Supporting Information

Mechanisms of the Thermal Cyclotrimerization of Fluoro- and Chloroacetylenes: Density Functional Theory Investigation and Intermediate Trapping Experiments

*Zhong-Ke Yao and Zhi-Xiang Yu**

Beijing National Laboratory for Molecular Sciences, Key Laboratory of Bioorganic Chemistry and Molecular Engineering of Ministry of Education, College of Chemistry, Peking University, Beijing 100871, China

E-mail: yuzx@pku.edu.cn

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1. General Methods of Synthesis

Unless otherwise noted, air- and moisture-sensitive reactions were carried out in oven-dried (110 ºC) glassware capped with rubber septa under a positive pressure of dry argon from a balloon. Teflon-coated magnetic stir bars cooled under a stream of dry nitrogen or argon. Reaction temperatures refer to the external temperature or to the temperature of the bath in which the reaction vessel was partially immersed. Reactions were stirred using Teflon-coated magnetic stir bars. Organic solutions were concentrated using a Büchi rotary evaporator with a membrane vacuum pump.

Analytical TLC was performed with 0.25 mm silica gel 60F plates with a 254 nm fluorescent indicator. The TLC plates were visualized by ultraviolet light and treatment with acidic *p*-anisaldehyde stain followed by gentle heating. Purification of products was accomplished by flash chromatography on silica gel and the purified compounds show a single spot by analytical TLC.

NMR spectra were measured on Bruker ARX400 (^{1}H at 400 MHz, ^{13}C at 100 MHz) nuclear magnetic resonance spectrometers. Data for ^{1}H-NMR spectra are reported as follows: chemical shift (ppm, referenced to TMS; s = singlet, dt = doublet of triplets, tt = triplet of triplets, m = multiplet), coupling constant (Hz), and integration. Data for ^{13}C-NMR are reported in terms of chemical shift (ppm) relative to residual solvent peak ($CDCl_3$: 77.0 ppm). Infrared spectra were recorded on an AVATAR 330 Fourier transform spectrometer (FT-IR) with an OMNI sampler and are reported in wavenumbers (cm^{-1}). Mass spectra (MS) and high-resolution mass spectra (HRMS) were recorded on Waters micromass GCT (EI, 70 eV) and Bruker APEX IV (ESI) mass spectrometers.

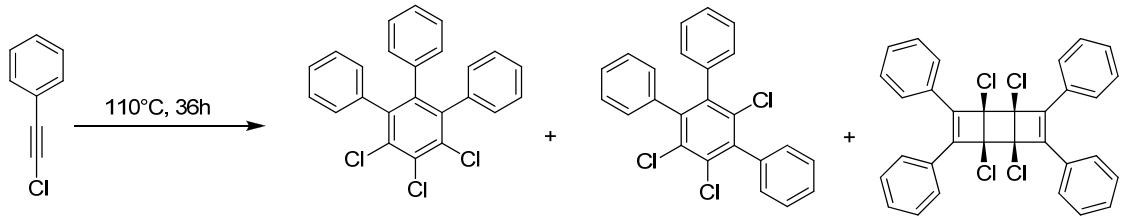
Abbreviations:

DCM = dichloromethane

Et_2O = diethyl ether

2. The Thermal Reactions of Phenylchloroacetylene and Cyclohexylchloroacetylene

The Thermal Reaction of Phenylchloroacetylene

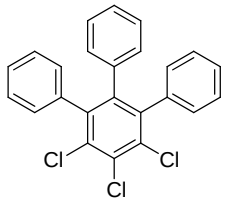


1d → **P-3** 7.3% + **P-4** 14.7% + **12** 6.6%

To an oven-dried Schlenk tube with stir bar was added 1.0 g (7.3 mmol) phenylchloroacetylene (prepared by the literature[1] method), and the tube was purged with Ar gas three times. Then the net

phenylchloroacetylene was stirred under balloon pressured Ar gas at 110 ℃ for 36 hours. The resulted brown mixture was cooled to room temperature and dissolved with 10 mL DCM, and then 10 mL Et_2O and 10 mL pentane were added. Colorless crystal formed from the solution after 24 hours at room temperature, and 66 mg (6.6%) tetramer **12** was afforded after filtration. The filtrate was condensed to about 2 mL, then 2 mL DCM and 10 mL pentane were added, light brown crystal formed from the solution after 24 hours at room temperature, and 215 mg mixture of **P-3** and **P-4** was afforded after filtration. Again, the filtrate was condensed to about 2 mL, then 1 mL DCM and 10 mL pentane were added, light brown crystal formed from the solution after 24 hours at room temperature, and 44 mg mixture of **P-3** and **P-4** was afforded after filtration. The combined mixture of **P-3** and **P-4** was dissolved in 3 mL DCM, and 20 mL pentane was added to assist crystallization, affording 147 mg (14.7%) colorless crystal of **P-4**, and the filtrate was condensed and purified by flash chromatography to afford 73 mg (7.3%) **P-3**.

1,2,3-Trichloro-4,5,6-triphenylbenzene (P3)



P3

Melting point: 164-165 ºC.

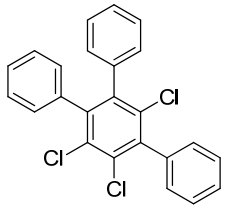
IR (film): 1444, 1384, 1373, 1265, 1249, 1075, 1030 cm^{-1}.

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.19-7.13 (m, 6H), 7.03-7.00 (dd, J = 8.0 and 1.6 Hz, 4H), 6.85-6.82 (m, 3H), 6.69-6.66 (m, 2H).

^{13}C-NMR (100 MHz, $CDCl_3$): δ 141.9, 140.5, 138.2, 132.8, 131.4, 130.5, 130.3, 130.0, 129.9, 127.6, 127.5, 127.2, 126.9, 126.2.

HRMS (EI+) for $C_{24}H_{15}Cl_3$ $(M)^+$: calculated: 408.0239, found: 408.0245.

1,2,4-Trichloro-3,5,6-triphenylbenzene (P4)



P4

Melting point: 226-227 ºC.

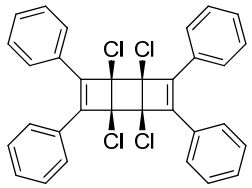
IR (film): 2917, 2849, 1602, 1444, 1404, 1360, 1302, 1234, 1074, 1048 cm^{-1}.

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.52-7.42 (m, 3H), 7.35-7.33 (m, 2H), 7.22-7.10 (m, 6H), 7.05-7.00 (m, 4H).

^{13}C-NMR (100 MHz, $CDCl_3$): δ 142.3, 140.7, 140.5, 138.2, 137.9, 133.0, 132.7, 131.6, 130.1, 129.9, 129.8, 129.2, 128.4, 128.2, 127.8, 127.6, 127.3, 127.2.

HRMS (EI+) for $C_{24}H_{15}Cl_3$ $(M)^+$: calculated: 408.0239, found: 408.0245.

cis-1,2,5,6-Tetrachloro-3,4,7,8-tetraphenyltricyclo[4.2.0.0^{2,5}]octa-3,7-diene (12)



12

Melting point: 213-214 ºC.

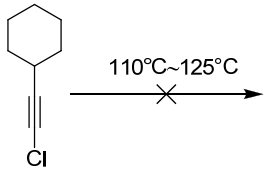
IR (film): 2925, 1444, 1343, 1179, 1084, 1026, 1002 cm^{-1}.

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.39-7.35 (dt, J = 6.8 and 1.6 Hz, 8H), 7.16-7.12 (tt, J = 7.2 and 1.6 Hz, 4H), 7.08-7.04 (tt, J = 7.2 and 1.6 Hz, 8H).

^{13}C-NMR (100 MHz, $CDCl_3$): δ 139.2, 130.4, 129.5, 128.1, 127.6, 75.8.

HRMS (ESI+) for $C_{32}H_{21}Cl_4$ $(M+H)^+$: calculated: 545.0392, found: 545.0399.

The Thermal Reaction of Cyclohexylchloroacetylene



1h

To an oven-dried Schlenk tube with stir bar was added 1.0 g (7.0 mmol) cyclohexylchloroacetylene (prepared by the literature[2] method), and the tube was purged with Ar gas three times. Then the net cyclohexylchloroacetylene was stirred under balloon pressured Ar gas at 110 ℃ for 36 hours. TLC indicated that there had not any product formed. Increased the temperature to 125 °C, unidentified dark polymers slowly appeared.

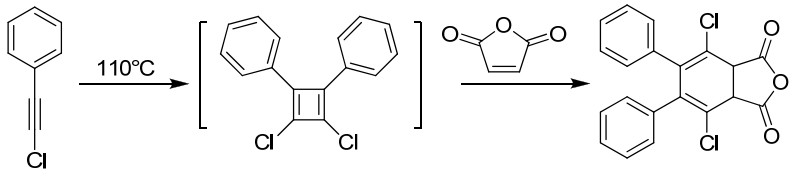
Preliminary Study of Cyclotrimerization of Bromophenylacetylene

Calculations showed that the barrier of the dimerization of bromophenylacetylene is close to that of chlorophenylacetylene (Table S10), suggesting that cyclotrimerization of bromophenylacetylene can also occur upon heating. However, preliminary experiments showed that, heating pure

bromophenylacetylene at 110-120 ℃ gave unidentified products, which did not include cyclotrimerization products. The reasons are not known to us at this stage.

3. Trapping the 1,2-Diphenyldichlorocyclobutadiene with Dienophiles

Trapping with Maleic anhydride

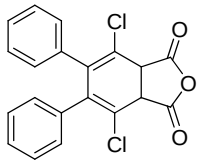


1d **INT2d-1** **13**

20%

To an oven-dried Schlenk tube with stir bar was added 410 mg (3 mmol, 1 equiv.) phenylchloroacetylene and 294 mg (3 mmol, 1 equiv.) maleic anhydride, and the tube was purged with Ar gas three times. Then the mixture of phenylchloroacetylene and maleic anhydride was stirred under balloon pressured Ar gas at 110 ℃ for 12 hours. The resulted brown mixture was cooled to room temperature and purified by flash chromatography to afford 114 mg (20% yield from **1d**) **13**.

4,7-Dichloro-5,6-diphenylisobenzofuran-1,3(3aH,7aH)-dione (13)



13

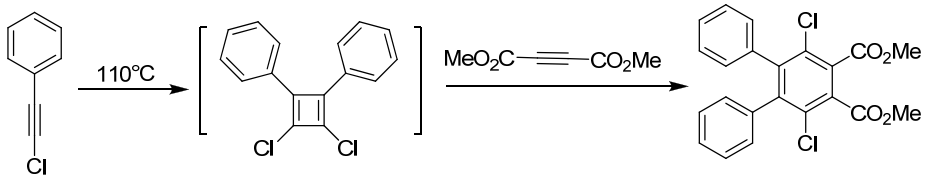
IR (film): 2955, 2923, 2850, 2360, 2340, 1869, 1789, 1460, 1444, 1378, 1269, 1204, 1100, 1041 cm^{-1}.

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.50-7.37 (m, 10H), 4.36 (s, 2H).

^{13}C-NMR (100 MHz, $CDCl_3$): δ 168.2, 136.2, 129.1, 129.0, 128.7, 128.3, 128.1, 48.5.

HRMS (ESI+) for $C_{20}H_{12}Cl_2NaO_3$ $(M+Na)^+$: calculated: 393.0056, found: 393.0051.

Trapping with Dimethyl acetylenedicarboxylate

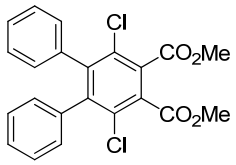


1d **INT2d-1** **14**

13%

To an oven-dried Schlenk tube with stir bar was added 410 mg (3 mmol, 1 equiv.) phenylchloroacetylene and 426 mg (3 mmol, 1 equiv.) dimethyl acetylenedicarboxylate, and the tube was purged with Ar gas three times. Then the mixture of phenylchloroacetylene and dimethyl acetylenedicarboxylate was stirred under balloon pressured Ar gas at 110 ℃ for 24 hours. The resulted brown mixture was cooled to room temperature and purified by flash chromatography to afford 100 mg (13% yield from **1d**) **14**.

Dimethyl 3,6-dichloro-4,5-diphenylphthalate (14)



14

Melting point: 246-247 ºC.

IR (film): 2955, 2917, 2850, 2358, 2337, 1745, 1727, 1466, 1378, 1321, 1257, 1210, 1088, 1018 cm^{-1}.

^{1}H-NMR (400 MHz, $CDCl_3$): δ 7.20-7.15 (m, 6H), 6.97-6.95 (m, 4H), 3.96 (s, 6H).

^{13}C-NMR (100 MHz, $CDCl_3$): δ 165.5, 144.6, 136.8, 132.5, 130.1, 129.6, 127.7, 127.6, 53.2.

HRMS (ESI+) for $C_{22}H_{16}Cl_2KO_4$ $(M+K)^+$: calculated: 453.0057, found: 453.0063.

4. Computational Methods and Discussion

All calculations were performed with the Gaussian 03 program.[3] The hybrid B3LYP functional in conjunction with the 6-31G(d) basis set were applied for the optimization of all the stationary points in the gas phase except for those singlet diradical transition states and intermediates, which were located at the UB3LYP/6-31G(d) level. This computational method has been successfully applied to study reactions involving singlet diradical intermediates and transition states. Frequency calculations were performed to confirm that each stationary point is either a minimum or a transition structure. Intrinsic reaction coordinate (IRC) calculations were used to confirm the connection between the reactants, products, and their transition states. For all singlet diradical transition states and intermediates, the YJH spin-projection[4] scheme has been used to reduce the spin contaminations. Orbital energies were computed using HF/6-31G(d) method and the orbital coefficients listed are the 2p orbitals of carbons, fluorines, and 3p orbitals of chlorines. ΔG, ΔH and ΔE_0 are the calculated relative free energies, relative

enthalpies and zero-point energy (ZPE) corrected relative electronic energies in the gas phase, respectively.

Scheme S1. Equation for the YJH Spin-Projection Energy Correction

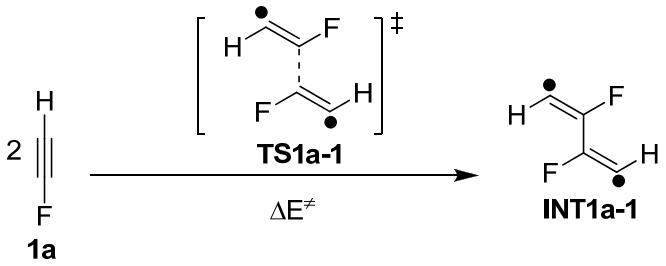
$$ {}^1E_{pure} = {}^1E_{mix} + \frac{{}^1\langle S^2 \rangle_{mix}}{{}^3\langle S^2 \rangle_{pure} - {}^1\langle S^2 \rangle_{mix}} ({}^1E_{mix} - {}^3E_{pure}) $$

${}^1E_{pure}$ is the corrected energy of the singlet diradical, ${}^1E_{mix}$ is the uncorrected energy of the singlet diradical, ${}^3E_{pure}$ is the energy of the triplet diradical, ${}^1\langle S^2 \rangle_{mix}$ is the total spin-squared operator of singlet diradical, ${}^3\langle S^2 \rangle_{pure}$ is the total spin-squared operator of triplet diradical.

Basis Set and DFT Functional Discussion

It has been shown that (U)B3LYP/6-31G(d) is adequate to describe the reaction mechanisms involving singlet diradical species. To evaluate how bigger basis sets affect the relative energies, we computed the dimerization of fluoroacetylenes and reaction of fluoroacetylene and 1,4-difluorocyclobutadiene using different basis sets based on the (U)B3LYP/6-31G(d) structures (Tables S1 and S2). It shows that (U)B3LYP/6-31G(d) method underestimates the activation barriers by about 4 kcal/mol. We also found that (U)mPW1WP91 gives similar results with those using (U)B3LYP method (Table S1). To evaluate the potential energy surfaces at high level DFT calculations, Figures S1 and S2 give these computed energies at the (U)B3LYP/6-311++G(d,p)//(U)B3LYP/6-31G(d) level (with spin contamination corrections). Figures S1 and S2 show that the conclusions from (U)B3LYP/6-31G(d) calculations are supported by the high level calculations.

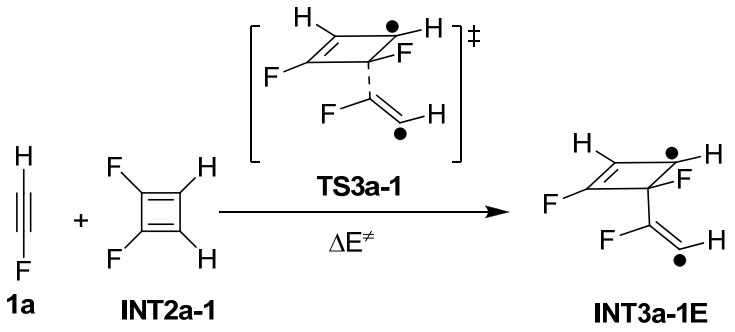
Table S1. The Computed Activation Energies of **TS1a-1** with Different Basis Sets[a]



basis set	Δ $E^{\neq}$ (kcal/mol)
(U)B3LYP/6-31G(d)	16.8
(U)B3LYP/6-311++G(d,P)	20.8
(U)B3LYP/cc-pVTZ	21.1
(U)B3LYP/cc-pVQZ	21.0
(U)B3LYP/cc-pV5Z	20.9
(U)B3LYP/aug-cc-pVTZ	20.5
(U)B3LYP/aug-cc-pVQZ	20.6
(U)B3LYP/aug-cc-pV5Z	20.7
(U)mPW1WP91/6-31G(d)	16.0
(U)mPW1WP91/6-311++G(d,p)	18.9

[a] All single-point energy calculations were carried out on the gas phase structures obtained at the (U)B3LYP/6-31G(d) level. All computed activation energies given in this Table were not corrected by spin contamination corrections and zero-point energy corrections.

Table S2. The Computed Activation Energies of **TS3a-1** with Different Basis Sets[a]



basis set	Δ $E^{\neq}$ (kcal/mol)
(U)B3LYP/6-31G(d)	10.2
(U)B3LYP/6-311++G(d,P)	13.7
(U)B3LYP/cc-pVTZ	14.3
(U)B3LYP/cc-pVQZ	14.4
(U)B3LYP/cc-pV5Z	14.5
(U)B3LYP/aug-cc-pVTZ	14.0
(U)B3LYP/aug-cc-pVQZ	14.3
(U)B3LYP/aug-cc-pV5Z	14.4

[a] All single-point energy calculations were carried out on the gas phase structures obtained at the (U)B3LYP/6-31G(d) level. All computed activation energies given in this Table were not corrected by spin contamination corrections and zero-point energy corrections.

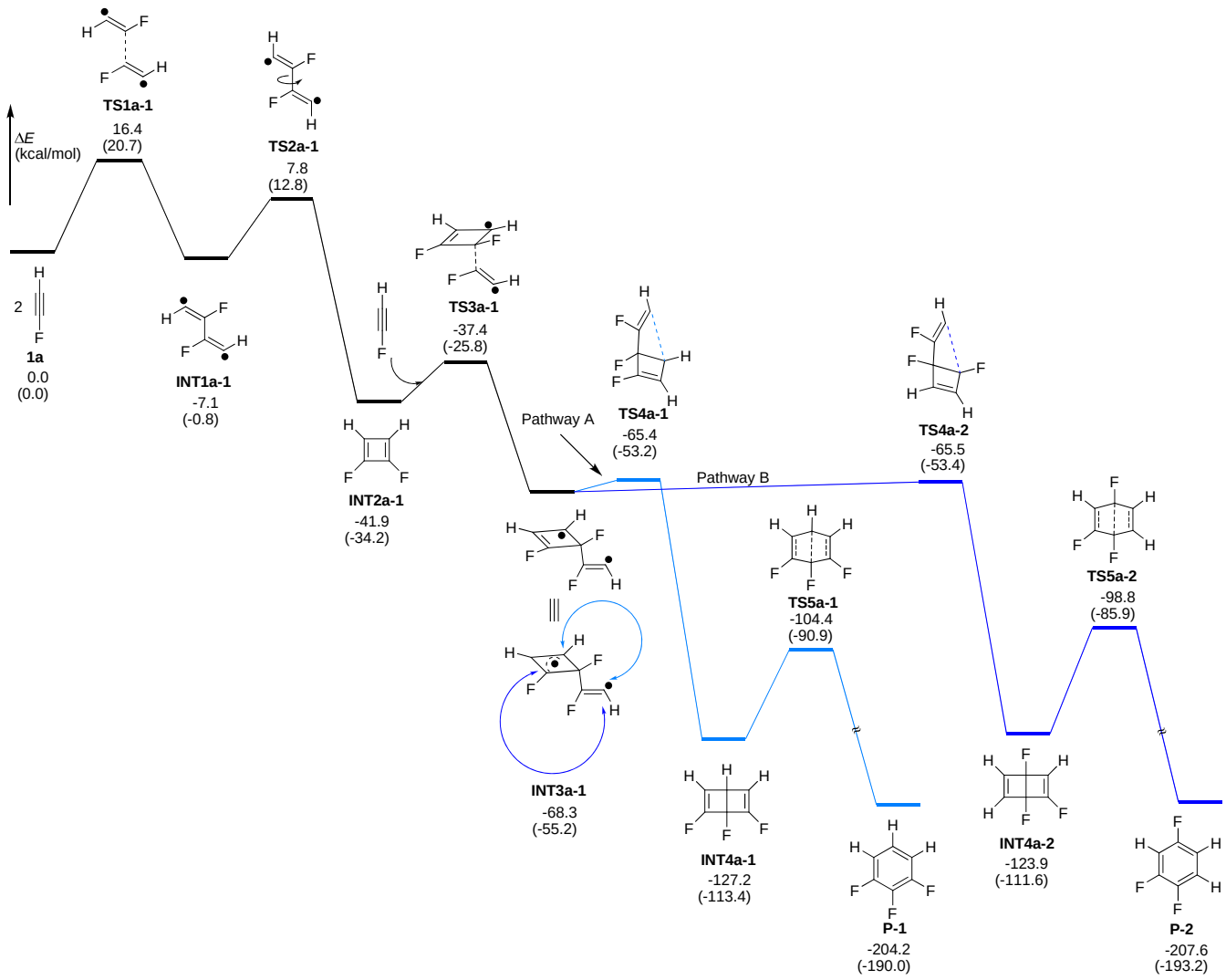


Figure S1. The computed potential energy surface at the (U)B3LYP/6-31G(d) level and the (U)B3LYP/6-311++G(d,p)//(U)B3LYP/6-31G(d) level (the energies given in parentheses). All computed energies are given with spin contamination corrections, but without zero-point energy corrections.

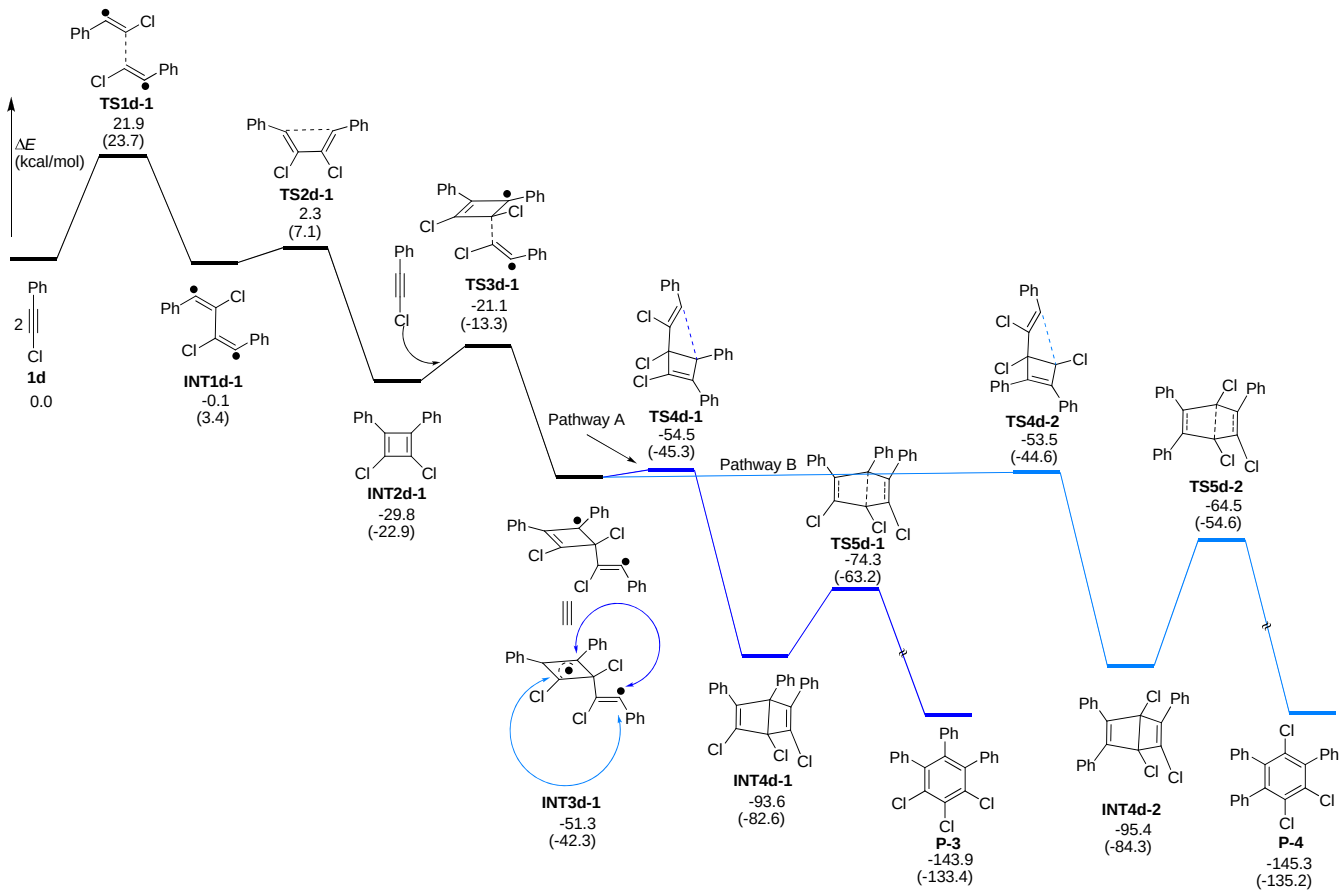


Figure S2. The computed potential energy surface at the (U)B3LYP/6-31G(d) level and the (U)B3LYP/6-311++G(d,p)//(U)B3LYP/6-31G(d) level (the energies given in parentheses). All computed energies are given with spin contamination corrections, but without zero-point energy corrections.

Basis Set Superposition Error (BSSE) Discussion

We evaluated the BSSE by computing the complex between two fluoroacetylenes at different distances, showing that the BSSE at the B3LYP/6-31G(d) level is about 1-2 kcal/mol, while this can be completely neglected at the B3LYP/6-311++G(d, p) level (Table S3).

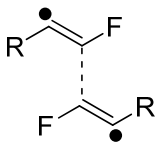
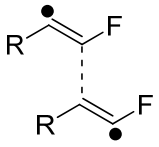
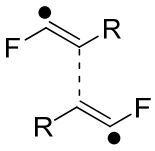
Table S3. BSSE at the (U)B3LYP/6-311++G(d,p)//(U)B3LYP/6-31G(d) Level

HC≡CF⋯⋯HC≡CF

Distance (Å)	BSSE (kcal/mol)	
	B3LYP/6-31G(d)	B3LYP/6-311++G(d,p)
1.3	1.9	0.7
1.4	1.7	0.6
1.5	1.6	0.6
1.6	1.5	0.5
1.7	1.3	0.5
1.8	1.2	0.4
1.9	1.15	0.4

5. Computational Results, Cartesian Coordinates, and Energies of All Discussed Species

Table S4. Energies[a] of **TS1a-1** to **TS1c-3** Before YJH Spin-projection Energy Corrections

Entry				
1	R = H	**TS1a-1**	**TS1a-2**	**TS1a-3**
	ΔE_0 (kcal/mol)	16.5	20.2	21.2
2	R = Me	**TS1b-1**	**TS1b-2**	**TS1b-3**
	ΔE_0 (kcal/mol)	14.3	22.1	26.7
3	R = ^{t}Bu	**TS1-1**	**TS1-2**	**TS1-3**
	ΔE_0 (kcal/mol)	12.9	25.0	31.8
4	R = Ph	**TS1c-1**	**TS1c-2**	**TS1c-3**
	ΔE_0 (kcal/mol)	8.4	20.5	28.7

[a] Computed at the (U)B3LYP/6-31G(d) level. The energies of the transition states are relative to the energies of the corresponding fluoroacetylenes.

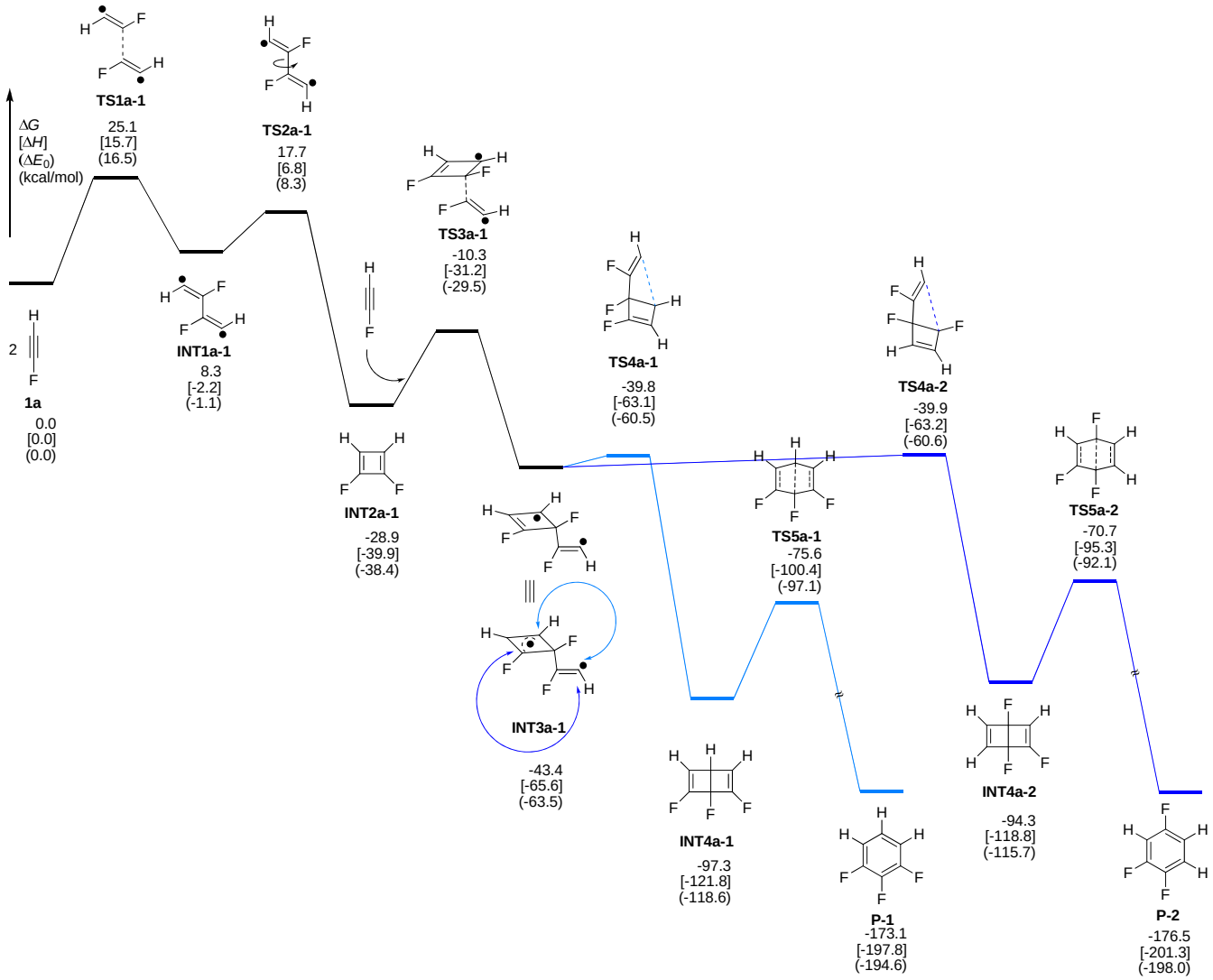


Figure S3. The (U)B3LYP/6-31G(d) computed energy surface of the favored pathways in the cyclotrimerization of fluoroacetylene before YJH spin-projection energy corrections.

Table S5. Energies[a] of **TS3a-1** to **TS3c-8** Before YJH Spin-projection Energy Corrections

entry									
1	R = H	**TS3a-1**	**TS3a-2**	**TS3a-3**	**TS3a-4**	**TS3a-5**	**TS3a-6**	**TS3a-7**	**TS3a-8**
	ΔE_0 (kcal/mol)	8.9	11.2	9.9	10.4	10.4	10.5	10.5	6.3
2	R = Me	**TS3b-1**	**TS3b-2**	**TS3b-3**	**TS3b-4**	**TS3b-5**	**TS3b-6**	**TS3b-7**	**TS3b-8**
	ΔE_0 (kcal/mol)	8.3	15.2	11.8	13.6	11.7	11.1	9.8	10.3
3	R = ^{t}Bu	**TS3-1**	**TS3-2**	**TS3-3**	**TS3-4**	**TS3-5**	**TS3-6**	**TS3-7**	**TS3-8**
	ΔE_0 (kcal/mol)	7.5	26.1	18.7	17.8	17.5	13.7	10.2	19.2
4	R = Ph	**TS3c-1**	**TS3c-2**	**TS3c-3**	**TS3c-4**	**TS3c-5**	**TS3dc-6**	**TS3c-7**	**TS3c-8**
	ΔE_0 (kcal/mol)	3.9	15.1	8.3	11.2	8.5	8.7	5.8	9.8

[a] Computed at the (U)B3LYP/6-31G(d) level. The energies of the transition states are relative to the energies of the corresponding difluorocyclobutadienes and fluoroacetylenes.

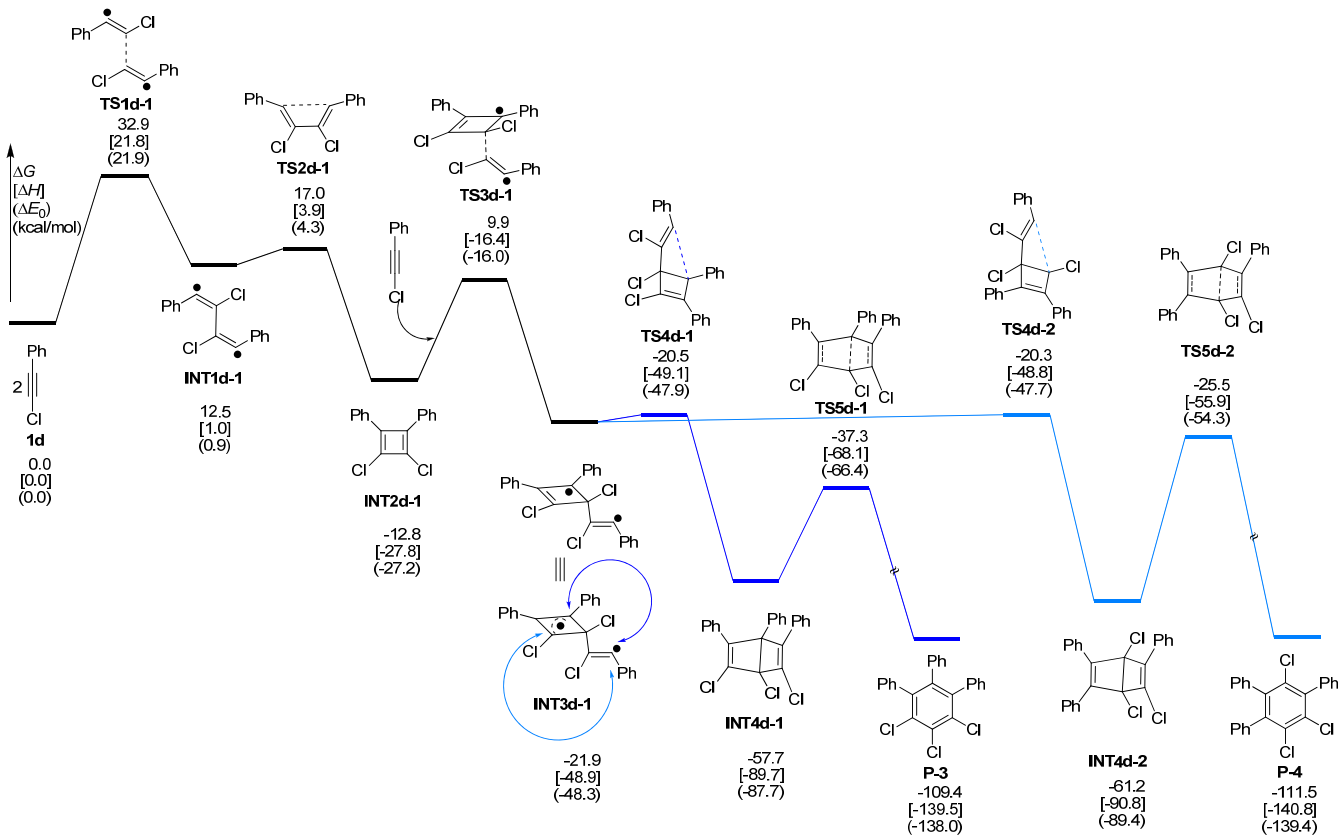
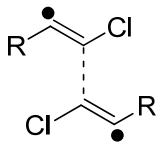
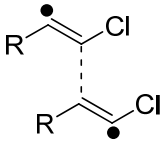
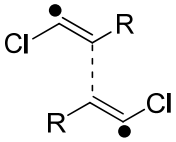


Figure S4. The (U)B3LYP/6-31G(d) computed energy surface of the favored pathway for the cyclotrimerization of phenylchloroacetylene before YJH spin-projection energy corrections.

Table S6. Energies[a] of **TS1d-1** to **TS1h-3** Before YJH Spin-projection Energy Corrections

Entry				
1	R = Ph	**TS1d-1**	**TS1d-2**	**TS1d-3**
	ΔE_0 (kcal/mol)	21.9	27.9	32.5
2	R = C_6Cl_5	**TS1e-1**	**TS1e-2**	**TS1e-3**
	ΔE_0 (kcal/mol)	22.1	30.1	39.5
3	R = Me	**TS1f-1**	**TS1f-2**	**TS1f-3**
	ΔE_0 (kcal/mol)	30.0	30.3	30.5
4	R = ^{t}Bu	**TS1g-1**	**TS1g-2**	**TS1g-3**
	ΔE_0 (kcal/mol)	31.2	33.3	38.1
5	R = Cy	**TS1h-1**	**TS1h-2**	**TS1h-3**
	ΔE_0 (kcal/mol)	30.0	30.4	30.5

[a] Computed at the (U)B3LYP/6-31G(d) level. The energies of the transition states are relative to the energies of the corresponding chloroacetylenes.

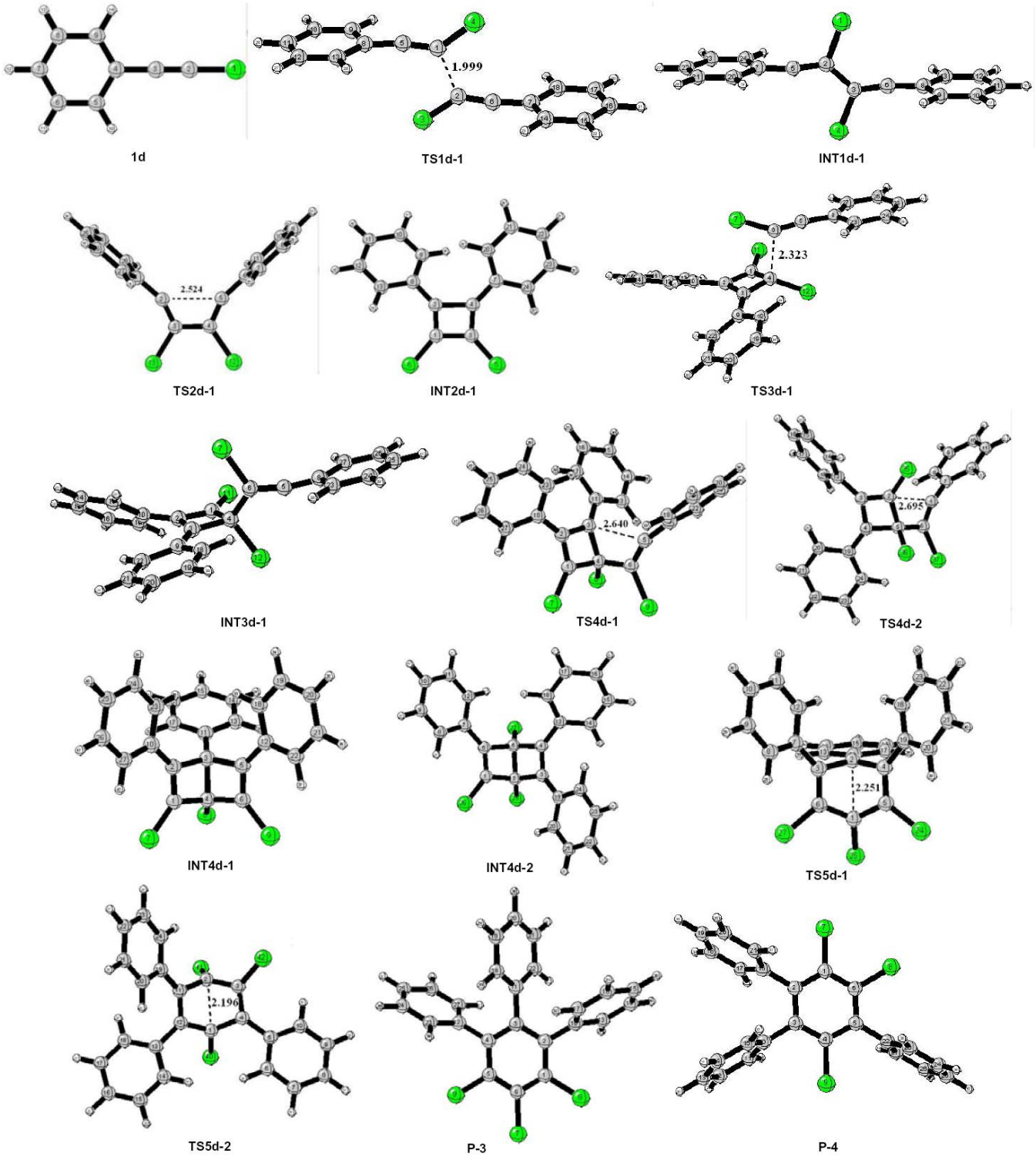
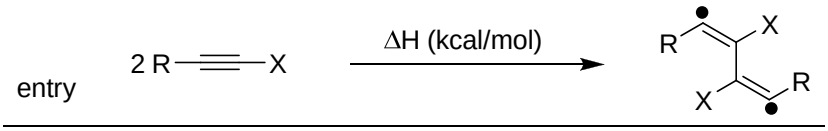


Figure S5. The (U)B3LYP/6-31G(d) computed geometries of the reactants, intermediates, transition states, and products in the cyclotrimerization of phenylchloroacetylene.

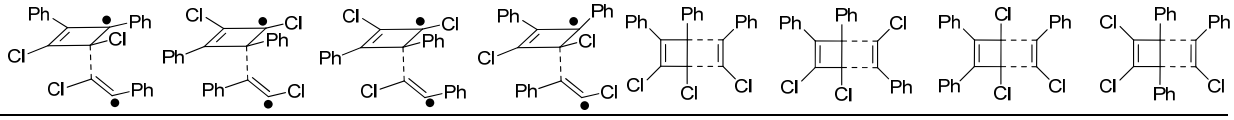
Table S7. Enthalpies[a] of the Dimerizations of **1b**, **1c**, **1d**, and **1f**



entry			
1	X=F, R=Me, **1b**	-8.7	**INT1b-1**
2	X=F, R=Ph, **1c**	-18.5	**INT1c-1**
3	X=Cl, R=Me, **1f**	10.8	**INT1f-1**
4	X=Cl, R=Ph, **1d**	0.0	**INT1d-1**

[a] Computed at the (U)B3LYP/6-31G(d) level. Enthalpies are given after YJH spin-projection energy corrections.

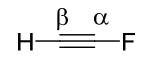
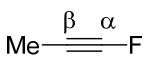
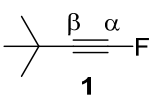
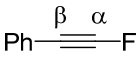
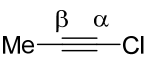
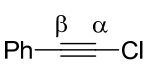
Table S8. Activation energies[a] of **TS3d-1** to **TS3d-8** Before/After YJH Spin-projection Energy Corrections



	TS3d-1	TS3d-2	TS3d-3	TS3d-4	TS3d-5	TS3d-6	TS3d-7	TS3d-8
Before correction:	11.2	22.8	13.7	17.4	13.7	14.9	15.2	14.9
After correction:	7.4	19.8	10.7	14.3	—	—	—	—

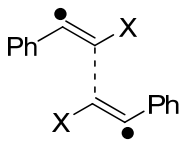
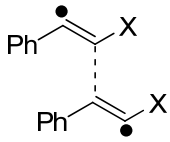
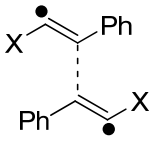
[a] Computed at the (U)B3LYP/6-31G(d) level. The activation energies of the transition states are relative to the energies of the corresponding dichlorocyclobutadienes and chloroacetylenes.

Table S9. Singlet-Triplet Energy Gaps[a] with the Ground State Closed-Shell Geometries

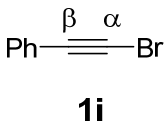
Compound	 **1a**	 **1b**	 **1**	 **1c**	 **1f**	 **1d**
$Gap_{triplet/singlet}$ (eV)	7.0	6.2	6.2	3.8	5.7	3.6

[a] Computed at the (U)B3LYP/6-31G(d) level.

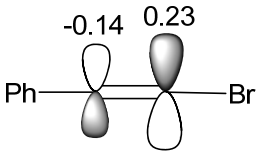
Table S10. Comparison of Barriers[a] of the Dimerizations of Fluoro-, Chloro-, and Bromo-phenylacetylenes Before YJH Spin-projection Energy Corrections

Entry				
1	X = F	**TS1c-1**	**TS1c-2**	**TS1c-3**
	ΔE_0 (kcal/mol)	8.4	20.5	28.7
2	X = Cl	**TS1d-1**	**TS1d-2**	**TS1d-3**
	ΔE_0 (kcal/mol)	21.9	27.9	32.5
3[b]	X = Br	**TS1i-1**	**TS1i-2**	**TS1i-3**
	ΔE_0 (kcal/mol)	21.8	26.9	32.8

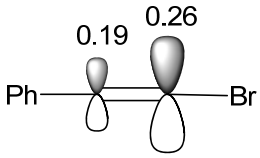
[a] Computed at the (U)B3LYP/6-31G(d) level. The energies of the transition states are relative to the energies of the corresponding haloacetylenes. [b] The molecular orbitals and energies of bromo-phenylacetylene are shown here:



1i



LUMO (2.7 eV)



HOMO (-8.5 eV)

Geometries and Associated Energies

All geometries and energies were calculated with the (U)B3LYP functional with the 6-31G(d) basis set using Gaussian 03 program.

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-0.095623
2	6	0	0.000000	0.000000	-1.296070
3	9	0	0.000000	0.000000	1.190061
4	1	0	0.000000	0.000000	-2.360386

Zero-point vibrational energy 53374.2 (Joules/Mol)
12.75675 (Kcal/Mol)
Zero-point correction= 0.020329 (Hartree/Particle)
Thermal correction to Energy= 0.023692
Thermal correction to Enthalpy= 0.024636
Thermal correction to Gibbs Free Energy= -0.001567
Sum of electronic and zero-point Energies= -176.515936
Sum of electronic and thermal Energies= -176.512573
Sum of electronic and thermal Enthalpies= -176.511629
Sum of electronic and thermal Free Energies= -176.537832

TS1a-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.040744	-0.946284	0.000000
2	6	0	0.040743	0.946283	0.000000
3	6	0	-1.209611	-1.369479	0.000000
4	6	0	1.209612	1.369473	0.000000
5	1	0	2.273198	1.267388	0.000000
6	9	0	1.209612	-1.347403	0.000000
7	9	0	-1.209611	1.347409	0.000000
8	1	0	-2.273199	-1.267399	0.000000

Zero-point vibrational energy 105673.1 (Joules/Mol)
25.25648 (Kcal/Mol)
Zero-point correction= 0.040249 (Hartree/Particle)
Thermal correction to Energy= 0.046654
Thermal correction to Enthalpy= 0.047598

Thermal correction to Gibbs Free Energy= 0.010147
Sum of electronic and zero-point Energies= -353.005576
Sum of electronic and thermal Energies= -352.999171
Sum of electronic and thermal Enthalpies= -352.998226
Sum of electronic and thermal Free Energies= -353.035677

INT1a-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.168208	1.414761	0.000000
2	6	0	-0.044962	0.738877	0.000000
3	6	0	0.044962	-0.738877	0.000000
4	6	0	1.168208	-1.414761	0.000000
5	9	0	1.168208	1.334082	0.000000
6	9	0	-1.168208	-1.334082	0.000000
7	1	0	-2.229220	1.233557	0.000000
8	1	0	2.229220	-1.233557	0.000000

Zero-point vibrational energy 112082.8 (Joules/Mol)
26.78843 (Kcal/Mol)
Zero-point correction= 0.042690 (Hartree/Particle)
Thermal correction to Energy= 0.048627
Thermal correction to Enthalpy= 0.049571
Thermal correction to Gibbs Free Energy= 0.013897
Sum of electronic and zero-point Energies= -353.033604
Sum of electronic and thermal Energies= -353.027667
Sum of electronic and thermal Enthalpies= -353.026723
Sum of electronic and thermal Free Energies= -353.062397

TS1a-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.230345	0.922637	0.000000
2	9	0	-2.199670	0.073072	0.000000
3	6	0	0.000000	1.177029	0.000000
4	6	0	1.142631	-0.391224	0.000000
5	9	0	0.251482	-1.359551	0.000000
6	6	0	2.374603	-0.201122	0.000000
7	1	0	0.607624	2.060577	0.000000
8	1	0	3.204735	0.473814	0.000000

Zero-point vibrational energy 106726.0 (Joules/Mol)
25.50813 (Kcal/Mol)
Zero-point correction= 0.040650 (Hartree/Particle)
Thermal correction to Energy= 0.047163
Thermal correction to Enthalpy= 0.048107
Thermal correction to Gibbs Free Energy= 0.009730
Sum of electronic and zero-point Energies= -352.999648
Sum of electronic and thermal Energies= -352.993135
Sum of electronic and thermal Enthalpies= -352.992190
Sum of electronic and thermal Free Energies= -353.030568

INT1a-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.014146	-0.094428	0.000000
2	6	0	-0.730175	-1.394183	0.000000
3	6	0	-0.257485	2.265506	0.000000
4	6	0	0.000000	0.973740	0.000000
5	9	0	0.413794	-2.028802	0.000000
6	9	0	1.273511	0.515856	0.000000
7	1	0	-2.056886	0.198708	0.000000
8	1	0	-1.118030	2.913993	0.000000

Zero-point vibrational energy 115811.3 (Joules/Mol)
27.67956 (Kcal/Mol)
Zero-point correction= 0.044110 (Hartree/Particle)
Thermal correction to Energy= 0.050005
Thermal correction to Enthalpy= 0.050949
Thermal correction to Gibbs Free Energy= 0.014356
Sum of electronic and zero-point Energies= -353.034246
Sum of electronic and thermal Energies= -353.028351
Sum of electronic and thermal Enthalpies= -353.027407
Sum of electronic and thermal Free Energies= -353.064000

TS1a-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.404907	1.867250	0.000000
2	9	0	1.650671	2.233290	0.000000
3	6	0	-0.404907	0.912424	0.000000
4	6	0	0.404907	-0.912424	0.000000

5	6	0	-0.404907	-1.867250	0.000000
6	9	0	-1.650671	-2.233290	0.000000
7	1	0	-1.465743	0.749980	0.000000
8	1	0	1.465743	-0.749980	0.000000

Zero-point vibrational energy 107113.9 (Joules/Mol)
25.60084 (Kcal/Mol)
Zero-point correction= 0.040798 (Hartree/Particle)
Thermal correction to Energy= 0.047550
Thermal correction to Enthalpy= 0.048494
Thermal correction to Gibbs Free Energy= 0.009357
Sum of electronic and zero-point Energies= -352.998154
Sum of electronic and thermal Energies= -352.991402
Sum of electronic and thermal Enthalpies= -352.990457
Sum of electronic and thermal Free Energies= -353.029595

INT1a-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.381480	0.630073	0.000117
2	6	0	1.708413	0.659623	0.000003
3	6	0	-1.708409	-0.659623	-0.000008
4	6	0	-0.381476	-0.630059	0.000097
5	9	0	2.561907	-0.344888	-0.000075
6	9	0	-2.561914	0.344876	-0.000068
7	1	0	-0.160310	1.569216	-0.000030
8	1	0	0.160321	-1.569199	0.000063

Zero-point vibrational energy 119327.3 (Joules/Mol)
28.51990 (Kcal/Mol)
Zero-point correction= 0.045449 (Hartree/Particle)
Thermal correction to Energy= 0.051352
Thermal correction to Enthalpy= 0.052296
Thermal correction to Gibbs Free Energy= 0.015400
Sum of electronic and zero-point Energies= -353.038144
Sum of electronic and thermal Energies= -353.032241
Sum of electronic and thermal Enthalpies= -353.031297
Sum of electronic and thermal Free Energies= -353.068193

TS1a-1EZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	1	0	1.874607	-2.166356	0.000009
2	6	0	1.320293	-1.254134	0.000004
3	6	0	0.721183	-0.104271	0.000000
4	9	0	1.375314	1.092917	-0.000003
5	6	0	-0.747993	0.082746	0.000000
6	9	0	-1.422260	-1.087584	0.000003
7	6	0	-1.352966	1.246716	-0.000004
8	1	0	-1.095198	2.292017	-0.000008

Zero-point vibrational energy 107676.5 (Joules/Mol)
25.73531 (Kcal/Mol)
Zero-point correction= 0.041012 (Hartree/Particle)
Thermal correction to Energy= 0.046892
Thermal correction to Enthalpy= 0.047836
Thermal correction to Gibbs Free Energy= 0.011558
Sum of electronic and zero-point Energies= -353.030157
Sum of electronic and thermal Energies= -353.024277
Sum of electronic and thermal Enthalpies= -353.023333
Sum of electronic and thermal Free Energies= -353.059611

INT1a-1EZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.011004	-1.544567	0.000000
2	6	0	-0.041658	-0.756165	0.000000
3	9	0	-1.301063	-1.245777	0.000000
4	6	0	0.000000	0.714577	0.000000
5	6	0	-1.051274	1.495318	0.000000
6	9	0	1.276888	1.189258	0.000000
7	1	0	2.084805	-1.467294	0.000000
8	1	0	-1.375661	2.520990	0.000000

Zero-point vibrational energy 111505.6 (Joules/Mol)
26.65048 (Kcal/Mol)
Zero-point correction= 0.042470 (Hartree/Particle)
Thermal correction to Energy= 0.048490
Thermal correction to Enthalpy= 0.049434
Thermal correction to Gibbs Free Energy= 0.012951
Sum of electronic and zero-point Energies= -353.030766
Sum of electronic and thermal Energies= -353.024747
Sum of electronic and thermal Enthalpies= -353.023803
Sum of electronic and thermal Free Energies= -353.060285

TS1a-1ZZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.426941	1.150503	-0.000377
2	1	0	1.989834	2.057142	0.001221
3	6	0	0.744794	0.042377	0.000057
4	9	0	1.334556	-1.186558	0.000061
5	6	0	-0.724768	-0.057716	-0.000007
6	9	0	-1.321292	1.164866	0.000045
7	6	0	-1.399492	-1.180323	-0.000036
8	1	0	-2.394056	-1.590962	0.000000

Zero-point vibrational energy 107145.4 (Joules/Mol)
25.60838 (Kcal/Mol)
Zero-point correction= 0.040810 (Hartree/Particle)
Thermal correction to Energy= 0.046770
Thermal correction to Enthalpy= 0.047714
Thermal correction to Gibbs Free Energy= 0.011290
Sum of electronic and zero-point Energies= -353.027652
Sum of electronic and thermal Energies= -353.021692
Sum of electronic and thermal Enthalpies= -353.020748
Sum of electronic and thermal Free Energies= -353.057171

INT1a-1ZZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.405080	1.184626	-0.000009
2	6	0	0.729852	0.056599	-0.000074
3	6	0	-0.729850	-0.056600	-0.000080
4	6	0	-1.405079	-1.184627	-0.000008
5	9	0	1.345713	-1.155952	0.000049
6	9	0	-1.345714	1.155952	0.000050
7	1	0	2.414673	1.559384	0.000069
8	1	0	-2.414677	-1.559374	0.000073

Zero-point vibrational energy 111862.4 (Joules/Mol)
26.73575 (Kcal/Mol)
Zero-point correction= 0.042606 (Hartree/Particle)
Thermal correction to Energy= 0.048612
Thermal correction to Enthalpy= 0.049556

Thermal correction to Gibbs Free Energy= 0.013095
Sum of electronic and zero-point Energies= -353.029697
Sum of electronic and thermal Energies= -353.023691
Sum of electronic and thermal Enthalpies= -353.022747
Sum of electronic and thermal Free Energies= -353.059208

TS2a-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.458048	0.882202	0.790616
2	6	0	-1.458135	-0.882155	0.790608
3	6	0	-0.741968	-0.024995	0.108046
4	6	0	0.741966	0.024957	0.108070
5	9	0	1.315679	-0.909523	-0.706381
6	9	0	-1.315605	0.909494	-0.706455
7	1	0	-2.477257	-1.186851	0.965753
8	1	0	2.477127	1.187058	0.965730

Zero-point vibrational energy 110790.5 (Joules/Mol)
26.47957 (Kcal/Mol)
Zero-point correction= 0.042198 (Hartree/Particle)
Thermal correction to Energy= 0.047569
Thermal correction to Enthalpy= 0.048513
Thermal correction to Gibbs Free Energy= 0.013395
Sum of electronic and zero-point Energies= -353.018682
Sum of electronic and thermal Energies= -353.013312
Sum of electronic and thermal Enthalpies= -353.012367
Sum of electronic and thermal Free Energies= -353.047486

INT2a-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.269423	0.802242	0.000000
2	6	0	-0.056662	0.782104	0.000000
3	6	0	-0.056662	-0.782104	0.000000
4	6	0	1.269423	-0.802242	0.000000
5	9	0	-1.036677	1.670051	0.000000
6	9	0	-1.036677	-1.670051	0.000000
7	1	0	2.053529	1.543773	0.000000
8	1	0	2.053529	-1.543773	0.000000

Zero-point vibrational energy 121611.4 (Joules/Mol)
29.06583 (Kcal/Mol)
Zero-point correction= 0.046319 (Hartree/Particle)
Thermal correction to Energy= 0.051632
Thermal correction to Enthalpy= 0.052577
Thermal correction to Gibbs Free Energy= 0.017560
Sum of electronic and zero-point Energies= -353.093028
Sum of electronic and thermal Energies= -353.087715
Sum of electronic and thermal Enthalpies= -353.086771
Sum of electronic and thermal Free Energies= -353.121788

TS3a-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.625139	-0.496591	-0.017589
2	6	0	-0.244174	0.751753	-0.279156
3	6	0	-1.278953	-0.084037	0.465381
4	6	0	-1.773220	-0.565413	-0.713993
5	6	0	-0.859817	0.339409	-1.473897
6	6	0	2.521675	0.174601	0.493231
7	1	0	2.968378	1.062006	0.883955
8	9	0	1.175043	-1.630248	-0.477309
9	9	0	0.238820	1.954190	0.048855
10	9	0	-1.376555	-0.444564	1.735113
11	1	0	-2.410300	-1.392882	-0.994754
12	1	0	-0.837752	0.698147	-2.492989

Zero-point vibrational energy 169414.9 (Joules/Mol)
40.49114 (Kcal/Mol)
Zero-point correction= 0.064527 (Hartree/Particle)
Thermal correction to Energy= 0.073892
Thermal correction to Enthalpy= 0.074836
Thermal correction to Gibbs Free Energy= 0.029539
Sum of electronic and zero-point Energies= -529.594812
Sum of electronic and thermal Energies= -529.585447
Sum of electronic and thermal Enthalpies= -529.584502
Sum of electronic and thermal Free Energies= -529.629799

INT3a-1E

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.230086	-0.123169	-0.391754
2	6	0	1.806004	0.088565	0.856937
3	6	0	0.691097	0.803042	1.319176
4	6	0	-0.083401	0.541377	0.021613
5	6	0	-1.291006	-0.362591	0.120674
6	6	0	-2.483386	-0.109377	-0.358102
7	9	0	-1.005128	-1.513120	0.777124
8	1	0	-2.980057	0.676398	-0.901049
9	9	0	-0.450507	1.665647	-0.696166
10	1	0	0.460270	1.394350	2.193368
11	1	0	2.746506	-0.206917	1.307034
12	9	0	1.517515	-0.918184	-1.415470

Zero-point vibrational energy 180521.2 (Joules/Mol)
43.14560 (Kcal/Mol)
Zero-point correction= 0.068757 (Hartree/Particle)
Thermal correction to Energy= 0.077279
Thermal correction to Enthalpy= 0.078223
Thermal correction to Gibbs Free Energy= 0.035160
Sum of electronic and zero-point Energies= -529.649899
Sum of electronic and thermal Energies= -529.641377
Sum of electronic and thermal Enthalpies= -529.640433
Sum of electronic and thermal Free Energies= -529.683496

TS3a-1EZ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.475346	-0.063481	-0.353849
2	6	0	-1.298405	-0.315756	0.127235
3	9	0	-1.015709	-1.449398	0.840589
4	1	0	-3.444315	0.143676	-0.749594
5	6	0	-0.068531	0.553512	-0.009545
6	9	0	-0.403532	1.649970	-0.780385
7	6	0	1.231261	-0.160211	-0.383762
8	6	0	1.808886	0.099017	0.854651
9	6	0	0.708335	0.858878	1.277445
10	1	0	0.488762	1.497902	2.120446
11	1	0	2.741262	-0.195277	1.322100
12	9	0	1.505585	-1.009245	-1.367537

Zero-point vibrational energy 175986.0 (Joules/Mol)
42.06167 (Kcal/Mol)
Zero-point correction= 0.067030 (Hartree/Particle)

Thermal correction to Energy=	0.075502
Thermal correction to Enthalpy=	0.076446
Thermal correction to Gibbs Free Energy=	0.033404
Sum of electronic and zero-point Energies=	-529.646425
Sum of electronic and thermal Energies=	-529.637953
Sum of electronic and thermal Enthalpies=	-529.637009
Sum of electronic and thermal Free Energies=	-529.680051

INT3a-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.302280	-0.259192	0.114389
2	6	0	-0.049093	0.560728	-0.033759
3	6	0	1.233960	-0.206136	-0.362274
4	6	0	1.803552	0.082647	0.872680
5	6	0	0.721199	0.888864	1.253366
6	6	0	-2.472181	0.020735	-0.402265
7	1	0	-3.475854	-0.367405	-0.455640
8	9	0	-1.089333	-1.376381	0.868537
9	9	0	-0.337503	1.638337	-0.848524
10	1	0	0.510608	1.565128	2.069168
11	1	0	2.722280	-0.219192	1.361857
12	9	0	1.497061	-1.095779	-1.312037

Zero-point vibrational energy	180432.2 (Joules/Mol)
	43.12432 (Kcal/Mol)
Zero-point correction=	0.068723 (Hartree/Particle)
Thermal correction to Energy=	0.077285
Thermal correction to Enthalpy=	0.078229
Thermal correction to Gibbs Free Energy=	0.035075
Sum of electronic and zero-point Energies=	-529.648941
Sum of electronic and thermal Energies=	-529.640379
Sum of electronic and thermal Enthalpies=	-529.639435
Sum of electronic and thermal Free Energies=	-529.682589

TS3a-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.590593	-0.597708	-0.708563
2	6	0	0.017189	0.055663	0.756920
3	6	0	-0.921811	-1.198334	0.721459

4	6	0	-1.858782	-0.456169	0.081654
5	6	0	-0.996670	0.755397	0.123702
6	6	0	2.789048	-0.359486	-0.491607
7	1	0	0.926315	-1.116366	-1.372007
8	9	0	3.738490	0.203004	0.190541
9	1	0	0.707547	0.370056	1.527554
10	1	0	-0.759539	-2.244167	0.934118
11	9	0	-1.224468	2.033939	-0.136799
12	9	0	-3.024214	-0.704243	-0.497192

Zero-point vibrational energy 170530.1 (Joules/Mol)
40.75767 (Kcal/Mol)
Zero-point correction= 0.064951 (Hartree/Particle)
Thermal correction to Energy= 0.074420
Thermal correction to Enthalpy= 0.075364
Thermal correction to Gibbs Free Energy= 0.028480
Sum of electronic and zero-point Energies= -529.591189
Sum of electronic and thermal Energies= -529.581721
Sum of electronic and thermal Enthalpies= -529.580777
Sum of electronic and thermal Free Energies= -529.627661

TS3a-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.019241	-0.132806	0.277550
2	6	0	-0.242765	0.306516	-1.020422
3	6	0	0.769085	0.790493	-0.201946
4	6	0	1.444875	-0.531671	-0.185513
5	6	0	0.508449	-1.064158	-1.011280
6	6	0	-3.116249	-0.102849	-0.288642
7	9	0	-1.348929	-0.366352	1.375403
8	1	0	-3.763288	0.068621	-1.121081
9	1	0	-0.764146	0.788450	-1.835849
10	1	0	0.225633	-2.056259	-1.330265
11	9	0	2.466354	-1.004498	0.510924
12	9	0	1.131116	1.993743	0.210198

Zero-point vibrational energy 170238.5 (Joules/Mol)
40.68797 (Kcal/Mol)
Zero-point correction= 0.064840 (Hartree/Particle)
Thermal correction to Energy= 0.074192
Thermal correction to Enthalpy= 0.075137
Thermal correction to Gibbs Free Energy= 0.029181

Sum of electronic and zero-point Energies= -529.593201
Sum of electronic and thermal Energies= -529.583849
Sum of electronic and thermal Enthalpies= -529.582905
Sum of electronic and thermal Free Energies= -529.628860

TS3a-4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.077213	0.236728	1.145145
2	6	0	0.458675	-0.589059	-0.265032
3	6	0	1.369282	-1.414907	0.428642
4	6	0	2.313938	-0.275157	0.580319
5	6	0	1.509562	0.508142	-0.205910
6	6	0	-2.215479	0.314203	0.670152
7	9	0	-3.142459	0.152663	-0.212697
8	1	0	-0.464707	0.452858	1.997337
9	9	0	-0.355256	-0.903223	-1.280873
10	1	0	1.445272	-2.480317	0.590462
11	1	0	3.178653	-0.095917	1.204928
12	9	0	1.463070	1.799857	-0.496720

Zero-point vibrational energy 169779.8 (Joules/Mol)
40.57835 (Kcal/Mol)
Zero-point correction= 0.064666 (Hartree/Particle)
Thermal correction to Energy= 0.074113
Thermal correction to Enthalpy= 0.075058
Thermal correction to Gibbs Free Energy= 0.028909
Sum of electronic and zero-point Energies= -529.592350
Sum of electronic and thermal Energies= -529.582902
Sum of electronic and thermal Enthalpies= -529.581958
Sum of electronic and thermal Free Energies= -529.628106

TS3a-5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.891292	1.295847	-0.492031
2	6	0	-0.528452	1.411955	0.742023
3	6	0	-1.430507	1.347556	-0.251444
4	6	0	-1.303261	-0.152508	-0.295029
5	6	0	-0.313937	-0.153336	0.636033
6	6	0	1.655031	0.098079	-0.418899

7	9	0	-1.968929	-1.081199	-0.962007
8	9	0	0.049232	-1.045313	1.563920
9	9	0	1.937301	-1.171016	-0.539258
10	1	0	-1.931738	2.068705	-0.883227
11	1	0	-0.066801	2.173156	1.352444
12	1	0	2.019110	2.350321	-0.557025

Zero-point vibrational energy 175669.8 (Joules/Mol)
41.98608 (Kcal/Mol)
Zero-point correction= 0.066909 (Hartree/Particle)
Thermal correction to Energy= 0.075988
Thermal correction to Enthalpy= 0.076932
Thermal correction to Gibbs Free Energy= 0.032548
Sum of electronic and zero-point Energies= -529.592431
Sum of electronic and thermal Energies= -529.583352
Sum of electronic and thermal Enthalpies= -529.582408
Sum of electronic and thermal Free Energies= -529.626793

TS3a-6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.355057	1.099894	1.053523
2	6	0	-0.826574	0.545408	-0.430894
3	6	0	-1.411761	-0.528555	0.123467
4	6	0	-0.371559	-1.451686	-0.459312
5	6	0	0.286899	-0.410648	-1.032035
6	6	0	1.852294	0.195192	0.395279
7	9	0	2.829662	-0.595437	0.031859
8	1	0	0.940809	-0.316239	-1.888114
9	1	0	0.827133	1.877096	1.554907
10	9	0	-1.135675	1.818611	-0.629350
11	9	0	-2.458775	-0.750300	0.909314
12	1	0	-0.190986	-2.514353	-0.373372

Zero-point vibrational energy 175948.1 (Joules/Mol)
42.05260 (Kcal/Mol)
Zero-point correction= 0.067015 (Hartree/Particle)
Thermal correction to Energy= 0.076089
Thermal correction to Enthalpy= 0.077034
Thermal correction to Gibbs Free Energy= 0.032483
Sum of electronic and zero-point Energies= -529.592239
Sum of electronic and thermal Energies= -529.583164
Sum of electronic and thermal Enthalpies= -529.582220

Sum of electronic and thermal Free Energies= -529.626771

TS3a-7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.769156	1.859759	0.323689
2	6	0	-1.348719	0.780690	0.216231
3	9	0	-2.458141	0.083238	0.155248
4	6	0	0.050146	-0.770169	-0.207187
5	9	0	-0.531522	-1.298894	-1.286925
6	6	0	1.339629	0.119036	-0.085844
7	9	0	1.949038	0.945044	-0.914053
8	6	0	1.561230	-0.363823	1.147119
9	6	0	0.378741	-1.300619	1.006850
10	1	0	2.213736	-0.110676	1.970511
11	1	0	-0.032335	-2.077279	1.635719
12	1	0	-0.087002	2.674216	0.400187

Zero-point vibrational energy 175559.4 (Joules/Mol)
41.95971 (Kcal/Mol)
Zero-point correction= 0.066867 (Hartree/Particle)
Thermal correction to Energy= 0.075910
Thermal correction to Enthalpy= 0.076854
Thermal correction to Gibbs Free Energy= 0.032680
Sum of electronic and zero-point Energies= -529.592179
Sum of electronic and thermal Energies= -529.583136
Sum of electronic and thermal Enthalpies= -529.582192
Sum of electronic and thermal Free Energies= -529.626366

TS3a-8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.699206	-1.543635	-0.492858
2	6	0	0.577217	-1.048559	0.905989
3	6	0	1.453449	-0.470863	0.076105
4	6	0	0.759475	0.855175	0.187349
5	6	0	-0.194791	0.351774	1.001370
6	6	0	-1.922834	-0.367483	-0.246523
7	9	0	2.490359	-0.870012	-0.645981
8	9	0	1.028786	2.041494	-0.328808
9	9	0	-2.632016	0.730616	-0.253764

10	1	0	-0.816668	0.778066	1.775676
11	1	0	0.433046	-2.000171	1.391022
12	1	0	-1.440405	-2.555222	-0.698303

Zero-point vibrational energy 176218.7 (Joules/Mol)
42.11727 (Kcal/Mol)
Zero-point correction= 0.067118 (Hartree/Particle)
Thermal correction to Energy= 0.076128
Thermal correction to Enthalpy= 0.077072
Thermal correction to Gibbs Free Energy= 0.032572
Sum of electronic and zero-point Energies= -529.598891
Sum of electronic and thermal Energies= -529.589881
Sum of electronic and thermal Enthalpies= -529.588937
Sum of electronic and thermal Free Energies= -529.633437

TS4a-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.495981	-0.320065	-0.300308
2	6	0	0.556195	-1.462273	-0.753901
3	6	0	1.687420	-0.648575	-0.919732
4	6	0	1.255800	0.254279	0.044764
5	6	0	-0.057750	-0.486121	0.262296
6	6	0	-1.316612	0.231640	-0.170432
7	9	0	-1.115931	1.561362	-0.418955
8	9	0	-0.249751	-1.013251	1.531027
9	9	0	1.696063	1.426770	0.476352
10	1	0	2.553837	-0.691681	-1.569447
11	1	0	0.214819	-2.408207	-1.146722
12	1	0	-3.516511	-0.087348	-0.555778

Zero-point vibrational energy 179171.5 (Joules/Mol)
42.82301 (Kcal/Mol)
Zero-point correction= 0.068243 (Hartree/Particle)
Thermal correction to Energy= 0.076132
Thermal correction to Enthalpy= 0.077076
Thermal correction to Gibbs Free Energy= 0.035630
Sum of electronic and zero-point Energies= -529.644277
Sum of electronic and thermal Energies= -529.636388
Sum of electronic and thermal Enthalpies= -529.635444
Sum of electronic and thermal Free Energies= -529.676890

INT4a-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.320457	1.279090	-0.220815
2	6	0	-1.308264	-0.056365	-0.261062
3	6	0	0.000000	-0.246333	0.478791
4	6	0	0.000000	1.325802	0.564945
5	6	0	1.308264	-0.056365	-0.261062
6	6	0	1.320456	1.279090	-0.220816
7	9	0	-2.090810	-0.970609	-0.827657
8	9	0	0.000000	-1.059684	1.577822
9	9	0	2.090810	-0.970608	-0.827657
10	1	0	-1.938552	2.044730	-0.672236
11	1	0	0.000000	1.769136	1.562019
12	1	0	1.938552	2.044730	-0.672237

Zero-point vibrational energy 196163.7 (Joules/Mol)
46.88425 (Kcal/Mol)
Zero-point correction= 0.074715 (Hartree/Particle)
Thermal correction to Energy= 0.081706
Thermal correction to Enthalpy= 0.082651
Thermal correction to Gibbs Free Energy= 0.043042
Sum of electronic and zero-point Energies= -529.736865
Sum of electronic and thermal Energies= -529.729873
Sum of electronic and thermal Enthalpies= -529.728929
Sum of electronic and thermal Free Energies= -529.768537

TS4a-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.280990	0.342692	-0.189594
2	6	0	1.859005	1.351142	-0.150955
3	6	0	1.300373	0.167867	-0.181751
4	6	0	-0.012759	-0.195339	0.475445
5	6	0	-0.622633	-1.543735	0.091564
6	6	0	-1.707225	-0.924021	-0.557637
7	1	0	-2.538899	-1.294011	-1.145844
8	9	0	-1.643530	1.576434	-0.514712
9	1	0	2.736230	1.883665	-0.479110
10	9	0	1.887241	-0.881788	-0.831428
11	9	0	0.079443	0.058683	1.836734
12	1	0	-0.320342	-2.561256	0.287178

Zero-point vibrational energy	179354.7 (Joules/Mol)				
	42.86680 (Kcal/Mol)				
Zero-point correction=			0.068313 (Hartree/Particle)		
Thermal correction to Energy=			0.076193		
Thermal correction to Enthalpy=			0.077137		
Thermal correction to Gibbs Free Energy=			0.035595		
Sum of electronic and zero-point Energies=			-529.644432		
Sum of electronic and thermal Energies=			-529.636552		
Sum of electronic and thermal Enthalpies=			-529.635607		
Sum of electronic and thermal Free Energies=			-529.677149		

INT4a-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.407308	-1.432798	-0.258166
2	6	0	0.834377	-0.577309	-0.033590
3	6	0	1.434243	0.225067	-1.195890
4	6	0	0.610391	1.270507	-1.030391
5	6	0	-0.119327	0.647858	0.161659
6	6	0	-1.213650	-0.377825	-0.076531
7	9	0	-0.155258	1.358826	1.328384
8	9	0	1.689789	-0.957612	0.966812
9	9	0	-2.523459	-0.206288	-0.216786
10	1	0	2.185339	-0.022789	-1.939585
11	1	0	0.441582	2.189340	-1.582782
12	1	0	-0.558915	-2.453891	-0.585875

Zero-point vibrational energy	194583.8 (Joules/Mol)				
	46.50664 (Kcal/Mol)				
Zero-point correction=			0.074113 (Hartree/Particle)		
Thermal correction to Energy=			0.081151		
Thermal correction to Enthalpy=			0.082095		
Thermal correction to Gibbs Free Energy=			0.042554		
Sum of electronic and zero-point Energies=			-529.732206		
Sum of electronic and thermal Energies=			-529.725168		
Sum of electronic and thermal Enthalpies=			-529.724224		
Sum of electronic and thermal Free Energies=			-529.763765		

TS5a-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.000001	-0.534854	0.230955
2	6	0	0.000001	1.571773	0.672245
3	6	0	1.257260	1.418893	-0.057613
4	6	0	1.281757	0.062026	-0.109375
5	6	0	-1.281758	0.062026	-0.109374
6	6	0	-1.257257	1.418895	-0.057614
7	1	0	-1.795963	2.125203	-0.679221
8	1	0	0.000001	1.221848	1.700947
9	1	0	1.795973	2.125202	-0.679213
10	9	0	2.273796	-0.735834	-0.547024
11	9	0	-0.000001	-1.802202	0.676507
12	9	0	-2.273798	-0.735831	-0.547023

Zero-point vibrational energy 190636.5 (Joules/Mol)
45.56322 (Kcal/Mol)
Zero-point correction= 0.072610 (Hartree/Particle)
Thermal correction to Energy= 0.079376
Thermal correction to Enthalpy= 0.080320
Thermal correction to Gibbs Free Energy= 0.041304
Sum of electronic and zero-point Energies= -529.702610
Sum of electronic and thermal Energies= -529.695843
Sum of electronic and thermal Enthalpies= -529.694899
Sum of electronic and thermal Free Energies= -529.733915

P-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.200145	0.014332	-0.000001
2	6	0	1.213915	-1.375479	-0.000001
3	6	0	0.000000	-2.064928	0.000003
4	6	0	-1.213915	-1.375479	-0.000001
5	6	0	-1.200145	0.014332	-0.000001
6	6	0	0.000000	0.722216	0.000001
7	9	0	0.000000	2.062118	0.000001
8	9	0	2.349033	0.709047	0.000000
9	9	0	-2.349033	0.709047	0.000000
10	1	0	2.168083	-1.890872	-0.000002
11	1	0	0.000000	-3.150129	0.000005
12	1	0	-2.168083	-1.890872	-0.000002

Zero-point vibrational energy 200067.4 (Joules/Mol)
47.81725 (Kcal/Mol)

Zero-point correction= 0.076202 (Hartree/Particle)
Thermal correction to Energy= 0.083078
Thermal correction to Enthalpy= 0.084022
Thermal correction to Gibbs Free Energy= 0.044774
Sum of electronic and zero-point Energies= -529.857979
Sum of electronic and thermal Energies= -529.851103
Sum of electronic and thermal Enthalpies= -529.850159
Sum of electronic and thermal Free Energies= -529.889406

TS5a-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.387304	0.744672	-0.038298
2	6	0	1.113758	-0.649070	0.063003
3	6	0	1.702068	0.336015	-0.865636
4	6	0	0.755482	1.301125	-0.771036
5	6	0	-0.945778	-0.577541	-0.217343
6	6	0	0.024102	-1.519802	-0.359769
7	1	0	0.042698	-2.421173	-0.964187
8	9	0	-2.278297	-0.752163	-0.228396
9	9	0	-1.086754	1.599203	0.747561
10	1	0	0.761531	2.318652	-1.162297
11	1	0	2.483924	0.193131	-1.605902
12	9	0	1.491483	-0.614041	1.354931

Zero-point vibrational energy 187947.8 (Joules/Mol)
44.92059 (Kcal/Mol)
Zero-point correction= 0.071586 (Hartree/Particle)
Thermal correction to Energy= 0.078550
Thermal correction to Enthalpy= 0.079494
Thermal correction to Gibbs Free Energy= 0.040113
Sum of electronic and zero-point Energies= -529.694618
Sum of electronic and thermal Energies= -529.687654
Sum of electronic and thermal Enthalpies= -529.686709
Sum of electronic and thermal Free Energies= -529.726091

P-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.116458	0.564749	0.000001
2	6	0	0.173162	1.583077	0.000002

3	6	0	-1.188446	1.271267	-0.000002
4	6	0	-1.567302	-0.065981	0.000002
5	6	0	-0.638237	-1.102673	0.000001
6	6	0	0.709492	-0.769718	-0.000003
7	9	0	2.431397	0.846639	0.000000
8	9	0	1.641150	-1.735847	0.000000
9	9	0	-2.877992	-0.377813	0.000000
10	1	0	0.514923	2.612625	0.000003
11	1	0	-1.946117	2.046504	-0.000005
12	1	0	-0.950568	-2.140259	0.000002

Zero-point vibrational energy 200035.3 (Joules/Mol)
47.80958 (Kcal/Mol)
Zero-point correction= 0.076189 (Hartree/Particle)
Thermal correction to Energy= 0.082999
Thermal correction to Enthalpy= 0.083943
Thermal correction to Gibbs Free Energy= 0.044777
Sum of electronic and zero-point Energies= -529.863363
Sum of electronic and thermal Energies= -529.856554
Sum of electronic and thermal Enthalpies= -529.855609
Sum of electronic and thermal Free Energies= -529.894776

1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.691734	-0.000030	0.000025
2	6	0	-0.510074	0.000013	0.000022
3	9	0	1.983887	0.000010	-0.000016
4	6	0	-1.973143	0.000001	-0.000012
5	1	0	-2.368737	-0.141055	1.012364
6	1	0	-2.368672	0.947288	-0.384059
7	1	0	-2.368679	-0.806229	-0.628374

Zero-point vibrational energy 129268.8 (Joules/Mol)
30.89599 (Kcal/Mol)
Zero-point correction= 0.049236 (Hartree/Particle)
Thermal correction to Energy= 0.053930
Thermal correction to Enthalpy= 0.054874
Thermal correction to Gibbs Free Energy= 0.023035
Sum of electronic and zero-point Energies= -215.812615
Sum of electronic and thermal Energies= -215.807921
Sum of electronic and thermal Enthalpies= -215.806976
Sum of electronic and thermal Free Energies= -215.838816

1b-triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.646330	0.436070	-0.033811
2	6	0	-0.454590	-0.402373	-0.047880
3	6	0	-1.859657	0.041210	0.013008
4	9	0	1.857964	-0.102430	0.025859
5	1	0	-2.533121	-0.685900	-0.453856
6	1	0	-2.165384	0.124227	1.068968
7	1	0	-2.015668	1.034100	-0.435744

Zero-point vibrational energy 119706.3 (Joules/Mol)
28.61048 (Kcal/Mol)
Zero-point correction= 0.045594 (Hartree/Particle)
Thermal correction to Energy= 0.050506
Thermal correction to Enthalpy= 0.051451
Thermal correction to Gibbs Free Energy= 0.017639
Sum of electronic and zero-point Energies= -215.706560
Sum of electronic and thermal Energies= -215.701647
Sum of electronic and thermal Enthalpies= -215.700703
Sum of electronic and thermal Free Energies= -215.734515

TS1b-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.529253	-0.804979	0.015348
2	6	0	0.529298	0.805170	0.015305
3	6	0	1.751440	0.595143	-0.005296
4	6	0	3.053771	-0.060234	-0.037368
5	9	0	-0.371691	1.771728	0.034813
6	6	0	-1.751418	-0.595102	-0.005014
7	6	0	-3.053959	0.059832	-0.037446
8	1	0	-3.012697	1.002505	-0.597728
9	1	0	-3.801956	-0.579136	-0.525697
10	1	0	-3.416667	0.281636	0.973461
11	9	0	0.371844	-1.771450	0.034756
12	1	0	3.802823	0.579694	-0.522746
13	1	0	3.414783	-0.284746	0.973553
14	1	0	3.013059	-1.001440	-0.600141

Zero-point vibrational energy 257554.2 (Joules/Mol)
61.55694 (Kcal/Mol)
Zero-point correction= 0.098097 (Hartree/Particle)
Thermal correction to Energy= 0.108195
Thermal correction to Enthalpy= 0.109139
Thermal correction to Gibbs Free Energy= 0.060210
Sum of electronic and zero-point Energies= -431.602442
Sum of electronic and thermal Energies= -431.592344
Sum of electronic and thermal Enthalpies= -431.591400
Sum of electronic and thermal Free Energies= -431.640329

INT1b-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.410232	0.614061	-0.000094
2	6	0	1.720195	0.683263	0.000281
3	6	0	-1.720195	-0.683266	-0.000398
4	6	0	-0.410229	-0.614046	-0.000094
5	9	0	-0.359191	1.742727	-0.000112
6	9	0	0.359206	-1.742705	0.000058
7	6	0	2.982453	-0.057906	0.000010
8	6	0	-2.982468	0.057878	0.000216
9	1	0	2.795777	-1.140971	0.001301
10	1	0	3.584826	0.179800	-0.886405
11	1	0	3.586353	0.181657	0.884876
12	1	0	-2.795816	1.140946	-0.001909
13	1	0	-3.586956	-0.182268	-0.884089
14	1	0	-3.584245	-0.179263	0.887189

Zero-point vibrational energy 262026.8 (Joules/Mol)
62.62590 (Kcal/Mol)
Zero-point correction= 0.099801 (Hartree/Particle)
Thermal correction to Energy= 0.109248
Thermal correction to Enthalpy= 0.110192
Thermal correction to Gibbs Free Energy= 0.064871
Sum of electronic and zero-point Energies= -431.631975
Sum of electronic and thermal Energies= -431.622528
Sum of electronic and thermal Enthalpies= -431.621584
Sum of electronic and thermal Free Energies= -431.666905

TS1b-2

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.619356	0.825707	-0.000012
2	6	0	-1.855175	0.570126	-0.000012
3	6	0	1.691702	-0.654973	0.000004
4	6	0	0.453227	-0.775653	0.000016
5	6	0	0.247371	2.033357	0.000022
6	9	0	-0.474750	-1.723597	0.000023
7	9	0	-2.807092	-0.310956	-0.000020
8	6	0	3.051275	-0.124035	-0.000023
9	1	0	0.893573	2.043636	0.884807
10	1	0	0.893605	2.043667	-0.884738
11	1	0	-0.358676	2.943070	0.000027
12	1	0	3.253865	0.487456	0.888685
13	1	0	3.786143	-0.941556	-0.000080
14	1	0	3.253805	0.487524	-0.888698

Zero-point vibrational energy 256982.2 (Joules/Mol)
61.42023 (Kcal/Mol)
Zero-point correction= 0.097879 (Hartree/Particle)
Thermal correction to Energy= 0.107845
Thermal correction to Enthalpy= 0.108790
Thermal correction to Gibbs Free Energy= 0.060703
Sum of electronic and zero-point Energies= -431.589997
Sum of electronic and thermal Energies= -431.580031
Sum of electronic and thermal Enthalpies= -431.579087
Sum of electronic and thermal Free Energies= -431.627173

TS1b-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.494470	-0.866695	0.223942
2	6	0	-1.646775	-0.735359	-0.274473
3	6	0	1.646776	0.735361	-0.274487
4	6	0	0.494476	0.866692	0.223944
5	6	0	0.366725	-1.899020	0.857072
6	6	0	-0.366712	1.899020	0.857079
7	9	0	-2.441408	0.111196	-0.877950
8	9	0	2.441390	-0.111196	-0.877987
9	1	0	0.624070	-1.621548	1.885259
10	1	0	-0.148139	-2.863836	0.875164
11	1	0	1.302730	-2.017151	0.302043
12	1	0	-1.302713	2.017173	0.302048

13	1	0	-0.624069	1.621538	1.885260
14	1	0	0.148165	2.863829	0.875185

Zero-point vibrational energy 258712.0 (Joules/Mol)
61.83366 (Kcal/Mol)
Zero-point correction= 0.098538 (Hartree/Particle)
Thermal correction to Energy= 0.108149
Thermal correction to Enthalpy= 0.109093
Thermal correction to Gibbs Free Energy= 0.063530
Sum of electronic and zero-point Energies= -431.582764
Sum of electronic and thermal Energies= -431.573153
Sum of electronic and thermal Enthalpies= -431.572209
Sum of electronic and thermal Free Energies= -431.617772

INT2b-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000082	-0.773700	-0.723907
2	6	0	0.000082	-0.815588	0.603658
3	6	0	-0.000082	0.815588	0.603658
4	6	0	-0.000082	0.773700	-0.723907
5	9	0	0.000174	-1.663982	-1.711352
6	9	0	-0.000174	1.663982	-1.711352
7	6	0	0.000178	-1.819328	1.693100
8	6	0	-0.000178	1.819328	1.693100
9	1	0	0.000278	-2.835007	1.284151
10	1	0	0.882437	-1.714574	2.340455
11	1	0	-0.882103	-1.714746	2.340452
12	1	0	-0.000278	2.835007	1.284151
13	1	0	-0.882437	1.714574	2.340455
14	1	0	0.882103	1.714746	2.340452

Zero-point vibrational energy 269464.1 (Joules/Mol)
64.40346 (Kcal/Mol)
Zero-point correction= 0.102633 (Hartree/Particle)
Thermal correction to Energy= 0.111433
Thermal correction to Enthalpy= 0.112377
Thermal correction to Gibbs Free Energy= 0.069840
Sum of electronic and zero-point Energies= -431.684878
Sum of electronic and thermal Energies= -431.676079
Sum of electronic and thermal Enthalpies= -431.675135
Sum of electronic and thermal Free Energies= -431.717672

TS3b-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.005265	0.383837	-0.629552
2	6	0	-1.375308	-0.218317	1.026375
3	6	0	-2.554636	-0.195669	0.674610
4	6	0	-3.763780	-0.002180	-0.121213
5	6	0	0.868423	-0.859585	-0.786743
6	6	0	1.890422	-0.276824	-0.115725
7	6	0	1.099619	1.030609	-0.087737
8	6	0	1.472241	2.448082	0.136333
9	6	0	3.123651	-0.738862	0.573239
10	1	0	3.332602	-1.787064	0.338024
11	1	0	4.000046	-0.143432	0.286829
12	1	0	3.015770	-0.649414	1.663648
13	1	0	2.307317	2.744025	-0.516359
14	1	0	1.799917	2.631691	1.169127
15	1	0	0.625883	3.109139	-0.074782
16	9	0	-0.908564	0.875187	-1.501159
17	9	0	0.563019	-2.117570	-1.093627
18	9	0	-0.470731	-0.478562	1.942629
19	1	0	-3.513447	0.398741	-1.111803
20	1	0	-4.304002	-0.945796	-0.265464
21	1	0	-4.449805	0.704072	0.362671

Zero-point vibrational energy 393843.9 (Joules/Mol)
94.13095 (Kcal/Mol)
Zero-point correction= 0.150007 (Hartree/Particle)
Thermal correction to Energy= 0.164656
Thermal correction to Enthalpy= 0.165600
Thermal correction to Gibbs Free Energy= 0.107389
Sum of electronic and zero-point Energies= -647.484264
Sum of electronic and thermal Energies= -647.469616
Sum of electronic and thermal Enthalpies= -647.468671
Sum of electronic and thermal Free Energies= -647.526883

TS3b-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.437857	-0.917627	-0.698802
2	6	0	0.111056	-0.151952	0.772678

3	6	0	1.334355	-0.665034	0.365133
4	6	0	1.733895	0.616646	-0.251821
5	6	0	0.566372	1.210443	0.090360
6	6	0	-0.607578	-0.323913	2.075257
7	6	0	-0.138532	2.485517	-0.180049
8	6	0	-0.808249	-2.033879	-1.435231
9	6	0	-2.481381	-0.229925	-0.599997
10	9	0	-3.044156	0.765408	0.050103
11	1	0	-0.496537	-2.834742	-0.755440
12	1	0	0.084035	-1.693988	-1.973763
13	1	0	-1.509233	-2.454135	-2.164594
14	1	0	-0.339351	3.039595	0.747656
15	1	0	-1.111254	2.306424	-0.655333
16	1	0	0.458233	3.129849	-0.833564
17	9	0	2.767953	0.958842	-1.018479
18	9	0	2.014523	-1.761154	0.696001
19	1	0	-1.620070	0.084854	2.034297
20	1	0	-0.676766	-1.382665	2.345756
21	1	0	-0.066422	0.195296	2.881198

Zero-point vibrational energy 395439.7 (Joules/Mol)
94.51235 (Kcal/Mol)
Zero-point correction= 0.150615 (Hartree/Particle)
Thermal correction to Energy= 0.164883
Thermal correction to Enthalpy= 0.165827
Thermal correction to Gibbs Free Energy= 0.108946
Sum of electronic and zero-point Energies= -647.473317
Sum of electronic and thermal Energies= -647.459049
Sum of electronic and thermal Enthalpies= -647.458105
Sum of electronic and thermal Free Energies= -647.514986

TS3b-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.366089	-0.105290	-0.946328
2	6	0	1.190733	-0.985056	0.120256
3	6	0	1.931462	0.287979	-0.017550
4	6	0	0.920193	0.998369	0.528319
5	6	0	0.096086	-0.357187	0.691166
6	6	0	-2.556679	0.033065	-0.647601
7	6	0	-3.850416	0.115667	0.026243
8	6	0	-0.725723	-0.781364	1.864657
9	6	0	0.523937	2.420327	0.655978

10	1	0	-0.353872	2.634744	0.029516
11	1	0	1.338925	3.083564	0.349344
12	1	0	0.247482	2.674715	1.688212
13	1	0	-1.639866	-0.184629	1.945327
14	1	0	-0.157913	-0.662043	2.798985
15	1	0	-1.014525	-1.833980	1.776339
16	9	0	3.062796	0.602715	-0.644570
17	9	0	1.569262	-2.255979	0.045334
18	9	0	-0.494979	-0.112228	-1.939699
19	1	0	-3.935589	1.025667	0.633758
20	1	0	-4.027930	-0.746699	0.681910
21	1	0	-4.671449	0.139042	-0.703822

Zero-point vibrational energy 394861.9 (Joules/Mol)
94.37426 (Kcal/Mol)
Zero-point correction= 0.150395 (Hartree/Particle)
Thermal correction to Energy= 0.164799
Thermal correction to Enthalpy= 0.165743
Thermal correction to Gibbs Free Energy= 0.107961
Sum of electronic and zero-point Energies= -647.478735
Sum of electronic and thermal Energies= -647.464331
Sum of electronic and thermal Enthalpies= -647.463387
Sum of electronic and thermal Free Energies= -647.521169

TS3b-4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.501021	-0.626316	0.838970
2	6	0	0.058799	0.479388	-0.488146
3	6	0	-1.018494	1.068633	0.208934
4	6	0	-1.895568	-0.102377	-0.137858
5	6	0	-0.903706	-0.601289	-0.937489
6	6	0	0.674822	-1.463186	1.734203
7	6	0	2.651464	-0.317231	0.482448
8	6	0	-1.281290	2.440479	0.714653
9	6	0	-3.197996	-0.603694	0.377771
10	1	0	-3.459764	-1.560300	-0.084863
11	1	0	-4.012318	0.104765	0.177861
12	1	0	-3.162785	-0.748242	1.466802
13	1	0	-1.713305	2.436563	1.724553
14	1	0	-0.355194	3.023033	0.743763
15	1	0	-1.994121	2.975124	0.067957
16	1	0	-0.082987	-0.857067	2.242945

17	1	0	1.296442	-1.947045	2.494219
18	1	0	0.153144	-2.244744	1.169628
19	9	0	3.480024	0.362244	-0.251032
20	9	0	0.965639	1.127815	-1.246742
21	9	0	-0.690487	-1.804339	-1.475979

Zero-point vibrational energy 393871.6 (Joules/Mol)
94.13757 (Kcal/Mol)
Zero-point correction= 0.150018 (Hartree/Particle)
Thermal correction to Energy= 0.164555
Thermal correction to Enthalpy= 0.165499
Thermal correction to Gibbs Free Energy= 0.107604
Sum of electronic and zero-point Energies= -647.475882
Sum of electronic and thermal Energies= -647.461345
Sum of electronic and thermal Enthalpies= -647.460401
Sum of electronic and thermal Free Energies= -647.518296

TS3b-5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.438859	-0.500944	-0.288017
2	6	0	1.239181	0.984611	-0.130157
3	6	0	0.366806	0.769257	0.878173
4	6	0	0.473320	-0.795244	0.623063
5	6	0	-1.968870	0.159629	-0.634956
6	6	0	-1.435106	-0.933298	-0.479359
7	9	0	2.272471	-1.203095	-1.043732
8	9	0	0.333601	-1.818223	1.479840
9	9	0	-1.419476	-2.245503	-0.599854
10	6	0	-2.570955	1.476978	-0.825647
11	6	0	-0.356596	1.554528	1.904923
12	6	0	1.738561	2.154019	-0.901482
13	1	0	-3.584045	1.394010	-1.244039
14	1	0	-2.660903	2.026366	0.120425
15	1	0	-1.981769	2.097216	-1.512649
16	1	0	0.148523	1.477485	2.879369
17	1	0	-0.397049	2.616358	1.637813
18	1	0	-1.378018	1.184433	2.046155
19	1	0	1.349966	3.090988	-0.490219
20	1	0	1.437752	2.091604	-1.956215
21	1	0	2.834972	2.205707	-0.886175

Zero-point vibrational energy 399772.6 (Joules/Mol)

95.54794 (Kcal/Mol)

Zero-point correction=	0.152265 (Hartree/Particle)
Thermal correction to Energy=	0.166400
Thermal correction to Enthalpy=	0.167344
Thermal correction to Gibbs Free Energy=	0.111247
Sum of electronic and zero-point Energies=	-647.478871
Sum of electronic and thermal Energies=	-647.464736
Sum of electronic and thermal Enthalpies=	-647.463792
Sum of electronic and thermal Free Energies=	-647.519889

TS3b-6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.875420	-1.372504	-0.174435
2	6	0	1.482513	0.010581	-0.161663
3	6	0	0.554468	0.447141	0.748673
4	6	0	-0.042648	-1.021815	0.735142
5	6	0	-0.971052	1.318808	-0.524636
6	6	0	-1.904009	0.533378	-0.669365
7	9	0	1.141490	-2.452488	-0.906958
8	9	0	-1.003986	-1.623784	1.428342
9	6	0	-2.961175	-0.469759	-0.757792
10	9	0	-0.419546	2.503397	-0.731528
11	6	0	0.607181	1.441465	1.863457
12	6	0	2.626263	0.612153	-0.888840
13	1	0	-2.952373	-1.136685	0.113731
14	1	0	-3.954711	-0.004628	-0.810906
15	1	0	-2.836830	-1.094532	-1.650882
16	1	0	1.130500	1.014499	2.731672
17	1	0	1.142655	2.343916	1.552408
18	1	0	-0.394641	1.735031	2.192648
19	1	0	2.777597	1.653275	-0.588705
20	1	0	3.555290	0.057576	-0.695424
21	1	0	2.469128	0.590740	-1.976491

Zero-point vibrational energy 400844.2 (Joules/Mol)
95.80407 (Kcal/Mol)

Zero-point correction=	0.152673 (Hartree/Particle)
Thermal correction to Energy=	0.166597
Thermal correction to Enthalpy=	0.167542
Thermal correction to Gibbs Free Energy=	0.112199
Sum of electronic and zero-point Energies=	-647.479819
Sum of electronic and thermal Energies=	-647.465895

Sum of electronic and thermal Enthalpies= -647.464951
Sum of electronic and thermal Free Energies= -647.520294

TS3b-7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.469412	-0.315733	-0.087977
2	6	0	1.138468	1.188853	-0.121314
3	6	0	0.179904	0.983021	0.791793
4	6	0	0.404592	-0.552954	0.737019
5	6	0	-2.052130	-0.281473	-0.673248
6	6	0	-1.194413	-1.149699	-0.511132
7	6	0	2.564003	-1.131499	-0.663400
8	9	0	0.254234	-1.464650	1.713963
9	9	0	-0.795462	-2.392577	-0.724276
10	6	0	-2.927477	0.884521	-0.708530
11	9	0	-0.721585	1.744964	1.403960
12	6	0	1.601384	2.310686	-0.980294
13	1	0	3.546248	-0.754278	-0.343335
14	1	0	2.476513	-2.173933	-0.343168
15	1	0	2.562393	-1.110542	-1.762674
16	1	0	-2.694181	1.583686	0.106261
17	1	0	-3.982680	0.598945	-0.605276
18	1	0	-2.821856	1.430951	-1.654178
19	1	0	2.681001	2.480120	-0.877640
20	1	0	1.408724	2.100605	-2.041390
21	1	0	1.086696	3.240484	-0.718921

Zero-point vibrational energy 399464.8 (Joules/Mol)
95.47438 (Kcal/Mol)
Zero-point correction= 0.152148 (Hartree/Particle)
Thermal correction to Energy= 0.166305
Thermal correction to Enthalpy= 0.167249
Thermal correction to Gibbs Free Energy= 0.110960
Sum of electronic and zero-point Energies= -647.481955
Sum of electronic and thermal Energies= -647.467799
Sum of electronic and thermal Enthalpies= -647.466854
Sum of electronic and thermal Free Energies= -647.523143

TS3b-8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.477609	-0.075103	-0.360849
2	6	0	-0.774832	-1.376640	-0.238641
3	6	0	-0.019934	-0.944569	0.783810
4	6	0	-0.749477	0.499963	0.631184
5	6	0	1.873919	0.544186	-0.584619
6	6	0	0.983342	1.377108	-0.458506
7	9	0	-2.461123	0.332522	-1.152705
8	6	0	-1.045263	1.547270	1.654137
9	9	0	0.497725	2.595657	-0.608769
10	6	0	2.936950	-0.440509	-0.777303
11	6	0	0.887859	-1.500292	1.815521
12	9	0	-0.855403	-2.503118	-0.944952
13	1	0	-1.661536	1.135157	2.466923
14	1	0	-0.132479	1.951668	2.102845
15	1	0	-1.595345	2.378200	1.201828
16	1	0	3.838426	0.026139	-1.198708
17	1	0	3.232385	-0.913842	0.167518
18	1	0	2.625704	-1.238855	-1.461949
19	1	0	0.350816	-1.679213	2.759274
20	1	0	1.712507	-0.815354	2.040861
21	1	0	1.309007	-2.457922	1.490830

Zero-point vibrational energy 401018.7 (Joules/Mol)
95.84577 (Kcal/Mol)
Zero-point correction= 0.152740 (Hartree/Particle)
Thermal correction to Energy= 0.166700
Thermal correction to Enthalpy= 0.167644
Thermal correction to Gibbs Free Energy= 0.111998
Sum of electronic and zero-point Energies= -647.481089
Sum of electronic and thermal Energies= -647.467130
Sum of electronic and thermal Enthalpies= -647.466185
Sum of electronic and thermal Free Energies= -647.521831

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.630628	0.000333	-0.000984
2	6	0	-1.833812	-0.000884	-0.000366
3	6	0	0.846566	0.000025	-0.000066
4	9	0	-3.126679	0.000364	-0.000048
5	6	0	1.356968	-0.255748	1.436735
6	6	0	1.358262	1.371922	-0.496433

7	6	0	1.358486	-1.116228	-0.939414
8	1	0	2.453585	-0.257614	1.451464
9	1	0	1.006194	-1.223305	1.811000
10	1	0	1.005006	0.522336	2.122301
11	1	0	2.454847	1.385599	-0.500731
12	1	0	1.007914	1.576479	-1.513658
13	1	0	1.007008	2.180236	0.153621
14	1	0	1.007360	-2.099116	-0.607848
15	1	0	1.008095	-0.957592	-1.964773
16	1	0	2.455056	-1.126814	-0.947784

Zero-point vibrational energy 352871.7 (Joules/Mol)
84.33836 (Kcal/Mol)
Zero-point correction= 0.134402 (Hartree/Particle)
Thermal correction to Energy= 0.142829
Thermal correction to Enthalpy= 0.143773
Thermal correction to Gibbs Free Energy= 0.102123
Sum of electronic and zero-point Energies= -333.669108
Sum of electronic and thermal Energies= -333.660681
Sum of electronic and thermal Enthalpies= -333.659737
Sum of electronic and thermal Free Energies= -333.701386

TS1-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.534322	-0.818722	-0.000313
2	6	0	-0.534324	0.818729	-0.000379
3	6	0	-1.758700	0.626342	-0.000094
4	6	0	1.758700	-0.626344	-0.000010
5	6	0	3.112437	-0.047543	0.000163
6	6	0	4.137432	-1.212528	0.000336
7	6	0	3.319409	0.815521	-1.267363
8	6	0	3.319042	0.815585	1.267704
9	6	0	-3.112437	0.047541	0.000162
10	6	0	-3.319492	-0.815489	-1.267373
11	6	0	-3.318959	-0.815621	1.267694
12	6	0	-4.137432	1.212526	0.000432
13	1	0	-4.017035	1.842701	-0.886720
14	1	0	-4.016664	1.842617	0.887594
15	1	0	-5.156483	0.807471	0.000626
16	1	0	-3.187270	-0.216040	2.174585
17	1	0	-4.333069	-1.233089	1.275194
18	1	0	-2.601070	-1.639859	1.294503

19	1	0	-4.333610	-1.232944	-1.274497
20	1	0	-2.601624	-1.639731	-1.294578
21	1	0	-3.188175	-0.215811	-2.174255
22	9	0	0.382667	1.774479	-0.000571
23	9	0	-0.382665	-1.774475	-0.000582
24	1	0	2.601156	1.639823	1.294586
25	1	0	3.187409	0.215976	2.174586
26	1	0	4.333154	1.233048	1.275151
27	1	0	2.601533	1.639758	-1.294500
28	1	0	3.188044	0.215868	-2.174255
29	1	0	4.333523	1.232988	-1.274535
30	1	0	5.156483	-0.807472	0.000455
31	1	0	4.016969	-1.842691	-0.886815
32	1	0	4.016732	-1.842630	0.887498

Zero-point vibrational energy 706818.4 (Joules/Mol)
168.93365 (Kcal/Mol)
Zero-point correction= 0.269213 (Hartree/Particle)
Thermal correction to Energy= 0.286630
Thermal correction to Enthalpy= 0.287575
Thermal correction to Gibbs Free Energy= 0.224206
Sum of electronic and zero-point Energies= -667.317713
Sum of electronic and thermal Energies= -667.300295
Sum of electronic and thermal Enthalpies= -667.299351
Sum of electronic and thermal Free Energies= -667.362719

TS1-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.158584	0.578628	-0.014388
2	6	0	-0.212745	-0.190351	1.184099
3	6	0	-1.354436	-0.382801	0.724050
4	6	0	-2.496409	-0.312392	-0.206692
5	6	0	-2.008736	-0.556431	-1.656912
6	6	0	-3.151107	1.085403	-0.103711
7	6	0	-3.532162	-1.400646	0.171986
8	1	0	-3.895711	-1.257610	1.194878
9	1	0	-4.390927	-1.351871	-0.508147
10	1	0	-3.093787	-2.401715	0.103082
11	1	0	-3.521843	1.268739	0.910380
12	1	0	-3.998096	1.158209	-0.796567
13	1	0	-2.427883	1.869041	-0.347416
14	1	0	-2.858350	-0.502000	-2.348254

15	1	0	-1.270193	0.194832	-1.952777
16	1	0	-1.550632	-1.546275	-1.754021
17	9	0	0.507915	-0.351824	2.286115
18	6	0	0.940322	1.818563	-0.159461
19	9	0	-0.003738	2.710464	0.012376
20	6	0	2.269392	-0.395901	-0.340442
21	6	0	1.736291	-1.835751	-0.492009
22	1	0	2.560727	-2.497465	-0.780811
23	1	0	1.312747	-2.212008	0.443485
24	1	0	0.963538	-1.895766	-1.265214
25	6	0	3.333904	-0.355884	0.781066
26	1	0	2.905703	-0.648284	1.743191
27	1	0	4.155146	-1.043537	0.544213
28	1	0	3.746586	0.653077	0.883308
29	6	0	2.915670	0.039066	-1.676009
30	1	0	2.183910	0.017671	-2.490406
31	1	0	3.311263	1.056496	-1.600590
32	1	0	3.738802	-0.638326	-1.934205

Zero-point vibrational energy 704404.2 (Joules/Mol)
168.35665 (Kcal/Mol)
Zero-point correction= 0.268293 (Hartree/Particle)
Thermal correction to Energy= 0.285893
Thermal correction to Enthalpy= 0.286837
Thermal correction to Gibbs Free Energy= 0.222666
Sum of electronic and zero-point Energies= -667.298391
Sum of electronic and thermal Energies= -667.280792
Sum of electronic and thermal Enthalpies= -667.279848
Sum of electronic and thermal Free Energies= -667.344018

TS1-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.843582	-0.555572	-0.263327
2	6	0	0.843777	0.555596	-0.263243
3	6	0	2.021727	-0.025657	0.498473
4	6	0	1.597864	-0.802139	1.760112
5	6	0	2.817509	-0.968244	-0.435576
6	6	0	2.938572	1.144589	0.925986
7	1	0	2.403131	1.845643	1.574262
8	1	0	3.298195	1.696621	0.052418
9	1	0	3.804971	0.757649	1.476113
10	1	0	1.108805	-0.146337	2.486620

11	1	0	0.914296	-1.620883	1.519926
12	1	0	2.487438	-1.227488	2.238718
13	1	0	2.218980	-1.826606	-0.748705
14	1	0	3.706676	-1.343601	0.085411
15	1	0	3.144427	-0.435684	-1.334812
16	6	0	0.676499	1.582031	-0.988076
17	9	0	-0.147032	2.174249	-1.814409
18	6	0	-0.676871	-1.581747	-0.988762
19	9	0	0.146853	-2.172791	-1.815780
20	6	0	-2.021632	0.025309	0.498549
21	6	0	-2.818027	0.967285	-0.435599
22	6	0	-1.597876	0.802349	1.759887
23	6	0	-2.937814	-1.145239	0.926640
24	1	0	-2.401906	-1.845770	1.575096
25	1	0	-3.297279	-1.697769	0.053324
26	1	0	-3.804314	-0.758524	1.476776
27	1	0	-3.145235	0.434214	-1.334426
28	1	0	-3.707025	1.342779	0.085580
29	1	0	-2.219745	1.825584	-0.749408
30	1	0	-2.487584	1.227278	2.238613
31	1	0	-1.108274	0.146981	2.486420
32	1	0	-0.914821	1.621418	1.519383

Zero-point vibrational energy 706628.3 (Joules/Mol)
168.88821 (Kcal/Mol)
Zero-point correction= 0.269140 (Hartree/Particle)
Thermal correction to Energy= 0.286315
Thermal correction to Enthalpy= 0.287259
Thermal correction to Gibbs Free Energy= 0.224959
Sum of electronic and zero-point Energies= -667.287572
Sum of electronic and thermal Energies= -667.270397
Sum of electronic and thermal Enthalpies= -667.269453
Sum of electronic and thermal Free Energies= -667.331753

7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000273	1.280054	0.726309
2	6	0	0.763791	0.219258	0.000508
3	6	0	-0.763780	0.219243	-0.000502
4	6	0	0.000264	1.280055	-0.726312
5	9	0	0.001451	1.999501	-1.852685
6	9	0	-0.001471	1.999493	1.852687

7	6	0	-2.031316	-0.581378	-0.000310
8	6	0	2.031322	-0.581371	0.000301
9	6	0	-3.230032	0.393724	-0.001406
10	6	0	-2.089363	-1.468933	-1.261329
11	6	0	-2.090031	-1.466979	1.262055
12	6	0	2.089497	-1.467912	-1.261420
13	6	0	2.089897	-1.467986	1.261966
14	6	0	3.230046	0.393723	0.000136
15	1	0	-3.214642	1.037510	0.885263
16	1	0	-3.214061	1.036226	-0.888994
17	1	0	-4.175345	-0.162176	-0.001306
18	1	0	-2.042750	-0.862249	-2.172695
19	1	0	-1.255544	-2.179398	-1.282293
20	1	0	-3.023690	-2.042786	-1.282385
21	1	0	-2.044496	-0.858847	2.172510
22	1	0	-3.024090	-2.041257	1.283194
23	1	0	-1.255880	-2.177008	1.284846
24	1	0	2.043146	-0.860494	-2.172311
25	1	0	3.023754	-2.041865	-1.282750
26	1	0	1.255593	-2.178256	-1.283118
27	1	0	2.044174	-0.860583	2.172896
28	1	0	1.255785	-2.178082	1.284053
29	1	0	3.023990	-2.042224	1.282799
30	1	0	3.214517	1.036845	0.887285
31	1	0	3.214224	1.036891	-0.886973
32	1	0	4.175355	-0.162184	-0.000023

Zero-point vibrational energy 713918.4 (Joules/Mol)
170.63060 (Kcal/Mol)
Zero-point correction= 0.271917 (Hartree/Particle)
Thermal correction to Energy= 0.287823
Thermal correction to Enthalpy= 0.288768
Thermal correction to Gibbs Free Energy= 0.229434
Sum of electronic and zero-point Energies= -667.310402
Sum of electronic and thermal Energies= -667.294496
Sum of electronic and thermal Enthalpies= -667.293552
Sum of electronic and thermal Free Energies= -667.352885

7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.834497	0.266539	0.062211
2	6	0	0.761067	1.594837	0.064879

3	6	0	-0.761066	1.594829	-0.064895
4	6	0	-0.834488	0.266529	-0.062261
5	6	0	1.945297	-0.744331	-0.010472
6	6	0	-1.945293	-0.744333	0.010467
7	6	0	1.733382	-1.891135	1.002033
8	6	0	3.277505	-0.033402	0.318250
9	6	0	2.031604	-1.330052	-1.441949
10	6	0	-1.733389	-1.891190	-1.001978
11	6	0	-3.277499	-0.033411	-0.318285
12	6	0	-2.031600	-1.329977	1.441977
13	9	0	1.637182	2.599561	0.060333
14	9	0	-1.637192	2.599542	-0.060337
15	1	0	1.643646	-1.504782	2.023392
16	1	0	2.586488	-2.579804	0.973062
17	1	0	0.833061	-2.471327	0.776879
18	1	0	3.474844	0.787368	-0.378113
19	1	0	3.265188	0.379462	1.332733
20	1	0	4.107879	-0.745751	0.249462
21	1	0	2.251774	-0.542417	-2.170540
22	1	0	1.096262	-1.813392	-1.740129
23	1	0	2.830688	-2.080032	-1.495976
24	1	0	-0.833154	-2.471470	-0.776704
25	1	0	-2.586567	-2.579773	-0.973078
26	1	0	-1.643501	-1.504891	-2.023344
27	1	0	-3.265171	0.379442	-1.332774
28	1	0	-3.474850	0.787363	0.378067
29	1	0	-4.107868	-0.745765	-0.249499
30	1	0	-1.096238	-1.813251	1.740208
31	1	0	-2.251836	-0.542318	2.170522
32	1	0	-2.830647	-2.079998	1.496015

Zero-point vibrational energy 716735.9 (Joules/Mol)
171.30400 (Kcal/Mol)
Zero-point correction= 0.272990 (Hartree/Particle)
Thermal correction to Energy= 0.289596
Thermal correction to Enthalpy= 0.290540
Thermal correction to Gibbs Free Energy= 0.230402
Sum of electronic and zero-point Energies= -667.392482
Sum of electronic and thermal Energies= -667.375877
Sum of electronic and thermal Enthalpies= -667.374933
Sum of electronic and thermal Free Energies= -667.435070

7c

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.083193	-0.976468	-0.000065
2	6	0	1.081132	-0.094878	-0.000208
3	6	0	-0.083199	0.976517	0.000134
4	6	0	-1.081130	0.094919	0.000211
5	9	0	0.000475	-2.305844	0.000081
6	6	0	-2.573467	0.005470	0.000015
7	6	0	2.573472	-0.005482	-0.000002
8	9	0	-0.000496	2.305892	0.000024
9	6	0	-3.036768	-0.764101	1.260484
10	6	0	-3.036264	-0.765171	-1.260043
11	6	0	-3.175994	1.423531	-0.000730
12	6	0	3.036462	0.763554	1.260907
13	6	0	3.036642	0.765658	-1.259615
14	6	0	3.175942	-1.423568	-0.001170
15	1	0	-2.590975	-1.764852	1.296086
16	1	0	-2.748044	-0.231297	2.173182
17	1	0	-4.127615	-0.879673	1.260655
18	1	0	-2.590437	-1.765946	-1.294564
19	1	0	-4.127107	-0.880740	-1.260529
20	1	0	-2.747196	-0.233158	-2.173089
21	1	0	-2.862317	1.986873	0.885021
22	1	0	-4.270924	1.370811	-0.000681
23	1	0	-2.862334	1.985912	-0.887097
24	1	0	2.590681	1.764301	1.296821
25	1	0	2.747504	0.230370	2.173308
26	1	0	4.127311	0.879113	1.261398
27	1	0	2.590870	1.766469	-1.293830
28	1	0	4.127491	0.881172	-1.259774
29	1	0	2.747778	0.234045	-2.172958
30	1	0	2.862018	-1.987263	0.884267
31	1	0	2.862486	-1.985571	-0.887850
32	1	0	4.270874	-1.370890	-0.000824

Zero-point vibrational energy 715716.9 (Joules/Mol)
171.06045 (Kcal/Mol)
Zero-point correction= 0.272602 (Hartree/Particle)
Thermal correction to Energy= 0.289496
Thermal correction to Enthalpy= 0.290441
Thermal correction to Gibbs Free Energy= 0.228159
Sum of electronic and zero-point Energies= -667.401817
Sum of electronic and thermal Energies= -667.384923
Sum of electronic and thermal Enthalpies= -667.383979
Sum of electronic and thermal Free Energies= -667.446261

7c’

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.835231	0.314783	-0.000006
2	6	0	0.000001	0.991099	0.970614
3	6	0	0.000001	0.991086	-0.970638
4	6	0	0.835233	0.314782	0.000002
5	6	0	2.024005	-0.613063	-0.000001
6	6	0	-2.024007	-0.613060	0.000005
7	9	0	0.000007	2.307638	1.301524
8	9	0	-0.000004	2.307640	-1.301517
9	6	0	3.286659	0.282829	-0.000037
10	6	0	2.015360	-1.488504	-1.265569
11	6	0	2.015404	-1.488451	1.265599
12	6	0	-2.015408	-1.488430	1.265623
13	6	0	-3.286658	0.282833	-0.000061
14	6	0	-2.015360	-1.488523	-1.265545
15	1	0	3.313917	0.926043	0.886433
16	1	0	3.313900	0.925996	-0.886542
17	1	0	4.189962	-0.338742	-0.000030
18	1	0	1.158826	-2.171347	-1.272121
19	1	0	1.963003	-0.872526	-2.169647
20	1	0	2.928049	-2.093329	-1.314061
21	1	0	1.158919	-2.171354	1.272169
22	1	0	1.962993	-0.872439	2.169652
23	1	0	2.928134	-2.093210	1.314138
24	1	0	-1.963054	-0.872404	2.169669
25	1	0	-2.928114	-2.093229	1.314132
26	1	0	-1.158892	-2.171294	1.272228
27	1	0	-3.313924	0.926066	0.886394
28	1	0	-3.313890	0.925980	-0.886580
29	1	0	-4.189963	-0.338737	-0.000047
30	1	0	-1.158919	-2.171481	-1.272011
31	1	0	-2.928125	-2.093227	-1.314120
32	1	0	-1.962840	-0.872564	-2.169629

Zero-point vibrational energy 711604.7 (Joules/Mol)
170.07759 (Kcal/Mol)
Zero-point correction= 0.271036 (Hartree/Particle)
Thermal correction to Energy= 0.287693
Thermal correction to Enthalpy= 0.288637
Thermal correction to Gibbs Free Energy= 0.227785

Sum of electronic and zero-point Energies=	-667.340371
Sum of electronic and thermal Energies=	-667.323713
Sum of electronic and thermal Enthalpies=	-667.322769
Sum of electronic and thermal Free Energies=	-667.383621

7d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.645034	-0.065784	-0.306964
2	6	0	-0.350711	-1.493359	0.807765
3	6	0	0.044434	-1.315020	-0.581328
4	6	0	-0.684221	-0.146027	0.218164
5	6	0	-2.016584	0.552960	0.049248
6	6	0	-1.999735	1.380790	-1.249556
7	6	0	-2.251123	1.475825	1.264352
8	6	0	-3.124455	-0.516007	-0.015015
9	6	0	1.988015	0.579416	-0.106682
10	6	0	1.981576	1.325882	1.242971
11	6	0	2.235189	1.572489	-1.267872
12	6	0	3.067287	-0.522999	-0.112241
13	1	0	4.057410	-0.083597	0.052827
14	1	0	3.084501	-1.051772	-1.072081
15	1	0	2.872512	-1.253505	0.678153
16	1	0	2.226287	1.062598	-2.237359
17	1	0	1.474891	2.360995	-1.288780
18	1	0	3.215048	2.047516	-1.141008
19	1	0	2.963174	1.776006	1.428666
20	1	0	1.232975	2.126281	1.247902
21	1	0	1.752150	0.636476	2.060527
22	9	0	-0.307325	-1.961849	-1.706202
23	9	0	0.647834	-1.609267	1.788307
24	1	0	-1.817693	0.741941	-2.121409
25	1	0	-2.962834	1.883562	-1.393472
26	1	0	-1.218776	2.149658	-1.222081
27	1	0	-1.474718	2.246459	1.336778
28	1	0	-3.221101	1.979700	1.175920
29	1	0	-2.247031	0.901658	2.197054
30	1	0	-4.109249	-0.038097	-0.067577
31	1	0	-3.095623	-1.161497	0.868362
32	1	0	-3.004735	-1.153340	-0.898418

Zero-point vibrational energy 710575.6 (Joules/Mol)
169.83165 (Kcal/Mol)

Zero-point correction= 0.270644 (Hartree/Particle)
Thermal correction to Energy= 0.287325
Thermal correction to Enthalpy= 0.288269
Thermal correction to Gibbs Free Energy= 0.227586
Sum of electronic and zero-point Energies= -667.333244
Sum of electronic and thermal Energies= -667.316563
Sum of electronic and thermal Enthalpies= -667.315619
Sum of electronic and thermal Free Energies= -667.376301

TS3-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.409995	-0.268949	1.077526
2	6	0	-0.171682	0.271448	-0.667795
3	6	0	0.511205	-1.042896	-0.984502
4	6	0	1.671798	-0.659082	-0.407512
5	6	0	1.046885	0.762234	-0.219164
6	6	0	1.562416	2.160990	-0.009494
7	6	0	0.375788	3.149750	-0.014396
8	1	0	-0.342291	2.908790	0.776997
9	1	0	-0.157004	3.130789	-0.968795
10	1	0	0.741177	4.168883	0.155660
11	6	0	2.527478	2.528424	-1.165410
12	1	0	2.009553	2.499706	-2.130227
13	1	0	2.917474	3.543085	-1.017940
14	1	0	3.379306	1.843763	-1.217853
15	6	0	2.300058	2.288515	1.343677
16	1	0	3.191780	1.655862	1.385762
17	1	0	1.642329	2.005312	2.172729
18	1	0	2.620733	3.325760	1.499770
19	6	0	2.852516	-1.422547	0.144441
20	6	0	2.822445	-2.862314	-0.414917
21	1	0	3.677300	-3.429331	-0.029022
22	1	0	1.907652	-3.387450	-0.124809
23	1	0	2.880185	-2.864267	-1.509046
24	6	0	4.192736	-0.770321	-0.259739
25	1	0	5.029640	-1.372509	0.114048
26	1	0	4.300978	0.237215	0.153609
27	1	0	4.285491	-0.702451	-1.349595
28	6	0	2.745736	-1.481935	1.687694
29	1	0	3.591252	-2.046214	2.100209
30	1	0	1.818262	-1.974783	1.995677
31	1	0	2.756654	-0.483089	2.133929

32	9	0	-0.011433	-2.215970	-1.342203
33	9	0	-1.095704	0.896093	-1.438785
34	9	0	-0.448257	-0.452633	1.960273
35	6	0	-2.616030	-0.313284	0.821741
36	6	0	-3.920233	-0.236202	0.136152
37	6	0	-5.008666	-0.835317	1.061288
38	1	0	-4.793348	-1.883344	1.294810
39	1	0	-5.072588	-0.281921	2.004218
40	1	0	-5.986326	-0.786417	0.566719
41	1	0	-3.614888	-2.096351	-0.982878
42	6	0	-3.860366	-1.047675	-1.180689
43	1	0	-4.832034	-1.009753	-1.688099
44	1	0	-3.099616	-0.637895	-1.850468
45	6	0	-4.258570	1.240864	-0.173301
46	1	0	-5.225197	1.306613	-0.687544
47	1	0	-3.489753	1.682444	-0.813189
48	1	0	-4.319308	1.829902	0.748175

Zero-point vibrational energy 1066965.5 (Joules/Mol)
255.01088 (Kcal/Mol)
Zero-point correction= 0.406386 (Hartree/Particle)
Thermal correction to Energy= 0.432376
Thermal correction to Enthalpy= 0.433320
Thermal correction to Gibbs Free Energy= 0.351138
Sum of electronic and zero-point Energies= -1001.049615
Sum of electronic and thermal Energies= -1001.023625
Sum of electronic and thermal Enthalpies= -1001.022681
Sum of electronic and thermal Free Energies= -1001.104863

TS3-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.594121	-0.192006	0.810441
2	6	0	-0.226253	0.697703	-0.308239
3	6	0	-0.000711	0.342711	-1.674687
4	6	0	-1.065368	-0.626211	-1.658693
5	6	0	-1.326914	-0.454239	-0.325837
6	6	0	-2.213302	-1.204573	0.644071
7	6	0	-2.438743	-2.636377	0.101024
8	1	0	-3.092604	-3.192663	0.782478
9	1	0	-2.908435	-2.626622	-0.886863
10	1	0	-1.491390	-3.180639	0.019793
11	6	0	-3.590937	-0.497890	0.736521

12	1	0	-3.501556	0.516162	1.139183
13	1	0	-4.064994	-0.431333	-0.248854
14	1	0	-4.257676	-1.064028	1.398712
15	6	0	-1.596366	-1.305100	2.051146
16	1	0	-2.282740	-1.848704	2.711413
17	1	0	-1.413214	-0.323159	2.492467
18	1	0	-0.646064	-1.846493	2.028434
19	6	0	-0.448424	2.173470	0.076947
20	6	0	-1.523084	2.745283	-0.890552
21	1	0	-1.186577	2.716913	-1.931249
22	1	0	-2.462541	2.186266	-0.819147
23	1	0	-1.733363	3.789636	-0.632420
24	6	0	-0.961758	2.385491	1.511788
25	1	0	-0.234373	2.083810	2.263736
26	1	0	-1.175720	3.450276	1.663053
27	1	0	-1.891527	1.837657	1.694199
28	6	0	0.860486	2.969082	-0.111010
29	1	0	0.682549	4.030977	0.097011
30	1	0	1.637329	2.611409	0.571098
31	1	0	1.238461	2.885862	-1.134265
32	6	0	1.534703	-0.034633	2.066424
33	9	0	0.863135	0.447471	3.083194
34	9	0	0.508756	1.063385	-2.687697
35	9	0	-1.446396	-1.522431	-2.573562
36	6	0	2.622881	-0.905771	-0.055968
37	6	0	3.750905	-1.420926	0.873598
38	1	0	3.354636	-2.114920	1.621126
39	1	0	4.231692	-0.591092	1.400586
40	1	0	4.511258	-1.944023	0.280499
41	6	0	3.265329	0.043516	-1.089721
42	1	0	3.743075	0.893637	-0.590715
43	1	0	4.038261	-0.497396	-1.649298
44	1	0	2.545546	0.432161	-1.810849
45	6	0	2.004830	-2.132895	-0.763045
46	1	0	2.791623	-2.691253	-1.284089
47	1	0	1.253263	-1.852525	-1.503317
48	1	0	1.537247	-2.805539	-0.035377

Zero-point vibrational energy 1068791.4 (Joules/Mol)
255.44728 (Kcal/Mol)

Zero-point correction= 0.407081 (Hartree/Particle)
Thermal correction to Energy= 0.432359
Thermal correction to Enthalpy= 0.433303
Thermal correction to Gibbs Free Energy= 0.355081
Sum of electronic and zero-point Energies= -1001.020023

Sum of electronic and thermal Energies= -1000.994745
Sum of electronic and thermal Enthalpies= -1000.993801
Sum of electronic and thermal Free Energies= -1001.072024

TS3-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.969315	-0.276514	-1.111135
2	6	0	-0.710196	0.836163	-0.024389
3	6	0	-1.493736	1.262617	-1.114755
4	6	0	-2.477885	0.220170	-0.912184
5	6	0	-1.793675	-0.337898	0.130224
6	6	0	-1.902406	-1.727415	0.724215
7	6	0	-3.358686	-1.924561	1.212023
8	1	0	-3.489525	-2.938089	1.610481
9	1	0	-3.608278	-1.210852	2.005159
10	1	0	-4.072739	-1.785625	0.393902
11	6	0	-1.606085	-2.768107	-0.388706
12	1	0	-2.282505	-2.633508	-1.239055
13	1	0	-1.744194	-3.784292	0.001463
14	1	0	-0.579184	-2.678704	-0.754070
15	6	0	-0.940942	-1.965302	1.898570
16	1	0	-1.027912	-3.003305	2.240735
17	1	0	0.098265	-1.790831	1.604987
18	1	0	-1.176237	-1.316966	2.749143
19	9	0	-1.564856	2.426898	-1.764733
20	9	0	-3.496582	-0.207893	-1.664692
21	9	0	0.171389	-0.604574	-2.121415
22	6	0	2.124480	-0.426079	-0.696498
23	6	0	3.505100	-0.565779	-0.191172
24	6	0	4.112479	0.805830	0.185202
25	1	0	5.155318	0.676802	0.498592
26	1	0	3.565815	1.275004	1.008439
27	1	0	4.094577	1.489285	-0.670212
28	6	0	3.549994	-1.515942	1.028299
29	1	0	4.587837	-1.659760	1.351541
30	1	0	3.130351	-2.495309	0.775792
31	1	0	2.985362	-1.110788	1.873897
32	6	0	4.348802	-1.185411	-1.339287
33	1	0	3.957207	-2.165759	-1.629070
34	1	0	4.342049	-0.539195	-2.222856
35	1	0	5.387795	-1.311203	-1.010252
36	6	0	-0.179433	1.797932	1.040418

37	6	0	0.653834	1.110459	2.134231
38	1	0	0.043228	0.448758	2.753307
39	1	0	1.465501	0.521157	1.703666
40	1	0	1.093510	1.867669	2.794540
41	6	0	0.682417	2.883131	0.356728
42	1	0	1.048631	3.594695	1.106285
43	1	0	0.109562	3.443081	-0.387321
44	1	0	1.545826	2.438907	-0.146548
45	6	0	-1.400860	2.475554	1.714760
46	1	0	-2.068940	1.732353	2.164548
47	1	0	-1.980905	3.060069	0.992229
48	1	0	-1.065075	3.153446	2.508976

Zero-point vibrational energy 1066206.8 (Joules/Mol)
254.82955 (Kcal/Mol)
Zero-point correction= 0.406097 (Hartree/Particle)
Thermal correction to Energy= 0.431997
Thermal correction to Enthalpy= 0.432942
Thermal correction to Gibbs Free Energy= 0.351256
Sum of electronic and zero-point Energies= -1001.031760
Sum of electronic and thermal Energies= -1001.005860
Sum of electronic and thermal Enthalpies= -1001.004916
Sum of electronic and thermal Free Energies= -1001.086602

TS3-4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.350845	0.632323	-0.844650
2	6	0	-2.391048	-0.034001	-0.084049
3	6	0	-2.404192	-1.060415	1.018323
4	6	0	-3.877815	-1.321938	1.410999
5	6	0	-1.646325	-0.542807	2.258462
6	6	0	-1.782100	-2.388232	0.533536
7	6	0	-3.200138	0.598824	-0.799305
8	6	0	0.755275	0.798006	0.047947
9	6	0	1.368331	-0.487669	-0.493416
10	6	0	0.362818	-0.554645	-1.416161
11	6	0	2.484048	-1.433213	-0.106278
12	6	0	2.391861	-1.792375	1.394041
13	6	0	2.367913	-2.729905	-0.938321
14	6	0	3.858120	-0.787161	-0.405103
15	6	0	1.273829	2.087257	0.647072
16	6	0	2.100429	2.827938	-0.438563

17	6	0	2.150584	1.857478	1.894026
18	6	0	0.074410	2.973102	1.055713
19	9	0	-0.832095	1.647026	-1.614704
20	9	0	-0.067123	-1.504918	-2.249789
21	9	0	-3.475254	1.459180	-1.730812
22	1	0	-2.107191	0.374447	2.641701
23	1	0	-0.599930	-0.326149	2.025860
24	1	0	-1.673849	-1.296687	3.054526
25	1	0	-0.721710	-2.273976	0.297595
26	1	0	-1.874956	-3.149055	1.317916
27	1	0	-2.291594	-2.754438	-0.363615
28	1	0	-3.925770	-2.061735	2.219721
29	1	0	-4.444986	-1.703658	0.556126
30	1	0	-4.358555	-0.400705	1.754622
31	1	0	-0.532830	2.482563	1.824006
32	1	0	-0.571455	3.191920	0.202047
33	1	0	0.436976	3.923361	1.464631
34	1	0	1.484442	3.028927	-1.320927
35	1	0	2.966321	2.236114	-0.755121
36	1	0	2.468337	3.785417	-0.048897
37	1	0	2.475369	2.821354	2.304015
38	1	0	3.050373	1.278462	1.666279
39	1	0	1.594388	1.331014	2.678011
40	1	0	3.947342	-0.534539	-1.467433
41	1	0	4.016691	0.127436	0.174095
42	1	0	4.664241	-1.486845	-0.152871
43	1	0	2.482748	-0.909194	2.032142
44	1	0	3.199541	-2.484930	1.660385
45	1	0	1.439433	-2.281396	1.625826
46	1	0	2.423993	-2.523879	-2.012144
47	1	0	1.424204	-3.250792	-0.745934
48	1	0	3.187740	-3.410021	-0.680440

Zero-point vibrational energy 1066349.3 (Joules/Mol)
254.86360 (Kcal/Mol)
Zero-point correction= 0.406151 (Hartree/Particle)
Thermal correction to Energy= 0.431927
Thermal correction to Enthalpy= 0.432872
Thermal correction to Gibbs Free Energy= 0.352109
Sum of electronic and zero-point Energies= -1001.033191
Sum of electronic and thermal Energies= -1001.007414
Sum of electronic and thermal Enthalpies= -1001.006470
Sum of electronic and thermal Free Energies= -1001.087232

TS3-5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.100632	-0.265409	0.508566
2	6	0	-1.529950	0.044367	1.551165
3	6	0	0.512703	0.815779	1.462790
4	6	0	0.868374	0.803846	-0.096330
5	6	0	1.263466	-0.310430	1.554928
6	6	0	1.462402	-0.410415	0.058652
7	6	0	-2.989476	-0.692542	-0.595474
8	6	0	-2.227276	-0.945592	-1.915042
9	6	0	-4.076754	0.383130	-0.829468
10	6	0	-3.673127	-2.013978	-0.156848
11	6	0	0.759481	2.004899	-0.997109
12	6	0	0.990383	1.714552	-2.488817
13	6	0	1.860411	2.994329	-0.508553
14	6	0	-0.613000	2.692242	-0.813699
15	6	0	2.091347	-1.578830	-0.663554
16	6	0	1.343267	-2.862346	-0.220705
17	6	0	3.570675	-1.682675	-0.210854
18	6	0	2.039770	-1.475077	-2.194847
19	9	0	-1.535792	0.139570	2.875332
20	9	0	0.404377	1.876268	2.287389
21	9	0	1.722428	-1.061193	2.549730
22	1	0	-1.741555	-0.032516	-2.272322
23	1	0	-1.456277	-1.711342	-1.782007
24	1	0	-2.921078	-1.289112	-2.692305
25	1	0	-4.651089	0.560407	0.085405
26	1	0	-3.633450	1.335066	-1.139859
27	1	0	-4.768921	0.057051	-1.615766
28	1	0	-4.248576	-1.869320	0.763019
29	1	0	-4.355796	-2.363971	-0.941472
30	1	0	-2.929633	-2.796786	0.026937
31	1	0	2.005590	1.356705	-2.680301
32	1	0	0.853221	2.639056	-3.061752
33	1	0	0.284928	0.972534	-2.874347
34	1	0	1.723899	3.248947	0.546795
35	1	0	2.858991	2.562066	-0.633328
36	1	0	1.808669	3.920528	-1.093566
37	1	0	-0.813376	2.910618	0.238781
38	1	0	-0.626629	3.637352	-1.369172
39	1	0	-1.424516	2.061463	-1.184666
40	1	0	1.379030	-2.992550	0.865494
41	1	0	1.804793	-3.743081	-0.682694

42	1	0	0.291021	-2.827148	-0.522006
43	1	0	3.649969	-1.777569	0.877249
44	1	0	4.138543	-0.797378	-0.518363
45	1	0	4.041998	-2.564170	-0.661890
46	1	0	1.015263	-1.342151	-2.555795
47	1	0	2.436380	-2.396510	-2.636938
48	1	0	2.647106	-0.645087	-2.566012

Zero-point vibrational energy 1070754.1 (Joules/Mol)
255.91637 (Kcal/Mol)
Zero-point correction= 0.407829 (Hartree/Particle)
Thermal correction to Energy= 0.433658
Thermal correction to Enthalpy= 0.434602
Thermal correction to Gibbs Free Energy= 0.353400
Sum of electronic and zero-point Energies= -1001.033692
Sum of electronic and thermal Energies= -1001.007863
Sum of electronic and thermal Enthalpies= -1001.006919
Sum of electronic and thermal Free Energies= -1001.088121

TS3-6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.332550	-0.569045	-0.306075
2	6	0	0.389623	-0.980600	-1.415290
3	6	0	-0.204124	0.213859	-1.422550
4	6	0	0.765518	0.691719	-0.251439
5	6	0	-1.832386	-0.047939	0.828822
6	6	0	-0.757319	0.253980	1.339576
7	6	0	2.308249	-1.483700	0.388825
8	9	0	0.201510	-2.152946	-2.029481
9	6	0	1.196182	2.143960	-0.094763
10	9	0	-1.084100	0.850334	-2.197560
11	9	0	0.001574	0.442260	2.413690
12	6	0	-3.192273	-0.387557	0.353606
13	6	0	3.268720	-2.061614	-0.682799
14	6	0	1.492668	-2.651409	1.009292
15	6	0	3.128545	-0.811263	1.499027
16	6	0	2.172769	2.405525	1.064140
17	6	0	-0.040661	3.054127	0.088620
18	6	0	1.889125	2.535265	-1.429434
19	6	0	-4.017497	-0.857802	1.580069
20	6	0	-3.155452	-1.523019	-0.693925
21	6	0	-3.861613	0.864797	-0.259067

22	1	0	3.865152	-1.267609	-1.146073
23	1	0	3.957004	-2.777902	-0.218824
24	1	0	2.719555	-2.582619	-1.473580
25	1	0	0.828570	-2.284440	1.798367
26	1	0	2.174765	-3.390020	1.447830
27	1	0	0.882420	-3.157889	0.254978
28	1	0	2.480629	-0.325876	2.233665
29	1	0	3.726612	-1.568624	2.019176
30	1	0	3.820937	-0.066188	1.096530
31	1	0	1.753776	2.089045	2.022097
32	1	0	2.379794	3.480665	1.123133
33	1	0	3.127621	1.895948	0.915221
34	1	0	-0.784275	2.887466	-0.696343
35	1	0	-0.524803	2.881038	1.054046
36	1	0	0.267883	4.105262	0.046026
37	1	0	1.222303	2.394553	-2.287338
38	1	0	2.789963	1.934430	-1.593844
39	1	0	2.178727	3.592685	-1.402091
40	1	0	-4.068642	-0.072890	2.341731
41	1	0	-3.570375	-1.747300	2.036642
42	1	0	-5.040379	-1.107312	1.271154
43	1	0	-2.629697	-1.208335	-1.599338
44	1	0	-2.648556	-2.408510	-0.296080
45	1	0	-4.177250	-1.808558	-0.971973
46	1	0	-3.301315	1.219274	-1.128088
47	1	0	-3.914731	1.677401	0.473313
48	1	0	-4.882294	0.623780	-0.579997

Zero-point vibrational energy 1072603.5 (Joules/Mol)
256.35839 (Kcal/Mol)
Zero-point correction= 0.408533 (Hartree/Particle)
Thermal correction to Energy= 0.434058
Thermal correction to Enthalpy= 0.435002
Thermal correction to Gibbs Free Energy= 0.355170
Sum of electronic and zero-point Energies= -1001.039722
Sum of electronic and thermal Energies= -1001.014197
Sum of electronic and thermal Enthalpies= -1001.013253
Sum of electronic and thermal Free Energies= -1001.093085

TS3-7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.204509	-0.707747	-0.251869

2	6	0	-1.349621	0.860675	-0.363558
3	6	0	-0.126702	0.877371	-0.910086
4	6	0	0.104780	-0.618381	-0.666134
5	6	0	2.516660	-0.330635	0.785987
6	6	0	1.343716	-0.665692	0.999449
7	6	0	-2.133477	-1.876490	-0.079583
8	6	0	-2.253454	1.927957	0.205317
9	9	0	0.728589	1.834358	-1.276853
10	9	0	0.500534	-1.041970	1.954767
11	6	0	3.766623	0.120619	0.149375
12	6	0	-1.313667	-3.185590	-0.080159
13	6	0	-3.125544	-1.899673	-1.272772
14	6	0	-2.921621	-1.793772	1.247998
15	6	0	4.957707	-0.634842	0.788991
16	6	0	3.929265	1.642044	0.380355
17	6	0	3.733293	-0.169597	-1.372647
18	9	0	0.778984	-1.444915	-1.505488
19	6	0	-3.714425	1.743490	-0.260350
20	6	0	-1.757348	3.308958	-0.277585
21	6	0	-2.188195	1.883391	1.751029
22	1	0	-0.609614	-3.202946	0.758015
23	1	0	-1.986539	-4.044790	0.020306
24	1	0	-0.743135	-3.300721	-1.005372
25	1	0	-2.592094	-2.028079	-2.220581
26	1	0	-3.825418	-2.736495	-1.157841
27	1	0	-3.710222	-0.976775	-1.334272
28	1	0	-2.236503	-1.734802	2.099886
29	1	0	-3.543967	-2.688838	1.368338
30	1	0	-3.583829	-0.923467	1.278862
31	1	0	4.866891	-1.714744	0.632006
32	1	0	5.899080	-0.298568	0.337659
33	1	0	5.007446	-0.449746	1.867188
34	1	0	3.086832	2.187185	-0.056102
35	1	0	4.855395	1.998384	-0.086779
36	1	0	3.971935	1.874535	1.449848
37	1	0	3.585962	-1.236169	-1.565056
38	1	0	4.680894	0.142785	-1.828743
39	1	0	2.919956	0.378999	-1.855417
40	1	0	-3.784485	1.760262	-1.353884
41	1	0	-4.141336	0.799820	0.092634
42	1	0	-4.338274	2.556013	0.131275
43	1	0	-0.733629	3.506591	0.054339
44	1	0	-1.777760	3.377986	-1.370794
45	1	0	-2.403131	4.097915	0.124433
46	1	0	-1.167343	2.066158	2.103496

47	1	0	-2.509865	0.914773	2.144757
48	1	0	-2.841096	2.654951	2.177428

Zero-point vibrational energy 1071640.3 (Joules/Mol)
256.12818 (Kcal/Mol)
Zero-point correction= 0.408166 (Hartree/Particle)
Thermal correction to Energy= 0.433756
Thermal correction to Enthalpy= 0.434700
Thermal correction to Gibbs Free Energy= 0.354266
Sum of electronic and zero-point Energies= -1001.045282
Sum of electronic and thermal Energies= -1001.019693

TS3-8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.618709	-0.985795	-0.387840
2	6	0	0.521935	-1.526912	-0.537486
3	6	0	-1.262397	-0.414449	0.219549
4	6	0	-0.436434	1.033634	0.339547
5	6	0	-1.007516	-0.507502	1.561683
6	6	0	-0.232279	0.728640	1.635401
7	6	0	3.071843	-0.718824	-0.240565
8	9	0	-0.122319	-2.630755	-0.921379
9	6	0	-0.207160	2.254024	-0.516630
10	6	0	-2.550769	-0.811428	-0.502586
11	9	0	0.480912	1.264193	2.629986
12	6	0	3.673009	-1.952107	0.485424
13	6	0	3.382096	0.541161	0.596123
14	6	0	3.730096	-0.588507	-1.634038
15	6	0	-1.558279	2.941963	-0.847423
16	6	0	0.642969	3.270030	0.281197
17	6	0	0.495253	1.913186	-1.848617
18	9	0	-1.351105	-1.372092	2.506698
19	6	0	-3.689966	0.148703	-0.068519
20	6	0	-2.977613	-2.235412	-0.068169
21	6	0	-2.406140	-0.769593	-2.036155
22	1	0	3.239140	-2.067016	1.484108
23	1	0	4.758576	-1.832200	0.592246
24	1	0	3.480368	-2.870356	-0.078521
25	1	0	2.850131	0.525184	1.552223
26	1	0	4.458498	0.603766	0.797314
27	1	0	3.091494	1.449369	0.060578
28	1	0	3.569235	-1.494763	-2.226891

29	1	0	4.810793	-0.430676	-1.529207
30	1	0	3.317137	0.258063	-2.192504
31	1	0	-2.131039	3.157866	0.060636
32	1	0	-2.175052	2.332964	-1.513349
33	1	0	-1.359961	3.892217	-1.357228
34	1	0	0.116219	3.605293	1.180863
35	1	0	0.844557	4.149422	-0.340987
36	1	0	1.600077	2.845599	0.591909
37	1	0	-0.045107	1.142482	-2.405286
38	1	0	0.552613	2.812444	-2.474195
39	1	0	1.508559	1.545594	-1.676049
40	1	0	-3.468757	1.193689	-0.294492
41	1	0	-3.876352	0.068036	1.008226
42	1	0	-4.616833	-0.115069	-0.592766
43	1	0	-3.124015	-2.293706	1.014726
44	1	0	-3.931029	-2.486348	-0.547861
45	1	0	-2.241152	-2.985786	-0.355060
46	1	0	-2.148595	0.233263	-2.392957
47	1	0	-3.355120	-1.052720	-2.507100
48	1	0	-1.635933	-1.463581	-2.381494

Zero-point vibrational energy 1072816.6 (Joules/Mol)
256.40932 (Kcal/Mol)
Zero-point correction= 0.408614 (Hartree/Particle)
Thermal correction to Energy= 0.434049
Thermal correction to Enthalpy= 0.434994
Thermal correction to Gibbs Free Energy= 0.356235
Sum of electronic and zero-point Energies= -1001.030959
Sum of electronic and thermal Energies= -1001.005524
Sum of electronic and thermal Enthalpies= -1001.004580

1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.706670	-1.212488	-0.000122
2	6	0	-0.008107	-0.000097	-0.000250
3	6	0	0.706485	1.212404	-0.000129
4	6	0	2.099519	1.208188	0.000090
5	6	0	2.800789	0.000116	0.000185
6	6	0	2.099703	-1.208062	0.000083
7	6	0	-1.440142	-0.000200	-0.000377
8	6	0	-2.645015	0.000031	0.000139
9	9	0	-3.933790	0.000046	0.000215

10	1	0	0.158953	2.149921	-0.000189
11	1	0	2.639389	2.151279	0.000188
12	1	0	3.887356	0.000199	0.000359
13	1	0	2.639719	-2.151069	0.000183
14	1	0	0.159282	-2.150089	-0.000184

Zero-point vibrational energy 269747.6 (Joules/Mol)
64.47122 (Kcal/Mol)
Zero-point correction= 0.102741 (Hartree/Particle)
Thermal correction to Energy= 0.110080
Thermal correction to Enthalpy= 0.111024
Thermal correction to Gibbs Free Energy= 0.070423
Sum of electronic and zero-point Energies= -407.499425
Sum of electronic and thermal Energies= -407.492086
Sum of electronic and thermal Enthalpies= -407.491142
Sum of electronic and thermal Free Energies= -407.531744

1c-triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.605661	1.224686	-0.171031
2	6	0	-0.113188	-0.000038	-0.332551
3	6	0	0.605741	-1.224735	-0.170989
4	6	0	1.956025	-1.215019	0.136301
5	6	0	2.640523	0.000053	0.291939
6	6	0	1.955962	1.215060	0.136270
7	6	0	-1.453246	-0.000058	-0.721061
8	6	0	-2.731164	-0.000002	-0.429885
9	9	0	-3.290188	0.000022	0.788948
10	1	0	0.069769	-2.160634	-0.293537
11	1	0	2.487410	-2.154734	0.259937
12	1	0	3.699714	0.000084	0.532814
13	1	0	2.487262	2.154827	0.259892
14	1	0	0.069654	2.160563	-0.293594

Zero-point vibrational energy 263741.3 (Joules/Mol)
63.03569 (Kcal/Mol)
Zero-point correction= 0.100454 (Hartree/Particle)
Thermal correction to Energy= 0.108025
Thermal correction to Enthalpy= 0.108969
Thermal correction to Gibbs Free Energy= 0.066235
Sum of electronic and zero-point Energies= -407.409968
Sum of electronic and thermal Energies= -407.402397

Sum of electronic and thermal Enthalpies= -407.401453
Sum of electronic and thermal Free Energies= -407.444187

TS1c-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.445813	-0.001773	-0.958874
2	6	0	0.445836	-0.004801	0.958961
3	6	0	1.676997	-0.003793	0.869084
4	6	0	-1.676976	-0.000498	-0.869020
5	6	0	-3.034178	0.000597	-0.459440
6	6	0	-3.726563	1.216384	-0.264522
7	6	0	-5.064203	1.211960	0.116266
8	6	0	-5.739355	0.002909	0.308076
9	6	0	-5.066475	-1.207292	0.115512
10	6	0	-3.728859	-1.214007	-0.265316
11	6	0	3.034183	-0.001112	0.459460
12	6	0	3.725993	1.215470	0.267463
13	6	0	5.063611	1.212599	-0.113406
14	6	0	5.739322	0.004331	-0.308179
15	6	0	5.067019	-1.206647	-0.118517
16	6	0	3.729420	-1.214915	0.262351
17	9	0	-0.605339	-0.007056	1.737079
18	9	0	0.605377	-0.001856	-1.736976
19	1	0	-3.198409	2.152884	-0.414542
20	1	0	-5.583857	2.154647	0.264905
21	1	0	-6.784362	0.003795	0.605491
22	1	0	-5.587903	-2.149089	0.263580
23	1	0	-3.202474	-2.151408	-0.415919
24	1	0	3.197402	2.151353	0.419775
25	1	0	5.582813	2.155888	-0.259789
26	1	0	6.784313	0.006426	-0.605641
27	1	0	5.588884	-2.147837	-0.268889
28	1	0	3.203485	-2.152928	0.410705

Zero-point vibrational energy 539064.8 (Joules/Mol)
128.83959 (Kcal/Mol)
Zero-point correction= 0.205319 (Hartree/Particle)
Thermal correction to Energy= 0.221085
Thermal correction to Enthalpy= 0.222029
Thermal correction to Gibbs Free Energy= 0.157259
Sum of electronic and zero-point Energies= -814.985412
Sum of electronic and thermal Energies= -814.969646

Sum of electronic and thermal Enthalpies= -814.968702
Sum of electronic and thermal Free Energies= -815.033472

INT1c-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.848199	-1.224325	-0.144426
2	6	0	3.121261	-0.000237	-0.263809
3	6	0	3.847214	1.224478	-0.144738
4	6	0	5.214081	1.213668	0.082026
5	6	0	5.908144	0.000950	0.196847
6	6	0	5.215062	-1.212352	0.082330
7	6	0	1.760648	-0.000789	-0.507551
8	6	0	0.462010	-0.000955	-0.576676
9	9	0	-0.212696	-0.001438	-1.763657
10	6	0	-0.462125	-0.000667	0.577325
11	9	0	0.212607	0.000155	1.764300
12	6	0	-1.760772	-0.001612	0.508281
13	6	0	-3.121291	-0.000643	0.264092
14	6	0	-3.846710	1.224321	0.144185
15	6	0	-5.213488	1.213971	-0.083093
16	6	0	-5.908012	0.001493	-0.197686
17	6	0	-5.215461	-1.212048	-0.082452
18	6	0	-3.848697	-1.224483	0.144833
19	1	0	-3.305958	2.161142	0.233343
20	1	0	-5.749061	2.155199	-0.173468
21	1	0	-6.979550	0.002320	-0.375474
22	1	0	-5.752562	-2.152452	-0.172323
23	1	0	-3.309475	-2.162138	0.234492
24	1	0	3.306822	2.161486	-0.234096
25	1	0	5.750077	2.154712	0.171801
26	1	0	6.979752	0.001405	0.374214
27	1	0	5.751816	-2.152941	0.172339
28	1	0	3.308574	-2.161800	-0.233545

Zero-point vibrational energy 540079.9 (Joules/Mol)
129.08219 (Kcal/Mol)
Zero-point correction= 0.205706 (Hartree/Particle)
Thermal correction to Energy= 0.221309
Thermal correction to Enthalpy= 0.222253
Thermal correction to Gibbs Free Energy= 0.158711
Sum of electronic and zero-point Energies= -815.023757
Sum of electronic and thermal Energies= -815.008154

Sum of electronic and thermal Enthalpies= -815.007210
Sum of electronic and thermal Free Energies= -815.070751

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.097890	-0.311990	0.022975
2	6	0	-0.905927	-1.816082	-0.455861
3	6	0	0.323632	-1.655651	-0.335547
4	6	0	1.615602	-1.156195	-0.057643
5	6	0	2.109508	-1.138723	1.268228
6	6	0	3.392494	-0.675934	1.536636
7	6	0	4.211925	-0.223551	0.497728
8	6	0	3.738970	-0.238401	-0.818249
9	6	0	2.458216	-0.699963	-1.098485
10	6	0	-3.231253	-0.764141	0.349712
11	6	0	-1.457554	0.998934	-0.056541
12	6	0	-1.656888	1.936384	0.971775
13	6	0	-1.077379	3.200777	0.897654
14	6	0	-0.287979	3.548981	-0.200729
15	6	0	-0.084254	2.623603	-1.225710
16	6	0	-0.662023	1.356959	-1.155521
17	1	0	-0.505782	0.639635	-1.953954
18	1	0	0.524950	2.888509	-2.085660
19	1	0	0.165561	4.534865	-0.256680
20	1	0	-1.241469	3.914658	1.700484
21	1	0	-2.272018	1.660437	1.822741
22	9	0	-3.983265	-1.793691	0.582595
23	9	0	-1.784830	-2.752783	-0.767620
24	1	0	2.091159	-0.720314	-2.119966
25	1	0	4.374537	0.109483	-1.628105
26	1	0	5.214225	0.136796	0.712120
27	1	0	3.757038	-0.665836	2.560242
28	1	0	1.469462	-1.490009	2.071470

Zero-point vibrational energy 537564.0 (Joules/Mol)
128.48088 (Kcal/Mol)
Zero-point correction= 0.204747 (Hartree/Particle)
Thermal correction to Energy= 0.220349
Thermal correction to Enthalpy= 0.221293
Thermal correction to Gibbs Free Energy= 0.158722
Sum of electronic and zero-point Energies= -814.966641
Sum of electronic and thermal Energies= -814.951040

Sum of electronic and thermal Enthalpies= -814.950096
Sum of electronic and thermal Free Energies= -815.012667

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.672830	-0.695194	0.628128
2	6	0	0.676860	0.796649	0.508314
3	6	0	1.947005	0.375730	-0.070802
4	6	0	3.135921	1.013578	0.333346
5	6	0	4.358571	0.650754	-0.223550
6	6	0	4.422656	-0.358969	-1.187294
7	6	0	3.250736	-1.000153	-1.590692
8	6	0	2.022308	-0.638391	-1.039735
9	6	0	0.165992	1.844071	1.006265
10	6	0	-0.155511	-1.649653	1.281757
11	6	0	-1.947084	-0.377936	-0.005617
12	6	0	-2.039811	0.503666	-1.095210
13	6	0	-3.272954	0.763674	-1.691589
14	6	0	-4.432519	0.151737	-1.214454
15	6	0	-4.351278	-0.725933	-0.130151
16	6	0	-3.124364	-0.986403	0.472249
17	1	0	-3.057750	-1.666407	1.315697
18	1	0	-5.248012	-1.206511	0.251893
19	1	0	-5.392040	0.357814	-1.680690
20	1	0	-3.324610	1.447803	-2.534289
21	1	0	-1.143751	0.986931	-1.468981
22	9	0	-0.882215	2.295637	1.631421
23	1	0	3.082332	1.796605	1.083206
24	1	0	5.265132	1.155319	0.099849
25	1	0	5.378679	-0.644348	-1.617543
26	1	0	3.289428	-1.786386	-2.339803
27	1	0	1.115628	-1.143535	-1.354454
28	9	0	0.896968	-1.995707	1.964059

Zero-point vibrational energy 536424.7 (Joules/Mol)
128.20858 (Kcal/Mol)
Zero-point correction= 0.204313 (Hartree/Particle)
Thermal correction to Energy= 0.220101
Thermal correction to Enthalpy= 0.221045
Thermal correction to Gibbs Free Energy= 0.157323
Sum of electronic and zero-point Energies= -814.953063
Sum of electronic and thermal Energies= -814.937275
Sum of electronic and thermal Enthalpies= -814.936331

Sum of electronic and thermal Free Energies= -815.000053

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.169115	0.176942	0.432577
2	6	0	1.865403	-0.156574	-0.002860
3	6	0	1.649001	-1.440116	-0.545668
4	6	0	2.696361	-2.354818	-0.641821
5	6	0	3.976598	-2.014504	-0.203332
6	6	0	4.206416	-0.740962	0.330375
7	6	0	0.813666	0.824793	0.078473
8	6	0	0.749333	2.165996	0.095679
9	9	0	1.643387	3.146201	0.104164
10	6	0	-0.813666	0.824793	-0.078473
11	6	0	-1.865403	-0.156574	0.002859
12	6	0	-1.649001	-1.440115	0.545669
13	6	0	-2.696361	-2.354817	0.641822
14	6	0	-3.976598	-2.014504	0.203332
15	6	0	-4.206416	-0.740962	-0.330376
16	6	0	-3.169115	0.176942	-0.432578
17	6	0	-0.749333	2.165996	-0.095678
18	9	0	-1.643387	3.146200	-0.104164
19	1	0	-0.664182	-1.706875	0.913484
20	1	0	-2.509928	-3.337188	1.067744
21	1	0	-4.789733	-2.731140	0.277167
22	1	0	-5.200563	-0.466346	-0.673118
23	1	0	-3.350846	1.161196	-0.854108
24	1	0	0.664181	-1.706876	-0.913483
25	1	0	2.509927	-3.337188	-1.067742
26	1	0	4.789733	-2.731140	-0.277167
27	1	0	5.200563	-0.466346	0.673117
28	1	0	3.350847	1.161196	0.854106

Zero-point vibrational energy 550240.7 (Joules/Mol)
131.51069 (Kcal/Mol)
Zero-point correction= 0.209576 (Hartree/Particle)
Thermal correction to Energy= 0.224139
Thermal correction to Enthalpy= 0.225084
Thermal correction to Gibbs Free Energy= 0.166558
Sum of electronic and zero-point Energies= -815.065634
Sum of electronic and thermal Energies= -815.051070
Sum of electronic and thermal Enthalpies= -815.050126

Sum of electronic and thermal Free Energies= -815.108652

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.252013	-0.916605	1.152594
2	6	0	-0.260708	-0.182007	-0.834420
3	6	0	0.650423	-1.313505	-1.155191
4	6	0	1.736616	-0.670159	-0.616953
5	6	0	0.858539	0.580881	-0.450591
6	6	0	-2.475071	-0.885465	1.041307
7	6	0	-3.826224	-0.730797	0.633939
8	6	0	-4.501614	-1.776984	-0.031730
9	6	0	-5.829785	-1.625389	-0.416243
10	6	0	-6.512516	-0.436278	-0.143812
11	6	0	-5.856071	0.605246	0.518381
12	6	0	-4.527562	0.464264	0.905902
13	6	0	1.070653	1.988953	-0.313467
14	6	0	-0.044574	2.853659	-0.168943
15	6	0	0.133977	4.224535	-0.046324
16	6	0	1.419927	4.778665	-0.070168
17	6	0	2.528220	3.941274	-0.225465
18	6	0	2.362982	2.565143	-0.344038
19	6	0	3.028923	-1.111665	-0.146393
20	6	0	3.589836	-2.302922	-0.659328
21	6	0	4.821677	-2.758610	-0.204982
22	6	0	5.524662	-2.043933	0.770990
23	6	0	4.977054	-0.870417	1.293633
24	6	0	3.744240	-0.404851	0.842265
25	1	0	3.315759	0.494379	1.272141
26	1	0	5.509818	-0.316026	2.061695
27	1	0	6.488641	-2.401636	1.121876
28	1	0	5.238472	-3.675410	-0.613471
29	1	0	3.047664	-2.860944	-1.416795
30	1	0	-3.968169	-2.698874	-0.241573
31	1	0	-6.336048	-2.437633	-0.930839
32	1	0	-7.550155	-0.322192	-0.445113
33	1	0	-6.383146	1.531028	0.732993
34	1	0	-4.015185	1.270215	1.422405
35	1	0	-1.043109	2.428637	-0.151833
36	1	0	-0.733014	4.869952	0.067656
37	1	0	1.554454	5.852260	0.027145
38	1	0	3.528727	4.364453	-0.258853

39	1	0	3.228866	1.927546	-0.485682
40	9	0	-1.369026	0.216711	-1.469695
41	9	0	-0.155676	-1.174900	1.811899
42	9	0	0.407688	-2.582250	-1.469706

Zero-point vibrational energy 814412.8 (Joules/Mol)
194.64933 (Kcal/Mol)
Zero-point correction= 0.310193 (Hartree/Particle)
Thermal correction to Energy= 0.333572
Thermal correction to Enthalpy= 0.334516
Thermal correction to Gibbs Free Energy= 0.252114
Sum of electronic and zero-point Energies= -1222.558855
Sum of electronic and thermal Energies= -1222.535476
Sum of electronic and thermal Enthalpies= -1222.534532
Sum of electronic and thermal Free Energies= -1222.616934

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.604788	-0.498324	0.588036
2	6	0	0.427550	-0.937006	-1.406511
3	6	0	1.818111	-1.208734	-1.106216
4	6	0	2.768449	-0.172112	-1.153414
5	6	0	4.105364	-0.426952	-0.852329
6	6	0	4.512437	-1.713871	-0.494115
7	6	0	3.575108	-2.748618	-0.436958
8	6	0	2.237612	-2.499611	-0.735292
9	6	0	0.010418	0.866844	0.942389
10	6	0	0.827269	0.205425	1.886719
11	6	0	0.306024	-1.059087	1.560471
12	6	0	-2.001304	-0.886234	0.402845
13	6	0	-3.034939	0.064070	0.298035
14	6	0	-4.360883	-0.341962	0.160010
15	6	0	-4.685081	-1.699140	0.121062
16	6	0	-3.668181	-2.653351	0.229500
17	6	0	-2.343606	-2.254878	0.368960
18	6	0	-0.028644	2.191237	0.411199
19	6	0	-0.754206	2.515637	-0.762789
20	6	0	-0.768506	3.818695	-1.248174
21	6	0	-0.066937	4.833299	-0.589384
22	6	0	0.663111	4.527386	0.566104
23	6	0	0.687040	3.231370	1.061622
24	1	0	1.506693	-3.301262	-0.690541

25	1	0	3.887173	-3.751774	-0.159349
26	1	0	5.555094	-1.910149	-0.259276
27	1	0	4.830468	0.381096	-0.898525
28	1	0	2.446576	0.825566	-1.434893
29	1	0	1.215428	5.308302	1.082329
30	1	0	-0.084809	5.849613	-0.972558
31	1	0	-1.327451	4.044346	-2.152569
32	1	0	-1.283827	1.735514	-1.298008
33	1	0	1.255299	3.001345	1.957645
34	9	0	-1.629726	-0.467355	-2.619073
35	6	0	-0.385899	-0.781045	-2.356907
36	9	0	0.454306	-2.283129	2.048204
37	9	0	1.810825	0.614493	2.681339
38	1	0	-1.559090	-3.000910	0.453730
39	1	0	-2.798571	1.121468	0.345337
40	1	0	-5.144612	0.407512	0.087474
41	1	0	-5.719462	-2.012453	0.010023
42	1	0	-3.910673	-3.712513	0.205764

Zero-point vibrational energy 813631.6 (Joules/Mol)
194.46261 (Kcal/Mol)
Zero-point correction= 0.309896 (Hartree/Particle)
Thermal correction to Energy= 0.333144
Thermal correction to Enthalpy= 0.334089
Thermal correction to Gibbs Free Energy= 0.254541
Sum of electronic and zero-point Energies= -1222.540970
Sum of electronic and thermal Energies= -1222.517722
Sum of electronic and thermal Enthalpies= -1222.516778
Sum of electronic and thermal Free Energies= -1222.596325

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.860877	-1.304064	-0.058212
2	6	0	-0.076270	-0.352186	-1.932239
3	6	0	-1.146090	0.251008	-1.781776
4	6	0	-2.322867	0.858142	-1.279908
5	6	0	-3.496285	0.101436	-1.057333
6	6	0	-4.650806	0.715599	-0.585383
7	6	0	-4.667174	2.090339	-0.328410
8	6	0	-3.515039	2.851666	-0.547278
9	6	0	-2.354153	2.248482	-1.019434
10	6	0	-0.256832	-1.604709	0.829372

11	6	0	-1.103099	-2.694995	0.534254
12	6	0	-2.165134	-3.017135	1.371609
13	6	0	-2.414105	-2.259329	2.521166
14	6	0	-1.582333	-1.181829	2.825872
15	6	0	-0.514546	-0.853895	1.990424
16	6	0	2.094844	-0.347685	0.118299
17	6	0	2.888628	-1.349536	-0.425091
18	6	0	1.772082	-2.223736	-0.629205
19	6	0	2.294141	1.033481	0.434850
20	6	0	1.214324	1.914590	0.680340
21	6	0	1.447172	3.251088	0.989270
22	6	0	2.751534	3.748419	1.059303
23	6	0	3.830264	2.890933	0.810013
24	6	0	3.611575	1.555099	0.503064
25	9	0	4.161795	-1.401131	-0.806337
26	9	0	1.661799	-3.495784	-0.984124
27	9	0	0.858007	-0.718643	-2.780006
28	1	0	-3.476537	-0.966555	-1.247890
29	1	0	-5.543862	0.120530	-0.414411
30	1	0	-5.572686	2.565364	0.038922
31	1	0	-3.524508	3.920738	-0.352068
32	1	0	-1.459337	2.836530	-1.199418
33	1	0	-0.916813	-3.286359	-0.357433
34	1	0	-2.802620	-3.863459	1.128880
35	1	0	-3.246808	-2.510363	3.172394
36	1	0	-1.760418	-0.592054	3.721211
37	1	0	0.136468	-0.026321	2.249944
38	1	0	0.603275	3.910961	1.173413
39	1	0	0.197287	1.546311	0.606942
40	1	0	2.927781	4.792360	1.302745
41	1	0	4.847791	3.269802	0.857987
42	1	0	4.452327	0.895430	0.311579

Zero-point vibrational energy 813907.5 (Joules/Mol)
194.52856 (Kcal/Mol)
Zero-point correction= 0.310001 (Hartree/Particle)
Thermal correction to Energy= 0.333315
Thermal correction to Enthalpy= 0.334259
Thermal correction to Gibbs Free Energy= 0.253727
Sum of electronic and zero-point Energies= -1222.551819
Sum of electronic and thermal Energies= -1222.528506
Sum of electronic and thermal Enthalpies= -1222.527561
Sum of electronic and thermal Free Energies= -1222.608094

TS3c-4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.191509	-2.361892	0.216564
2	6	0	-1.214691	-0.691189	-1.310272
3	6	0	-0.873781	0.556980	-0.682505
4	6	0	0.541160	0.388540	-1.164776
5	6	0	1.840878	0.941382	-0.848018
6	6	0	2.929513	0.697857	-1.713686
7	6	0	4.190657	1.208370	-1.427138
8	6	0	4.399108	1.967872	-0.271441
9	6	0	3.333631	2.203965	0.600440
10	6	0	2.066803	1.698443	0.319244
11	6	0	-1.678399	1.590114	-0.111902
12	6	0	-3.027291	1.312791	0.233525
13	6	0	-3.835722	2.297630	0.784187
14	6	0	-3.336514	3.587500	1.002406
15	6	0	-2.014502	3.881910	0.653485
16	6	0	-1.193022	2.903469	0.105156
17	6	0	0.131261	-0.702303	-1.914521
18	6	0	-2.182603	-3.087618	-0.023277
19	6	0	-0.039439	-2.160203	1.071644
20	6	0	1.241353	-2.560633	0.652091
21	6	0	2.347201	-2.357789	1.475356
22	6	0	2.193180	-1.748632	2.722403
23	6	0	0.925615	-1.339030	3.143632
24	6	0	-0.183523	-1.536776	2.323851
25	1	0	-1.170280	-1.218289	2.645628
26	1	0	0.800057	-0.864280	4.113122
27	1	0	3.057279	-1.591277	3.362172
28	1	0	3.331559	-2.673269	1.140719
29	1	0	1.358780	-3.024596	-0.322191
30	9	0	-3.247040	-3.314817	-0.732832
31	9	0	0.801684	-1.650726	-2.569676
32	9	0	-2.382082	-0.998706	-1.905490
33	1	0	-3.422451	0.316800	0.061489
34	1	0	-4.864460	2.062465	1.044416
35	1	0	-3.972968	4.355016	1.433688
36	1	0	-1.623525	4.884749	0.804773
37	1	0	-0.177378	3.151702	-0.183283
38	1	0	2.771506	0.108764	-2.612051
39	1	0	1.251598	1.861228	1.016062
40	1	0	5.015479	1.015760	-2.108044
41	1	0	3.490778	2.780375	1.508274

42	1	0	5.384784	2.368560	-0.051465

Zero-point vibrational energy 814023.0 (Joules/Mol)
194.55616 (Kcal/Mol)
Zero-point correction= 0.310045 (Hartree/Particle)
Thermal correction to Energy= 0.333282
Thermal correction to Enthalpy= 0.334227
Thermal correction to Gibbs Free Energy= 0.253581
Sum of electronic and zero-point Energies= -1222.547295
Sum of electronic and thermal Energies= -1222.524058
Sum of electronic and thermal Enthalpies= -1222.523114
Sum of electronic and thermal Free Energies= -1222.603759

TS3c-5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.015350	1.279237	0.871590
2	6	0	-2.263690	-0.095103	0.676093
3	6	0	-3.603214	-0.537972	0.654017
4	6	0	-4.651002	0.355463	0.857823
5	6	0	-4.389522	1.710342	1.074458
6	6	0	-3.068345	2.166794	1.071819
7	6	0	-1.200787	-1.058038	0.464792
8	6	0	0.153429	-1.191572	0.660572
9	6	0	0.997979	-0.290162	-2.077815
10	6	0	0.884179	-1.512583	-2.152316
11	6	0	0.134539	-2.485961	-0.241820
12	6	0	-1.218139	-2.384106	-0.248903
13	9	0	1.033231	-2.638809	-2.809473
14	6	0	1.031221	1.114051	-1.867894
15	6	0	2.148852	1.734775	-1.266890
16	6	0	2.177970	3.114760	-1.087483
17	6	0	1.106117	3.907363	-1.506928
18	6	0	-0.004764	3.305317	-2.105665
19	6	0	-0.048403	1.926069	-2.283355
20	6	0	1.245333	-0.611696	1.390234
21	6	0	1.073187	0.435229	2.325098
22	6	0	2.158058	0.939052	3.032171
23	6	0	3.439783	0.414300	2.835205
24	6	0	3.624480	-0.632514	1.927973
25	6	0	2.544226	-1.145621	1.217712
26	9	0	0.955244	-3.547753	-0.243565
27	9	0	-2.218211	-3.129818	-0.697556

28	1	0	2.982344	1.120691	-0.942115
29	1	0	3.044946	3.575080	-0.620870
30	1	0	1.136775	4.985007	-1.370934
31	1	0	-0.842389	3.914324	-2.435629
32	1	0	-0.911998	1.457920	-2.745387
33	1	0	0.081700	0.833929	2.506930
34	1	0	2.003713	1.742419	3.747474
35	1	0	4.284320	0.812000	3.391020
36	1	0	4.613983	-1.056256	1.778928
37	1	0	2.690387	-1.969479	0.527930
38	1	0	-3.813636	-1.588459	0.479670
39	1	0	-5.675389	-0.006992	0.845662
40	1	0	-5.208262	2.406771	1.232937
41	1	0	-2.857167	3.223408	1.213036
42	1	0	-0.998528	1.652511	0.823768

Zero-point vibrational energy 820388.0 (Joules/Mol)
196.07743 (Kcal/Mol)
Zero-point correction= 0.312469 (Hartree/Particle)
Thermal correction to Energy= 0.335455
Thermal correction to Enthalpy= 0.336399
Thermal correction to Gibbs Free Energy= 0.257130
Sum of electronic and zero-point Energies= -1222.551525
Sum of electronic and thermal Energies= -1222.528539
Sum of electronic and thermal Enthalpies= -1222.527595
Sum of electronic and thermal Free Energies= -1222.606864

TS3c-6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.080819	-0.718364	-0.624071
2	6	0	-0.086520	-1.076773	-1.515600
3	6	0	-0.618795	0.141324	-1.384404
4	6	0	0.569607	0.569770	-0.449151
5	6	0	-1.723207	0.076700	1.295439
6	6	0	-0.543882	0.377660	1.485387
7	6	0	2.194409	-1.513587	-0.185086
8	9	0	-0.438074	-2.224781	-2.090845
9	6	0	1.126011	1.910208	-0.311987
10	9	0	-1.690629	0.782262	-1.826573
11	9	0	0.422975	0.702620	2.315412
12	6	0	-3.034568	-0.291266	0.896866
13	6	0	2.950594	-1.191555	0.965826

14	6	0	4.025921	-1.984300	1.349472
15	6	0	4.371977	-3.118478	0.607227
16	6	0	3.616151	-3.465588	-0.515987
17	6	0	2.533898	-2.683389	-0.904299
18	6	0	0.293297	3.017995	-0.576254
19	6	0	0.782380	4.318147	-0.481981
20	6	0	2.110393	4.546495	-0.117519
21	6	0	2.947835	3.457564	0.143684
22	6	0	2.466114	2.156222	0.049829
23	6	0	-3.951836	0.680363	0.439114
24	6	0	-5.240326	0.312792	0.064049
25	6	0	-5.645787	-1.022281	0.139359
26	6	0	-4.747866	-1.993380	0.593211
27	6	0	-3.456189	-1.638329	0.966224
28	1	0	2.653726	-0.345966	1.576461
29	1	0	4.590417	-1.725313	2.241213
30	1	0	5.213474	-3.734473	0.911563
31	1	0	3.868846	-4.353806	-1.088744
32	1	0	1.944658	-2.963548	-1.771574
33	1	0	-0.739940	2.848733	-0.860687
34	1	0	0.122868	5.155559	-0.693758
35	1	0	2.491228	5.561021	-0.039538
36	1	0	3.986593	3.624024	0.416730
37	1	0	3.135666	1.324337	0.235633
38	1	0	-3.637744	1.717900	0.384451
39	1	0	-5.933182	1.072407	-0.288279
40	1	0	-6.653499	-1.304310	-0.152886
41	1	0	-5.056857	-3.033516	0.654711
42	1	0	-2.757280	-2.391671	1.316687

Zero-point vibrational energy 820757.3 (Joules/Mol)
196.16570 (Kcal/Mol)

Zero-point correction= 0.312610 (Hartree/Particle)
Thermal correction to Energy= 0.335516
Thermal correction to Enthalpy= 0.336460
Thermal correction to Gibbs Free Energy= 0.257447
Sum of electronic and zero-point Energies= -1222.551134
Sum of electronic and thermal Energies= -1222.528228
Sum of electronic and thermal Enthalpies= -1222.527283
Sum of electronic and thermal Free Energies= -1222.606297

TS3c-7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.542770	-0.373914	0.482611
2	6	0	0.362844	0.573560	0.880620
3	6	0	-0.206797	-0.471563	1.512591
4	6	0	0.844285	-1.440071	0.996869
5	6	0	-1.409184	-2.062087	-0.812406
6	6	0	-0.239131	-2.428578	-0.698340
7	6	0	2.900268	-0.204536	0.048020
8	6	0	-0.080094	1.898071	0.493187
9	9	0	-1.359902	-0.668493	2.133373
10	9	0	0.747347	-3.215723	-1.060376
11	6	0	-2.690925	-1.459761	-0.736828
12	9	0	1.304350	-2.570601	1.554697
13	6	0	3.656305	-1.333153	-0.351438
14	6	0	4.984680	-1.193681	-0.730563
15	6	0	5.596561	0.065474	-0.722118
16	6	0	4.862941	1.186774	-0.328369
17	6	0	3.528602	1.060707	0.048524
18	6	0	-1.114138	2.530997	1.215257
19	6	0	-1.569098	3.790605	0.842579
20	6	0	-1.006460	4.450439	-0.255215
21	6	0	0.011729	3.831654	-0.981686
22	6	0	0.474079	2.568677	-0.614333
23	6	0	-3.038561	-0.390612	-1.592714
24	6	0	-4.303195	0.183364	-1.524206
25	6	0	-5.244849	-0.287567	-0.603904
26	6	0	-4.911449	-1.341279	0.251469
27	6	0	-3.650714	-1.926150	0.189069
28	1	0	3.178159	-2.306935	-0.375553
29	1	0	5.548597	-2.069812	-1.039337
30	1	0	6.635439	0.169717	-1.022318
31	1	0	5.333017	2.166493	-0.312670
32	1	0	2.972626	1.934643	0.370764
33	1	0	-1.553184	2.023204	2.068860
34	1	0	-2.365335	4.262843	1.411893
35	1	0	-1.361135	5.436959	-0.540551
36	1	0	0.448656	4.331822	-1.842024
37	1	0	1.253532	2.088771	-1.196982
38	1	0	-2.303574	-0.022557	-2.301687
39	1	0	-4.555958	1.004824	-2.189163
40	1	0	-6.231585	0.164524	-0.553625
41	1	0	-5.638746	-1.709653	0.970077
42	1	0	-3.389477	-2.745707	0.851014

Zero-point vibrational energy 820361.6 (Joules/Mol)

196.07112 (Kcal/Mol)

Zero-point correction=	0.312459 (Hartree/Particle)
Thermal correction to Energy=	0.335442
Thermal correction to Enthalpy=	0.336386
Thermal correction to Gibbs Free Energy=	0.256834
Sum of electronic and zero-point Energies=	-1222.555795
Sum of electronic and thermal Energies=	-1222.532812
Sum of electronic and thermal Enthalpies=	-1222.531868
Sum of electronic and thermal Free Energies=	-1222.611420

TS3c-8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.622879	-1.301827	-1.320266
2	6	0	-0.593845	-1.489175	-1.288640
3	6	0	-1.556255	-0.530893	0.505919
4	6	0	-0.137192	-0.030728	1.158852
5	6	0	-1.483738	-1.555358	1.414283
6	6	0	-0.189072	-1.134610	1.942721
7	6	0	2.023288	-1.069469	-1.293424
8	9	0	-1.674842	-2.002464	-1.830531
9	6	0	0.718411	1.121670	1.072028
10	6	0	-2.701962	0.150336	-0.097730
11	9	0	0.626608	-1.677138	2.841504
12	9	0	-2.281457	-2.567274	1.723344
13	6	0	2.891534	-1.967701	-0.633278
14	6	0	4.266448	-1.756088	-0.640308
15	6	0	4.808730	-0.646093	-1.295080
16	6	0	3.960486	0.254017	-1.944395
17	6	0	2.583904	0.048496	-1.948279
18	6	0	2.016384	1.060029	1.633649
19	6	0	2.855468	2.165928	1.600536
20	6	0	2.429660	3.361745	1.011784
21	6	0	1.150697	3.437560	0.457876
22	6	0	0.300388	2.334218	0.486099
23	6	0	-4.004735	-0.132944	0.359084
24	6	0	-5.111443	0.489998	-0.211705
25	6	0	-4.945854	1.414387	-1.245835
26	6	0	-3.661353	1.696877	-1.715882
27	6	0	-2.552822	1.065870	-1.156919
28	1	0	2.470801	-2.830135	-0.124988
29	1	0	4.919633	-2.461283	-0.132879
30	1	0	5.883237	-0.484798	-1.298399

31	1	0	4.373557	1.120941	-2.453228
32	1	0	1.926273	0.746392	-2.456772
33	1	0	2.355943	0.132804	2.083717
34	1	0	3.850040	2.095747	2.032675
35	1	0	3.088301	4.225547	0.989840
36	1	0	0.806119	4.365495	0.008904
37	1	0	-0.702540	2.417273	0.084679
38	1	0	-4.142129	-0.840977	1.170491
39	1	0	-6.106532	0.259676	0.159570
40	1	0	-5.810039	1.903589	-1.686544
41	1	0	-3.522493	2.401074	-2.531887
42	1	0	-1.562969	1.253051	-1.560570

Zero-point vibrational energy 820472.1 (Joules/Mol)
196.09755 (Kcal/Mol)
Zero-point correction= 0.312501 (Hartree/Particle)
Thermal correction to Energy= 0.335429
Thermal correction to Enthalpy= 0.336373
Thermal correction to Gibbs Free Energy= 0.257269
Sum of electronic and zero-point Energies= -1222.549435
Sum of electronic and thermal Energies= -1222.526508
Sum of electronic and thermal Enthalpies= -1222.525564
Sum of electronic and thermal Free Energies= -1222.604667

1d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.109536	0.000005	-0.000010
2	6	0	-0.898695	-0.000029	-0.000781
3	17	0	-3.760337	0.000003	0.000138
4	6	0	0.530740	-0.000015	-0.000458
5	6	0	1.244825	-1.213685	-0.000195
6	6	0	2.637553	-1.208728	0.000280
7	6	0	3.338049	0.000017	0.000500
8	6	0	2.637525	1.208747	0.000280
9	6	0	1.244797	1.213673	-0.000196
10	1	0	0.696813	-2.150795	-0.000351
11	1	0	3.178037	-2.151379	0.000481
12	1	0	4.424591	0.000030	0.000879
13	1	0	3.177988	2.151410	0.000482
14	1	0	0.696763	2.150770	-0.000352

Zero-point vibrational energy 266011.3 (Joules/Mol)

63.57822 (Kcal/Mol)

Zero-point correction=	0.101318 (Hartree/Particle)
Thermal correction to Energy=	0.108987
Thermal correction to Enthalpy=	0.109931
Thermal correction to Gibbs Free Energy=	0.067960
Sum of electronic and zero-point Energies=	-767.879899
Sum of electronic and thermal Energies=	-767.872231
Sum of electronic and thermal Enthalpies=	-767.871287
Sum of electronic and thermal Free Energies=	-767.913258

1d-triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.112005	-1.230008	0.181695
2	6	0	-0.402248	-0.000105	0.388626
3	6	0	-1.111812	1.229916	0.181930
4	6	0	-2.439979	1.217147	-0.200500
5	6	0	-3.115672	0.000158	-0.394718
6	6	0	-2.440161	-1.216982	-0.200724
7	6	0	0.901616	-0.000307	0.843379
8	6	0	2.199630	-0.000231	0.836832
9	17	0	3.316353	0.000123	-0.534029
10	1	0	-0.582858	2.165352	0.332988
11	1	0	-2.964347	2.156125	-0.355123
12	1	0	-4.159179	0.000268	-0.695550
13	1	0	-2.964677	-2.155846	-0.355524
14	1	0	-0.583158	-2.165530	0.332589

Zero-point vibrational energy 259280.1 (Joules/Mol)
61.96942 (Kcal/Mol)

Zero-point correction=	0.098755 (Hartree/Particle)
Thermal correction to Energy=	0.106717
Thermal correction to Enthalpy=	0.107662
Thermal correction to Gibbs Free Energy=	0.063352
Sum of electronic and zero-point Energies=	-767.786252
Sum of electronic and thermal Energies=	-767.778289
Sum of electronic and thermal Enthalpies=	-767.777345
Sum of electronic and thermal Free Energies=	-767.821655

TS1d-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.513209	-0.857560	-0.059472
2	6	0	-0.513208	0.857563	-0.059344
3	17	0	0.629316	2.126678	-0.099204
4	17	0	-0.629315	-2.126669	-0.099517
5	6	0	1.756882	-0.753827	-0.029670
6	6	0	-1.756881	0.753826	-0.029554
7	6	0	-3.123940	0.425100	0.010744
8	6	0	3.123941	-0.425104	0.010677
9	6	0	3.863673	-0.258089	-1.185886
10	6	0	5.221054	0.033555	-1.137131
11	6	0	5.873115	0.163664	0.093779
12	6	0	5.155428	-0.000806	1.283278
13	6	0	3.797478	-0.292102	1.249830
14	6	0	-3.797481	0.291928	1.249877
15	6	0	-5.155433	0.000633	1.283280
16	6	0	-5.873117	-0.163669	0.093756
17	6	0	-5.221052	-0.033391	-1.137133
18	6	0	-3.863670	0.258255	-1.185844
19	1	0	-3.352946	0.359776	-2.138157
20	1	0	-5.776513	-0.160795	-2.062280
21	1	0	-6.934854	-0.391583	0.125723
22	1	0	-5.659740	-0.100303	2.240442
23	1	0	-3.235895	0.419672	2.169858
24	1	0	3.352952	-0.359479	-2.138215
25	1	0	5.776517	0.161090	-2.062258
26	1	0	6.934851	0.391578	0.125780
27	1	0	5.659732	0.099999	2.240454
28	1	0	3.235889	-0.419975	2.169791

Zero-point vibrational energy 531909.7 (Joules/Mol)
127.12948 (Kcal/Mol)
Zero-point correction= 0.202594 (Hartree/Particle)
Thermal correction to Energy= 0.218789
Thermal correction to Enthalpy= 0.219733
Thermal correction to Gibbs Free Energy= 0.153480
Sum of electronic and zero-point Energies= -1535.724981
Sum of electronic and thermal Energies= -1535.708786
Sum of electronic and thermal Enthalpies= -1535.707841
Sum of electronic and thermal Free Energies= -1535.774095

INT1d-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.565524	-0.475900	-0.001394
2	6	0	-1.832576	-0.197996	-0.001601
3	6	0	1.832594	0.198227	-0.000962
4	6	0	0.565543	0.476138	-0.001093
5	17	0	-0.028317	-2.204715	-0.001079
6	17	0	0.028335	2.204944	-0.000349
7	6	0	-3.211692	-0.107936	-0.000535
8	6	0	3.211693	0.107970	-0.000195
9	6	0	-3.943124	-0.048386	-1.225569
10	6	0	-5.324703	0.055227	-1.212012
11	6	0	-6.024361	0.106988	0.001784
12	6	0	-5.322779	0.054176	1.214429
13	6	0	-3.941185	-0.049451	1.225720
14	6	0	3.941441	0.048715	1.225867
15	6	0	5.323021	-0.055092	1.214226
16	6	0	6.024335	-0.107334	0.001405
17	6	0	5.324422	-0.054810	-1.212216
18	6	0	3.942858	0.049000	-1.225425
19	1	0	-3.397862	-0.087077	-2.163048
20	1	0	-5.867770	0.096650	-2.152248
21	1	0	-7.107374	0.189028	0.002683
22	1	0	-5.864365	0.094785	2.155555
23	1	0	-3.394431	-0.088962	2.162295
24	1	0	3.394898	0.087782	2.162584
25	1	0	5.864798	-0.096294	2.155217
26	1	0	7.107338	-0.189522	0.002020
27	1	0	5.867288	-0.095790	-2.152588
28	1	0	3.397397	0.088286	-2.162763

Zero-point vibrational energy 531846.0 (Joules/Mol)
127.11424 (Kcal/Mol)
Zero-point correction= 0.202569 (Hartree/Particle)
Thermal correction to Energy= 0.218981
Thermal correction to Enthalpy= 0.219925
Thermal correction to Gibbs Free Energy= 0.154245
Sum of electronic and zero-point Energies= -1535.758349
Sum of electronic and thermal Energies= -1535.741938
Sum of electronic and thermal Enthalpies= -1535.740994
Sum of electronic and thermal Free Energies= -1535.806674

TS1d-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.112553	-1.098363	1.043149
2	6	0	-1.415436	-0.612268	-0.314882
3	6	0	-1.737326	-1.606832	-1.031144
4	6	0	1.041470	-0.671006	0.825599
5	6	0	2.214151	-0.086452	0.312345
6	6	0	3.075202	-0.825595	-0.535482
7	6	0	4.245105	-0.252261	-1.018311
8	6	0	4.580869	1.062535	-0.678595
9	6	0	3.736624	1.805131	0.153843
10	6	0	2.568024	1.242339	0.651673
11	6	0	-1.760404	0.806825	-0.231886
12	6	0	-2.300173	1.438502	-1.369523
13	6	0	-2.665496	2.780571	-1.330876
14	6	0	-2.502684	3.522325	-0.158051
15	6	0	-1.972317	2.905756	0.975546
16	6	0	-1.602232	1.561635	0.941982
17	17	0	-0.935498	-2.020545	2.232883
18	17	0	-1.424922	-3.188653	-1.450283
19	1	0	-1.195858	1.094115	1.831678
20	1	0	-2.426022	0.859148	-2.278590
21	1	0	-3.076797	3.249257	-2.220979
22	1	0	-2.787225	4.570590	-0.129144
23	1	0	-1.848213	3.470675	1.895653
24	1	0	1.908717	1.814951	1.296078
25	1	0	3.994222	2.827602	0.416000
26	1	0	5.495495	1.506639	-1.061252
27	1	0	2.807482	-1.843803	-0.799481
28	1	0	4.898388	-0.829865	-1.666492

Zero-point vibrational energy 530278.4 (Joules/Mol)
126.73958 (Kcal/Mol)
Zero-point correction= 0.201972 (Hartree/Particle)
Thermal correction to Energy= 0.218297
Thermal correction to Enthalpy= 0.219241
Thermal correction to Gibbs Free Energy= 0.153300
Sum of electronic and zero-point Energies= -1535.715302
Sum of electronic and thermal Energies= -1535.698978
Sum of electronic and thermal Enthalpies= -1535.698033
Sum of electronic and thermal Free Energies= -1535.763974

TS1d-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.260136	1.164669	1.683789
2	6	0	0.650582	0.451356	0.709195
3	6	0	-0.650527	0.451436	-0.709066
4	6	0	-0.260204	1.164885	-1.683624
5	17	0	-0.861695	2.240950	2.277997
6	17	0	0.861548	2.241237	-2.277846
7	6	0	1.828957	-0.358054	0.391545
8	6	0	-1.828899	-0.358032	-0.391532
9	6	0	3.002443	-0.174055	1.150525
10	6	0	4.136890	-0.938251	0.899154
11	6	0	4.127882	-1.902764	-0.112518
12	6	0	2.971690	-2.093207	-0.868810
13	6	0	1.831301	-1.328577	-0.623277
14	6	0	-3.002321	-0.174065	-1.150619
15	6	0	-4.136763	-0.938305	-0.899360
16	6	0	-4.127814	-1.902829	0.112303
17	6	0	-2.971686	-2.093238	0.868701
18	6	0	-1.831302	-1.328564	0.623281
19	1	0	3.005720	0.574960	1.936044
20	1	0	5.032410	-0.778704	1.493845
21	1	0	5.015393	-2.498020	-0.308914
22	1	0	2.952389	-2.840860	-1.657100
23	1	0	0.940307	-1.483099	-1.220793
24	1	0	-3.005549	0.574958	-1.936131
25	1	0	-5.032234	-0.778784	-1.494132
26	1	0	-5.015322	-2.498118	0.308612
27	1	0	-2.952432	-2.840897	1.656987
28	1	0	-0.940356	-1.483050	1.220880

Zero-point vibrational energy 530377.6 (Joules/Mol)
126.76330 (Kcal/Mol)
Zero-point correction= 0.202010 (Hartree/Particle)
Thermal correction to Energy= 0.218266
Thermal correction to Enthalpy= 0.219210
Thermal correction to Gibbs Free Energy= 0.154290
Sum of electronic and zero-point Energies= -1535.707990
Sum of electronic and thermal Energies= -1535.691734
Sum of electronic and thermal Enthalpies= -1535.690790
Sum of electronic and thermal Free Energies= -1535.755710

TS2d-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.421315	0.365301	0.003632
2	6	0	1.421159	0.365157	-0.003804
3	6	0	0.733224	1.471912	0.082564
4	6	0	-0.733270	1.471996	-0.082611
5	6	0	-2.480759	-0.534957	0.008327
6	6	0	-3.226493	-0.777924	1.198841
7	6	0	-4.261030	-1.701024	1.202560
8	6	0	-4.581289	-2.414823	0.039988
9	6	0	-3.854232	-2.194588	-1.137696
10	6	0	-2.817767	-1.274183	-1.163118
11	6	0	2.480672	-0.535034	-0.008410
12	6	0	3.226445	-0.778031	-1.198889
13	6	0	4.261055	-1.701052	-1.202518
14	6	0	4.581339	-2.414743	-0.039888
15	6	0	3.854233	-2.194487	1.137761
16	6	0	2.817693	-1.274161	1.163088
17	17	0	1.555020	3.025737	0.474858
18	17	0	-1.554902	3.025935	-0.474808
19	1	0	-2.252198	-1.100212	-2.072953
20	1	0	-4.103838	-2.746484	-2.039773
21	1	0	-5.391618	-3.138041	0.051605
22	1	0	-4.826169	-1.869701	2.115129
23	1	0	-2.974262	-0.222914	2.096778
24	1	0	2.974192	-0.223105	-2.096872
25	1	0	4.826230	-1.869753	-2.115061
26	1	0	5.391725	-3.137899	-0.051433
27	1	0	4.103858	-2.746302	2.039882
28	1	0	2.252084	-1.100168	2.072894

Zero-point vibrational energy 531645.9 (Joules/Mol)
127.06642 (Kcal/Mol)
Zero-point correction= 0.202493 (Hartree/Particle)
Thermal correction to Energy= 0.218082
Thermal correction to Enthalpy= 0.219026
Thermal correction to Gibbs Free Energy= 0.155985
Sum of electronic and zero-point Energies= -1535.752884
Sum of electronic and thermal Energies= -1535.737295
Sum of electronic and thermal Enthalpies= -1535.736351
Sum of electronic and thermal Free Energies= -1535.799392

INT2d-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.049368	0.760550	1.780687
2	6	0	-0.071233	0.806530	0.434416
3	6	0	0.071233	-0.806530	0.434416
4	6	0	0.049368	-0.760550	1.780687
5	17	0	-0.250829	1.880010	3.062680
6	17	0	0.250829	-1.880010	3.062680
7	6	0	-0.296712	1.810382	-0.578255
8	6	0	0.296712	-1.810382	-0.578255
9	6	0	-0.848630	1.471673	-1.831933
10	6	0	-1.096309	2.455601	-2.786862
11	6	0	-0.797852	3.792294	-2.517908
12	6	0	-0.250829	4.141896	-1.278500
13	6	0	-0.001080	3.167905	-0.319103
14	6	0	0.848630	-1.471673	-1.831933
15	6	0	1.096309	-2.455601	-2.786862
16	6	0	0.797852	-3.792294	-2.517908
17	6	0	0.250829	-4.141896	-1.278500
18	6	0	0.001080	-3.167905	-0.319103
19	1	0	-1.104139	0.438877	-2.042684
20	1	0	-1.528576	2.175633	-3.743801
21	1	0	-0.988730	4.556810	-3.265849
22	1	0	-0.012300	5.179931	-1.062707
23	1	0	0.437346	3.444687	0.634221
24	1	0	1.104139	-0.438877	-2.042684
25	1	0	1.528576	-2.175633	-3.743801
26	1	0	0.988730	-4.556810	-3.265849
27	1	0	0.012300	-5.179931	-1.062707
28	1	0	-0.437346	-3.444687	0.634221

Zero-point vibrational energy 542878.0 (Joules/Mol)
129.75096 (Kcal/Mol)
Zero-point correction= 0.206771 (Hartree/Particle)
Thermal correction to Energy= 0.221996
Thermal correction to Enthalpy= 0.222940
Thermal correction to Gibbs Free Energy= 0.162944
Sum of electronic and zero-point Energies= -1535.803084
Sum of electronic and thermal Energies= -1535.787859
Sum of electronic and thermal Enthalpies= -1535.786915
Sum of electronic and thermal Free Energies= -1535.846911

TS3d-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.562649	-1.239893	-0.970282
2	6	0	1.730044	-0.637872	-0.514262
3	6	0	1.016393	0.674298	-0.451323
4	6	0	-0.220126	0.007211	-0.775172
5	6	0	-2.560383	-0.407881	1.057979
6	6	0	-1.332353	-0.406343	1.222276
7	17	0	-0.086228	-0.634213	2.341804
8	6	0	-3.916982	-0.369828	0.671043
9	6	0	1.384834	2.053617	-0.339157
10	6	0	3.032772	-1.129396	-0.106145
11	17	0	0.064150	-2.852201	-1.273921
12	17	0	-1.488116	0.582842	-1.825730
13	6	0	3.791441	-0.455024	0.872628
14	6	0	5.028766	-0.950620	1.275094
15	6	0	5.537801	-2.121935	0.708780
16	6	0	4.795140	-2.800078	-0.261967
17	6	0	3.555596	-2.313876	-0.665812
18	6	0	0.392297	3.035067	-0.093063
19	6	0	0.731925	4.378180	0.005612
20	6	0	2.062268	4.786814	-0.141826
21	6	0	3.052840	3.832032	-0.392350
22	6	0	2.725731	2.484236	-0.488853
23	6	0	-4.671218	0.820444	0.798978
24	6	0	-6.013791	0.842717	0.440531
25	6	0	-6.633242	-0.311379	-0.050296
26	6	0	-5.898771	-1.494556	-0.181114
27	6	0	-4.555838	-1.530895	0.175032
28	1	0	3.393257	0.444346	1.330687
29	1	0	5.595757	-0.422769	2.037181
30	1	0	6.505350	-2.504463	1.021865
31	1	0	5.185177	-3.711046	-0.707850
32	1	0	2.988556	-2.840144	-1.426715
33	1	0	-0.639263	2.723778	0.034273
34	1	0	-0.043732	5.113843	0.201248
35	1	0	2.323320	5.838541	-0.064340
36	1	0	4.086831	4.141973	-0.519002
37	1	0	3.499894	1.755912	-0.705275
38	1	0	-4.185972	1.713294	1.180590
39	1	0	-6.582145	1.763179	0.542542
40	1	0	-7.682949	-0.288752	-0.329519
41	1	0	-6.377414	-2.391831	-0.563782
42	1	0	-3.980170	-2.445362	0.073501

Zero-point vibrational energy 803483.7 (Joules/Mol)

192.03720 (Kcal/Mol)

Zero-point correction=	0.306031 (Hartree/Particle)
Thermal correction to Energy=	0.330264
Thermal correction to Enthalpy=	0.331208
Thermal correction to Gibbs Free Energy=	0.247201
Sum of electronic and zero-point Energies=	-2303.665198
Sum of electronic and thermal Energies=	-2303.640965
Sum of electronic and thermal Enthalpies=	-2303.640021
Sum of electronic and thermal Free Energies=	-2303.724028

TS3d-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.563115	-1.318137	-1.248860
2	6	0	1.681407	-1.735454	-1.648126
3	6	0	-0.643090	0.556271	0.768740
4	6	0	0.731954	0.091234	0.437161
5	6	0	-0.722500	-0.481869	1.793779
6	6	0	0.570971	-0.893992	1.560179
7	6	0	-0.858345	-1.582608	-1.438637
8	17	0	3.342823	-1.770355	-1.617067
9	6	0	1.940896	0.914542	0.192850
10	6	0	-1.494860	1.638210	0.382610
11	17	0	1.536345	-2.174081	2.156170
12	17	0	-1.946917	-1.078850	2.845037
13	6	0	-1.445330	-2.710628	-0.839939
14	6	0	-2.800450	-2.981609	-1.025516
15	6	0	-3.585800	-2.134242	-1.808934
16	6	0	-3.009799	-1.010370	-2.406090
17	6	0	-1.657740	-0.731738	-2.219580
18	6	0	2.864458	1.114236	1.234365
19	6	0	3.993082	1.911484	1.046960
20	6	0	4.227982	2.520486	-0.186338
21	6	0	3.327379	2.318387	-1.234319
22	6	0	2.200703	1.520111	-1.048702
23	6	0	-1.090070	2.606739	-0.570769
24	6	0	-1.932858	3.650222	-0.931377
25	6	0	-3.205488	3.767177	-0.362245
26	6	0	-3.623115	2.822334	0.581045
27	6	0	-2.788436	1.775676	0.950783
28	1	0	-0.829199	-3.373537	-0.240512
29	1	0	-3.241145	-3.858483	-0.558941
30	1	0	-4.641452	-2.347523	-1.953518

31	1	0	-3.615353	-0.346390	-3.016814
32	1	0	-1.213302	0.145707	-2.678744
33	1	0	2.688374	0.653001	2.201327
34	1	0	4.688829	2.056428	1.869164
35	1	0	5.108752	3.139599	-0.333081
36	1	0	3.508560	2.773030	-2.204653
37	1	0	1.531925	1.331264	-1.882636
38	1	0	-0.101851	2.543919	-1.008374
39	1	0	-1.594225	4.382113	-1.660176
40	1	0	-3.861820	4.584171	-0.648585
41	1	0	-4.609192	2.902744	1.030994
42	1	0	-3.131543	1.051067	1.679941

Zero-point vibrational energy 802574.6 (Joules/Mol)
191.81993 (Kcal/Mol)
Zero-point correction= 0.305685 (Hartree/Particle)
Thermal correction to Energy= 0.329966
Thermal correction to Enthalpy= 0.330910
Thermal correction to Gibbs Free Energy= 0.247418
Sum of electronic and zero-point Energies= -2303.646696
Sum of electronic and thermal Energies= -2303.622414
Sum of electronic and thermal Enthalpies= -2303.621470
Sum of electronic and thermal Free Energies= -2303.704962

TS3d-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.802485	0.273695	0.359071
2	6	0	2.790957	-0.686652	0.032358
3	6	0	1.844546	-1.741193	-0.021737
4	6	0	0.758410	-0.844264	0.324069
5	6	0	-1.442839	-0.058427	-1.606027
6	6	0	-0.249315	-0.396080	-1.700095
7	6	0	1.759301	1.697511	0.497176
8	17	0	4.466486	-0.634962	-0.348637
9	6	0	-0.358173	-1.128968	1.227901
10	17	0	1.991274	-3.430033	-0.222154
11	17	0	0.979823	-0.624395	-2.850911
12	6	0	-2.762263	0.322563	-1.288767
13	6	0	0.524795	2.391520	0.555510
14	6	0	0.492450	3.774672	0.689966
15	6	0	1.679861	4.509366	0.767959
16	6	0	2.907660	3.840303	0.709044

17	6	0	2.953486	2.458574	0.576446
18	6	0	-0.652624	-0.295418	2.322256
19	6	0	-1.694533	-0.608495	3.194794
20	6	0	-2.463204	-1.755298	2.993893
21	6	0	-2.179805	-2.592716	1.910890
22	6	0	-1.143018	-2.284058	1.036014
23	6	0	-3.791607	-0.641541	-1.162911
24	6	0	-5.092937	-0.246538	-0.878665
25	6	0	-5.402966	1.107998	-0.715204
26	6	0	-4.397242	2.071958	-0.841096
27	6	0	-3.091519	1.691158	-1.126401
28	1	0	-0.401935	1.834095	0.480546
29	1	0	-0.466106	4.285562	0.732116
30	1	0	1.649778	5.590184	0.873364
31	1	0	3.835855	4.402304	0.769925
32	1	0	3.912218	1.952969	0.539585
33	1	0	-0.048667	0.587128	2.502286
34	1	0	-1.900362	0.045493	4.038036
35	1	0	-3.275221	-1.996694	3.674317
36	1	0	-2.771318	-3.489764	1.747202
37	1	0	-0.937364	-2.932745	0.190539
38	1	0	-3.547126	-1.691315	-1.286647
39	1	0	-5.872793	-0.997122	-0.782709
40	1	0	-6.422584	1.410321	-0.493293
41	1	0	-4.635434	3.125142	-0.719003
42	1	0	-2.309287	2.436049	-1.235999

Zero-point vibrational energy 802452.8 (Joules/Mol)
191.79081 (Kcal/Mol)
Zero-point correction= 0.305638 (Hartree/Particle)
Thermal correction to Energy= 0.329923
Thermal correction to Enthalpy= 0.330867
Thermal correction to Gibbs Free Energy= 0.247265
Sum of electronic and zero-point Energies= -2303.661162
Sum of electronic and thermal Energies= -2303.636878
Sum of electronic and thermal Enthalpies= -2303.635933
Sum of electronic and thermal Free Energies= -2303.719535

TS3d-4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.215613	0.006678	-0.971467
2	6	0	-2.053738	-0.766229	0.906412

3	6	0	-0.926205	-0.847185	1.828091
4	6	0	-0.228581	-2.056604	1.983657
5	6	0	0.836043	-2.144838	2.879428
6	6	0	1.218861	-1.030842	3.629086
7	6	0	0.532417	0.176211	3.476547
8	6	0	-0.529484	0.272278	2.578165
9	6	0	-0.029061	0.819873	-0.694500
10	6	0	0.833528	-0.335849	-1.015660
11	6	0	-0.283813	-1.058174	-1.424582
12	6	0	2.857724	-1.594987	-1.713458
13	6	0	2.243963	-0.658870	-0.857885
14	1	0	2.547193	0.633206	0.845927
15	1	0	4.663609	-2.636066	-2.232198
16	6	0	4.359857	-0.396185	0.311165
17	6	0	0.150470	2.217397	-0.446865
18	6	0	-0.948510	3.013967	-0.034176
19	6	0	-0.792355	4.373762	0.202237
20	6	0	0.454470	4.985957	0.030807
21	6	0	1.546768	4.217552	-0.385474
22	6	0	1.403975	2.855264	-0.621185
23	6	0	-3.272369	-1.043293	0.828643
24	17	0	-4.780025	-1.192189	0.166032
25	17	0	-0.567370	-2.677143	-1.917894
26	17	0	-2.586602	0.555773	-1.931203
27	1	0	-1.060678	1.211005	2.458533
28	1	0	0.821392	1.046312	4.060066
29	1	0	2.046524	-1.103053	4.329532
30	1	0	1.365851	-3.086762	2.992093
31	1	0	-0.532923	-2.922784	1.404501
32	1	0	2.276827	-2.054879	-2.506561
33	1	0	6.010241	-1.572316	-0.431034
34	1	0	4.939713	0.064175	1.106635
35	1	0	2.254680	2.276048	-0.963381
36	1	0	2.516060	4.686628	-0.533153
37	1	0	0.572014	6.050068	0.215350
38	1	0	-1.647909	4.963274	0.521150
39	1	0	-1.919350	2.548607	0.101486
40	6	0	3.015808	-0.064568	0.159760
41	6	0	4.960104	-1.319251	-0.548731
42	6	0	4.203191	-1.917559	-1.559488

Zero-point vibrational energy 803650.6 (Joules/Mol)
192.07709 (Kcal/Mol)
Zero-point correction= 0.306094 (Hartree/Particle)
Thermal correction to Energy= 0.330260

Thermal correction to Enthalpy=	0.331205
Thermal correction to Gibbs Free Energy=	0.248058
Sum of electronic and zero-point Energies=	-2303.655216
Sum of electronic and thermal Energies=	-2303.631050
Sum of electronic and thermal Enthalpies=	-2303.630106
Sum of electronic and thermal Free Energies=	-2303.713252

TS3d-5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.150769	0.888244	0.222558
2	6	0	0.727930	1.151576	0.599063
3	6	0	0.565184	-0.179200	0.919860
4	6	0	2.023970	-0.464837	0.382302
5	6	0	0.100170	-1.172173	-1.710836
6	6	0	1.328112	-1.293452	-1.627856
7	17	0	3.467542	1.889521	-0.217776
8	17	0	3.218218	-1.595557	0.943296
9	17	0	2.743862	-1.823251	-2.391378
10	6	0	-0.095309	2.350481	0.537215
11	6	0	-0.347442	-1.023827	1.647071
12	6	0	-1.302050	-1.022827	-1.846733
13	6	0	-0.154768	-2.424002	1.664676
14	6	0	-1.002563	-3.249650	2.396682
15	6	0	-2.059679	-2.704758	3.129950
16	6	0	-2.258693	-1.320346	3.128992
17	6	0	-1.415419	-0.487922	2.402858
18	6	0	-2.192015	-2.005175	-1.355869
19	6	0	-3.565072	-1.860760	-1.529609
20	6	0	-4.082243	-0.749240	-2.200493
21	6	0	-3.211721	0.227250	-2.694983
22	6	0	-1.837840	0.100688	-2.518990
23	6	0	-1.490138	2.274003	0.345967
24	6	0	-2.263070	3.430295	0.292641
25	6	0	-1.665992	4.686997	0.424068
26	6	0	-0.284122	4.777173	0.602621
27	6	0	0.495881	3.624299	0.654882
28	1	0	0.662096	-2.855288	1.097115
29	1	0	-0.835270	-4.323387	2.397507
30	1	0	-2.719366	-3.351270	3.702030
31	1	0	-3.070988	-0.887187	3.706442
32	1	0	-1.564407	0.585881	2.431418
33	1	0	-1.791650	-2.871191	-0.840107

34	1	0	-4.235841	-2.623865	-1.143992
35	1	0	-5.154753	-0.645804	-2.340242
36	1	0	-3.606307	1.092860	-3.220473
37	1	0	-1.161451	0.859783	-2.898798
38	1	0	-1.959221	1.305754	0.210032
39	1	0	-3.335513	3.349528	0.136519
40	1	0	-2.272072	5.587810	0.382117
41	1	0	0.190291	5.749652	0.702964
42	1	0	1.567577	3.707594	0.800831

Zero-point vibrational energy 809767.2 (Joules/Mol)
193.53900 (Kcal/Mol)
Zero-point correction= 0.308424 (Hartree/Particle)
Thermal correction to Energy= 0.332251
Thermal correction to Enthalpy= 0.333195
Thermal correction to Gibbs Free Energy= 0.251706
Sum of electronic and zero-point Energies= -2303.661179
Sum of electronic and thermal Energies= -2303.637352
Sum of electronic and thermal Enthalpies= -2303.636408
Sum of electronic and thermal Free Energies= -2303.717897

TS3d-6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.617787	0.390184	1.254184
2	6	0	0.582631	0.236160	-1.277734
3	6	0	0.237943	-1.064353	-1.331937
4	6	0	-1.019912	-0.834269	-0.543131
5	6	0	-0.725895	0.530896	-0.445462
6	6	0	0.431579	0.665759	1.487203
7	6	0	2.971078	0.055335	1.011626
8	6	0	3.921777	1.055748	0.705565
9	6	0	5.255305	0.718650	0.494904
10	6	0	5.671576	-0.611585	0.588661
11	6	0	4.740896	-1.610336	0.894336
12	6	0	3.405033	-1.288081	1.100872
13	6	0	-2.046533	-1.727658	-0.063829
14	6	0	-2.923631	-1.349989	0.979620
15	6	0	-3.909115	-2.220869	1.428776
16	6	0	-4.050355	-3.489154	0.855907
17	6	0	-3.187890	-3.879622	-0.170852
18	6	0	-2.195133	-3.016274	-0.624424
19	6	0	-2.931933	1.719057	-0.568739

20	6	0	-1.528597	1.754163	-0.456335
21	6	0	-0.894451	3.011083	-0.401807
22	6	0	-1.637214	4.187169	-0.454175
23	6	0	-3.029213	4.137455	-0.556227
24	6	0	-3.671259	2.897939	-0.613443
25	17	0	-0.657952	1.139978	2.703813
26	17	0	1.725251	1.206579	-2.092797
27	17	0	1.004982	-2.454395	-1.998469
28	1	0	-1.536219	-3.331330	-1.425725
29	1	0	-3.287973	-4.863294	-0.621750
30	1	0	-4.821723	-4.166951	1.210768
31	1	0	-4.566834	-1.912721	2.237135
32	1	0	-2.807141	-0.378846	1.448021
33	1	0	-3.440065	0.763536	-0.642008
34	1	0	-4.753050	2.848114	-0.705190
35	1	0	-3.608471	5.055987	-0.593272
36	1	0	-1.127683	5.145996	-0.410289
37	1	0	0.185355	3.057543	-0.304987
38	1	0	3.598643	2.089860	0.643336
39	1	0	5.974569	1.498620	0.259928
40	1	0	6.714318	-0.869614	0.425996
41	1	0	5.060170	-2.646334	0.969157
42	1	0	2.680484	-2.061767	1.334236

Zero-point vibrational energy 809332.0 (Joules/Mol)
193.43499 (Kcal/Mol)
Zero-point correction= 0.308258 (Hartree/Particle)
Thermal correction to Energy= 0.332147
Thermal correction to Enthalpy= 0.333091
Thermal correction to Gibbs Free Energy= 0.251424
Sum of electronic and zero-point Energies= -2303.659176
Sum of electronic and thermal Energies= -2303.635287
Sum of electronic and thermal Enthalpies= -2303.634343
Sum of electronic and thermal Free Energies= -2303.716010

TS3d-7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.288264	-1.771448	-0.794827
2	6	0	0.344509	-0.200525	1.392395
3	6	0	-0.254255	0.831765	0.750820
4	6	0	-1.482055	-0.055845	0.480129
5	6	0	-0.832813	-1.136346	1.060454

6	6	0	0.132294	-2.192495	-0.648466
7	6	0	2.600318	-1.270299	-0.950316
8	6	0	2.866537	-0.208318	-1.847665
9	6	0	4.165053	0.257095	-2.021857
10	6	0	5.224374	-0.312416	-1.306971
11	6	0	4.974143	-1.358485	-0.414815
12	6	0	3.680728	-1.838626	-0.235651
13	6	0	0.111252	2.223182	0.512609
14	6	0	-0.852877	3.249131	0.546918
15	6	0	-0.477453	4.580195	0.376378
16	6	0	0.862400	4.913822	0.168480
17	6	0	1.828076	3.904652	0.136032
18	6	0	1.460577	2.572442	0.306742
19	6	0	-2.753376	0.145149	-0.171145
20	6	0	-3.846392	-0.715015	0.088908
21	6	0	-5.063655	-0.527838	-0.554048
22	6	0	-5.228038	0.514501	-1.472742
23	6	0	-4.156737	1.366974	-1.747412
24	6	0	-2.933657	1.188331	-1.107040
25	17	0	-1.426092	-2.447058	2.033878
26	17	0	1.702628	-0.387779	2.409284
27	17	0	-1.028803	-3.286436	-1.231083
28	1	0	2.043253	0.233105	-2.400543
29	1	0	4.354124	1.068467	-2.719775
30	1	0	6.236925	0.055771	-1.446586
31	1	0	5.793194	-1.805709	0.142045
32	1	0	3.485696	-2.656084	0.450824
33	1	0	2.212974	1.791938	0.261599
34	1	0	2.872692	4.154972	-0.028563
35	1	0	1.152181	5.952360	0.033913
36	1	0	-1.234114	5.359358	0.412819
37	1	0	-1.893399	3.002076	0.731108
38	1	0	-2.101079	1.839887	-1.347346
39	1	0	-4.271061	2.170811	-2.469704
40	1	0	-6.182205	0.656656	-1.972554
41	1	0	-5.892181	-1.196578	-0.336905
42	1	0	-3.731759	-1.522862	0.802872

Zero-point vibrational energy 809473.6 (Joules/Mol)
193.46882 (Kcal/Mol)

Zero-point correction= 0.308312 (Hartree/Particle)
Thermal correction to Energy= 0.332211
Thermal correction to Enthalpy= 0.333156
Thermal correction to Gibbs Free Energy= 0.251052
Sum of electronic and zero-point Energies= -2303.658836

Sum of electronic and thermal Energies= -2303.634937
Sum of electronic and thermal Enthalpies= -2303.633993
Sum of electronic and thermal Free Energies= -2303.716096

TS3d-8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.709651	-0.763111	1.520353
2	6	0	0.054478	0.047310	-0.992630
3	6	0	-0.004424	-1.185234	-1.577070
4	6	0	-1.348462	-1.455055	-1.074538
5	6	0	-1.413314	-0.269066	-0.370023
6	6	0	-0.519490	-0.903042	1.596240
7	6	0	2.122134	-0.649049	1.509935
8	6	0	2.756839	0.542434	1.924980
9	6	0	4.145639	0.630903	1.945459
10	6	0	4.929635	-0.457991	1.557293
11	6	0	4.312845	-1.642110	1.139964
12	6	0	2.926233	-1.741404	1.110306
13	6	0	0.886295	1.217089	-1.131420
14	6	0	0.376410	2.516730	-0.923275
15	6	0	1.185592	3.635053	-1.108845
16	6	0	2.517368	3.488903	-1.501556
17	6	0	3.037081	2.207295	-1.707504
18	6	0	2.238768	1.084187	-1.525301
19	6	0	-2.532169	0.586289	0.033533
20	6	0	-2.362714	1.638939	0.954449
21	6	0	-3.435101	2.450025	1.315246
22	6	0	-4.704568	2.220062	0.779284
23	6	0	-4.891224	1.170536	-0.122318
24	6	0	-3.818346	0.363630	-0.494797
25	17	0	-2.356455	-2.831780	-1.236742
26	17	0	-1.807170	-1.397887	2.585724
27	17	0	1.040997	-2.127584	-2.563765
28	1	0	2.659162	0.095304	-1.670537
29	1	0	4.073961	2.081869	-2.007425
30	1	0	3.144679	4.363921	-1.647869
31	1	0	0.768555	4.626807	-0.954678
32	1	0	-0.663705	2.647159	-0.650697
33	1	0	2.446065	-2.659314	0.786041
34	1	0	4.917352	-2.492797	0.836744
35	1	0	6.013530	-0.385924	1.578763
36	1	0	4.618230	1.554828	2.267671

37	1	0	2.147492	1.387699	2.228304
38	1	0	-1.387919	1.798132	1.404197
39	1	0	-3.282098	3.256225	2.027647
40	1	0	-5.541522	2.850903	1.065822
41	1	0	-5.874188	0.983671	-0.546293
42	1	0	-3.969850	-0.435163	-1.212984

Zero-point vibrational energy 809417.6 (Joules/Mol)
193.45544 (Kcal/Mol)
Zero-point correction= 0.308291 (Hartree/Particle)
Thermal correction to Energy= 0.332137
Thermal correction to Enthalpy= 0.333081
Thermal correction to Gibbs Free Energy= 0.251357
Sum of electronic and zero-point Energies= -2303.659178
Sum of electronic and thermal Energies= -2303.635332
Sum of electronic and thermal Enthalpies= -2303.634388
Sum of electronic and thermal Free Energies= -2303.716112

INT3d-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.801267	-1.439012	-0.575349
2	6	0	1.866224	-0.610546	-0.248322
3	6	0	1.035082	0.557811	-0.291241
4	6	0	-0.204094	-0.307739	-0.586723
5	6	0	-2.605480	-0.338937	0.203719
6	6	0	-1.330342	-0.365423	0.426372
7	17	0	-0.728907	-0.535368	2.133280
8	6	0	-3.988480	-0.346204	0.258588
9	6	0	1.188319	1.976632	-0.245233
10	6	0	3.269155	-0.890685	0.073679
11	17	0	0.573477	-3.129839	-0.708448
12	17	0	-0.928482	-0.011905	-2.244602
13	6	0	3.919636	-0.208421	1.115921
14	6	0	5.241141	-0.510037	1.438800
15	6	0	5.932819	-1.490854	0.724233
16	6	0	5.293309	-2.176086	-0.310782
17	6	0	3.968908	-1.884338	-0.631393
18	6	0	0.044169	2.814297	-0.211867
19	6	0	0.173923	4.196302	-0.169501
20	6	0	1.440165	4.791119	-0.165044
21	6	0	2.580617	3.981056	-0.210694
22	6	0	2.464014	2.597900	-0.251932

23	6	0	-4.726142	0.868927	0.384302
24	6	0	-6.111241	0.847452	0.415871
25	6	0	-6.807598	-0.365464	0.319697
26	6	0	-6.099603	-1.568552	0.190530
27	6	0	-4.714393	-1.571024	0.156780
28	1	0	3.378545	0.543212	1.682547
29	1	0	5.730151	0.019309	2.251955
30	1	0	6.964538	-1.721853	0.974938
31	1	0	5.825987	-2.940412	-0.869845
32	1	0	3.474888	-2.416626	-1.438342
33	1	0	-0.942865	2.364119	-0.214420
34	1	0	-0.717757	4.816986	-0.140299
35	1	0	1.537495	5.872588	-0.131914
36	1	0	3.568446	4.434336	-0.221194
37	1	0	3.356870	1.985073	-0.308476
38	1	0	-4.184136	1.806324	0.458070
39	1	0	-6.659470	1.780197	0.516272
40	1	0	-7.893424	-0.372869	0.343944
41	1	0	-6.638819	-2.508907	0.115776
42	1	0	-4.162205	-2.499612	0.054589

Zero-point vibrational energy 810695.6 (Joules/Mol)
193.76089 (Kcal/Mol)
Zero-point correction= 0.308778 (Hartree/Particle)
Thermal correction to Energy= 0.332679
Thermal correction to Enthalpy= 0.333623
Thermal correction to Gibbs Free Energy= 0.250758
Sum of electronic and zero-point Energies= -2303.716622
Sum of electronic and thermal Energies= -2303.692721
Sum of electronic and thermal Enthalpies= -2303.691776
Sum of electronic and thermal Free Energies= -2303.774642

TS4d-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.608598	0.013222	1.238932
2	6	0	-1.683800	0.721379	0.468948
3	6	0	0.482583	-0.045611	-0.828910
4	6	0	1.669303	0.250784	-0.061400
5	6	0	1.437003	1.611364	-0.138836
6	6	0	0.147896	1.456598	-0.911837
7	6	0	-1.126887	1.715973	-0.157009
8	6	0	-2.394794	-0.195415	2.629967

9	6	0	-3.305017	-0.927560	3.377817
10	6	0	-4.438695	-1.484267	2.771680
11	6	0	-4.657138	-1.299222	1.401101
12	6	0	-3.761150	-0.564624	0.637348
13	6	0	-0.096791	-1.198480	-1.465682
14	6	0	-1.081253	-1.053855	-2.474526
15	6	0	-1.636009	-2.168749	-3.090770
16	6	0	-1.242054	-3.458571	-2.718715
17	6	0	-0.284466	-3.619164	-1.713284
18	6	0	0.282046	-2.510856	-1.093532
19	6	0	2.743817	-0.524424	0.576717
20	6	0	3.157907	-0.207086	1.880720
21	6	0	4.199793	-0.911145	2.482086
22	6	0	4.849999	-1.932051	1.786284
23	6	0	4.453925	-2.246218	0.484378
24	6	0	3.407064	-1.550265	-0.117462
25	17	0	2.219668	2.998844	0.477542
26	17	0	0.194629	2.232053	-2.560663
27	17	0	-1.726247	3.408772	-0.070068
28	1	0	-1.514131	0.234653	3.096642
29	1	0	-3.134271	-1.069145	4.441615
30	1	0	-3.926057	-0.420716	-0.425440
31	1	0	-5.535694	-1.730357	0.928840
32	1	0	-5.145738	-2.058637	3.363390
33	1	0	3.111256	-1.787312	-1.134810
34	1	0	4.963480	-3.032257	-0.066107
35	1	0	5.664223	-2.478226	2.254624
36	1	0	4.504875	-0.660472	3.494277
37	1	0	2.653797	0.586643	2.423614
38	1	0	-1.392589	-0.060453	-2.777478
39	1	0	-2.380475	-2.031481	-3.870613
40	1	0	-1.679873	-4.326828	-3.203058
41	1	0	0.019544	-4.616212	-1.405484
42	1	0	1.006706	-2.654106	-0.299892

Zero-point vibrational energy 811219.1 (Joules/Mol)
193.88601 (Kcal/Mol)
Zero-point correction= 0.308977 (Hartree/Particle)
Thermal correction to Energy= 0.332105
Thermal correction to Enthalpy= 0.333049
Thermal correction to Gibbs Free Energy= 0.252699
Sum of electronic and zero-point Energies= -2303.716096
Sum of electronic and thermal Energies= -2303.692968
Sum of electronic and thermal Enthalpies= -2303.692024
Sum of electronic and thermal Free Energies= -2303.772374

TS4d-2 (conver=6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.066666	-0.741559	-0.075048
2	6	0	0.130983	0.470173	1.356279
3	6	0	-0.938782	0.878184	0.559340
4	6	0	-1.288035	-0.468543	0.241589
5	6	0	-0.083258	-0.999659	1.048931
6	6	0	1.109720	-1.537932	0.293309
7	6	0	3.238848	-0.250279	-0.642535
8	6	0	3.251810	0.244856	-1.978138
9	6	0	4.417979	0.760128	-2.523122
10	6	0	5.595445	0.812385	-1.765268
11	6	0	5.597728	0.338040	-0.447243
12	6	0	4.443087	-0.185457	0.115332
13	6	0	-1.423157	2.212707	0.180000
14	6	0	-1.516421	3.229524	1.144725
15	6	0	-1.942471	4.506814	0.784268
16	6	0	-2.268425	4.790352	-0.543344
17	6	0	-2.168498	3.788725	-1.511738
18	6	0	-1.751361	2.508182	-1.154103
19	6	0	-2.368013	-1.134952	-0.422980
20	6	0	-3.502497	-0.417920	-0.884811
21	6	0	-4.555901	-1.075148	-1.505982
22	6	0	-4.520666	-2.462471	-1.686512
23	6	0	-3.417489	-3.186934	-1.225502
24	6	0	-2.358191	-2.541029	-0.599422
25	1	0	-1.512534	-3.118008	-0.245447
26	1	0	-3.382870	-4.265537	-1.352805
27	1	0	-5.346385	-2.972281	-2.174960
28	1	0	-5.415136	-0.503819	-1.847393
29	1	0	-3.556547	0.654265	-0.735097
30	1	0	-1.663850	1.733537	-1.910155
31	1	0	-2.412977	4.005294	-2.548040
32	1	0	-2.596814	5.787638	-0.822983
33	1	0	-2.018480	5.281802	1.541921
34	1	0	-1.264614	3.012396	2.177942
35	17	0	1.170753	1.258681	2.465302
36	17	0	-0.532142	-2.028455	2.483627
37	17	0	1.153580	-3.301740	-0.101921
38	1	0	2.337534	0.204398	-2.561704
39	1	0	4.415463	1.125798	-3.546384

40	1	0	6.504073	1.220062	-2.198855
41	1	0	6.510361	0.376699	0.141213
42	1	0	4.440940	-0.555622	1.135451

Zero-point vibrational energy 810605.8 (Joules/Mol)
193.73943 (Kcal/Mol)
Zero-point correction= 0.308743 (Hartree/Particle)
Thermal correction to Energy= 0.331938
Thermal correction to Enthalpy= 0.332882
Thermal correction to Gibbs Free Energy= 0.252420
Sum of electronic and zero-point Energies= -2303.715730
Sum of electronic and thermal Energies= -2303.692536
Sum of electronic and thermal Enthalpies= -2303.691592
Sum of electronic and thermal Free Energies= -2303.772054

INT4d-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.284592	-1.337941	-1.068830
2	6	0	1.307589	-0.145735	-0.432405
3	6	0	-0.001510	-0.468525	0.343529
4	6	0	-0.006358	-1.837363	-0.480560
5	6	0	-1.309882	-0.137871	-0.430359
6	6	0	-1.295423	-1.330566	-1.066248
7	17	0	2.259165	-2.087306	-2.284742
8	17	0	-0.009946	-3.448603	0.280977
9	17	0	-2.275995	-2.074294	-2.280815
10	6	0	2.127128	1.058262	-0.491050
11	6	0	-0.000885	-0.531448	1.846697
12	6	0	-2.121409	1.071423	-0.488136
13	6	0	-1.206529	-0.586638	2.562965
14	6	0	-1.205553	-0.706528	3.952447
15	6	0	-0.000102	-0.774532	4.652160
16	6	0	1.204997	-0.724969	3.950205
17	6	0	1.205157	-0.605125	2.560770
18	6	0	-1.898049	2.122268	0.421328
19	6	0	-2.664963	3.283930	0.373015
20	6	0	-3.671676	3.421437	-0.583875
21	6	0	-3.906650	2.385689	-1.492156
22	6	0	-3.144055	1.222674	-1.447430
23	6	0	1.928437	2.100353	0.434131
24	6	0	2.703975	3.256278	0.385459
25	6	0	3.694495	3.396915	-0.587728

26	6	0	3.904671	2.369989	-1.511947
27	6	0	3.133616	1.212546	-1.466720
28	1	0	-2.151441	-0.535947	2.031084
29	1	0	-2.150760	-0.746465	4.487156
30	1	0	0.000211	-0.864408	5.735053
31	1	0	2.150481	-0.779445	4.483137
32	1	0	2.149714	-0.568956	2.026994
33	1	0	-1.129511	2.018977	1.179227
34	1	0	-2.476130	4.082166	1.085605
35	1	0	-4.269668	4.327829	-0.622158
36	1	0	-4.687459	2.485255	-2.241279
37	1	0	-3.333020	0.429056	-2.161262
38	1	0	1.173930	1.993748	1.205607
39	1	0	2.534650	4.047541	1.110632
40	1	0	4.299081	4.298907	-0.626339
41	1	0	4.672526	2.472137	-2.273999
42	1	0	3.302902	0.425934	-2.193164

Zero-point vibrational energy 822768.9 (Joules/Mol)
196.64649 (Kcal/Mol)
Zero-point correction= 0.313376 (Hartree/Particle)
Thermal correction to Energy= 0.335039
Thermal correction to Enthalpy= 0.335983
Thermal correction to Gibbs Free Energy= 0.260981
Sum of electronic and zero-point Energies= -2303.779378
Sum of electronic and thermal Energies= -2303.757715
Sum of electronic and thermal Enthalpies= -2303.756771
Sum of electronic and thermal Free Energies= -2303.831773

INT4d-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.533827	-1.926995	0.089137
2	6	0	-0.498928	-1.233786	0.942041
3	6	0	-1.413085	-0.189280	0.292354
4	6	0	-0.500232	0.815523	0.438708
5	6	0	0.564891	-0.097360	1.059860
6	6	0	1.475642	-0.955403	0.160194
7	6	0	2.783235	-0.700833	-0.427918
8	6	0	3.304951	-1.535873	-1.436902
9	6	0	4.556219	-1.280345	-1.989344
10	6	0	5.314950	-0.192252	-1.549370
11	6	0	4.812274	0.639363	-0.547655

12	6	0	3.560004	0.389443	0.010388
13	6	0	-0.444752	2.249806	0.150724
14	6	0	-1.550081	3.077419	0.423531
15	6	0	-1.489250	4.447583	0.180197
16	6	0	-0.324053	5.018505	-0.337305
17	6	0	0.782963	4.209755	-0.601921
18	6	0	0.728100	2.839693	-0.353150
19	6	0	-2.693114	-0.381883	-0.383451
20	6	0	-3.384878	-1.600112	-0.240355
21	6	0	-4.592933	-1.816002	-0.900535
22	6	0	-5.132852	-0.826276	-1.722404
23	6	0	-4.450607	0.383052	-1.884183
24	6	0	-3.246169	0.605151	-1.224603
25	17	0	-1.087547	-2.106397	2.389999
26	17	0	0.390957	-3.406128	-0.791558
27	17	0	1.214869	0.391326	2.660591
28	1	0	-2.449119	2.640240	0.847504
29	1	0	-2.350097	5.071957	0.403612
30	1	0	-0.277201	6.087496	-0.526147
31	1	0	1.694007	4.646692	-1.001797
32	1	0	1.591939	2.218261	-0.567184
33	1	0	-2.720969	1.542312	-1.371445
34	1	0	-4.856655	1.155114	-2.532307
35	1	0	-6.074854	-0.995488	-2.236897
36	1	0	-5.111456	-2.762233	-0.772474
37	1	0	-2.976413	-2.377645	0.395699
38	1	0	2.724219	-2.380327	-1.790461
39	1	0	4.940569	-1.932327	-2.769000
40	1	0	6.292011	0.002961	-1.982752
41	1	0	5.398307	1.482823	-0.193069
42	1	0	3.188252	1.027179	0.804953

Zero-point vibrational energy 823306.7 (Joules/Mol)
196.77502 (Kcal/Mol)

Zero-point correction= 0.313581 (Hartree/Particle)
Thermal correction to Energy= 0.336143
Thermal correction to Enthalpy= 0.337087
Thermal correction to Gibbs Free Energy= 0.258360
Sum of electronic and zero-point Energies= -2303.782114
Sum of electronic and thermal Energies= -2303.759552
Sum of electronic and thermal Enthalpies= -2303.758607
Sum of electronic and thermal Free Energies= -2303.837334

TS5d-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000787	-1.777993	-1.117332
2	6	0	0.000035	-0.209831	0.497158
3	6	0	-1.254539	0.038354	-0.293752
4	6	0	-1.269023	-1.059668	-1.102108
5	6	0	1.270367	-1.059235	-1.101394
6	6	0	1.255361	0.038434	-0.292634
7	6	0	2.064100	1.250109	-0.220526
8	6	0	1.962135	2.067746	0.924211
9	6	0	2.705148	3.239966	1.037815
10	6	0	3.570271	3.622967	0.012063
11	6	0	3.681943	2.823948	-1.130122
12	6	0	2.940700	1.653425	-1.250342
13	6	0	-0.000359	-0.935936	1.744491
14	6	0	1.215262	-1.272580	2.391915
15	6	0	1.208816	-1.939505	3.610264
16	6	0	-0.001139	-2.278621	4.225904
17	6	0	-1.210680	-1.938142	3.610240
18	6	0	-1.216389	-1.271017	2.391974
19	6	0	-2.063839	1.249648	-0.221834
20	6	0	-1.961047	2.068283	0.922116
21	6	0	-2.705109	3.239802	1.036008
22	6	0	-3.572325	3.621069	0.011374
23	6	0	-3.684903	2.821059	-1.130019
24	6	0	-2.942524	1.651266	-1.250561
25	17	0	-2.580726	-1.583835	-2.161788
26	17	0	0.001062	-3.500029	-1.347691
27	17	0	2.582759	-1.582761	-2.160534
28	1	0	3.025933	1.055394	-2.149363
29	1	0	4.346893	3.119933	-1.937049
30	1	0	4.153025	4.535823	0.099533
31	1	0	2.610944	3.852020	1.930720
32	1	0	1.304993	1.766558	1.734049
33	1	0	2.157496	-1.004150	1.925218
34	1	0	2.151337	-2.192958	4.087877
35	1	0	-0.001458	-2.792112	5.183261
36	1	0	-2.153490	-2.190432	4.087905
37	1	0	-2.158287	-1.001323	1.925326
38	1	0	-1.302272	1.768430	1.731110
39	1	0	-2.610133	3.852625	1.928302
40	1	0	-4.156049	4.533276	0.099120
41	1	0	-4.351460	3.115651	-1.936130
42	1	0	-3.028379	1.052606	-2.149092

Zero-point vibrational energy	814624.5 (Joules/Mol)	
	194.69992 (Kcal/Mol)	
Zero-point correction=		0.310274 (Hartree/Particle)
Thermal correction to Energy=		0.332797
Thermal correction to Enthalpy=		0.333741
Thermal correction to Gibbs Free Energy=		0.255960
Sum of electronic and zero-point Energies=		-2303.747561
Sum of electronic and thermal Energies=		-2303.725038
Sum of electronic and thermal Enthalpies=		-2303.724094
Sum of electronic and thermal Free Energies=		-2303.801875

TS5d-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.729349	0.553045	0.726563
2	6	0	-0.187839	-1.427180	0.969206
3	6	0	1.074020	-1.638091	0.252693
4	6	0	1.698057	-0.438377	0.166143
5	6	0	3.018869	-0.084013	-0.378609
6	6	0	3.232027	1.166328	-0.983458
7	6	0	4.475675	1.497433	-1.515641
8	6	0	5.532414	0.587449	-1.446170
9	6	0	5.336858	-0.654286	-0.837606
10	6	0	4.093418	-0.987814	-0.306114
11	6	0	-1.233977	-0.600100	0.304355
12	6	0	-0.697774	0.663950	0.347287
13	6	0	-1.359654	1.965452	0.112224
14	6	0	-0.731636	2.980934	-0.627514
15	6	0	-1.362633	4.206584	-0.833048
16	6	0	-2.629685	4.441167	-0.295267
17	6	0	-3.262258	3.442145	0.448805
18	6	0	-2.632672	2.216548	0.652983
19	6	0	-2.408416	-1.169380	-0.353987
20	6	0	-3.113108	-0.488604	-1.368999
21	6	0	-4.207815	-1.079804	-1.989402
22	6	0	-4.624551	-2.363603	-1.621085
23	6	0	-3.931329	-3.053636	-0.626118
24	6	0	-2.835951	-2.464098	0.001479
25	1	0	-2.307580	-3.003262	0.782068
26	1	0	-4.243920	-4.052662	-0.334751
27	1	0	-5.479926	-2.821360	-2.110381
28	1	0	-4.733844	-0.541877	-2.773638

29	1	0	-2.787215	0.498074	-1.678898
30	1	0	-3.117527	1.444817	1.243354
31	1	0	-4.244390	3.621198	0.877935
32	1	0	-3.119806	5.398321	-0.451512
33	1	0	-0.864641	4.978645	-1.413345
34	1	0	0.250232	2.800603	-1.055829
35	1	0	2.415007	1.878745	-1.042267
36	1	0	4.620016	2.467058	-1.984354
37	1	0	6.503723	0.846443	-1.858753
38	1	0	6.157160	-1.363629	-0.770099
39	1	0	3.953321	-1.946897	0.180704
40	17	0	1.367666	1.724462	1.864022
41	17	0	-0.275001	-1.752483	2.692745
42	17	0	1.446808	-3.138832	-0.580446

Zero-point vibrational energy 813691.7 (Joules/Mol)
194.47699 (Kcal/Mol)
Zero-point correction= 0.309919 (Hartree/Particle)
Thermal correction to Energy= 0.332774
Thermal correction to Enthalpy= 0.333718
Thermal correction to Gibbs Free Energy= 0.254305
Sum of electronic and zero-point Energies= -2303.729874
Sum of electronic and thermal Energies= -2303.707019
Sum of electronic and thermal Enthalpies= -2303.706075
Sum of electronic and thermal Free Energies= -2303.785488

P-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.208202	1.887274	-0.017869
2	6	0	1.227954	0.482452	-0.010412
3	6	0	0.000008	-0.216661	-0.000013
4	6	0	-1.227742	0.482841	0.010379
5	6	0	-1.207564	1.887622	0.017739
6	6	0	0.000437	2.599509	-0.000100
7	17	0	0.000735	4.339571	-0.000192
8	17	0	2.716769	2.770974	-0.085823
9	17	0	-2.715920	2.771726	0.085667
10	6	0	2.531715	-0.254026	-0.043568
11	6	0	-0.000291	-1.716211	-0.000077
12	6	0	-2.531697	-0.253273	0.043713
13	6	0	3.351701	-0.307639	1.092020
14	6	0	4.562652	-0.998306	1.059622

15	6	0	4.973352	-1.638871	-0.110867
16	6	0	4.165642	-1.585976	-1.247601
17	6	0	2.951661	-0.899664	-1.213612
18	6	0	-0.441478	-2.430605	-1.122625
19	6	0	-0.438742	-3.825209	-1.124324
20	6	0	-0.000986	-4.527331	-0.000319
21	6	0	0.437068	-3.825620	1.123806
22	6	0	0.440453	-2.430998	1.122360
23	6	0	-3.351624	-0.307161	-1.091890
24	6	0	-4.562765	-0.997502	-1.059263
25	6	0	-4.973697	-1.637460	0.111468
26	6	0	-4.166024	-1.584302	1.248224
27	6	0	-2.951869	-0.898323	1.214010
28	1	0	3.038377	0.195689	2.002755
29	1	0	5.186112	-1.033856	1.949044
30	1	0	5.918013	-2.175371	-0.136643
31	1	0	4.478854	-2.079872	-2.163460
32	1	0	2.324145	-0.862686	-2.099335
33	1	0	-0.789099	-1.889496	-1.997922
34	1	0	-0.781060	-4.362660	-2.004664
35	1	0	-0.001257	-5.614006	-0.000412
36	1	0	0.779104	-4.363370	2.004072
37	1	0	0.788282	-1.890233	1.997784
38	1	0	-3.038129	0.195693	-2.002828
39	1	0	-5.186176	-1.033251	-1.948711
40	1	0	-5.918497	-2.173704	0.137430
41	1	0	-4.479411	-2.077738	2.164272
42	1	0	-2.324385	-0.861114	2.099750

Zero-point vibrational energy 823023.7 (Joules/Mol)
196.70740 (Kcal/Mol)
Zero-point correction= 0.313473 (Hartree/Particle)
Thermal correction to Energy= 0.335973
Thermal correction to Enthalpy= 0.336917
Thermal correction to Gibbs Free Energy= 0.258966
Sum of electronic and zero-point Energies= -2303.859559
Sum of electronic and thermal Energies= -2303.837059
Sum of electronic and thermal Enthalpies= -2303.836115
Sum of electronic and thermal Free Energies= -2303.914067

P-4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.005334	-1.767246	-0.046832
2	6	0	0.978748	-0.754007	-0.020039
3	6	0	0.565597	0.596372	0.007261
4	6	0	-0.810476	0.878603	0.017212
5	6	0	-1.797689	-0.119283	-0.004175
6	6	0	-1.360996	-1.453498	-0.040155
7	17	0	0.508596	-3.441042	-0.121042
8	17	0	-2.552896	-2.731483	-0.084083
9	17	0	-1.333410	2.555510	0.094778
10	6	0	1.578566	1.698474	0.036372
11	6	0	1.835869	2.459154	-1.112316
12	6	0	2.783894	3.481457	-1.087500
13	6	0	3.483132	3.760638	0.088077
14	6	0	3.229110	3.011701	1.237810
15	6	0	2.283990	1.986033	1.211826
16	6	0	2.435885	-1.100287	-0.031217
17	6	0	3.193598	-0.947630	-1.199159
18	6	0	4.551110	-1.268701	-1.208940
19	6	0	5.168002	-1.743146	-0.050654
20	6	0	4.419631	-1.898684	1.117474
21	6	0	3.061607	-1.582176	1.126482
22	6	0	-3.255216	0.216585	0.015710
23	6	0	-3.948482	0.284197	1.230567
24	6	0	-5.307830	0.595697	1.249529
25	6	0	-5.987346	0.841392	0.055253
26	6	0	-5.301642	0.774853	-1.158717
27	6	0	-3.941972	0.464408	-1.179220
28	1	0	1.288581	2.248302	-2.027077
29	1	0	2.974634	4.060773	-1.986949
30	1	0	4.220897	4.558239	0.108019
31	1	0	3.767082	3.224217	2.157760
32	1	0	2.089528	1.404555	2.108402
33	1	0	2.717076	-0.577580	-2.102363
34	1	0	5.125979	-1.146958	-2.123012
35	1	0	6.225932	-1.991291	-0.058039
36	1	0	4.892122	-2.268693	2.023463
37	1	0	2.480164	-1.710572	2.035460
38	1	0	-3.420141	0.092666	2.160376
39	1	0	-5.835321	0.645861	2.198236
40	1	0	-7.046607	1.083463	0.070473
41	1	0	-5.824507	0.964392	-2.092269
42	1	0	-3.408905	0.412445	-2.124492

Zero-point vibrational energy 822709.9 (Joules/Mol)
196.63239 (Kcal/Mol)

Zero-point correction= 0.313354 (Hartree/Particle)
Thermal correction to Energy= 0.335989
Thermal correction to Enthalpy= 0.336934
Thermal correction to Gibbs Free Energy= 0.257705
Sum of electronic and zero-point Energies= -2303.861888
Sum of electronic and thermal Energies= -2303.839252
Sum of electronic and thermal Enthalpies= -2303.838308
Sum of electronic and thermal Free Energies= -2303.917537

1e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.270501	1.218102	0.000024
2	6	0	-1.972024	-0.000143	0.000321
3	6	0	-1.270227	-1.218225	0.000026
4	6	0	0.130114	-1.212900	-0.000558
5	6	0	0.853252	0.000170	-0.000755
6	6	0	0.129834	1.213074	-0.000562
7	6	0	2.273494	0.000355	-0.001324
8	6	0	3.483240	0.000076	0.000694
9	17	0	5.127593	0.000113	0.001445
10	17	0	1.010906	2.709200	-0.001066
11	17	0	-2.138330	2.720928	0.000264
12	17	0	-3.705880	-0.000337	0.000915
13	17	0	-2.137725	-2.721245	0.000263
14	17	0	1.011489	-2.708839	-0.001067

Zero-point vibrational energy 138135.4 (Joules/Mol)
33.01515 (Kcal/Mol)
Zero-point correction= 0.052613 (Hartree/Particle)
Thermal correction to Energy= 0.066425
Thermal correction to Enthalpy= 0.067369
Thermal correction to Gibbs Free Energy= 0.009401
Sum of electronic and zero-point Energies= -3065.873008
Sum of electronic and thermal Energies= -3065.859197
Sum of electronic and thermal Enthalpies= -3065.858253
Sum of electronic and thermal Free Energies= -3065.916221

TS1e-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.469336	-0.289116	0.888490
2	6	0	1.710176	-0.196994	0.808534
3	6	0	-1.710176	-0.196995	-0.808533
4	6	0	-0.469336	-0.289117	-0.888489
5	17	0	-0.709855	-0.408448	2.103416
6	17	0	0.709855	-0.408450	-2.103415
7	6	0	3.069265	-0.078523	0.500834
8	6	0	-3.069265	-0.078524	-0.500834
9	6	0	-3.684432	1.198701	-0.390543
10	6	0	-5.048939	1.320419	-0.117604
11	6	0	-5.835389	0.164166	0.050952
12	6	0	-5.249763	-1.112484	-0.056088
13	6	0	-3.885391	-1.230324	-0.330827
14	6	0	3.885391	-1.230324	0.330827
15	6	0	5.249762	-1.112484	0.056088
16	6	0	5.835389	0.164165	-0.050953
17	6	0	5.048940	1.320419	0.117603
18	6	0	3.684432	1.198701	0.390543
19	17	0	-3.148322	-2.793125	-0.468314
20	17	0	-6.224590	-2.532846	0.152138
21	17	0	-7.526982	0.312267	0.388931
22	17	0	-5.776876	2.890248	0.013921
23	17	0	-2.701583	2.611019	-0.601798
24	17	0	2.701584	2.611020	0.601798
25	17	0	5.776877	2.890247	-0.013922
26	17	0	7.526982	0.312266	-0.388932
27	17	0	6.224590	-2.532847	-0.152139
28	17	0	3.148321	-2.793124	0.468315

Zero-point vibrational energy 275755.6 (Joules/Mol)
65.90718 (Kcal/Mol)
Zero-point correction= 0.105030 (Hartree/Particle)
Thermal correction to Energy= 0.133708
Thermal correction to Enthalpy= 0.134652
Thermal correction to Gibbs Free Energy= 0.037421
Sum of electronic and zero-point Energies= -6131.710840
Sum of electronic and thermal Energies= -6131.682162
Sum of electronic and thermal Enthalpies= -6131.681218
Sum of electronic and thermal Free Energies= -6131.778448

TS1e-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.867097	1.937756	0.319397
2	6	0	-0.668886	2.278187	-1.146904
3	6	0	0.400966	1.626855	-1.129347
4	6	0	1.511070	0.818939	-0.870239
5	6	0	2.596160	1.297117	-0.083052
6	6	0	3.721027	0.504141	0.153273
7	6	0	3.793262	-0.792564	-0.392435
8	6	0	2.735867	-1.286971	-1.181075
9	6	0	1.614998	-0.489191	-1.419735
10	6	0	-2.285602	2.974938	0.906653
11	6	0	-2.048246	0.497593	0.510682
12	6	0	-1.383084	-0.182259	1.547944
13	6	0	-1.554459	-1.562661	1.733632
14	6	0	-2.401264	-2.280918	0.873422
15	6	0	-3.074146	-1.617592	-0.166454
16	6	0	-2.890025	-0.239462	-0.341592
17	17	0	-3.722988	0.593678	-1.618430
18	17	0	-4.126728	-2.501430	-1.225227
19	17	0	-2.618463	-3.986934	1.095868
20	17	0	-0.726431	-2.382507	3.019836
21	17	0	-0.341904	0.707798	2.620265
22	17	0	-2.311361	4.602076	1.172142
23	17	0	-1.371042	3.465891	-2.160712
24	17	0	2.497444	2.899531	0.573658
25	17	0	5.029399	1.110978	1.118758
26	17	0	5.185714	-1.778610	-0.097027
27	17	0	2.831658	-2.882815	-1.856164
28	17	0	0.309805	-1.077271	-2.400908

Zero-point vibrational energy 273639.5 (Joules/Mol)
65.40141 (Kcal/Mol)
Zero-point correction= 0.104224 (Hartree/Particle)
Thermal correction to Energy= 0.133049
Thermal correction to Enthalpy= 0.133994
Thermal correction to Gibbs Free Energy= 0.037345
Sum of electronic and zero-point Energies= -6131.697978
Sum of electronic and thermal Energies= -6131.669152
Sum of electronic and thermal Enthalpies= -6131.668208
Sum of electronic and thermal Free Energies= -6131.764857

TS1e-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.480164	0.000087	0.817561
2	6	0	0.480159	-0.000059	-0.817526
3	6	0	-0.168933	-0.000380	-1.910455
4	6	0	0.168921	0.000076	1.910494
5	6	0	-1.932979	0.000120	0.584917
6	6	0	-2.644167	1.208287	0.471748
7	6	0	-4.027649	1.216706	0.240598
8	6	0	-4.719282	0.000132	0.119863
9	6	0	-4.027777	-1.216446	0.241307
10	6	0	-2.644292	-1.208042	0.472442
11	6	0	1.932975	-0.000012	-0.584888
12	6	0	2.644186	1.208159	-0.471924
13	6	0	4.027673	1.216591	-0.240805
14	6	0	4.719287	0.000024	-0.119892
15	6	0	4.027757	-1.216561	-0.241127
16	6	0	2.644268	-1.208170	-0.472235
17	17	0	1.787914	-2.711485	-0.635460
18	17	0	4.884245	-2.719923	-0.105750
19	17	0	6.429222	0.000045	0.172114
20	17	0	4.884055	2.719978	-0.105045
21	17	0	1.787733	2.711450	-0.634835
22	17	0	-1.571054	-0.001235	-2.790055
23	17	0	1.571054	0.000331	2.790078
24	17	0	-1.787966	-2.711345	0.635930
25	17	0	-4.884290	-2.719813	0.106149
26	17	0	-6.429211	0.000139	-0.172182
27	17	0	-4.884002	2.720087	0.104586
28	17	0	-1.787695	2.711590	0.634443

Zero-point vibrational energy 273473.3 (Joules/Mol)
65.36168 (Kcal/Mol)
Zero-point correction= 0.104160 (Hartree/Particle)
Thermal correction to Energy= 0.132942
Thermal correction to Enthalpy= 0.133886
Thermal correction to Gibbs Free Energy= 0.038595
Sum of electronic and zero-point Energies= -6131.683143
Sum of electronic and thermal Energies= -6131.654362
Sum of electronic and thermal Enthalpies= -6131.653418
Sum of electronic and thermal Free Energies= -6131.748708

1f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.113144	0.000001	0.000051
2	6	0	1.094176	-0.000031	0.000024
3	17	0	-1.768601	0.000003	-0.000014
4	6	0	2.554831	0.000011	-0.000018
5	1	0	2.950404	-0.509076	0.886825
6	1	0	2.950331	-0.513485	-0.884353
7	1	0	2.950299	1.022627	-0.002582

Zero-point vibrational energy 125372.2 (Joules/Mol)
29.96467 (Kcal/Mol)
Zero-point correction= 0.047752 (Hartree/Particle)
Thermal correction to Energy= 0.052753
Thermal correction to Enthalpy= 0.053697
Thermal correction to Gibbs Free Energy= 0.020452
Sum of electronic and zero-point Energies= -576.192894
Sum of electronic and thermal Energies= -576.187893
Sum of electronic and thermal Enthalpies= -576.186949
Sum of electronic and thermal Free Energies= -576.220194

1f-triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.439109	-0.005442	-0.000159
2	6	0	1.000574	-0.331072	0.000016
3	6	0	-0.060324	0.535164	0.000117
4	17	0	-1.692766	-0.076485	-0.000035
5	1	0	2.914600	-0.482576	-0.870088
6	1	0	2.912474	-0.475746	0.874715
7	1	0	2.673788	1.066660	-0.003875

Zero-point vibrational energy 117351.6 (Joules/Mol)
28.04770 (Kcal/Mol)
Zero-point correction= 0.044697 (Hartree/Particle)
Thermal correction to Energy= 0.049941
Thermal correction to Enthalpy= 0.050885
Thermal correction to Gibbs Free Energy= 0.015312
Sum of electronic and zero-point Energies= -576.074186
Sum of electronic and thermal Energies= -576.068942
Sum of electronic and thermal Enthalpies= -576.067998
Sum of electronic and thermal Free Energies= -576.103571

TS1f-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.434139	0.859772	-0.003896
2	6	0	-1.683925	0.884995	0.024909
3	6	0	1.683930	-0.884994	0.024895
4	6	0	0.434144	-0.859768	-0.003884
5	17	0	0.801249	2.058819	-0.044191
6	17	0	-0.801259	-2.058801	-0.044192
7	6	0	-3.109647	0.594278	0.065618
8	6	0	3.109658	-0.594310	0.065621
9	1	0	-3.366806	-0.033332	0.927912
10	1	0	-3.694478	1.521907	0.147337
11	1	0	-3.438528	0.076659	-0.843791
12	1	0	3.438487	-0.076340	-0.843607
13	1	0	3.694481	-1.521981	0.146931
14	1	0	3.366886	0.032955	0.928145

Zero-point vibrational energy 248641.0 (Joules/Mol)
59.42662 (Kcal/Mol)
Zero-point correction= 0.094702 (Hartree/Particle)
Thermal correction to Energy= 0.105349
Thermal correction to Enthalpy= 0.106293
Thermal correction to Gibbs Free Energy= 0.055956
Sum of electronic and zero-point Energies= -1152.338026
Sum of electronic and thermal Energies= -1152.327379
Sum of electronic and thermal Enthalpies= -1152.326435
Sum of electronic and thermal Free Energies= -1152.376773

INT1f-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.309898	-0.674458	-0.001218
2	6	0	-1.571688	-0.998030	-0.011841
3	6	0	1.571252	0.997444	-0.010713
4	6	0	0.308836	0.676294	-0.000126
5	17	0	0.912657	-1.999060	0.018359
6	17	0	-0.911530	2.002075	0.018152
7	6	0	-3.009257	-0.738757	-0.025394
8	6	0	3.008173	0.732794	-0.025756
9	1	0	-3.268464	0.039765	-0.755021
10	1	0	-3.571964	-1.644625	-0.289333
11	1	0	-3.357639	-0.407683	0.961244

12	1	0	3.333793	0.269754	0.914507
13	1	0	3.580296	1.661912	-0.154026
14	1	0	3.280313	0.057900	-0.847767

Zero-point vibrational energy 250616.6 (Joules/Mol)
59.89880 (Kcal/Mol)
Zero-point correction= 0.095455 (Hartree/Particle)
Thermal correction to Energy= 0.104492
Thermal correction to Enthalpy= 0.105436
Thermal correction to Gibbs Free Energy= 0.059802
Sum of electronic and zero-point Energies= -1152.361660
Sum of electronic and thermal Energies= -1152.352623
Sum of electronic and thermal Enthalpies= -1152.351679
Sum of electronic and thermal Free Energies= -1152.397312

TS1f-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.344443	-0.089527	1.102123
2	6	0	-1.522994	-0.243351	0.667901
3	6	0	1.649948	-0.738437	-0.590931
4	6	0	0.950956	0.241336	-0.248120
5	6	0	0.371323	-0.013848	2.407884
6	17	0	-2.487930	-0.441992	-0.682729
7	6	0	2.117267	-2.114686	-0.697081
8	17	0	0.856508	1.924859	-0.604900
9	1	0	-0.337014	-0.121327	3.233818
10	1	0	1.124767	-0.805784	2.484487
11	1	0	0.890933	0.945246	2.514328
12	1	0	1.476671	-2.802347	-0.123851
13	1	0	2.101863	-2.451244	-1.741597
14	1	0	3.144605	-2.222216	-0.328143

Zero-point vibrational energy 249713.2 (Joules/Mol)
59.68289 (Kcal/Mol)
Zero-point correction= 0.095111 (Hartree/Particle)
Thermal correction to Energy= 0.105636
Thermal correction to Enthalpy= 0.106580
Thermal correction to Gibbs Free Energy= 0.056777
Sum of electronic and zero-point Energies= -1152.337168
Sum of electronic and thermal Energies= -1152.326642
Sum of electronic and thermal Enthalpies= -1152.325698
Sum of electronic and thermal Free Energies= -1152.375502

TS1f-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.564607	-0.012156	-0.768901
2	6	0	-0.486463	0.647440	-0.815556
3	6	0	0.486463	0.647440	0.815556
4	6	0	1.564607	-0.012156	0.768901
5	17	0	-2.528422	-1.062109	0.106238
6	17	0	2.528422	-1.062109	-0.106238
7	6	0	0.260215	1.508552	-1.777649
8	6	0	-0.260215	1.508551	1.777650
9	1	0	-0.299386	1.605484	-2.711938
10	1	0	0.427853	2.509403	-1.363465
11	1	0	1.242446	1.077954	-2.000324
12	1	0	0.299385	1.605482	2.711939
13	1	0	-0.427853	2.509403	1.363466
14	1	0	-1.242446	1.077953	2.000324

Zero-point vibrational energy 251933.8 (Joules/Mol)
60.21362 (Kcal/Mol)
Zero-point correction= 0.095957 (Hartree/Particle)
Thermal correction to Energy= 0.106124
Thermal correction to Enthalpy= 0.107068
Thermal correction to Gibbs Free Energy= 0.058855
Sum of electronic and zero-point Energies= -1152.337470
Sum of electronic and thermal Energies= -1152.327303
Sum of electronic and thermal Enthalpies= -1152.326359
Sum of electronic and thermal Free Energies= -1152.374572

1g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.332152	-0.000064	0.000103
2	6	0	0.123540	-0.000120	0.000261
3	17	0	2.988182	0.000001	0.000015
4	6	0	-1.351339	-0.000056	0.000030
5	6	0	-1.861174	-0.340347	1.420000
6	6	0	-1.860725	-1.059668	-1.004901
7	6	0	-1.860641	1.400102	-0.415346
8	1	0	-2.957554	-0.342817	1.433057

9	1	0	-1.509606	0.396117	2.149986
10	1	0	-1.510610	-1.328258	1.736225
11	1	0	-2.957131	-1.069621	-1.014167
12	1	0	-1.509555	-0.839963	-2.018449
13	1	0	-1.509594	-2.060180	-0.731800
14	1	0	-1.508528	1.664637	-1.417835
15	1	0	-1.510338	2.167930	0.282291
16	1	0	-2.957059	1.413052	-0.420445

Zero-point vibrational energy 349533.8 (Joules/Mol)
83.54059 (Kcal/Mol)
Zero-point correction= 0.133130 (Hartree/Particle)
Thermal correction to Energy= 0.141842
Thermal correction to Enthalpy= 0.142786
Thermal correction to Gibbs Free Energy= 0.099859
Sum of electronic and zero-point Energies= -694.049501
Sum of electronic and thermal Energies= -694.040790
Sum of electronic and thermal Enthalpies= -694.039846
Sum of electronic and thermal Free Energies= -694.082773

TS1g-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.586237	-0.747433	-0.631715
2	6	0	1.705932	-0.598605	-0.092080
3	6	0	-1.705958	0.598640	-0.091895
4	6	0	-0.586293	0.747738	-0.631511
5	17	0	-0.230104	-2.028302	-1.458336
6	17	0	0.230045	2.028910	-1.457659
7	6	0	2.859493	-0.067338	0.649129
8	6	0	-2.859465	0.067060	0.649173
9	6	0	3.556264	-1.243907	1.382030
10	6	0	3.853496	0.585942	-0.339937
11	6	0	2.389679	0.977457	1.693502
12	6	0	-3.556237	1.243337	1.382542
13	6	0	-3.853495	-0.585887	-0.340087
14	6	0	-2.389564	-0.978104	1.693135
15	1	0	4.421029	-0.867970	1.941710
16	1	0	2.873172	-1.728152	2.087532
17	1	0	3.906202	-1.998643	0.670516
18	1	0	4.722378	0.970788	0.206905
19	1	0	3.383242	1.417280	-0.873856
20	1	0	4.205751	-0.140636	-1.079332

21	1	0	1.901787	1.827189	1.206971
22	1	0	1.681749	0.531943	2.399992
23	1	0	3.252518	1.350402	2.258717
24	1	0	-4.420932	0.867158	1.942167
25	1	0	-2.873111	1.727374	2.088154
26	1	0	-3.906273	1.998298	0.671315
27	1	0	-4.722335	-0.970976	0.206651
28	1	0	-3.383243	-1.417007	-0.874348
29	1	0	-4.205819	0.140952	-1.079194
30	1	0	-1.901643	-1.827636	1.206279
31	1	0	-1.681630	-0.532822	2.399766
32	1	0	-3.252369	-1.351299	2.258241

Zero-point vibrational energy 696670.1 (Joules/Mol)
166.50815 (Kcal/Mol)
Zero-point correction= 0.265348 (Hartree/Particle)
Thermal correction to Energy= 0.283756
Thermal correction to Enthalpy= 0.284700
Thermal correction to Gibbs Free Energy= 0.217290
Sum of electronic and zero-point Energies= -1388.049280
Sum of electronic and thermal Energies= -1388.030872
Sum of electronic and thermal Enthalpies= -1388.029928
Sum of electronic and thermal Free Energies= -1388.097338

TS1g-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.267188	0.087051	-0.251121
2	6	0	1.544562	1.189244	-0.812187
3	6	0	-1.373672	-0.048554	0.496461
4	6	0	-0.242232	0.271358	0.919215
5	6	0	1.847642	-1.314805	-0.232166
6	17	0	1.037126	2.758587	-1.100229
7	17	0	0.389290	0.958705	2.379877
8	6	0	-2.596963	-0.365258	-0.255227
9	6	0	2.037316	-1.836458	1.207393
10	6	0	0.923002	-2.277844	-1.005780
11	6	0	3.224382	-1.266989	-0.933143
12	6	0	-3.090740	-1.788526	0.093375
13	6	0	-2.347770	-0.247938	-1.781050
14	6	0	-3.679294	0.668030	0.160507
15	1	0	2.503686	-2.828129	1.176627
16	1	0	2.683903	-1.172135	1.789073

17	1	0	1.082032	-1.928273	1.732112
18	1	0	1.363310	-3.281980	-1.023538
19	1	0	0.785942	-1.946144	-2.040705
20	1	0	-0.059522	-2.350044	-0.530243
21	1	0	3.126041	-0.917306	-1.965311
22	1	0	3.671380	-2.268648	-0.944614
23	1	0	3.904548	-0.588673	-0.409223
24	1	0	-4.030296	-1.995214	-0.432290
25	1	0	-3.268749	-1.890199	1.168823
26	1	0	-2.360871	-2.547862	-0.205631
27	1	0	-3.280611	-0.443618	-2.323581
28	1	0	-1.998407	0.755445	-2.043179
29	1	0	-1.597239	-0.969618	-2.115984
30	1	0	-3.893852	0.604461	1.232009
31	1	0	-3.354766	1.688702	-0.065194
32	1	0	-4.606133	0.469396	-0.390840

Zero-point vibrational energy 697457.2 (Joules/Mol)
166.69626 (Kcal/Mol)
Zero-point correction= 0.265647 (Hartree/Particle)
Thermal correction to Energy= 0.283857
Thermal correction to Enthalpy= 0.284801
Thermal correction to Gibbs Free Energy= 0.218479
Sum of electronic and zero-point Energies= -1388.045971
Sum of electronic and thermal Energies= -1388.027762
Sum of electronic and thermal Enthalpies= -1388.026818
Sum of electronic and thermal Free Energies= -1388.093139

TS1g-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.665628	1.545052	-0.763129
2	6	0	0.788015	0.545694	0.008381
3	6	0	-0.788133	-0.545774	0.007483
4	6	0	-0.665543	-1.544042	-0.765405
5	17	0	-0.225555	2.337473	-1.936095
6	17	0	0.226084	-2.334613	-1.939303
7	6	0	1.940666	0.045425	0.880509
8	6	0	-1.940900	-0.046725	0.880130
9	6	0	2.428891	1.227251	1.750736
10	6	0	1.560892	-1.128281	1.801833
11	6	0	3.091412	-0.402964	-0.052158
12	6	0	-1.560866	1.124815	1.804101

13	6	0	-3.091017	0.404251	-0.052059
14	6	0	-2.430124	-1.230121	1.747654
15	1	0	3.277437	0.910407	2.369417
16	1	0	2.747104	2.064746	1.123135
17	1	0	1.636634	1.584789	2.416681
18	1	0	2.435008	-1.408931	2.400577
19	1	0	1.240553	-2.006528	1.236216
20	1	0	0.757068	-0.859637	2.494560
21	1	0	2.781612	-1.231277	-0.696541
22	1	0	3.415095	0.424413	-0.691394
23	1	0	3.948897	-0.737168	0.544898
24	1	0	-2.435070	1.404703	2.403075
25	1	0	-0.757491	0.854250	2.496603
26	1	0	-1.239782	2.004070	1.240469
27	1	0	-3.948602	0.737552	0.545359
28	1	0	-3.414814	-0.421582	-0.693230
29	1	0	-2.780560	1.233823	-0.694498
30	1	0	-2.748609	-2.066093	1.118165
31	1	0	-1.638298	-1.589555	2.413094
32	1	0	-3.278692	-0.914093	2.366722

Zero-point vibrational energy 699019.9 (Joules/Mol)
167.06978 (Kcal/Mol)
Zero-point correction= 0.266243 (Hartree/Particle)
Thermal correction to Energy= 0.284117
Thermal correction to Enthalpy= 0.285061
Thermal correction to Gibbs Free Energy= 0.220091
Sum of electronic and zero-point Energies= -1388.038310
Sum of electronic and thermal Energies= -1388.020436
Sum of electronic and thermal Enthalpies= -1388.019491
Sum of electronic and thermal Free Energies= -1388.084462

1h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.272672	0.000311	0.095305
2	6	0	-1.079486	-0.000646	0.287366
3	17	0	-3.909557	0.000019	-0.154720
4	6	0	0.372266	-0.000361	0.492229
5	6	0	1.028892	1.273677	-0.095979
6	6	0	2.549553	1.268352	0.117719
7	6	0	3.199016	0.000403	-0.456688
8	6	0	2.550198	-1.267940	0.117573

9	6	0	1.029540	-1.273996	-0.096127
10	1	0	0.562093	-0.000390	1.577635
11	1	0	0.803258	1.318389	-1.170270
12	1	0	0.576908	2.162962	0.358487
13	1	0	2.990414	2.163653	-0.338304
14	1	0	2.764316	1.330014	1.194985
15	1	0	3.085839	0.000436	-1.550896
16	1	0	4.277359	0.000666	-0.253862
17	1	0	2.991504	-2.162967	-0.338556
18	1	0	2.764991	-1.329621	1.194832
19	1	0	0.803942	-1.318701	-1.170428
20	1	0	0.578013	-2.163574	0.358225

Zero-point vibrational energy 451115.5 (Joules/Mol)
107.81920 (Kcal/Mol)
Zero-point correction= 0.171821 (Hartree/Particle)
Thermal correction to Energy= 0.180783
Thermal correction to Enthalpy= 0.181727
Thermal correction to Gibbs Free Energy= 0.137095
Sum of electronic and zero-point Energies= -771.434238
Sum of electronic and thermal Energies= -771.425276
Sum of electronic and thermal Enthalpies= -771.424331
Sum of electronic and thermal Free Energies= -771.468964

TS1h-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.609404	0.860858	-0.099382
2	6	0	1.841808	0.652867	-0.152229
3	6	0	-1.788315	-0.481137	-0.195039
4	6	0	-0.577553	-0.608651	-0.482547
5	17	0	-0.374335	2.231392	0.256345
6	17	0	0.375904	-1.867000	-1.175119
7	6	0	3.204870	0.140253	-0.263472
8	6	0	-3.118795	-0.069351	0.244749
9	6	0	3.532362	-0.900904	0.837562
10	6	0	4.973291	-1.416115	0.709894
11	6	0	5.993265	-0.268088	0.725507
12	6	0	5.674574	0.774221	-0.356434
13	6	0	4.238360	1.303826	-0.231819
14	6	0	-3.912280	-1.275420	0.821781
15	6	0	-5.311560	-0.845570	1.286107
16	6	0	-6.098919	-0.160490	0.159606

17	6	0	-5.319488	1.027560	-0.423843
18	6	0	-3.917245	0.613879	-0.893623
19	1	0	3.305214	-0.356305	-1.242029
20	1	0	-3.001988	0.661820	1.061723
21	1	0	3.391167	-0.427180	1.818667
22	1	0	2.818605	-1.729196	0.777437
23	1	0	5.184247	-2.125135	1.520316
24	1	0	5.074456	-1.979218	-0.229759
25	1	0	5.975842	0.217841	1.712191
26	1	0	7.008983	-0.659564	0.587417
27	1	0	6.380941	1.612049	-0.300600
28	1	0	5.807229	0.319498	-1.349241
29	1	0	4.122247	1.849933	0.714081
30	1	0	4.015862	2.013117	-1.037074
31	1	0	-3.996951	-2.045762	0.043279
32	1	0	-3.349442	-1.721793	1.649593
33	1	0	-5.860208	-1.719534	1.659054
34	1	0	-5.213925	-0.152451	2.134721
35	1	0	-6.297026	-0.891121	-0.638556
36	1	0	-7.077306	0.171812	0.528859
37	1	0	-5.872314	1.472532	-1.260660
38	1	0	-5.228391	1.813067	0.341020
39	1	0	-3.998360	-0.088494	-1.734456
40	1	0	-3.358239	1.482973	-1.257726

Zero-point vibrational energy 900752.0 (Joules/Mol)
215.28489 (Kcal/Mol)
Zero-point correction= 0.343078 (Hartree/Particle)
Thermal correction to Energy= 0.361837
Thermal correction to Enthalpy= 0.362781
Thermal correction to Gibbs Free Energy= 0.293168
Sum of electronic and zero-point Energies= -1542.820695
Sum of electronic and thermal Energies= -1542.801937
Sum of electronic and thermal Enthalpies= -1542.800993
Sum of electronic and thermal Free Energies= -1542.870606

TS1h-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.209907	0.861487	-0.274763
2	6	0	-0.098102	1.023501	1.091956
3	6	0	-1.110669	0.293612	1.021329
4	6	0	-2.173161	-0.609202	0.583578

5	6	0	-2.303046	-0.670074	-0.963512
6	6	0	-3.434562	-1.616149	-1.391518
7	6	0	-4.774596	-1.231482	-0.747498
8	6	0	-4.657261	-1.159339	0.781689
9	6	0	-3.533817	-0.209822	1.222543
10	6	0	1.050656	1.657483	-1.248555
11	6	0	2.214658	-0.160119	0.173486
12	6	0	1.707878	-1.604710	-0.038905
13	6	0	2.746526	-2.636462	0.428219
14	6	0	3.571842	0.043368	-0.536252
15	6	0	4.608091	-0.991181	-0.072437
16	6	0	4.101494	-2.428649	-0.264001
17	1	0	3.992735	-2.633484	-1.339347
18	1	0	4.837957	-3.146796	0.118354
19	1	0	5.548509	-0.841896	-0.618057
20	1	0	4.836200	-0.825900	0.991025
21	1	0	3.930470	1.062178	-0.352273
22	1	0	3.414135	-0.042740	-1.619704
23	1	0	2.372571	-3.650847	0.239529
24	1	0	2.877333	-2.550033	1.517078
25	1	0	1.498058	-1.748305	-1.108381
26	1	0	2.376509	-0.021506	1.252640
27	1	0	0.762460	-1.748353	0.496401
28	17	0	-0.003112	2.741607	-1.971616
29	17	0	0.544140	2.192596	2.191728
30	1	0	-1.930701	-1.622588	0.942708
31	1	0	-1.348591	-0.985271	-1.399329
32	1	0	-2.499968	0.344092	-1.335159
33	1	0	-3.175369	-2.646053	-1.104024
34	1	0	-3.521703	-1.612377	-2.485298
35	1	0	-5.553720	-1.948640	-1.034663
36	1	0	-5.093306	-0.251589	-1.132281
37	1	0	-4.457749	-2.165445	1.179515
38	1	0	-5.607188	-0.833170	1.223421
39	1	0	-3.773077	0.818458	0.919568
40	1	0	-3.438072	-0.204741	2.314217

Zero-point vibrational energy 900347.2 (Joules/Mol)
215.18815 (Kcal/Mol)
Zero-point correction= 0.342924 (Hartree/Particle)
Thermal correction to Energy= 0.361814
Thermal correction to Enthalpy= 0.362758
Thermal correction to Gibbs Free Energy= 0.292099
Sum of electronic and zero-point Energies= -1542.820070
Sum of electronic and thermal Energies= -1542.801181

Sum of electronic and thermal Enthalpies= -1542.800237
Sum of electronic and thermal Free Energies= -1542.870895

TS1h-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.611447	1.297650	-1.570512
2	6	0	0.711431	0.464038	-0.621732
3	6	0	-0.711413	0.464021	0.621613
4	6	0	-0.611471	1.297435	1.570567
5	17	0	-0.182975	2.623421	-2.210425
6	17	0	0.182876	2.623146	2.210652
7	6	0	1.696720	-0.592013	-0.198864
8	6	0	-1.696697	-0.592036	0.198722
9	6	0	2.700712	-0.034413	0.837231
10	6	0	3.720513	-1.101412	1.264695
11	6	0	4.455204	-1.700444	0.056769
12	6	0	3.463343	-2.253326	-0.977225
13	6	0	2.444773	-1.188283	-1.412059
14	6	0	-2.700751	-0.034424	-0.837309
15	6	0	-3.720548	-1.101444	-1.264734
16	6	0	-4.455159	-1.700518	-0.056778
17	6	0	-3.463248	-2.253403	0.977161
18	6	0	-2.444645	-1.188366	1.411944
19	1	0	1.140741	-1.406814	0.287533
20	1	0	-1.140737	-1.406760	-0.287786
21	1	0	3.223474	0.820626	0.387075
22	1	0	2.160971	0.346781	1.710434
23	1	0	4.437812	-0.663686	1.970373
24	1	0	3.200289	-1.904099	1.808224
25	1	0	5.071362	-0.920962	-0.415052
26	1	0	5.144486	-2.489653	0.382774
27	1	0	3.999256	-2.631592	-1.857051
28	1	0	2.930600	-3.113514	-0.544811
29	1	0	2.957672	-0.372252	-1.937980
30	1	0	1.721066	-1.609562	-2.119765
31	1	0	-3.223496	0.820607	-0.387121
32	1	0	-2.161044	0.346783	-1.710532
33	1	0	-4.437899	-0.663738	-1.970371
34	1	0	-3.200314	-1.904098	-1.808303
35	1	0	-5.071325	-0.921061	0.415077
36	1	0	-5.144439	-2.489735	-0.382770
37	1	0	-3.999119	-2.631660	1.857018

38	1	0	-2.930541	-3.113603	0.544731
39	1	0	-2.957515	-0.372358	1.937927
40	1	0	-1.720882	-1.609655	2.119587

Zero-point vibrational energy 900531.6 (Joules/Mol)
215.23222 (Kcal/Mol)
Zero-point correction= 0.342994 (Hartree/Particle)
Thermal correction to Energy= 0.361845
Thermal correction to Enthalpy= 0.362789
Thermal correction to Gibbs Free Energy= 0.293203
Sum of electronic and zero-point Energies= -1542.819840
Sum of electronic and thermal Energies= -1542.800990
Sum of electronic and thermal Enthalpies= -1542.800046
Sum of electronic and thermal Free Energies= -1542.869632

1i

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.069367	1.213513	0.000217
2	6	0	-1.355177	-0.000012	0.000377
3	6	0	-2.069388	-1.213522	0.000217
4	6	0	-3.461862	-1.208530	-0.000178
5	6	0	-4.162364	0.000014	-0.000384
6	6	0	-3.461840	1.208546	-0.000178
7	6	0	0.072868	-0.000022	0.000702
8	6	0	1.284641	-0.000004	0.000124
9	35	0	3.075174	0.000002	-0.000138
10	1	0	-1.521409	-2.150639	0.000385
11	1	0	-4.002248	-2.151228	-0.000321
12	1	0	-5.248903	0.000024	-0.000686
13	1	0	-4.002211	2.151252	-0.000321
14	1	0	-1.521369	2.150619	0.000385

Zero-point vibrational energy 267141.0 (Joules/Mol)
63.84823 (Kcal/Mol)
Zero-point correction= 0.101749 (Hartree/Particle)
Thermal correction to Energy= 0.109224
Thermal correction to Enthalpy= 0.110168
Thermal correction to Gibbs Free Energy= 0.067709
Sum of electronic and zero-point Energies= -2879.390959
Sum of electronic and thermal Energies= -2879.383483
Sum of electronic and thermal Enthalpies= -2879.382539
Sum of electronic and thermal Free Energies= -2879.424999

TS1i-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.821043	-0.448445	1.222116
2	6	0	-3.109801	-0.561097	0.002238
3	6	0	-3.825386	-0.443684	-1.214647
4	6	0	-5.195350	-0.213726	-1.204107
5	6	0	-5.884490	-0.099753	0.008097
6	6	0	-5.191048	-0.218493	1.217373
7	6	0	-1.729845	-0.833994	-0.000586
8	6	0	-0.481837	-0.869455	-0.002627
9	35	0	0.801662	-2.216567	-0.005924
10	6	0	0.483672	0.880101	-0.002385
11	6	0	1.731733	0.843791	-0.000221
12	6	0	3.110203	0.563009	0.002452
13	6	0	3.820243	0.442441	1.222239
14	6	0	5.188173	0.200465	1.217352
15	6	0	5.880545	0.076376	0.007999
16	6	0	5.192377	0.196895	-1.204126
17	6	0	3.824488	0.438893	-1.214502
18	35	0	-0.800013	2.226871	-0.005566
19	1	0	-3.278233	-0.540517	2.157473
20	1	0	-5.724190	-0.131102	2.160149
21	1	0	-6.955974	0.079601	0.010355
22	1	0	-5.731846	-0.122629	-2.144626
23	1	0	-3.285899	-0.532037	-2.152282
24	1	0	3.278177	0.538205	2.157656
25	1	0	5.720455	0.107424	2.160074
26	1	0	6.950391	-0.112504	0.010135
27	1	0	5.727937	0.101079	-2.144710
28	1	0	3.285666	0.531873	-2.152071

Zero-point vibrational energy 528169.7 (Joules/Mol)
126.23558 (Kcal/Mol)
Zero-point correction= 0.201169 (Hartree/Particle)
Thermal correction to Energy= 0.217964
Thermal correction to Enthalpy= 0.218909
Thermal correction to Gibbs Free Energy= 0.149775
Sum of electronic and zero-point Energies= -5758.747109
Sum of electronic and thermal Energies= -5758.730314
Sum of electronic and thermal Enthalpies= -5758.729370
Sum of electronic and thermal Free Energies= -5758.798503

TS1i-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.274563	-0.429054	0.904253
2	6	0	-0.878553	0.772917	-0.502090
3	6	0	-1.792789	0.240438	-1.200751
4	6	0	0.868532	-0.903954	0.742140
5	6	0	2.139191	-1.292675	0.278851
6	6	0	2.279490	-2.410257	-0.579772
7	6	0	3.538324	-2.804533	-1.016051
8	6	0	4.677995	-2.098028	-0.617137
9	6	0	4.552417	-0.989535	0.227042
10	6	0	3.301021	-0.588393	0.677920
11	6	0	-0.146456	2.034385	-0.428868
12	6	0	0.101532	2.754982	-1.611544
13	6	0	0.770647	3.975492	-1.567902
14	6	0	1.203380	4.498688	-0.347126
15	6	0	0.957579	3.792087	0.831716
16	6	0	0.289834	2.569554	0.794555
17	35	0	-1.649518	-0.528683	2.163905
18	35	0	-2.712243	-1.302215	-1.477828
19	1	0	0.089590	2.029827	1.713730
20	1	0	-0.236833	2.343623	-2.557255
21	1	0	0.956815	4.517996	-2.491011
22	1	0	1.727057	5.450259	-0.315092
23	1	0	1.282458	4.195347	1.787189
24	1	0	3.197075	0.271229	1.332235
25	1	0	5.436562	-0.438267	0.535074
26	1	0	5.659523	-2.409134	-0.963617
27	1	0	1.389777	-2.948356	-0.891256
28	1	0	3.634142	-3.663756	-1.674127

Zero-point vibrational energy 527427.5 (Joules/Mol)
126.05820 (Kcal/Mol)
Zero-point correction= 0.200887 (Hartree/Particle)
Thermal correction to Energy= 0.217689
Thermal correction to Enthalpy= 0.218633
Thermal correction to Gibbs Free Energy= 0.150081
Sum of electronic and zero-point Energies= -5758.739125
Sum of electronic and thermal Energies= -5758.722322
Sum of electronic and thermal Enthalpies= -5758.721378
Sum of electronic and thermal Free Energies= -5758.789931

TS1i-3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.067545	0.157451	1.675499
2	6	0	-1.724238	-0.839772	0.748544
3	6	0	-2.629449	-1.898890	0.533203
4	6	0	-3.835493	-1.953626	1.223332
5	6	0	-4.166884	-0.955930	2.144558
6	6	0	-3.277693	0.095314	2.366039
7	6	0	-0.457317	-0.844996	0.014859
8	6	0	0.207706	-1.683293	-0.668346
9	35	0	1.643723	-1.982967	-1.727233
10	6	0	0.455239	0.845619	0.068336
11	6	0	1.721026	0.791213	0.802003
12	6	0	2.639547	1.847788	0.637170
13	6	0	3.844596	1.855711	1.331261
14	6	0	4.161519	0.812660	2.206082
15	6	0	3.259027	-0.236745	2.377285
16	6	0	2.049957	-0.252073	1.682320
17	6	0	-0.206112	1.726677	-0.562937
18	35	0	-1.638589	2.090452	-1.607656
19	1	0	2.389869	2.656721	-0.042068
20	1	0	4.539906	2.678450	1.187123
21	1	0	5.103859	0.819037	2.746978
22	1	0	3.493377	-1.052435	3.055946
23	1	0	1.358442	-1.074600	1.822106
24	1	0	-2.368546	-2.672474	-0.182019
25	1	0	-4.520205	-2.777431	1.039930
26	1	0	-5.110009	-0.998790	2.682418
27	1	0	-3.523278	0.875945	3.080989
28	1	0	-1.386406	0.980952	1.854470

Zero-point vibrational energy 527337.9 (Joules/Mol)
126.03678 (Kcal/Mol)
Zero-point correction= 0.200852 (Hartree/Particle)
Thermal correction to Energy= 0.217563
Thermal correction to Enthalpy= 0.218507
Thermal correction to Gibbs Free Energy= 0.150815
Sum of electronic and zero-point Energies= -5758.729624
Sum of electronic and thermal Energies= -5758.712913
Sum of electronic and thermal Enthalpies= -5758.711969
Sum of electronic and thermal Free Energies= -5758.779662

6. References

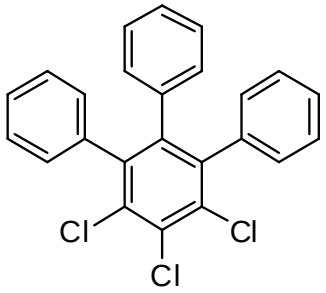
[1] Sud, D.; Wigglesworth, T. J.; Branda, N. R. *Angew. Chem. Int. Ed.* **2007**, *46*, 8017.

[2] Murray, R. E. *Synth. Commun.* **1980**, *10*, 345.

[3] Full citation of Gaussian 03: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A. Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Revision C.02; Gaussian Inc.: Wallingford CT, 2004.

[4] Yamaguchi, K.; Jensen, F. Dorigo, A.; Houk, K. N. *Chem. Phys. Lett.* **1988**, *149*, 537.

7. 1H and 13C Spectra for New Compounds



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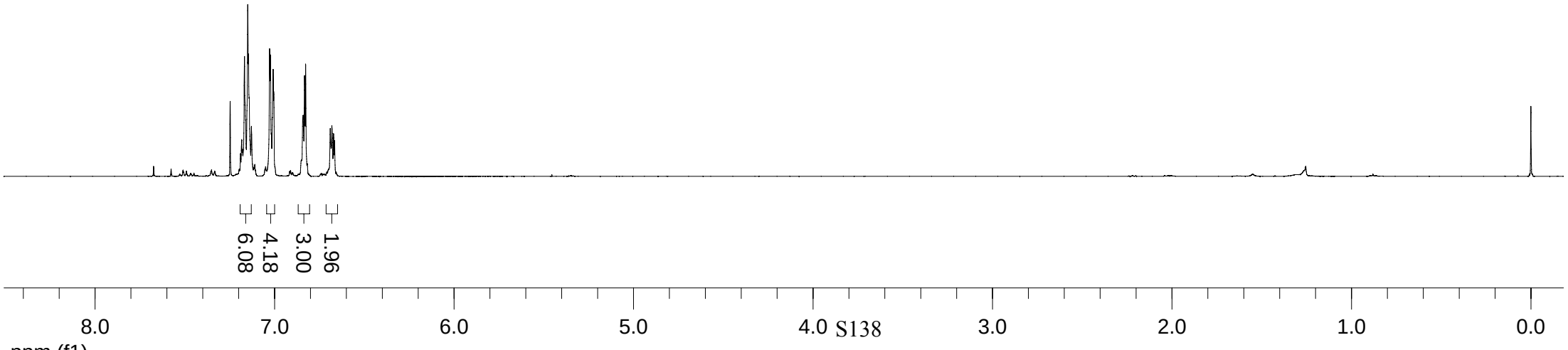

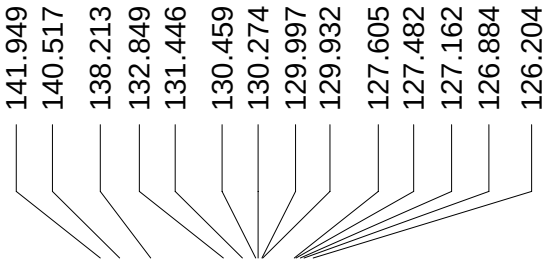
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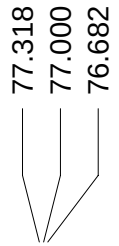
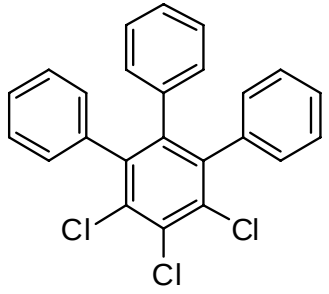
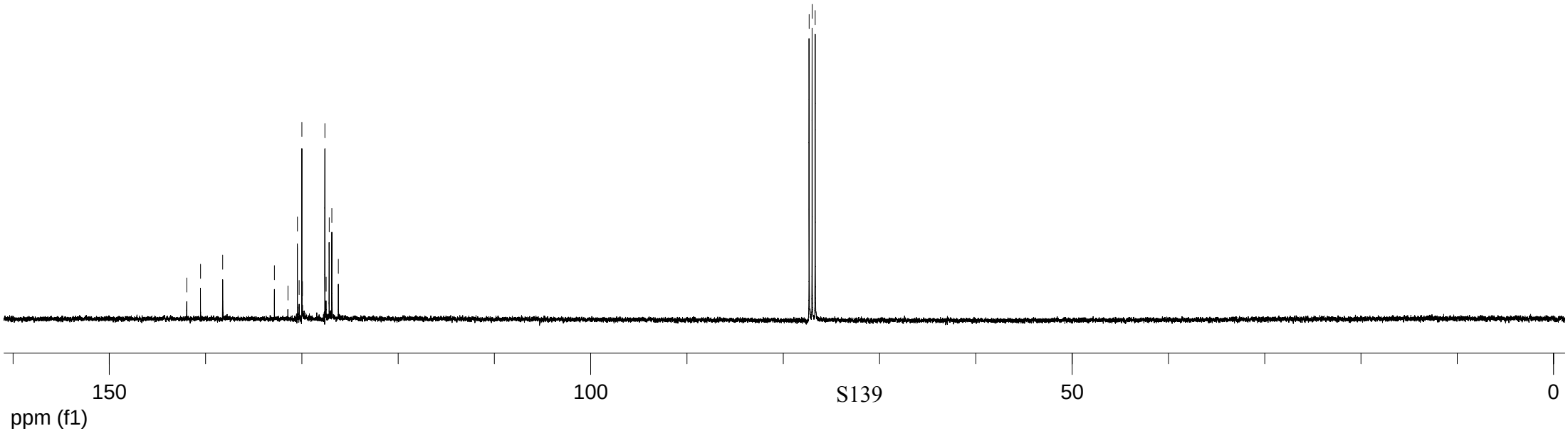
127.162
126.884
126.204


77.318
77.000
76.682


Cl
Cl
Cl

P3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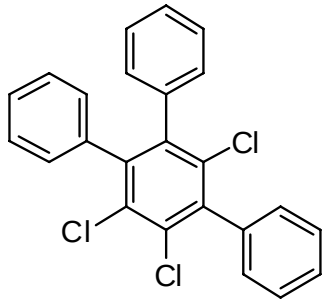
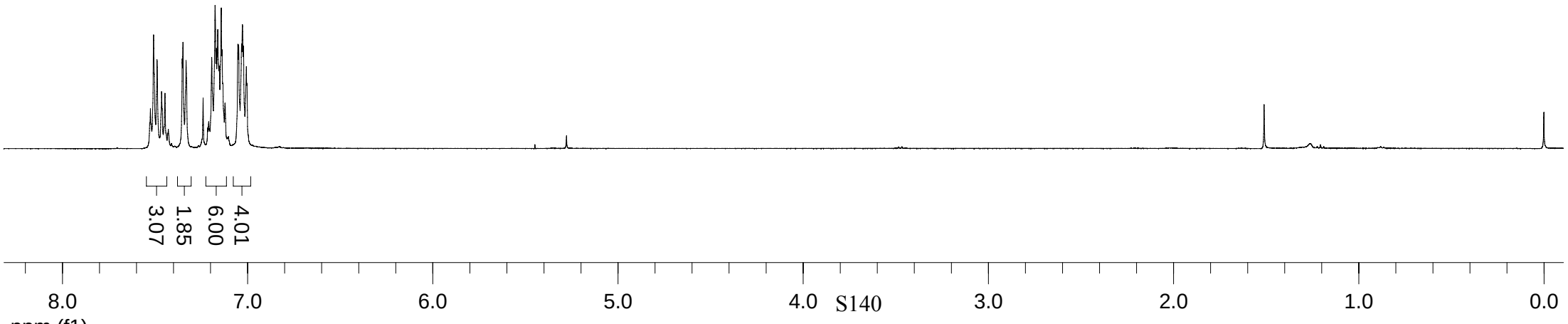
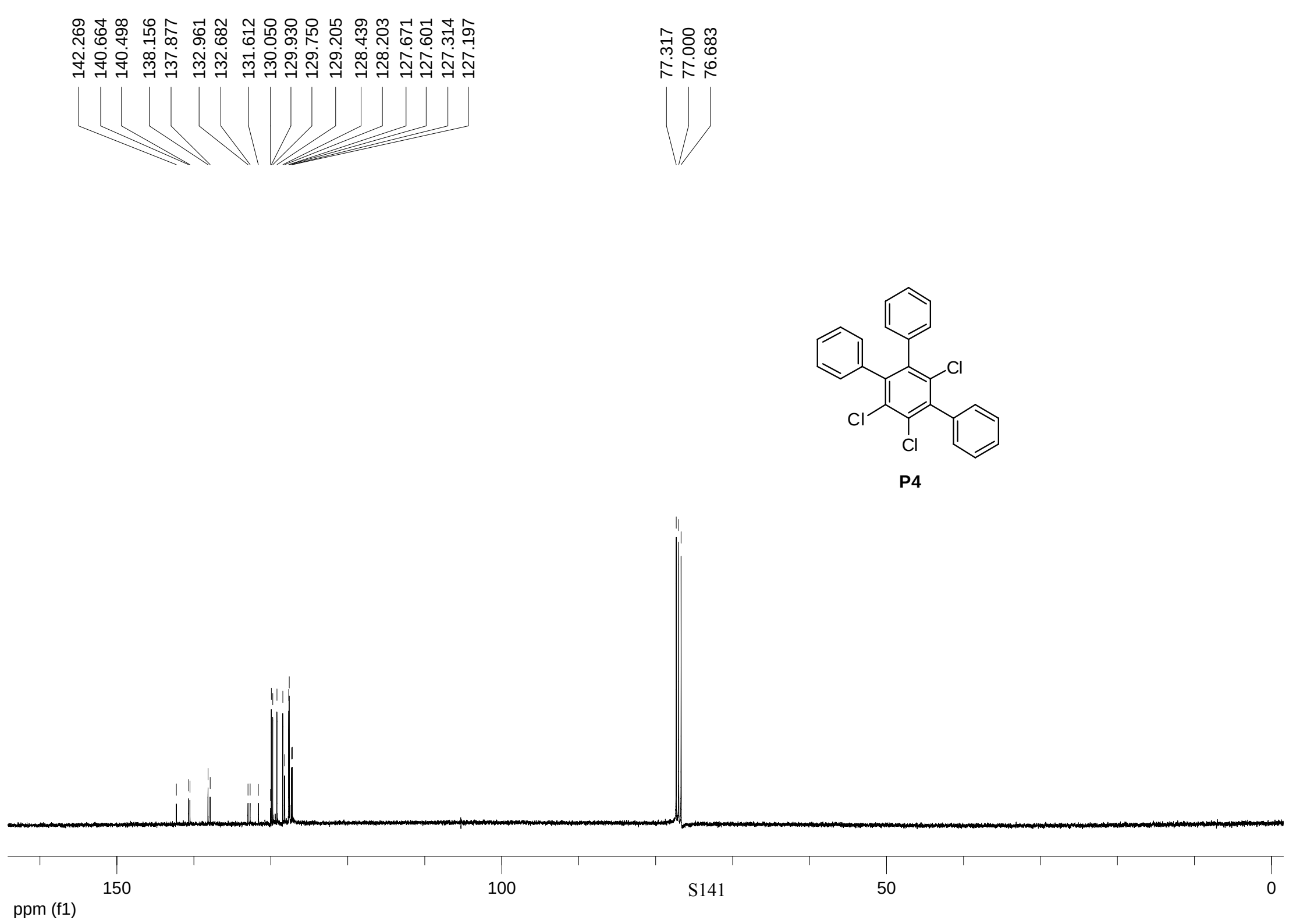
100
50
0
ppm (f1)



P4




142.269
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140.498
138.156
137.877
132.961
132.682
131.612
130.050
129.930
129.750
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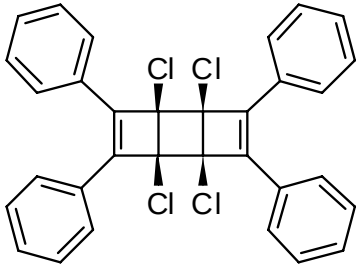
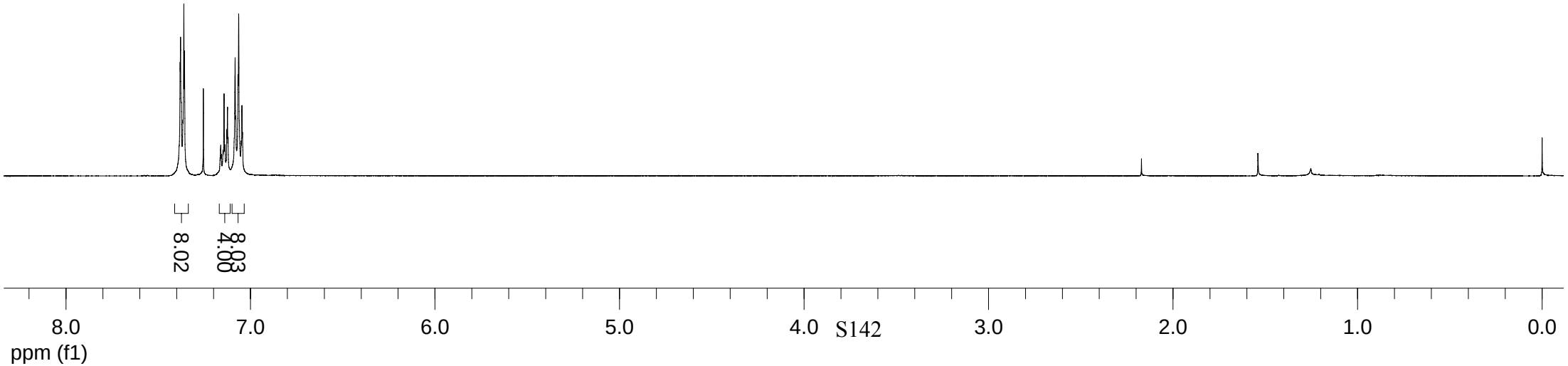
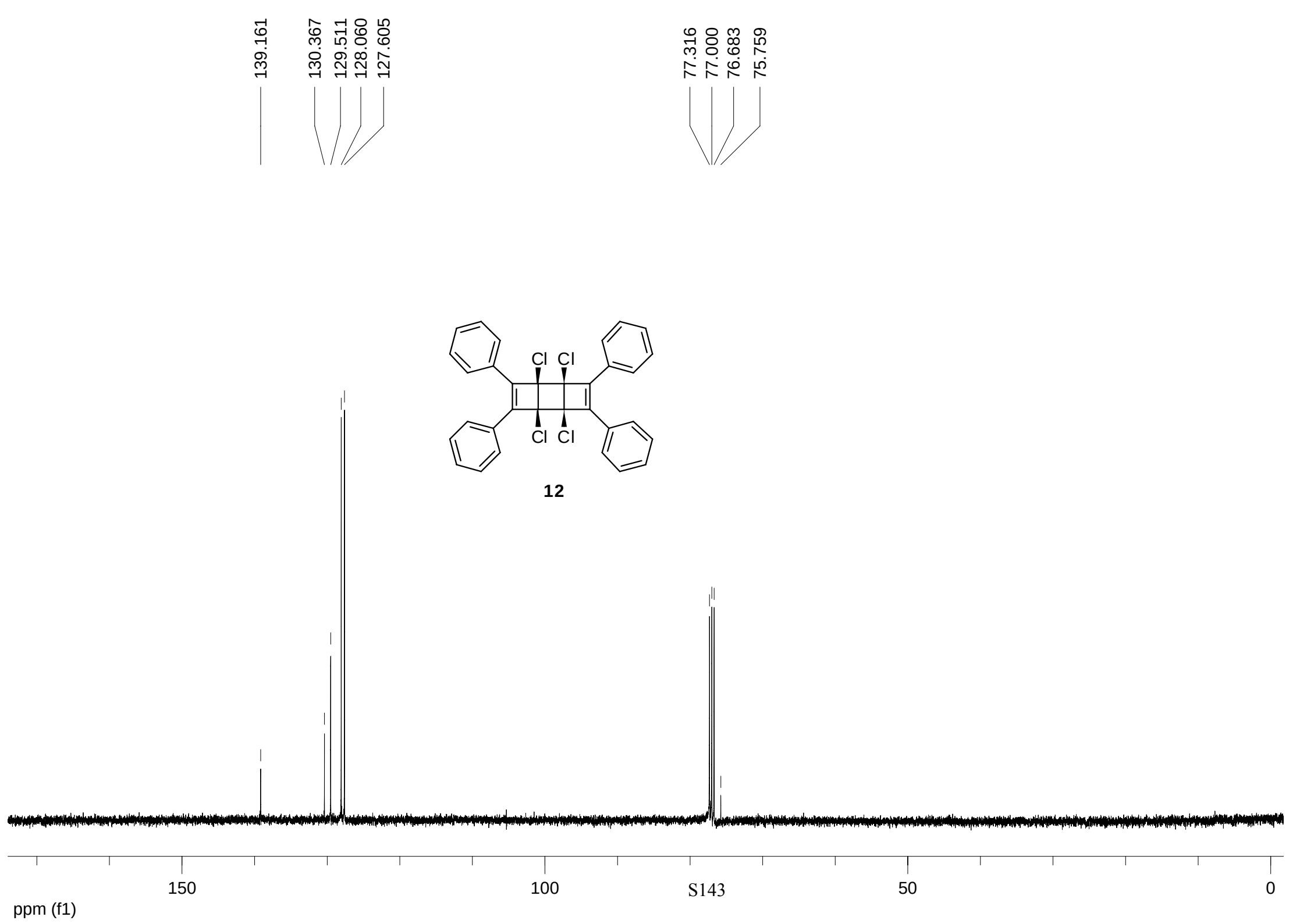
128.439
128.203
127.671
127.601
127.314
127.197
77.317
77.000
76.683
Cl
Cl
Cl
P4
150
100
50
0
ppm (f1)



12

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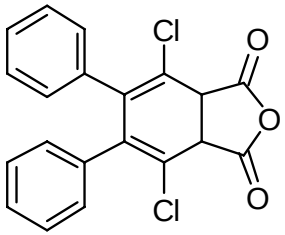
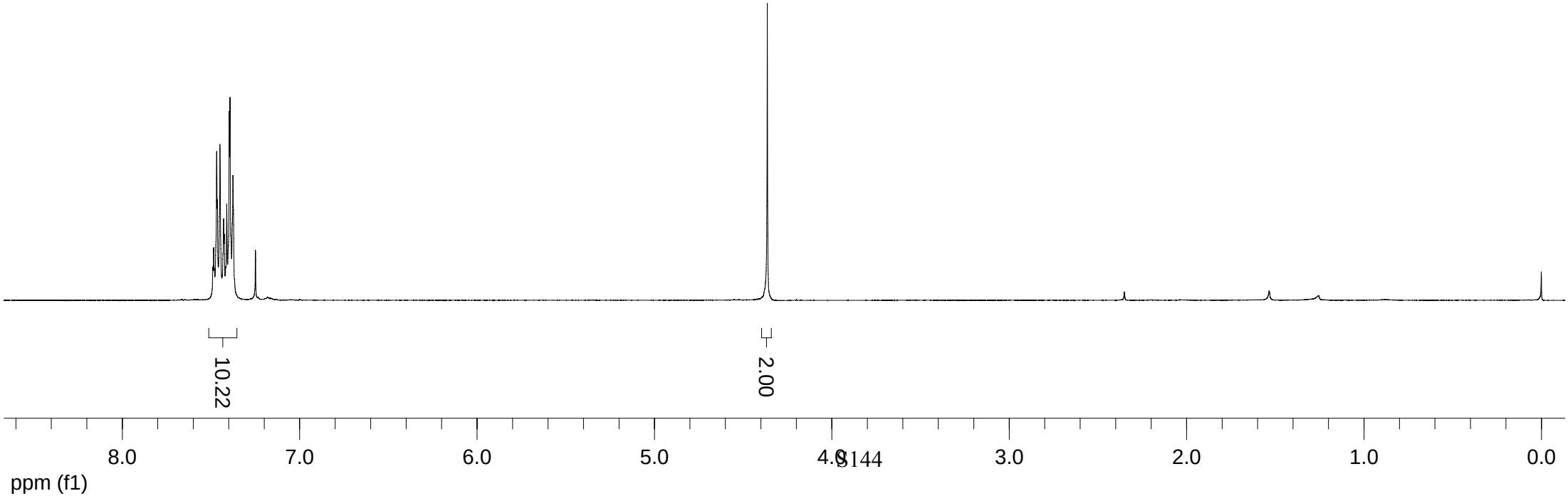
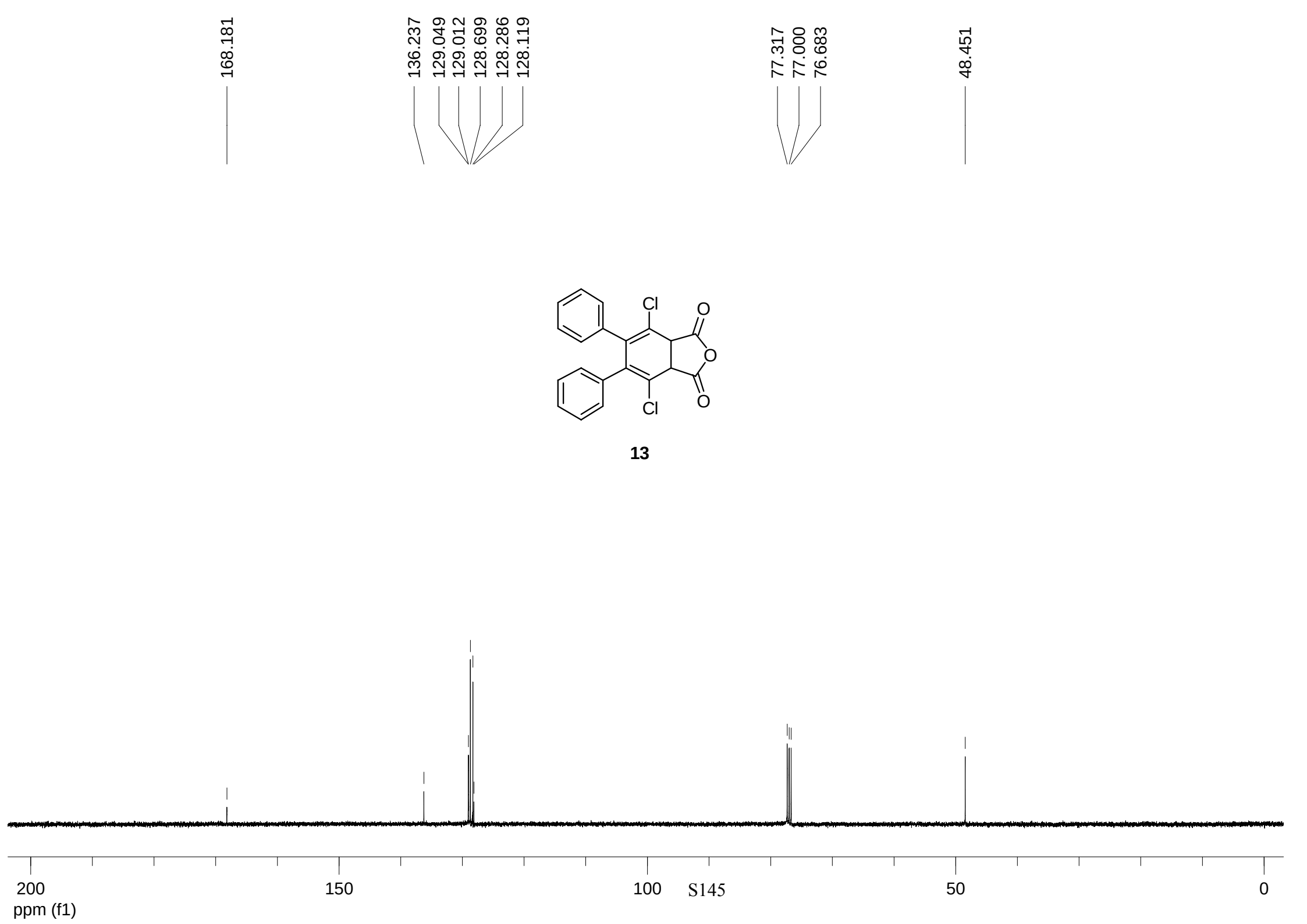
77.000
76.683
75.759
Cl Cl
Cl Cl
12
150
100
50
0
ppm (f1)

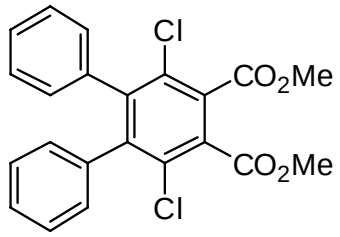


13




168.181
136.237
129.049
129.012
128.699
128.286
128.119
77.317
77.000
76.683
48.451
Cl
O
O
O
Cl
200
150
100
50
0
ppm (f1)

13



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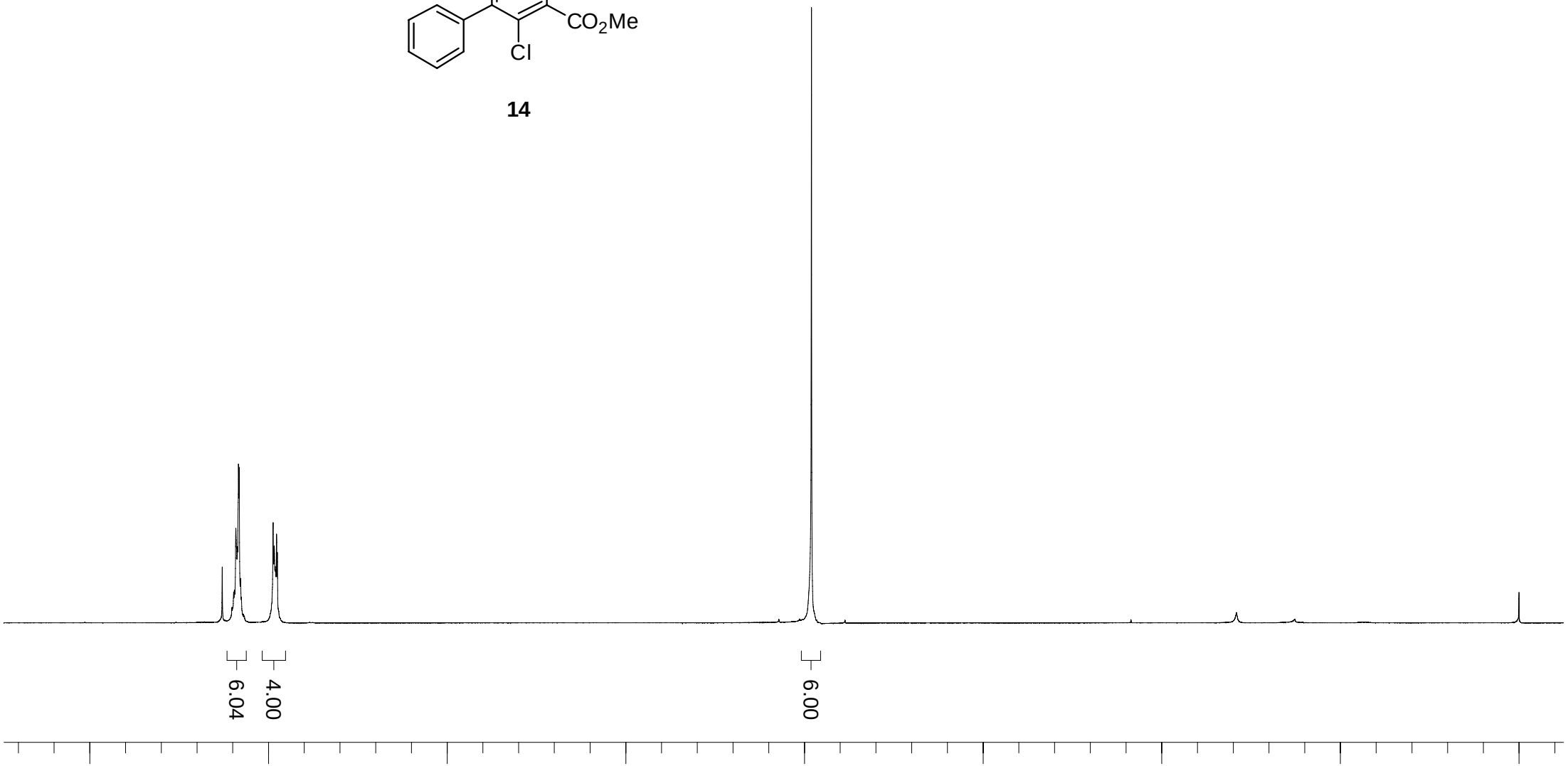

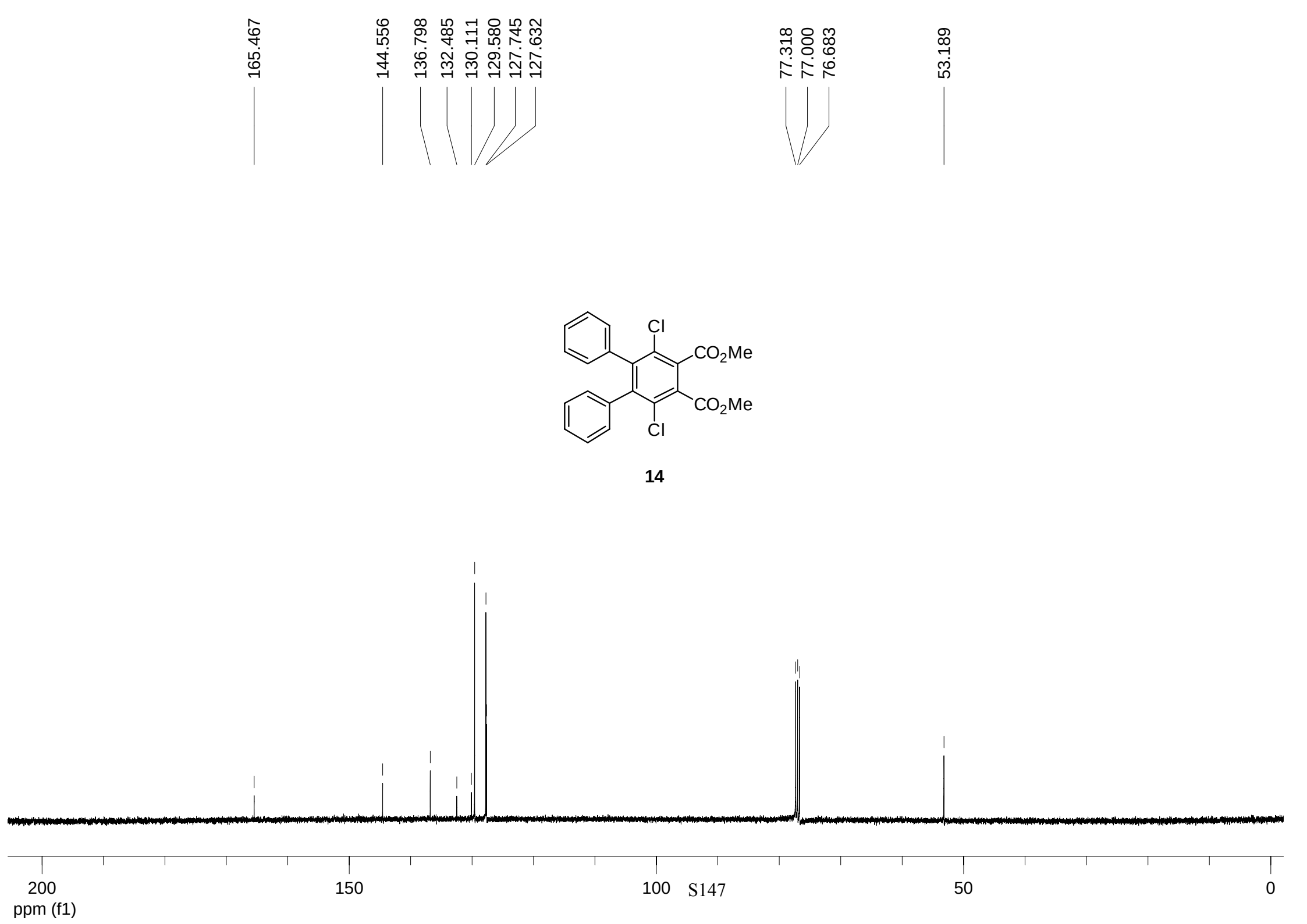
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144.556
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132.485
130.111
129.580
127.745
127.632
77.318
77.000
76.683
53.189
Cl
CO2Me
CO2Me
Cl
200
150
100
50
0
ppm (f1)

14