.944492	-0.714786
159	6	0	-2.460604	4.243433	2.373947
160	1	0	-0.383942	3.682571	2.404818
161	6	0	-3.685408	4.068174	1.737731
162	1	0	-4.778620	3.067324	0.165591
163	1	0	-2.378470	4.904668	3.228777
164	17	0	-5.085894	4.929151	2.323116
165	30	0	3.717739	2.536664	-0.815272
166	6	0	3.977221	3.951459	0.916477
167	1	0	3.807493	2.875582	1.139117
168	6	0	5.095264	1.653066	-1.950334
169	1	0	4.755444	1.926747	-2.962153
170	6	0	5.292301	0.133627	-1.938728
171	1	0	6.097333	-0.157103	-2.631974
172	1	0	5.582999	-0.227750	-0.947752
173	1	0	4.400087	-0.429599	-2.229706
174	6	0	6.461950	2.325166	-1.755323
175	1	0	7.179836	1.998826	-2.524657
176	1	0	6.384523	3.414580	-1.797390
177	1	0	6.906811	2.054293	-0.788404
178	6	0	3.005985	4.671898	1.840128
179	1	0	3.205603	4.440923	2.897119
180	1	0	3.101491	5.763377	1.747442
181	1	0	1.966766	4.408489	1.625436
182	6	0	5.429691	4.229582	1.275113
183	1	0	5.657539	5.298785	1.181910

184	1	0	5.661512	3.936120	2.308815
185	1	0	6.121228	3.700383	0.614858
186	8	0	4.753393	5.001432	-1.653333
187	6	0	3.840366	5.172958	-0.815036
188	1	0	3.885420	6.013336	-0.096432
189	6	0	2.429924	4.907429	-1.282002
190	6	0	1.228530	5.562686	-1.215124
191	7	0	2.210493	3.736308	-1.930285
192	1	0	0.943756	6.522902	-0.818411
193	7	0	0.963081	3.614957	-2.255360
194	7	0	0.349245	4.725367	-1.835969
195	6	0	-1.052106	4.859597	-2.022518
196	6	0	-1.674598	4.137073	-3.038293
197	6	0	-1.789881	5.680309	-1.175108
198	6	0	-3.050060	4.234751	-3.201560
199	1	0	-1.084536	3.511082	-3.696850
200	6	0	-3.163207	5.792464	-1.351123
201	1	0	-1.309625	6.212811	-0.362086
202	6	0	-3.783541	5.063106	-2.358709
203	1	0	-3.544408	3.683537	-3.993742
204	1	0	-3.747559	6.426106	-0.694418
205	17	0	-5.514460	5.174658	-2.560862

13(SSSS)-7(R)

Sum of electronic and zero-point Energies = -15309.678231

Sum of electronic and thermal Energies = -15309.565027

Sum of electronic and thermal Enthalpies = -15309.564083

Sum of electronic and thermal Free Energies = -15309.836576

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	2.908048	-0.520500	1.488901
2	6	0	4.315861	0.598199	2.277024
3	6	0	5.445783	0.811120	1.264451
4	6	0	-2.258512	-2.439574	1.687127
5	8	0	-2.757663	-1.765682	0.566441
6	30	0	-3.900484	-0.143189	0.712908
7	6	0	-4.976730	-0.129039	2.340094
8	6	0	-5.803388	1.099675	2.704350
9	8	0	2.362121	-0.776740	-0.437460
10	30	0	2.614791	-2.676489	-0.557382
11	8	0	3.056106	-2.521721	1.332278
12	6	0	4.046937	-3.271558	1.981840
13	6	0	1.795340	0.159465	-1.311877
14	6	0	1.222018	-0.505161	-2.571649
15	6	0	0.176799	-1.578698	-2.270010
16	6	0	0.711012	0.517799	-3.585357
17	6	0	2.834154	-4.165180	-1.804912
18	6	0	1.733341	-5.222819	-1.677735
19	6	0	3.694194	-4.773259	1.951639
20	6	0	4.766961	-5.629255	2.623114
21	6	0	2.326382	-4.990661	2.597064
22	6	0	4.888092	0.072870	3.597238
23	6	0	-1.982147	-3.928659	1.398505
24	6	0	-1.628855	-4.682072	2.680602
25	6	0	-0.922061	-4.153701	0.322301
26	30	0	-3.067186	-2.142266	-1.292922
27	8	0	-3.614301	-0.216499	-1.217039

28	6	0	-4.546350	0.359320	-2.115323
29	6	0	-3.370536	-3.710793	-2.417972
30	6	0	-2.650794	-3.731210	-3.767623
31	6	0	-4.864310	-4.000181	-2.610354
32	6	0	-5.873588	-1.370637	2.230881
33	6	0	-4.344092	-0.174436	-3.540227
34	6	0	-2.896226	0.043637	-3.976057
35	6	0	-5.316853	0.477204	-4.521858
36	1	0	2.585650	0.847117	-1.655703
37	1	0	2.083776	-1.011408	-3.027663
38	1	0	0.460593	0.025716	-4.530526
39	1	0	1.464891	1.284291	-3.786722
40	1	0	-0.187336	1.027725	-3.224557
41	1	0	-0.685238	-1.178034	-1.725561
42	1	0	-0.180140	-2.034223	-3.197967
43	1	0	0.594173	-2.373960	-1.651274
44	1	0	3.776734	-4.653081	-1.509902
45	1	0	1.642381	-5.611046	-0.656191
46	1	0	1.917430	-6.083974	-2.338210
47	1	0	0.752487	-4.816739	-1.957685
48	1	0	4.103656	-2.966553	3.039305
49	1	0	3.631239	-5.058443	0.890967
50	1	0	1.972224	-6.016348	2.451282
51	1	0	1.591078	-4.303126	2.173862
52	1	0	2.377870	-4.804272	3.677434
53	1	0	5.734636	-5.540514	2.121471
54	1	0	4.478783	-6.685470	2.615093
55	1	0	4.910078	-5.329405	3.667823
56	1	0	3.875605	1.581917	2.486474
57	1	0	5.621081	0.770827	4.033968
58	1	0	5.413150	-0.879994	3.460032
59	1	0	4.111190	-0.090429	4.354814
60	1	0	5.090111	1.273146	0.335053
61	1	0	6.243240	1.461245	1.656439
62	1	0	5.919424	-0.138964	0.987611
63	1	0	-1.116186	-3.542336	-0.561530
64	1	0	0.076650	-3.898523	0.686041
65	1	0	-0.910912	-5.201491	0.009242
66	1	0	-2.938052	-4.320506	1.021743

67	1	0	-0.690544	-4.313644	3.110124
68	1	0	-1.497756	-5.748978	2.477510
69	1	0	-2.412140	-4.579809	3.439880
70	1	0	-3.014614	-2.412017	2.488485
71	1	0	-5.024131	-4.971571	-3.100774
72	1	0	-5.345735	-3.251566	-3.254361
73	1	0	-5.411855	-4.028385	-1.659310
74	1	0	-2.883056	-4.646868	-4.332064
75	1	0	-2.938252	-2.885437	-4.405629
76	1	0	-1.562219	-3.697111	-3.652958
77	1	0	-2.964623	-4.546604	-1.829674
78	1	0	-4.278249	-0.310480	3.171781
79	1	0	-6.637218	-1.243692	1.453701
80	1	0	-6.412825	-1.569844	3.169007
81	1	0	-5.311887	-2.279761	1.979885
82	1	0	-5.166486	1.950877	2.960125
83	1	0	-6.447774	0.904182	3.576221
84	1	0	-6.458670	1.416318	1.885236
85	1	0	-4.388108	1.448701	-2.153626
86	1	0	-4.536770	-1.256409	-3.518725
87	1	0	-5.176522	1.564065	-4.549798
88	1	0	-6.360095	0.285646	-4.256169
89	1	0	-5.154062	0.093871	-5.533412
90	1	0	-2.734217	-0.303448	-5.000545
91	1	0	-2.638314	1.109341	-3.937532
92	1	0	-2.197499	-0.489231	-3.328651
93	6	0	2.984127	-3.743154	-3.269681
94	1	0	3.783787	-3.006458	-3.416748
95	1	0	3.207737	-4.600912	-3.922762
96	1	0	2.059960	-3.291579	-3.652491
97	6	0	5.400663	-2.987898	1.385486
98	6	0	5.741723	-2.812455	0.066928
99	1	0	5.175637	-2.818467	-0.849534
100	7	0	6.524428	-2.802868	2.132137
101	7	0	7.525259	-2.518186	1.353898
102	7	0	7.062791	-2.519130	0.092338
103	6	0	7.893353	-2.160969	-0.999475
104	6	0	7.710589	-2.781628	-2.230695
105	6	0	8.835906	-1.150508	-0.836389

106	6	0	8.464513	-2.373235	-3.323208
107	1	0	6.979635	-3.575586	-2.340970
108	6	0	9.601994	-0.751557	-1.923746
109	1	0	8.949771	-0.672221	0.129206
110	6	0	9.401781	-1.360382	-3.158068
111	1	0	8.325740	-2.841961	-4.290212
112	1	0	10.335181	0.038996	-1.815351
113	17	0	10.347190	-0.838562	-4.535626
114	6	0	-5.933556	0.160848	-1.578692
115	6	0	-6.719955	-0.965910	-1.533932
116	1	0	-6.586315	-1.967707	-1.909616
117	7	0	-6.585698	1.151498	-0.909675
118	7	0	-7.718068	0.703134	-0.462429
119	7	0	-7.814389	-0.584450	-0.834418
120	6	0	-8.943836	-1.363400	-0.465459
121	6	0	-9.405651	-2.354783	-1.325082
122	6	0	-9.560629	-1.126863	0.759450
123	6	0	-10.493992	-3.132643	-0.950847
124	1	0	-8.933895	-2.512651	-2.288780
125	6	0	-10.658289	-1.893617	1.127383
126	1	0	-9.180832	-0.352851	1.415926
127	6	0	-11.110887	-2.892363	0.271512
128	1	0	-10.864851	-3.907508	-1.611338
129	1	0	-11.149506	-1.721869	2.077791
130	17	0	-12.486005	-3.865145	0.740935
131	6	0	-1.060336	-1.695368	2.214237
132	6	0	-0.839760	-1.149103	3.459695
133	1	0	-1.430768	-1.116042	4.361205
134	7	0	0.014817	-1.411389	1.440711
135	7	0	0.868389	-0.732915	2.138905
136	7	0	0.372373	-0.561052	3.370731
137	6	0	1.100507	0.153684	4.366835
138	6	0	1.369852	-0.468618	5.580738
139	6	0	1.535779	1.446161	4.096528
140	6	0	2.080355	0.220275	6.555300
141	1	0	1.042742	-1.488053	5.755448
142	6	0	2.262076	2.127913	5.063801
143	1	0	1.318094	1.910366	3.140062
144	6	0	2.521041	1.511156	6.282946

145	1	0	2.304136	-0.248369	7.506148
146	1	0	2.625652	3.129404	4.867652
147	17	0	3.429314	2.374469	7.499526
148	6	0	0.840276	1.035224	-0.541894
149	6	0	-0.521128	1.209822	-0.522311
150	1	0	-1.338892	0.751812	-1.058898
151	7	0	1.372181	1.859929	0.402140
152	7	0	0.432315	2.520103	0.997036
153	7	0	-0.732759	2.137059	0.448350
154	6	0	-1.942937	2.750390	0.855874
155	6	0	-3.038209	2.739260	-0.000977
156	6	0	-2.013291	3.393427	2.090076
157	6	0	-4.220335	3.370741	0.369028
158	1	0	-2.957826	2.283857	-0.979894
159	6	0	-3.180006	4.056534	2.446359
160	1	0	-1.157493	3.391545	2.754085
161	6	0	-4.272072	4.042698	1.583019
162	1	0	-5.085121	3.335345	-0.284286
163	1	0	-3.243397	4.571652	3.397887
164	17	0	-5.733086	4.883485	2.037458
165	30	0	4.504062	2.560755	-1.779049
166	6	0	3.814952	4.239395	1.362610
167	1	0	3.515864	3.187330	1.285976
168	6	0	4.959930	1.082819	-2.968280
169	1	0	4.095408	0.939649	-3.636179
170	6	0	5.221198	-0.248383	-2.262745
171	1	0	5.441956	-1.050161	-2.986448
172	1	0	6.091083	-0.178602	-1.599605
173	1	0	4.375309	-0.568761	-1.645982
174	6	0	6.160844	1.452831	-3.848906
175	1	0	6.394700	0.659653	-4.576563
176	1	0	5.995311	2.375563	-4.417835
177	1	0	7.067562	1.602205	-3.249270
178	6	0	2.727237	5.001885	2.120711
179	1	0	2.764228	4.757237	3.187900
180	1	0	2.871733	6.087617	2.040088
181	1	0	1.722541	4.752404	1.768560
182	6	0	5.148657	4.316162	2.100928
183	1	0	5.432192	5.360451	2.286581

184	1	0	5.089853	3.806966	3.068981
185	1	0	5.936107	3.848653	1.508100
186	8	0	5.001262	4.010873	-0.736741
187	6	0	4.010434	4.728541	-0.097668
188	1	0	4.276709	5.801509	-0.052089
189	6	0	2.712788	4.606911	-0.875210
190	6	0	1.478109	5.202411	-0.834449
191	7	0	2.639318	3.632517	-1.816241
192	1	0	1.093263	6.018019	-0.247264
193	7	0	1.455660	3.574905	-2.342651
194	7	0	0.731960	4.523676	-1.747903
195	6	0	-0.640374	4.679149	-2.089864
196	6	0	-1.151630	3.977374	-3.180267
197	6	0	-1.461905	5.505569	-1.329541
198	6	0	-2.495775	4.101498	-3.504963
199	1	0	-0.499737	3.345771	-3.770596
200	6	0	-2.804389	5.638780	-1.662122
201	1	0	-1.080529	6.032670	-0.463481
202	6	0	-3.312978	4.929414	-2.742241
203	1	0	-2.899874	3.567432	-4.357350
204	1	0	-3.450767	6.272362	-1.066584
205	17	0	-5.009829	5.058482	-3.136848
