CHEMISTRY
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Supporting Information

WHY PLATINUM CATALYSTS FEATURING LARGE BITE ANGLE LIGANDS ARE SO EFFICIENT IN THE ALLYLATION OF AMINES? DESIGN OF A HIGHLY ACTIVE CATALYST AND COMPREHENSIVE EXPERIMENTAL AND DFT JOINT STUDY

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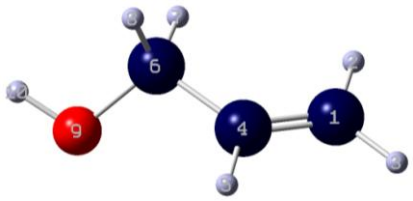
DFT Data

Complete reference 46

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

Computed Cartesian coordinates, three lower frequencies PCM energy for **allyl alcohol**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.840349	0.078411	-0.212304
2	1	0	1.952039	1.079034	-0.627371
3	1	0	2.732684	-0.542090	-0.187944
4	6	0	0.667641	-0.364012	0.245849
5	1	0	0.577351	-1.375384	0.642841
6	6	0	-0.586364	0.451408	0.282604
7	1	0	-0.429302	1.411035	-0.233304
8	1	0	-0.845544	0.670539	1.332262
9	8	0	-1.630601	-0.298594	-0.331633
10	1	0	-2.472173	0.150778	-0.170314

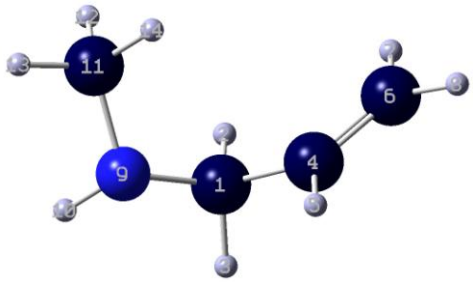
	1	2	3
	A	A	A
Frequencies --	114.9738	261.7225	330.7050
Red. masses --	2.7366	1.0825	2.1670
Frc consts --	0.0213	0.0437	0.1396
IR Inten --	2.0584	143.8978	11.2576

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.11	0.04	0.17	-0.02	0.02	-0.01	-0.02	0.10	0.01
2	1	0.25	0.15	0.47	-0.03	0.04	0.03	-0.36	0.03	-0.24
3	1	0.07	0.00	0.20	-0.01	0.03	-0.06	0.20	0.43	0.21
4	6	-0.01	-0.04	-0.21	0.00	-0.01	-0.01	0.08	-0.14	0.06
5	1	-0.14	-0.13	-0.49	0.01	-0.03	-0.05	0.30	-0.04	0.36
6	6	0.02	0.02	-0.15	0.00	-0.01	0.03	0.07	-0.13	-0.08
7	1	-0.02	-0.06	-0.32	0.01	-0.02	0.01	0.23	-0.19	-0.13
8	1	0.20	0.19	-0.14	0.01	0.01	0.03	0.12	-0.01	-0.09
9	8	-0.11	-0.03	0.15	0.01	-0.03	0.05	-0.13	0.10	-0.01
10	1	-0.05	0.07	0.15	0.13	0.52	-0.83	-0.01	0.29	0.12

Total free energy in solution:

with all non electrostatic terms (a.u.) = -193.046154

Computed Cartesian coordinates, three lower frequencies PCM energy for **allylmethylamine**



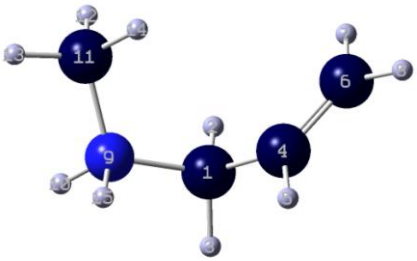
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.022235	0.841742	0.327317
2	1	0	0.100410	0.585041	1.402433
3	1	0	0.124177	1.933526	0.248283
4	6	0	1.155658	0.198309	-0.421429
5	1	0	1.139878	0.350225	-1.501754
6	6	0	2.139595	-0.508392	0.140418
7	1	0	2.173606	-0.686912	1.214571
8	1	0	2.949730	-0.929779	-0.450086
9	7	0	-1.270442	0.488164	-0.250012
10	1	0	-1.977357	1.140384	0.076311
11	6	0	-1.687634	-0.876034	0.033761
12	1	0	-1.730989	-1.114859	1.113612
13	1	0	-2.677541	-1.051030	-0.400718
14	1	0	-0.987943	-1.577500	-0.432970

	1	2	3
	A	A	A
Frequencies --	97.0082	134.8804	217.3573
Red. masses --	2.5492	1.7342	1.1770
Frc consts --	0.0141	0.0186	0.0328
IR Inten --	0.1126	2.4916	0.4397

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.01	-0.11	0.02	0.01	0.07	-0.04	0.00	-0.04	-0.03
2	1	0.00	-0.15	0.02	0.07	0.20	-0.01	-0.01	-0.08	-0.04
3	1	0.10	-0.12	0.06	0.06	0.06	-0.18	-0.03	-0.03	0.03
4	6	-0.03	-0.16	0.00	-0.07	-0.10	-0.01	0.06	0.05	-0.01
5	1	-0.22	-0.40	-0.03	-0.16	-0.32	-0.04	0.18	0.17	0.01
6	6	0.20	0.17	0.01	-0.04	0.00	0.05	0.01	0.01	0.03
7	1	0.41	0.43	0.05	0.04	0.22	0.09	-0.11	-0.10	0.01
8	1	0.19	0.18	-0.02	-0.10	-0.14	0.08	0.09	0.08	0.08
9	7	-0.02	0.03	0.02	-0.04	0.06	0.08	0.00	-0.03	-0.03
10	1	0.04	0.08	0.06	-0.05	-0.05	0.30	0.03	0.00	-0.02
11	6	-0.16	0.05	-0.05	0.13	-0.03	-0.09	-0.06	0.00	0.03
12	1	-0.19	0.00	-0.07	0.46	-0.27	-0.13	0.42	-0.09	0.02
13	1	-0.17	0.17	-0.07	0.01	0.01	0.16	-0.30	0.20	0.49
14	1	-0.22	0.01	-0.08	0.03	0.11	-0.44	-0.40	-0.07	-0.38

Total free energy in solution:
with all non electrostatic terms (a.u.) = -212.480062

Computed Cartesian coordinates, three lower frequencies PCM energy for **allylmethylammonium**



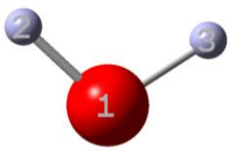
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.098859	-0.884741	0.394804
2	1	0	-0.116558	-0.574391	1.442985
3	1	0	-0.114037	-1.979473	0.349299
4	6	0	-1.207749	-0.275708	-0.399656
5	1	0	-1.320737	-0.620814	-1.428399
6	6	0	-2.086312	0.588438	0.115700
7	1	0	-2.031235	0.926232	1.149106
8	1	0	-2.911984	0.970651	-0.477958
9	7	0	1.268903	-0.474967	-0.149419
10	1	0	1.990962	-1.040301	0.310086
11	6	0	1.604140	0.976471	0.007075
12	1	0	1.628691	1.212505	1.072019
13	1	0	2.580629	1.162637	-0.443600
14	1	0	0.833454	1.564849	-0.491161
15	1	0	1.311177	-0.723888	-1.143982

	1	2	3
	A	A	A
Frequencies --	100.7614	113.5803	220.8753
Red. masses --	1.9089	2.0868	1.2216
Frc consts --	0.0114	0.0159	0.0351
IR Inten --	2.8472	0.4514	0.8127

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.02	0.04	-0.03	0.00	-0.12	-0.05	0.00	0.03	-0.02
2	1	-0.06	-0.03	-0.01	-0.05	-0.26	-0.01	0.02	0.05	-0.03
3	1	-0.09	0.04	-0.09	0.02	-0.11	-0.20	0.03	0.02	0.02
4	6	0.05	0.15	-0.04	0.03	-0.01	-0.01	-0.07	-0.06	0.01
5	1	0.23	0.41	-0.14	-0.04	0.03	-0.01	-0.18	-0.18	0.07
6	6	-0.12	-0.10	0.08	0.16	0.09	0.04	-0.02	0.00	0.01
7	1	-0.30	-0.37	0.17	0.24	0.06	0.05	0.09	0.12	-0.03
8	1	-0.09	-0.05	0.07	0.18	0.22	0.08	-0.09	-0.08	0.06
9	7	0.04	-0.04	0.08	0.02	-0.02	0.07	0.00	0.03	-0.04
10	1	-0.02	0.01	0.24	0.02	0.12	0.23	-0.03	-0.02	-0.06
11	6	0.04	-0.02	-0.10	-0.18	0.04	-0.06	0.08	0.00	0.03
12	1	-0.17	0.16	-0.13	-0.50	0.21	-0.09	-0.41	0.07	0.02
13	1	0.14	-0.12	0.07	-0.08	0.08	0.18	0.32	-0.14	0.49
14	1	0.16	-0.08	-0.34	-0.11	-0.11	-0.35	0.39	0.07	-0.39
15	1	0.16	-0.18	0.12	0.18	-0.12	0.10	-0.01	0.07	-0.05

Total free energy in solution:
with all non electrostatic terms (a.u.) = -212.908038

Computed Cartesian coordinates, three lower frequencies PCM energy for **water**



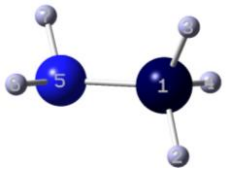
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.117169
2	1	0	0.000000	0.768778	-0.468677
3	1	0	0.000000	-0.768778	-0.468677

	1	2	3
	A1	A1	B2
Frequencies --	1674.7347	3765.6572	3892.9487
Red. masses --	1.0833	1.0446	1.0827
Frc consts --	1.7901	8.7273	9.6678
IR Inten --	100.1900	8.1389	56.0877

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	8	0.00	0.00	0.07	0.00	0.00	0.05	0.00	0.07	0.00
2	1	0.00	-0.42	-0.56	0.00	0.59	-0.39	0.00	-0.56	0.43
3	1	0.00	0.42	-0.56	0.00	-0.59	-0.39	0.00	-0.56	-0.43

Total free energy in solution:
with all non electrostatic terms (a.u.) = -76.398371

Computed Cartesian coordinates, three lower frequencies PCM energy for **methylamine**



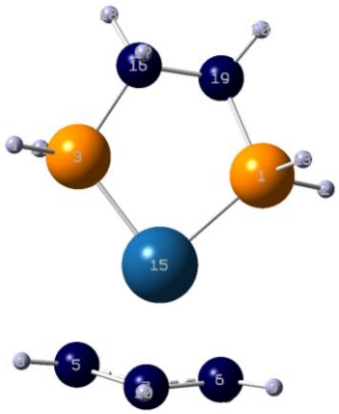
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.705665	0.000000	0.017872
2	1	0	-1.112285	0.881605	-0.489107
3	1	0	-1.081426	-0.000027	1.055425
4	1	0	-1.112291	-0.881577	-0.489155
5	7	0	0.747646	0.000000	-0.120311
6	1	0	1.153235	0.816721	0.328890
7	1	0	1.153236	-0.816723	0.328890

	1	2	3
	A	A	A
Frequencies --	320.6655	852.8192	982.6267
Red. masses --	1.0294	1.2040	1.0509
Frc consts --	0.0624	0.5159	0.5978
IR Inten --	45.7991	196.7206	0.1438

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	-0.03	0.00	-0.01	0.00	-0.06	0.00
2	1	-0.08	-0.20	-0.30	-0.13	0.02	0.12	0.46	0.15	-0.01
3	1	0.00	0.31	0.00	0.25	0.00	0.08	0.00	0.27	0.00
4	1	0.08	-0.20	0.30	-0.13	-0.02	0.12	-0.46	0.15	0.01
5	7	0.00	0.04	0.00	0.08	0.00	-0.09	0.00	-0.01	0.00
6	1	0.04	-0.25	0.50	-0.35	-0.10	0.54	-0.43	0.13	0.15
7	1	-0.04	-0.25	-0.50	-0.35	0.10	0.54	0.43	0.13	-0.15

Total free energy in solution:
with all non electrostatic terms (a.u.) = -95.826326

Computed Cartesian coordinates, three lower frequencies PCM energy for **I**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.235278	-1.563254	0.053940
2	1	0	1.231709	-2.661159	-0.827151
3	15	0	1.234298	1.564515	-0.046981
4	1	0	1.209966	2.666027	0.829017
5	6	0	-2.254886	1.218836	-0.225468
6	6	0	-2.253969	-1.227402	-0.164374
7	6	0	-2.588048	0.011632	0.438075
8	1	0	-2.359496	2.157558	0.311588
9	1	0	-2.359274	-2.137855	0.419165
10	1	0	-2.820526	0.038462	1.502244
11	1	0	-2.344242	1.287585	-1.310596
12	1	0	-2.344322	-1.350719	-1.244586
13	1	0	1.430034	-2.219056	1.286310
14	1	0	1.456155	2.217333	-1.276740
15	78	0	-0.447905	-0.000918	-0.006418
16	6	0	2.838494	0.706028	0.329639
17	1	0	2.921731	0.655764	1.422119
18	1	0	3.687086	1.294484	-0.034616
19	6	0	2.847824	-0.701756	-0.280526
20	1	0	3.687580	-1.288731	0.105831
21	1	0	2.960056	-0.651034	-1.370427

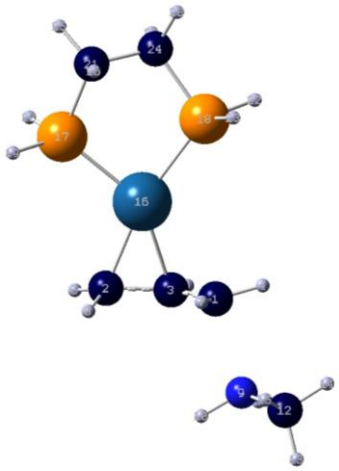
	1	2	3
	A	A	A
Frequencies --	61.6115	101.2650	120.7073
Red. masses --	3.3585	2.7003	4.4292
Frc consts --	0.0075	0.0163	0.0380
IR Inten --	1.4251	0.8237	7.2836

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	15	0.00	-0.01	-0.06	0.01	0.00	-0.07	0.08	0.01	0.03
2	1	0.08	0.09	-0.18	-0.02	0.08	-0.17	0.19	-0.04	0.09
3	15	0.00	-0.01	-0.07	-0.01	0.01	0.07	-0.08	0.01	0.00
4	1	-0.07	0.09	-0.19	-0.06	-0.07	0.17	-0.16	0.01	-0.01
5	6	-0.02	0.00	0.15	0.01	-0.01	-0.22	0.18	0.18	0.07
6	6	-0.02	0.00	0.14	-0.01	0.00	0.23	-0.19	0.18	-0.06
7	6	0.05	0.00	0.18	0.00	0.12	0.00	0.01	0.20	0.01
8	1	0.04	0.00	0.16	0.02	0.10	-0.40	0.34	0.17	0.13
9	1	0.04	0.00	0.15	-0.02	0.11	0.40	-0.33	0.16	-0.11
10	1	0.15	0.00	0.21	0.01	0.32	0.00	0.02	0.18	0.02
11	1	-0.14	0.00	0.16	0.06	-0.22	-0.24	0.16	0.26	0.08
12	1	-0.13	0.01	0.15	-0.07	-0.20	0.25	-0.19	0.26	-0.07
13	1	-0.14	-0.15	-0.11	0.05	-0.11	-0.14	0.12	0.10	0.07
14	1	0.15	-0.15	-0.12	0.03	0.13	0.14	-0.15	0.02	-0.01

15	78	0.00	0.00	-0.04	0.00	-0.01	0.00	0.00	-0.06	-0.01
16	6	-0.05	0.01	0.20	-0.02	0.00	0.05	-0.02	0.12	-0.02
17	1	-0.23	0.01	0.21	-0.04	-0.08	0.05	0.00	0.15	-0.02
18	1	0.00	0.01	0.33	-0.01	0.02	0.11	-0.06	0.16	-0.06
19	6	0.05	0.01	0.20	0.00	0.04	-0.05	0.03	0.11	0.01
20	1	-0.01	0.01	0.34	0.01	0.02	-0.10	0.07	0.16	0.01
21	1	0.23	0.01	0.22	-0.02	0.12	-0.05	0.02	0.10	0.00

Total free energy in solution:
with all non electrostatic terms (a.u.) = -999.993789

Computed Cartesian coordinates, three lower frequencies PCM energy for **TS_{I-II}**

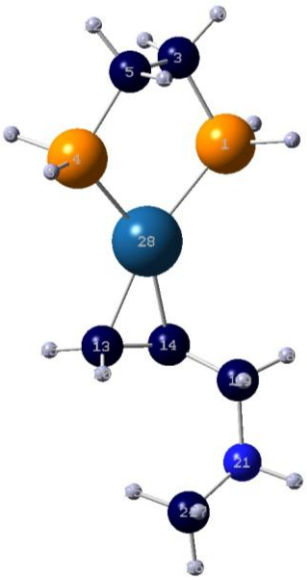


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.381049	0.382259	-0.068722
2	6	0	1.197305	-1.828688	-0.171886
3	6	0	1.814908	-0.684332	-0.803496
4	1	0	2.538708	1.340021	-0.553069
5	1	0	0.968165	-2.688761	-0.797724
6	1	0	1.886900	-0.647686	-1.889836
7	1	0	2.310440	0.399884	1.014708
8	1	0	1.488826	-2.092305	0.846645
9	7	0	4.473805	0.095466	0.072326
10	1	0	4.578683	-0.845494	0.447561
11	1	0	4.811650	0.071199	-0.888296
12	6	0	5.203888	1.083324	0.874974
13	1	0	6.280947	0.881614	0.919425
14	1	0	5.052936	2.077910	0.446020
15	1	0	4.806972	1.082796	1.894019
16	78	0	-0.201005	-0.254882	-0.141644
17	15	0	-2.208209	-1.118381	0.492095
18	15	0	-1.292892	1.783953	-0.245284
19	1	0	-2.338694	-1.942353	1.628661
20	1	0	-2.876944	-1.916556	-0.460065
21	6	0	-3.397058	0.276132	0.821763
22	1	0	-1.212823	2.661326	-1.348093
23	1	0	-1.073526	2.715756	0.794178
24	6	0	-3.123162	1.448767	-0.129101
25	1	0	-4.433213	-0.066809	0.731855
26	1	0	-3.243541	0.581630	1.864101
27	1	0	-3.463604	1.207780	-1.143648
28	1	0	-3.665158	2.344229	0.192143

			1			2			3		
			A			A			A		
Frequencies --			-248.3259			31.0082			42.5315		
Red. masses --			5.9134			2.8393			3.8378		
Frc consts --			0.2148			0.0016			0.0041		
IR Inten --			692.0517			0.1290			4.8863		
	Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6		0.50	-0.01	0.11	-0.01	0.04	-0.07	-0.03	-0.03	0.02
2	6		0.06	0.09	0.01	0.02	0.02	0.00	-0.01	-0.05	-0.01
3	6		0.03	0.17	0.08	0.00	0.01	-0.04	0.01	-0.05	0.00
4	1		0.21	0.09	0.17	-0.01	0.03	-0.10	-0.03	-0.04	0.01
5	1		0.10	0.12	-0.04	0.02	0.01	0.03	0.00	-0.04	-0.02
6	1		0.05	0.19	0.08	-0.02	-0.01	-0.05	0.04	-0.05	0.00
7	1		0.20	0.05	0.09	0.00	0.06	-0.07	-0.08	-0.02	0.01
8	1		0.06	0.02	0.00	0.04	0.05	0.00	-0.04	-0.05	-0.01
9	7		-0.28	-0.02	-0.04	0.00	0.03	-0.05	-0.05	0.05	0.13
10	1		-0.32	-0.03	-0.05	-0.03	-0.05	-0.26	-0.01	0.10	0.25
11	1		-0.34	-0.03	-0.06	0.06	0.26	-0.03	0.00	-0.04	0.15
12	6		-0.15	-0.05	-0.06	-0.05	-0.16	0.23	-0.16	0.19	0.06
13	1		-0.18	-0.19	-0.17	-0.06	-0.17	0.25	-0.15	0.27	0.14
14	1		-0.10	-0.05	-0.06	-0.02	-0.05	0.45	-0.20	0.13	-0.07
15	1		-0.08	-0.05	-0.04	-0.12	-0.40	0.20	-0.22	0.28	0.03
16	78		0.00	-0.01	-0.01	0.00	0.01	-0.02	0.00	-0.03	-0.04
17	15		0.00	0.01	0.02	0.04	0.00	0.10	-0.01	0.04	0.03
18	15		0.01	-0.01	-0.02	-0.04	-0.01	-0.07	0.07	0.01	-0.01
19	1		-0.08	0.00	0.02	0.11	0.05	0.14	0.01	0.00	0.00
20	1		-0.01	0.02	0.01	0.01	-0.05	0.17	-0.13	0.13	0.04
21	6		-0.01	0.01	0.00	0.04	0.00	0.10	0.09	0.10	0.17
22	1		-0.05	0.05	0.02	-0.10	-0.08	-0.13	0.02	-0.02	-0.03
23	1		-0.01	-0.02	0.00	0.00	0.05	-0.14	0.20	0.02	-0.04
24	6		0.00	0.00	0.00	-0.03	-0.04	0.03	0.06	0.10	0.16
25	1		-0.01	0.01	0.00	0.04	-0.02	0.17	0.07	0.15	0.26
26	1		-0.02	0.01	0.00	0.09	0.05	0.08	0.21	0.07	0.16
27	1		-0.01	0.00	0.00	-0.07	-0.09	0.06	-0.05	0.13	0.19
28	1		0.00	0.01	0.00	-0.02	-0.03	0.02	0.14	0.12	0.23

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1095.802046

Computed Cartesian coordinates, three lower frequencies PCM energy for **II**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.570317	1.671103	-0.005537
2	1	0	-1.621424	2.720279	-0.951481
3	6	0	-3.329505	1.044953	-0.043242
4	15	0	-2.024686	-1.414360	0.222656
5	6	0	-3.438571	-0.293383	0.698496
6	1	0	-2.555599	-2.142217	-0.866480
7	1	0	-1.562568	2.463673	1.167478
8	1	0	-2.095947	-2.423911	1.207326
9	1	0	-3.594009	0.917690	-1.100421
10	1	0	-4.019050	1.783506	0.378757
11	1	0	-3.366364	-0.136795	1.782042
12	1	0	-4.404007	-0.771539	0.502312
13	6	0	1.583364	-1.281283	-0.388049
14	6	0	1.896339	0.129086	-0.577815
15	1	0	1.577883	-1.938031	-1.257983
16	6	0	2.652264	0.910562	0.439726
17	1	0	2.031796	0.489250	-1.602187
18	1	0	2.441569	1.983410	0.393599
19	1	0	2.492777	0.554691	1.461236
20	1	0	1.899872	-1.782285	0.529605
21	7	0	4.193521	0.822954	0.220020
22	1	0	4.658245	1.517391	0.813980
23	1	0	4.377211	1.105621	-0.747819
24	6	0	4.799239	-0.519734	0.458677
25	1	0	4.305596	-1.238635	-0.194603
26	1	0	5.868757	-0.474901	0.243452
27	1	0	4.637000	-0.792346	1.502710
28	78	0	-0.147181	-0.145998	-0.148528

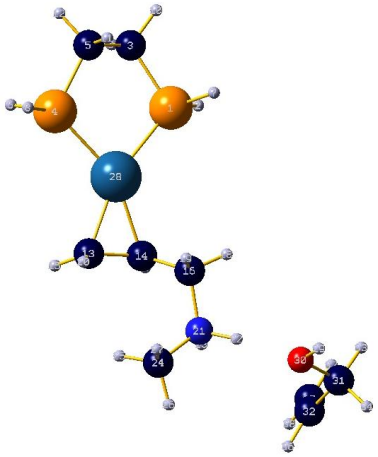
	1	2	3
	A	A	A
Frequencies --	41.3809	55.6041	65.9187
Red. masses --	3.9550	4.4086	2.4681
Frc consts --	0.0040	0.0080	0.0063
IR Inten --	6.6264	10.0865	4.2767

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	15	0.02	0.00	0.00	-0.11	-0.02	-0.06	0.02	0.01	-0.08
2	1	-0.07	-0.03	-0.04	-0.19	-0.08	-0.12	0.01	-0.07	-0.15

3	6	0.01	0.03	0.22	-0.07	-0.15	-0.03	0.01	0.02	0.02
4	15	0.01	0.01	0.04	0.10	-0.04	0.09	-0.01	0.02	0.03
5	6	0.08	0.03	0.23	0.03	-0.12	0.05	0.03	0.05	0.07
6	1	-0.12	0.07	0.06	0.12	-0.17	0.16	-0.07	0.01	0.07
7	1	0.16	0.05	-0.03	-0.18	0.04	-0.10	0.06	0.10	-0.14
8	1	0.08	-0.03	0.01	0.22	0.02	0.17	0.01	0.03	0.05
9	1	-0.13	0.04	0.25	-0.05	-0.24	-0.02	-0.04	-0.01	0.04
10	1	0.07	0.04	0.31	-0.12	-0.18	-0.08	0.03	0.04	0.02
11	1	0.22	0.02	0.22	0.03	-0.05	0.04	0.08	0.08	0.06
12	1	0.05	0.04	0.34	0.06	-0.19	0.09	0.01	0.06	0.14
13	6	0.01	-0.01	-0.03	-0.02	0.05	-0.06	0.01	0.00	0.01
14	6	0.01	-0.01	-0.03	0.02	0.05	-0.01	0.01	0.01	0.06
15	1	0.03	-0.01	-0.03	-0.05	0.08	-0.08	0.03	0.03	-0.01
16	6	-0.05	0.02	-0.01	0.05	-0.04	0.03	-0.04	-0.04	0.14
17	1	0.03	-0.01	-0.03	0.04	0.08	0.00	0.05	0.05	0.08
18	1	-0.05	0.02	-0.05	0.14	-0.02	0.06	-0.09	-0.04	0.24
19	1	-0.12	0.05	-0.01	0.00	-0.05	0.01	-0.04	-0.14	0.10
20	1	-0.02	0.00	-0.02	-0.01	0.01	-0.08	0.01	-0.03	0.00
21	7	-0.04	0.01	0.10	0.05	-0.16	0.07	-0.04	0.06	0.14
22	1	-0.08	0.06	0.07	0.09	-0.24	0.13	-0.07	-0.08	0.34
23	1	0.02	-0.07	0.08	0.11	-0.11	0.10	-0.02	0.32	0.22
24	6	-0.05	0.03	0.25	-0.07	-0.22	0.00	0.00	0.02	-0.20
25	1	0.00	-0.03	0.28	-0.09	-0.14	-0.08	0.04	0.18	-0.40
26	1	-0.03	0.02	0.32	-0.06	-0.29	0.07	0.01	0.12	-0.16
27	1	-0.12	0.12	0.27	-0.15	-0.29	-0.03	-0.01	-0.27	-0.28
28	78	0.00	-0.01	-0.06	0.00	0.06	-0.01	0.00	-0.01	-0.01

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1095.822962

Computed Cartesian coordinates, three lower frequencies PCM energy for **II'**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.996100	1.931494	-0.029052
2	1	0	-1.712235	2.926458	-0.993327
3	6	0	-3.864706	1.967913	-0.003930
4	15	0	-3.501984	-0.795016	0.259191
5	6	0	-4.416504	0.755318	0.756666
6	1	0	-4.292121	-1.288875	-0.804544
7	1	0	-1.674139	2.687314	1.124819
8	1	0	-3.908545	-1.707161	1.258395
9	1	0	-4.192472	1.941591	-1.050724
10	1	0	-4.234820	2.903001	0.429450

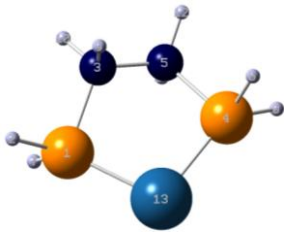
11	1	0	-4.261424	0.878952	1.835825
12	1	0	-5.493984	0.648594	0.592593
13	6	0	-0.070130	-1.928517	-0.417322
14	6	0	0.700099	-0.712158	-0.623025
15	1	0	-0.319132	-2.546440	-1.280186
16	6	0	1.712717	-0.241942	0.373016
17	1	0	0.939262	-0.433525	-1.654118
18	1	0	1.869789	0.840009	0.326837
19	1	0	1.449064	-0.513976	1.399213
20	1	0	0.068309	-2.502868	0.501248
21	7	0	3.104165	-0.842374	0.130575
22	1	0	3.808610	-0.348387	0.720543
23	1	0	3.370429	-0.632445	-0.836190
24	6	0	3.213576	-2.308242	0.354042
25	1	0	2.513685	-2.824110	-0.303177
26	1	0	4.238386	-2.622296	0.146583
27	1	0	2.967596	-2.520330	1.395967
28	78	0	-1.306770	-0.266761	-0.169632
29	1	0	5.219296	0.678357	2.494365
30	8	0	5.167313	0.448946	1.554390
31	6	0	6.093239	1.265251	0.802133
32	6	0	6.279747	0.645602	-0.546259
33	1	0	5.704727	2.287669	0.716352
34	1	0	7.050312	1.296598	1.338719
35	6	0	5.978258	1.258346	-1.695216
36	1	0	6.727924	-0.348904	-0.555722
37	1	0	5.557993	2.262905	-1.715729
38	1	0	6.177399	0.793652	-2.657750

			1			2			3	
			A			A			A	
Frequencies --			13.8596			19.9947			29.6361	
Red. masses --			4.2275			4.2701			4.0653	
Frc consts --			0.0005			0.0010			0.0021	
IR Inten --			0.2163			0.3898			0.5075	
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	15	0.07	0.01	-0.04	0.01	0.00	-0.11	0.09	0.00	0.06
2	1	0.10	-0.01	-0.05	-0.02	-0.07	-0.20	0.09	0.03	0.09
3	6	0.07	0.05	-0.06	0.01	0.02	-0.04	0.09	0.07	0.13
4	15	0.00	0.05	0.00	0.00	0.03	0.14	0.00	0.04	0.00
5	6	0.03	0.08	-0.04	0.04	0.07	0.07	0.07	0.05	0.10
6	1	0.00	0.05	0.00	-0.05	-0.04	0.21	-0.05	0.13	-0.01
7	1	0.07	0.02	-0.05	0.07	0.09	-0.18	0.16	-0.06	0.08
8	1	-0.03	0.08	0.01	0.04	0.11	0.22	-0.01	0.01	-0.04
9	1	0.08	0.04	-0.06	-0.03	-0.06	-0.02	0.05	0.13	0.14
10	1	0.09	0.07	-0.08	0.04	0.05	-0.09	0.14	0.06	0.19
11	1	0.02	0.10	-0.04	0.08	0.15	0.06	0.11	0.00	0.10
12	1	0.03	0.10	-0.05	0.03	0.07	0.13	0.06	0.10	0.13
13	6	-0.02	-0.04	0.04	-0.04	-0.04	0.04	-0.02	-0.04	-0.06
14	6	0.01	-0.06	0.02	-0.04	-0.06	-0.05	0.00	-0.05	-0.04
15	1	-0.03	-0.05	0.05	-0.08	-0.08	0.08	-0.03	-0.02	-0.07
16	6	0.01	-0.07	0.02	0.00	-0.02	-0.11	-0.01	-0.06	-0.03
17	1	0.02	-0.08	0.02	-0.07	-0.11	-0.08	0.00	-0.04	-0.03
18	1	0.03	-0.07	0.01	0.00	-0.02	-0.16	0.00	-0.06	-0.02
19	1	0.00	-0.05	0.02	0.04	0.02	-0.09	-0.03	-0.06	-0.03
20	1	-0.04	-0.03	0.05	-0.01	0.00	0.06	-0.04	-0.05	-0.07
21	7	0.00	-0.10	0.03	-0.01	-0.03	-0.13	-0.01	-0.07	0.00
22	1	0.01	-0.10	0.03	0.00	-0.03	-0.14	-0.02	-0.04	-0.01
23	1	0.01	-0.11	0.03	-0.02	-0.04	-0.14	-0.01	-0.10	-0.01
24	6	-0.03	-0.10	0.05	-0.01	-0.03	-0.13	-0.01	-0.06	0.04
25	1	-0.03	-0.09	0.05	-0.02	-0.03	-0.11	-0.02	-0.08	0.06

26	1	-0.03	-0.12	0.06	-0.01	-0.03	-0.14	-0.01	-0.07	0.05
27	1	-0.04	-0.08	0.05	0.01	-0.02	-0.12	-0.01	-0.03	0.05
28	78	0.02	-0.01	0.01	-0.01	-0.01	0.00	0.01	-0.02	-0.02
29	1	0.08	-0.18	0.02	-0.16	-0.09	0.00	-0.24	0.25	-0.01
30	8	0.02	-0.10	0.00	-0.07	-0.04	-0.02	-0.17	0.17	0.01
31	6	-0.08	0.01	0.00	-0.02	0.01	0.10	-0.18	0.16	-0.01
32	6	-0.15	0.15	-0.07	0.10	0.09	0.09	-0.03	0.03	0.07
33	1	-0.14	0.00	0.13	-0.04	0.01	0.12	-0.24	0.12	-0.14
34	1	-0.04	0.01	-0.07	-0.07	0.01	0.19	-0.22	0.28	0.05
35	6	-0.28	0.23	0.01	0.21	0.15	0.09	-0.01	-0.12	-0.02
36	1	-0.10	0.17	-0.19	0.11	0.09	0.07	0.04	0.06	0.20
37	1	-0.33	0.21	0.13	0.20	0.15	0.11	-0.08	-0.15	-0.15
38	1	-0.33	0.33	-0.05	0.30	0.20	0.08	0.09	-0.20	0.04

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1288.876803

Computed Cartesian coordinates, three lower frequencies PCM energy for **III**



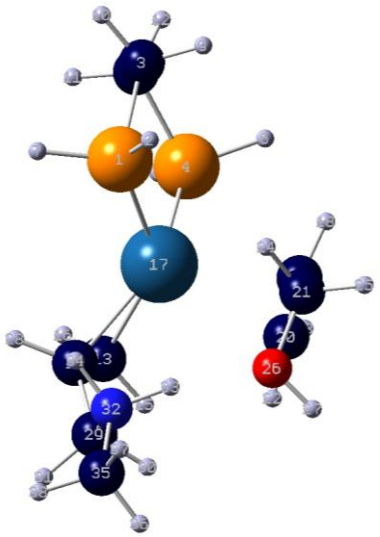
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.645841	1.691965	-0.055766
2	1	0	0.898097	2.800556	0.802429
3	6	0	2.216171	0.709467	0.302689
4	15	0	0.645977	-1.691928	0.055842
5	6	0	2.216190	-0.709327	-0.302793
6	1	0	1.010214	-2.345801	1.264739
7	1	0	1.010071	2.346260	-1.264437
8	1	0	0.898486	-2.800746	-0.801997
9	1	0	2.284173	0.647570	1.396389
10	1	0	3.098519	1.261600	-0.044878
11	1	0	2.284064	-0.647435	-1.396503
12	1	0	3.098619	-1.261390	0.044680
13	78	0	-0.776329	-0.000026	-0.000012

		1			2			3		
		A			A			A		
Frequencies --		115.5374			203.3553			211.6561		
Red. masses --		2.5003			7.5317			1.8047		
Frc consts --		0.0197			0.1835			0.0476		
IR Inten --		0.4201			0.0738			0.0060		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	15	-0.01	0.00	0.13	0.18	-0.15	0.02	0.02	-0.01	-0.03
2	1	-0.05	-0.18	0.37	0.28	-0.01	-0.18	0.00	0.07	-0.13
3	6	0.04	-0.01	-0.13	0.24	-0.03	0.03	-0.07	-0.07	0.15
4	15	0.01	0.00	0.13	0.18	0.15	-0.02	0.02	0.01	0.03
5	6	-0.04	-0.01	-0.13	0.24	0.03	-0.03	-0.07	0.07	-0.15
6	1	0.06	0.29	0.27	0.15	0.35	0.10	0.15	0.16	0.08
7	1	-0.06	0.29	0.27	0.15	-0.35	-0.10	0.15	-0.16	-0.08
8	1	0.05	-0.18	0.37	0.28	0.01	0.18	0.00	-0.07	0.13
9	1	0.22	-0.03	-0.14	0.28	-0.06	0.02	-0.31	-0.29	0.15
10	1	-0.01	-0.01	-0.26	0.18	0.06	0.01	0.02	-0.04	0.43

11	1	-0.22	-0.03	-0.14	0.28	0.06	-0.02	-0.31	0.29	-0.15
12	1	0.01	-0.01	-0.26	0.18	-0.06	-0.01	0.02	0.04	-0.43
13	78	0.00	0.00	-0.03	-0.10	0.00	0.00	0.00	0.00	0.00

Total free energy in solution:
with all non electrostatic terms (a.u.) = -882.834072

Computed Cartesian coordinates, three lower frequencies PCM energy for **$TS_{II'-IV}$**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.076517	0.642995	1.761164
2	1	0	-0.642536	1.869465	2.335758
3	6	0	-2.903846	1.004080	1.604654
4	15	0	-2.575987	-0.304641	-0.852370
5	6	0	-3.594960	-0.003467	0.681449
6	1	0	-3.130187	0.637284	-1.759611
7	1	0	-1.019733	-0.114028	2.957869
8	1	0	-3.207899	-1.452109	-1.382855
9	1	0	-2.981126	2.016559	1.188735
10	1	0	-3.380136	1.022765	2.590816
11	1	0	-3.696697	-0.973706	1.182250
12	1	0	-4.602824	0.338053	0.421590
13	6	0	0.366375	-2.234770	-0.856823
14	6	0	1.154492	-1.819300	0.264012
15	1	0	0.808748	-2.229939	-1.852617
16	1	0	-0.385810	-3.006469	-0.712552
17	78	0	-0.340776	-0.316515	-0.194981
18	1	0	-0.582977	2.328592	-1.439869
19	6	0	0.379929	1.836274	-1.312969
20	6	0	0.688133	0.769168	-2.115533
21	6	0	1.372028	2.645826	-0.521220
22	1	0	1.704539	0.388983	-2.179869
23	1	0	0.011771	0.442138	-2.897386
24	1	0	1.039979	2.803755	0.508534
25	1	0	1.473967	3.642139	-0.976001
26	8	0	2.670073	2.048951	-0.421818
27	1	0	3.140117	2.173755	-1.259835
28	1	0	0.917524	-2.286045	1.222788
29	6	0	2.620576	-1.534233	0.103477

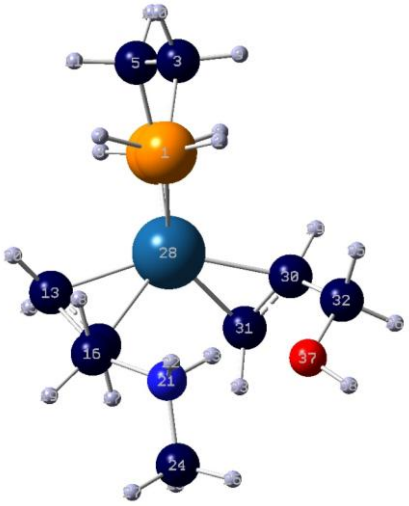
30	1	0	2.890819	-1.299554	-0.930070
31	1	0	3.240508	-2.376680	0.436905
32	7	0	3.037124	-0.347350	0.939578
33	1	0	2.753849	0.522852	0.430898
34	1	0	2.475840	-0.359778	1.795927
35	6	0	4.486017	-0.274699	1.265551
36	1	0	5.055781	-0.285629	0.334622
37	1	0	4.685470	0.652234	1.806489
38	1	0	4.766147	-1.135183	1.875993

	1	2	3
	A	A	A
Frequencies --	-95.7353	40.6497	57.4495
Red. masses --	8.5826	3.8992	4.1781
Frc consts --	0.0463	0.0038	0.0081
IR Inten --	5.8529	2.4018	1.8855

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	15	-0.02	-0.13	0.04	0.09	-0.01	0.00	0.03	-0.12	0.06
2	1	0.03	-0.14	0.03	0.10	0.00	-0.03	0.09	-0.19	0.17
3	6	0.00	-0.06	0.02	0.07	-0.05	0.10	0.06	0.02	0.06
4	15	-0.01	-0.03	0.00	-0.03	-0.01	0.07	0.02	0.18	-0.05
5	6	-0.02	-0.03	0.00	0.05	-0.05	0.13	0.00	0.16	-0.06
6	1	-0.01	-0.03	0.00	-0.11	-0.02	0.11	0.17	0.33	0.01
7	1	-0.06	-0.12	0.05	0.17	0.00	0.00	-0.03	-0.23	-0.01
8	1	-0.03	-0.03	0.00	-0.04	-0.02	0.09	-0.10	0.30	-0.17
9	1	0.04	-0.05	0.03	0.03	-0.04	0.12	0.14	0.07	0.16
10	1	-0.02	-0.06	0.01	0.13	-0.07	0.13	0.04	-0.05	0.05
11	1	-0.05	-0.03	-0.02	0.10	-0.06	0.13	-0.11	0.13	-0.14
12	1	-0.01	0.00	-0.01	0.03	-0.08	0.19	0.04	0.28	-0.06
13	6	-0.08	-0.10	0.20	0.01	0.03	-0.10	0.00	-0.05	0.02
14	6	-0.03	0.01	0.10	-0.03	-0.03	-0.05	0.00	-0.03	0.01
15	1	-0.15	-0.21	0.17	0.04	0.07	-0.08	-0.01	-0.05	0.02
16	1	-0.12	-0.03	0.33	-0.01	0.03	-0.16	0.00	-0.05	0.03
17	78	0.04	0.10	-0.06	0.01	0.02	-0.03	0.01	-0.03	0.01
18	1	-0.08	-0.20	0.09	-0.01	-0.01	-0.05	-0.04	-0.09	-0.14
19	6	-0.14	-0.28	0.23	-0.02	-0.01	-0.06	-0.03	-0.05	-0.07
20	6	-0.10	-0.28	0.15	-0.02	-0.02	-0.05	0.04	-0.08	-0.01
21	6	-0.10	-0.13	0.05	0.00	-0.01	-0.08	-0.09	0.03	-0.07
22	1	-0.06	-0.16	0.07	-0.02	-0.02	-0.06	0.06	-0.04	0.05
23	1	-0.02	-0.13	0.02	-0.03	-0.02	-0.04	0.09	-0.15	-0.02
24	1	-0.01	0.00	0.05	-0.01	0.05	-0.09	-0.14	0.05	-0.09
25	1	-0.16	-0.20	-0.10	0.03	-0.03	-0.12	-0.12	0.01	-0.10
26	8	-0.06	-0.06	0.02	-0.02	-0.04	-0.04	-0.07	0.08	0.00
27	1	-0.13	-0.13	-0.03	0.01	-0.06	-0.02	-0.04	0.10	0.02
28	1	-0.03	0.16	0.17	-0.08	-0.07	-0.08	0.00	-0.02	0.02
29	6	-0.03	-0.04	0.04	-0.03	0.00	0.04	-0.01	0.01	0.02
30	1	-0.06	-0.08	0.02	0.04	0.01	0.06	0.00	-0.02	0.01
31	1	-0.04	-0.04	0.05	-0.03	0.01	0.08	0.01	0.05	0.06
32	7	0.01	-0.02	-0.01	-0.12	0.00	0.08	-0.06	0.06	-0.02
33	1	-0.01	-0.03	-0.02	-0.07	-0.01	0.04	-0.08	0.04	-0.05
34	1	0.04	0.01	0.01	-0.23	0.01	0.01	-0.07	0.08	-0.03
35	6	0.02	-0.02	-0.05	-0.16	0.01	0.27	-0.07	0.13	-0.01
36	1	-0.01	-0.04	-0.07	-0.04	0.01	0.34	-0.05	0.10	0.00
37	1	0.03	-0.01	-0.08	-0.24	0.01	0.29	-0.11	0.16	-0.04
38	1	0.03	0.00	-0.04	-0.24	0.01	0.31	-0.05	0.16	0.04

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1288.854361

Computed Cartesian coordinates, three lower frequencies PCM energy for **IV**



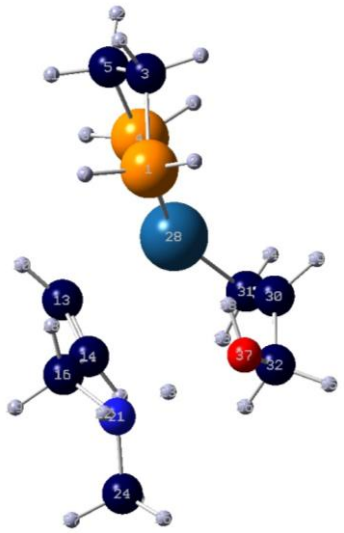
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.027813	-0.717687	1.740445
2	1	0	-0.590264	-0.227318	2.997077
3	6	0	-2.839288	-0.277503	1.850754
4	15	0	-2.547176	0.286569	-0.873736
5	6	0	-3.543145	-0.475307	0.504938
6	1	0	-3.114254	1.582491	-0.972966
7	1	0	-1.058525	-2.089409	2.112670
8	1	0	-3.171098	-0.277062	-2.009758
9	1	0	-2.879205	0.777369	2.149314
10	1	0	-3.331652	-0.858218	2.637985
11	1	0	-3.636029	-1.543745	0.274672
12	1	0	-4.556279	-0.060377	0.534005
13	6	0	0.136523	-1.905173	-1.354886
14	6	0	1.373839	-1.307068	-0.967585
15	1	0	-0.149665	-1.887076	-2.403264
16	6	0	2.194990	-1.940952	0.117782
17	1	0	1.960423	-0.849110	-1.765396
18	1	0	1.554204	-2.394432	0.878426
19	1	0	2.881436	-2.712353	-0.257222
20	1	0	-0.240792	-2.764875	-0.801732
21	7	0	3.057479	-0.911097	0.810252
22	1	0	3.246588	-1.206017	1.771130
23	1	0	2.524339	-0.007259	0.863735
24	6	0	4.352880	-0.639471	0.127431
25	1	0	4.147489	-0.276272	-0.879298
26	1	0	4.897730	0.123560	0.685739
27	1	0	4.939132	-1.559201	0.084290
28	78	0	-0.247475	0.004806	-0.373145
29	1	0	-0.698307	2.701032	0.004600
30	6	0	0.229592	2.139037	-0.116796
31	6	0	0.556918	1.713350	-1.435176
32	6	0	1.241775	2.597462	0.897493
33	1	0	1.603693	1.574297	-1.699313
34	1	0	-0.079926	1.994126	-2.270385
35	1	0	0.813611	2.566991	1.907792
36	1	0	1.519153	3.640633	0.682060
37	8	0	2.444613	1.805967	0.867396
38	1	0	3.162308	2.347787	1.225795

1	2	3
A	A	A

Frequencies --		30.2546			46.2140			57.9560		
Red. masses --		3.5461			4.1574			3.5410		
Frc consts --		0.0019			0.0052			0.0070		
IR Inten --		1.4645			2.6181			4.5242		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	15	0.05	-0.03	-0.01	0.08	0.00	0.00	-0.05	-0.07	-0.02
2	1	0.07	-0.04	-0.01	0.18	-0.02	-0.02	0.02	-0.18	0.00
3	6	0.04	-0.08	0.04	0.12	0.13	0.09	0.01	0.17	0.02
4	15	-0.02	-0.01	0.05	0.00	0.01	0.05	0.00	0.02	-0.01
5	6	0.02	-0.06	0.05	0.03	0.13	0.14	-0.06	0.21	0.04
6	1	-0.04	-0.02	0.09	0.05	0.03	0.01	0.12	0.07	-0.11
7	1	0.09	-0.03	-0.03	0.00	0.01	0.01	-0.22	-0.08	-0.09
8	1	-0.03	0.01	0.05	-0.08	-0.02	0.11	-0.04	-0.01	0.03
9	1	0.02	-0.08	0.07	0.21	0.15	0.05	0.16	0.18	-0.02
10	1	0.07	-0.11	0.04	0.12	0.20	0.14	-0.05	0.26	0.05
11	1	0.04	-0.06	0.03	-0.05	0.13	0.18	-0.21	0.21	0.09
12	1	0.01	-0.08	0.08	0.06	0.20	0.18	0.00	0.35	0.05
13	6	0.05	0.08	-0.11	0.00	-0.01	-0.07	0.10	0.01	-0.03
14	6	0.03	0.07	-0.01	0.00	-0.02	-0.06	0.07	0.07	0.02
15	1	0.09	0.14	-0.12	-0.01	0.01	-0.07	0.13	0.02	-0.04
16	6	-0.03	0.00	-0.02	-0.02	-0.04	-0.06	0.08	0.07	0.01
17	1	0.06	0.12	0.05	0.01	-0.02	-0.05	0.06	0.12	0.04
18	1	-0.06	-0.07	-0.09	-0.04	-0.10	-0.11	0.09	0.06	0.01
19	1	0.00	0.03	-0.04	0.04	0.02	-0.06	0.08	0.07	-0.01
20	1	0.03	0.04	-0.18	-0.01	-0.01	-0.08	0.13	-0.02	-0.06
21	7	-0.07	-0.04	0.10	-0.11	-0.03	0.04	0.10	0.06	0.00
22	1	-0.21	-0.05	0.13	-0.13	-0.07	0.03	0.07	0.08	0.01
23	1	-0.03	-0.02	0.02	-0.18	-0.07	0.07	0.13	0.08	-0.03
24	6	0.04	-0.10	0.28	-0.10	0.11	0.11	0.12	0.00	0.02
25	1	0.19	-0.11	0.25	-0.09	0.19	0.14	0.16	-0.05	-0.01
26	1	-0.01	-0.12	0.35	-0.17	0.09	0.20	0.12	0.02	0.00
27	1	0.01	-0.13	0.37	-0.05	0.15	0.05	0.11	-0.01	0.09
28	78	-0.01	0.02	-0.01	0.01	-0.02	-0.04	-0.02	-0.04	0.00
29	1	0.00	0.01	0.04	-0.06	-0.02	-0.10	-0.05	-0.05	0.14
30	6	0.00	0.02	-0.02	-0.04	-0.01	-0.04	-0.05	-0.03	0.08
31	6	-0.08	0.02	-0.04	0.03	-0.01	-0.01	-0.08	0.03	0.05
32	6	0.06	0.01	-0.08	-0.11	0.02	0.02	-0.02	-0.05	0.05
33	1	-0.09	0.02	-0.10	0.05	0.00	0.04	-0.09	0.06	0.01
34	1	-0.12	0.03	-0.01	0.07	-0.04	-0.05	-0.12	0.05	0.08
35	1	0.12	0.03	-0.06	-0.20	0.08	-0.01	0.06	-0.16	0.08
36	1	0.07	0.00	-0.11	-0.07	0.00	0.00	-0.10	-0.01	0.12
37	8	0.05	-0.01	-0.15	-0.13	-0.01	0.17	0.04	0.04	-0.09
38	1	0.09	0.00	-0.25	-0.17	-0.03	0.27	0.04	0.08	-0.17

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1288.856643

Computed Cartesian coordinates, three lower frequencies PCM energy for **TS_{IV-V}**



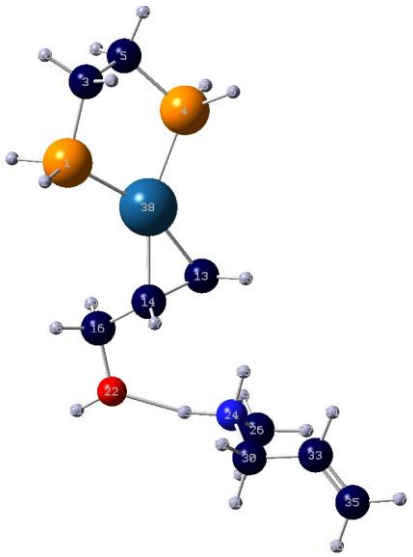
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.128193	-1.221110	1.422939
2	1	0	-0.921980	-1.142602	2.822317
3	6	0	-2.995993	-1.223642	1.377418
4	15	0	-2.572504	0.222668	-0.989695
5	6	0	-3.515842	-1.087381	-0.056141
6	1	0	-3.387463	1.368067	-0.840746
7	1	0	-0.845284	-2.610573	1.303068
8	1	0	-2.933301	-0.087347	-2.324726
9	1	0	-3.317510	-0.369842	1.985881
10	1	0	-3.388443	-2.130102	1.850767
11	1	0	-3.371739	-2.026560	-0.604746
12	1	0	-4.589789	-0.872433	-0.060379
13	6	0	0.482030	-0.912817	-2.037641
14	6	0	1.705244	-0.730173	-1.464760
15	1	0	0.135564	-0.233844	-2.809454
16	6	0	2.413985	-1.823429	-0.720685
17	1	0	2.284915	0.148521	-1.742433
18	1	0	1.700012	-2.443848	-0.171957
19	1	0	2.979028	-2.477759	-1.398953
20	1	0	-0.040173	-1.863584	-1.960464
21	7	0	3.414451	-1.302606	0.278768
22	1	0	3.635214	-2.050718	0.941379
23	1	0	2.969171	-0.513779	0.862679
24	6	0	4.693373	-0.817848	-0.310923
25	1	0	4.482288	-0.017480	-1.020168
26	1	0	5.325879	-0.434278	0.492002
27	1	0	5.195334	-1.641579	-0.823117
28	78	0	-0.439904	0.354801	-0.107410
29	1	0	0.095462	2.508797	1.498394
30	6	0	0.665079	2.082864	0.671610
31	6	0	0.191125	2.341797	-0.646761
32	6	0	2.117899	1.857369	0.980094
33	1	0	0.897404	2.352912	-1.478181
34	1	0	-0.654969	3.011473	-0.782792
35	1	0	2.534199	2.669087	1.586985
36	1	0	2.703820	1.785942	0.054760
37	8	0	2.311426	0.637878	1.749085
38	1	0	1.401362	0.268438	1.801900

1 2 3

		A			A			A		
Frequencies --		-117.6024			38.9899			58.6183		
Red. masses --		9.1429			3.7790			3.5346		
Frc consts --		0.0745			0.0034			0.0072		
IR Inten --		2.9855			3.4953			0.3895		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	15	-0.01	-0.01	-0.02	-0.09	0.02	0.02	-0.03	0.06	0.07
2	1	-0.01	-0.03	-0.02	-0.11	0.05	0.02	0.01	0.15	0.06
3	6	-0.01	-0.02	-0.02	-0.09	0.12	-0.01	-0.02	0.17	0.11
4	15	0.01	-0.10	-0.09	0.02	0.04	-0.04	0.01	-0.07	-0.03
5	6	-0.01	-0.05	-0.03	-0.06	0.11	-0.03	-0.04	0.06	0.11
6	1	0.03	-0.08	-0.10	0.07	0.08	-0.10	0.04	-0.03	-0.18
7	1	0.00	-0.01	-0.06	-0.16	0.01	0.05	-0.11	0.03	0.17
8	1	-0.04	-0.13	-0.07	0.04	0.02	-0.04	0.02	-0.22	0.00
9	1	-0.01	0.00	-0.04	-0.06	0.15	-0.04	0.04	0.24	0.04
10	1	-0.01	-0.01	0.00	-0.15	0.15	0.00	-0.07	0.24	0.20
11	1	-0.03	-0.07	0.00	-0.10	0.09	0.00	-0.10	0.00	0.19
12	1	-0.01	-0.04	-0.03	-0.05	0.16	-0.05	-0.03	0.12	0.10
13	6	0.27	-0.10	-0.14	-0.02	-0.13	0.07	0.07	0.15	-0.11
14	6	0.30	-0.20	-0.27	0.00	-0.05	0.01	0.06	0.12	-0.06
15	1	0.18	-0.02	-0.03	-0.07	-0.19	0.04	0.08	0.22	-0.05
16	6	0.16	-0.13	-0.05	0.09	0.01	0.02	0.06	0.06	-0.15
17	1	0.31	-0.20	-0.22	-0.05	-0.04	-0.07	0.05	0.15	0.04
18	1	0.06	0.01	-0.01	0.15	0.01	0.09	0.05	-0.04	-0.27
19	1	0.17	-0.28	0.11	0.08	0.01	0.01	0.12	0.16	-0.19
20	1	0.12	-0.01	0.00	0.02	-0.14	0.15	0.08	0.14	-0.20
21	7	0.09	-0.05	-0.03	0.13	0.09	-0.06	-0.02	-0.02	-0.03
22	1	0.10	-0.02	0.00	0.26	0.10	-0.10	-0.09	-0.06	-0.06
23	1	0.05	-0.05	-0.06	0.09	0.03	0.00	-0.04	-0.05	-0.02
24	6	0.10	-0.02	0.00	0.03	0.23	-0.16	0.04	0.00	0.11
25	1	0.10	-0.03	-0.01	-0.11	0.24	-0.11	0.10	0.03	0.13
26	1	0.07	-0.01	0.02	0.07	0.25	-0.21	-0.04	-0.04	0.18
27	1	0.13	-0.01	0.02	0.05	0.30	-0.24	0.08	0.02	0.12
28	78	-0.07	0.07	0.07	0.00	-0.03	0.01	0.00	-0.03	-0.01
29	1	0.12	-0.01	-0.01	-0.01	-0.03	0.01	-0.03	-0.05	0.02
30	6	0.07	-0.04	-0.04	0.01	-0.04	0.02	-0.02	-0.03	0.02
31	6	0.00	-0.01	-0.02	0.04	-0.03	0.01	-0.01	-0.01	0.02
32	6	0.07	-0.07	-0.09	0.00	-0.05	0.05	-0.02	-0.03	0.04
33	1	-0.04	-0.06	-0.06	0.06	-0.04	0.03	0.00	0.01	0.03
34	1	0.04	0.06	0.03	0.05	-0.03	-0.01	-0.02	-0.02	0.03
35	1	0.12	-0.07	-0.11	-0.01	-0.07	0.08	-0.04	-0.03	0.07
36	1	0.04	-0.10	-0.11	0.01	-0.03	0.05	0.00	0.01	0.05
37	8	0.04	-0.06	-0.08	-0.02	-0.07	0.02	-0.02	-0.04	0.01
38	1	0.02	-0.04	-0.09	-0.02	-0.10	-0.06	-0.02	-0.04	0.02

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1288.850566

Computed Cartesian coordinates, three lower frequencies PCM energy for **V**

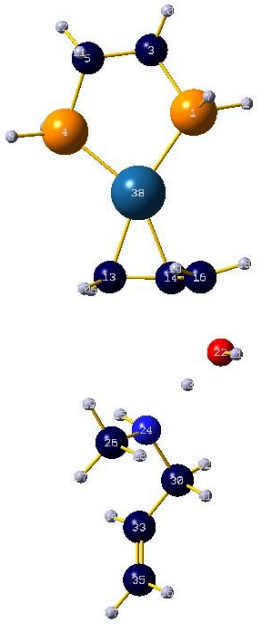


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.882191	1.115085	-0.842732
2	1	0	-2.936674	1.645635	-2.151737
3	6	0	-4.387394	0.008695	-0.821056
4	15	0	-2.650574	-1.626200	0.640725
5	6	0	-4.358905	-0.908481	0.408058
6	1	0	-2.729644	-2.833258	-0.093047
7	1	0	-3.343182	2.257656	-0.145968
8	1	0	-2.741126	-2.173681	1.940479
9	1	0	-4.351831	-0.586657	-1.742048
10	1	0	-5.310183	0.597701	-0.849032
11	1	0	-4.585696	-0.335911	1.316133
12	1	0	-5.112027	-1.698960	0.323944
13	6	0	0.895926	-0.479630	0.501083
14	6	0	0.822101	0.777093	-0.236081
15	1	0	1.252218	-1.385106	0.001471
16	6	0	1.039116	2.097119	0.439640
17	1	0	1.130915	0.770581	-1.285175
18	1	0	0.554416	2.903788	-0.120420
19	1	0	0.653562	2.089970	1.465699
20	1	0	1.072165	-0.465102	1.580208
21	1	0	2.611877	3.299930	0.807125
22	8	0	2.474741	2.394728	0.488678
23	1	0	3.561497	1.110572	0.531522
24	7	0	4.033587	0.170874	0.466573
25	1	0	3.227974	-0.468188	0.392794
26	6	0	4.791667	-0.115980	1.710893
27	1	0	5.234083	-1.111106	1.647900
28	1	0	5.579525	0.631499	1.823284
29	1	0	4.106279	-0.059494	2.558478
30	6	0	4.841896	0.106832	-0.802209
31	1	0	5.671597	0.810319	-0.687198
32	1	0	4.180665	0.481145	-1.591404
33	6	0	5.324768	-1.278665	-1.098850
34	1	0	4.557682	-2.029232	-1.296002
35	6	0	6.615140	-1.608507	-1.187306
36	1	0	7.409026	-0.881884	-1.023287
37	1	0	6.923834	-2.616997	-1.448145
38	78	0	-1.091851	-0.054247	0.005308

		A			A			A		
Frequencies --		17.4773			26.4520			38.8205		
Red. masses --		4.4028			4.3002			2.5321		
Frc consts --		0.0008			0.0018			0.0022		
IR Inten --		0.7993			0.9588			1.3816		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	15	-0.04	0.04	0.07	-0.05	0.03	0.14	0.01	0.04	0.03
2	1	-0.08	0.06	0.08	-0.12	0.13	0.18	0.02	0.08	0.05
3	6	-0.06	0.06	0.11	-0.03	0.00	0.13	0.00	0.05	-0.02
4	15	-0.02	0.01	0.02	0.07	-0.08	-0.08	-0.03	-0.01	-0.06
5	6	-0.02	0.04	0.10	0.05	-0.09	0.05	-0.02	0.01	-0.05
6	1	-0.07	0.02	0.00	0.07	-0.01	-0.19	-0.03	0.02	-0.10
7	1	0.01	0.03	0.11	-0.04	-0.03	0.25	0.01	0.01	0.07
8	1	0.02	-0.01	0.01	0.14	-0.19	-0.13	-0.05	-0.06	-0.08
9	1	-0.10	0.08	0.10	-0.06	0.07	0.08	0.00	0.08	-0.04
10	1	-0.05	0.08	0.16	-0.04	-0.01	0.22	0.00	0.06	-0.01
11	1	0.02	0.03	0.12	0.08	-0.17	0.11	-0.03	-0.02	-0.04
12	1	-0.04	0.06	0.11	0.06	-0.10	0.03	-0.03	0.02	-0.09
13	6	-0.01	-0.04	-0.09	0.04	0.03	-0.12	-0.01	-0.02	0.01
14	6	-0.02	-0.03	-0.07	-0.01	0.07	-0.05	-0.01	-0.01	0.02
15	1	-0.04	-0.03	-0.12	0.04	0.06	-0.18	-0.01	-0.02	0.00
16	6	0.01	-0.04	-0.06	-0.01	0.04	0.01	0.00	-0.02	0.03
17	1	-0.05	-0.01	-0.08	-0.05	0.12	-0.06	-0.01	-0.01	0.02
18	1	0.01	-0.02	-0.03	-0.06	0.05	0.07	-0.01	-0.02	0.05
19	1	0.04	-0.05	-0.05	0.04	-0.02	0.03	0.02	-0.03	0.04
20	1	0.02	-0.06	-0.10	0.06	-0.03	-0.12	-0.02	-0.03	0.01
21	1	0.04	-0.07	-0.08	-0.03	0.07	-0.05	0.01	-0.02	0.01
22	8	0.02	-0.06	-0.09	-0.02	0.07	-0.04	0.00	-0.02	0.01
23	1	-0.02	-0.08	-0.06	0.02	0.08	-0.06	0.00	-0.01	-0.06
24	7	0.02	-0.06	-0.05	-0.01	0.06	-0.01	0.03	0.00	-0.01
25	1	0.05	-0.09	-0.13	-0.04	0.10	0.00	0.05	-0.05	0.13
26	6	-0.08	-0.07	0.01	-0.06	0.09	0.02	0.16	0.17	-0.04
27	1	-0.03	-0.05	0.01	-0.11	0.06	0.08	0.18	0.18	0.04
28	1	-0.12	-0.04	0.10	-0.02	0.05	0.00	0.15	0.20	-0.21
29	1	-0.15	-0.13	-0.05	-0.07	0.17	0.00	0.24	0.27	0.02
30	6	0.13	0.01	0.02	0.01	-0.04	0.01	-0.08	-0.10	-0.07
31	1	0.08	0.05	0.11	0.05	-0.09	0.00	-0.15	0.01	-0.26
32	1	0.18	-0.01	-0.03	0.05	-0.03	-0.02	-0.20	-0.29	-0.07
33	6	0.24	0.04	0.03	-0.08	-0.09	0.09	0.05	-0.09	0.09
34	1	0.30	0.00	-0.05	-0.12	-0.04	0.09	0.12	-0.21	0.28
35	6	0.26	0.12	0.14	-0.10	-0.19	0.15	0.08	0.06	0.00
36	1	0.21	0.17	0.23	-0.05	-0.23	0.15	0.01	0.18	-0.20
37	1	0.35	0.15	0.14	-0.16	-0.22	0.21	0.18	0.06	0.11
38	78	-0.02	0.00	-0.02	0.01	0.01	-0.03	-0.01	-0.01	0.01

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1288.875509

Computed Cartesian coordinates, three lower frequencies PCM energy for **$TS_{V\text{-}I}$**

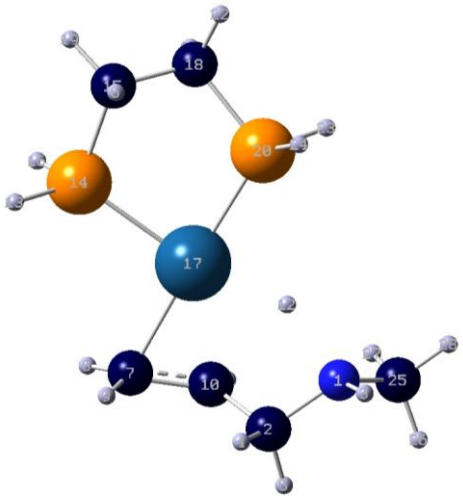


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-3.055598	1.436964	-0.059365
2	1	0	-3.278307	2.444659	-1.023060
3	6	0	-4.647529	0.467204	-0.128744
4	15	0	-2.880290	-1.676793	0.193509
5	6	0	-4.501866	-0.863411	0.620989
6	1	0	-3.203024	-2.495451	-0.910681
7	1	0	-3.216467	2.218417	1.107646
8	1	0	-2.749318	-2.671187	1.185687
9	1	0	-4.860165	0.287366	-1.189826
10	1	0	-5.480429	1.052032	0.275183
11	1	0	-4.493470	-0.695067	1.705003
12	1	0	-5.342386	-1.530230	0.401405
13	6	0	0.599784	-0.942679	-0.294727
14	6	0	0.722467	0.457076	-0.650804
15	1	0	0.734911	-1.683466	-1.081253
16	6	0	0.923125	1.483203	0.314314
17	1	0	0.804282	0.740680	-1.699147
18	1	0	0.670415	2.500670	0.036878
19	1	0	0.820449	1.238059	1.367760
20	1	0	0.954440	-1.271561	0.684502
21	1	0	2.954563	2.515476	1.098802
22	8	0	2.761121	1.900754	0.371703
23	1	0	3.453729	1.050152	0.426281
24	7	0	4.421229	-0.047063	0.379340
25	1	0	3.927057	-0.816530	-0.075223
26	6	0	4.834601	-0.479205	1.724533
27	1	0	5.560129	-1.299813	1.695310
28	1	0	5.292550	0.367666	2.245462
29	1	0	3.952347	-0.798064	2.286999
30	6	0	5.554650	0.360376	-0.491932
31	1	0	6.066048	1.192964	0.004398
32	1	0	5.112458	0.754895	-1.415566
33	6	0	6.521688	-0.745599	-0.802864
34	1	0	6.114573	-1.602454	-1.344213
35	6	0	7.818896	-0.724450	-0.488772
36	1	0	8.268398	0.116867	0.036451
37	1	0	8.483856	-1.540076	-0.760329
38	78	0	-1.301292	-0.069619	-0.147585

	1			2			3		
	A			A			A		
Frequencies --	-364.2561			0.9598			17.3499		
Red. masses --	6.1334			4.5199			4.8237		
Frc consts --	0.4795			0.0000			0.0009		
IR Inten --	1881.8572			0.8549			1.6425		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 15	0.02	0.00	-0.01	-0.03	-0.02	0.13	0.03	0.04	0.03
2 1	-0.07	0.03	0.03	-0.12	0.00	0.17	0.04	0.06	0.04
3 6	0.00	0.00	0.00	-0.02	-0.05	0.22	-0.01	0.11	0.07
4 15	-0.01	0.00	0.02	0.05	-0.03	-0.02	-0.08	0.04	0.02
5 6	-0.02	0.00	0.00	0.07	-0.08	0.15	-0.04	0.10	0.06
6 1	-0.03	0.01	0.01	-0.01	0.03	-0.04	-0.15	0.06	0.02
7 1	-0.01	-0.02	0.00	0.04	-0.06	0.16	0.08	0.05	0.04
8 1	-0.11	-0.04	0.00	0.14	-0.09	-0.09	-0.10	0.02	0.01
9 1	0.00	0.00	0.00	-0.10	-0.01	0.23	-0.04	0.12	0.07
10 1	0.00	0.01	0.00	0.01	-0.09	0.32	0.02	0.14	0.09
11 1	-0.02	0.00	0.00	0.16	-0.13	0.16	0.00	0.10	0.06
12 1	-0.03	0.01	0.00	0.07	-0.09	0.19	-0.07	0.13	0.08
13 6	0.02	0.06	0.02	0.01	0.05	-0.15	-0.06	-0.08	-0.05
14 6	-0.05	0.09	0.06	-0.03	0.07	-0.10	-0.02	-0.08	-0.04
15 1	0.00	0.08	0.00	-0.01	0.09	-0.19	-0.09	-0.08	-0.05
16 6	0.51	0.12	0.07	0.00	0.03	-0.07	0.02	-0.09	-0.04
17 1	-0.01	0.08	0.06	-0.07	0.11	-0.09	-0.04	-0.08	-0.04
18 1	0.14	0.05	0.13	-0.02	0.04	-0.02	0.03	-0.08	-0.03
19 1	0.18	0.07	0.04	0.04	-0.01	-0.07	0.03	-0.09	-0.04
20 1	0.02	0.02	0.01	0.05	0.02	-0.18	-0.05	-0.09	-0.06
21 1	-0.33	-0.11	-0.11	0.01	0.08	-0.16	0.03	-0.08	-0.11
22 8	-0.19	-0.25	-0.04	0.00	0.03	-0.12	0.02	-0.12	-0.08
23 1	0.21	-0.48	-0.03	-0.01	0.03	-0.07	0.05	-0.10	-0.07
24 7	-0.08	0.10	-0.01	-0.02	0.01	0.00	0.09	-0.05	-0.05
25 1	-0.08	0.09	-0.01	-0.02	0.01	0.00	0.16	-0.06	-0.10
26 6	-0.05	0.04	0.00	-0.09	0.04	0.03	0.04	-0.06	-0.04
27 1	-0.08	0.03	-0.11	-0.11	0.02	0.09	0.09	-0.02	-0.03
28 1	-0.01	0.01	0.00	-0.10	0.04	0.03	-0.03	-0.05	0.01
29 1	-0.04	0.03	0.00	-0.12	0.07	0.00	0.03	-0.12	-0.10
30 6	-0.01	0.04	-0.01	0.02	-0.04	0.04	0.11	0.04	0.02
31 1	-0.01	0.03	-0.01	0.02	-0.04	0.04	0.03	0.07	0.06
32 1	0.00	0.03	-0.02	0.07	-0.06	0.01	0.14	0.03	0.00
33 6	-0.04	0.00	0.02	0.01	-0.08	0.11	0.21	0.12	0.06
34 1	-0.04	0.01	0.01	0.01	-0.08	0.11	0.30	0.10	0.02
35 6	-0.03	0.01	0.00	-0.01	-0.11	0.18	0.19	0.21	0.13
36 1	-0.02	0.01	-0.01	-0.01	-0.11	0.18	0.10	0.24	0.16
37 1	-0.04	0.01	-0.02	-0.02	-0.13	0.23	0.27	0.26	0.15
38 78	0.00	-0.01	-0.01	0.00	0.02	-0.04	-0.03	-0.02	-0.01

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1288.847530

Computed Cartesian coordinates, three lower frequencies PCM energy for **$TS_{II\text{-}VI}$**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.915369	0.909764	0.616069
2	6	0	3.029313	-0.552538	0.545558
3	1	0	3.211223	1.260456	1.524811
4	1	0	2.849070	-0.958448	1.545437
5	1	0	4.035132	-0.859387	0.226520
6	1	0	-3.367121	0.320209	1.494039
7	6	0	1.095797	-2.127869	-0.116367
8	1	0	0.719550	-2.768748	-0.910383
9	1	0	1.094132	-2.570019	0.880108
10	6	0	2.001362	-1.094543	-0.427707
11	1	0	2.217765	-0.926754	-1.483807
12	1	0	1.392807	0.793930	0.291232
13	1	0	-2.552444	-2.179590	0.907607
14	15	0	-2.167046	-1.164931	0.007770
15	6	0	-3.342557	0.224187	0.401728
16	1	0	-2.690609	-1.706260	-1.186529
17	78	0	0.016808	-0.237703	-0.045076
18	6	0	-2.865906	1.530658	-0.244591
19	1	0	-4.358172	-0.020488	0.074045
20	15	0	-1.045689	1.780781	0.041170
21	1	0	-3.011481	1.499095	-1.331421
22	1	0	-3.435176	2.385967	0.134945
23	1	0	-0.712274	2.811512	-0.859344
24	1	0	-0.984542	2.493455	1.257285
25	6	0	3.565686	1.653431	-0.466317
26	1	0	4.634063	1.416700	-0.552228
27	1	0	3.073916	1.418264	-1.415607
28	1	0	3.454426	2.724897	-0.281161

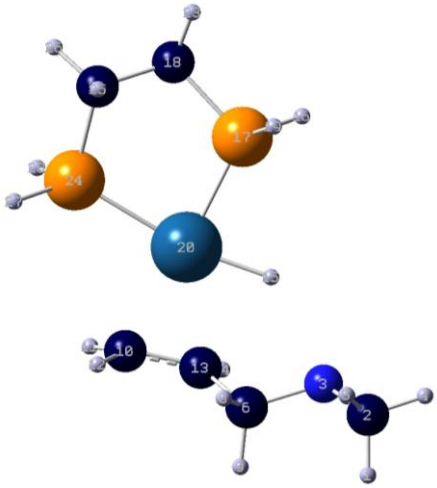
	1	2	3
	A	A	A
Frequencies --	-397.2689	45.1649	61.7174
Red. masses --	1.6597	3.8776	3.2059
Frc consts --	0.1543	0.0047	0.0072
IR Inten --	1591.4404	2.9793	1.4931

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	7	-0.18	-0.02	-0.05	-0.03	-0.01	0.10	-0.03	0.07	-0.04
2	6	0.00	-0.04	-0.01	-0.04	-0.01	0.10	-0.04	0.06	0.15
3	1	-0.40	0.08	0.00	-0.12	-0.02	0.14	-0.05	0.18	-0.08
4	1	0.01	-0.03	0.00	-0.12	-0.01	0.09	-0.12	0.18	0.18
5	1	0.05	0.13	0.03	-0.03	-0.02	0.17	-0.02	0.01	0.25

6	1	-0.01	0.01	0.00	0.19	0.03	0.22	0.09	-0.13	0.09
7	6	-0.04	0.02	0.00	-0.01	0.00	-0.02	0.00	-0.01	0.16
8	1	0.00	-0.01	0.01	0.03	0.02	-0.05	0.05	-0.07	0.18
9	1	-0.01	0.00	-0.01	-0.05	-0.01	-0.03	-0.07	0.07	0.19
10	6	-0.02	0.02	-0.01	0.01	0.01	0.03	0.02	-0.03	0.14
11	1	0.05	-0.05	-0.01	0.08	0.01	0.05	0.08	-0.12	0.13
12	1	0.75	0.12	0.33	-0.02	0.01	-0.04	0.01	0.04	-0.05
13	1	-0.01	0.01	-0.01	0.12	0.00	0.17	-0.02	-0.12	-0.27
14	15	0.01	0.02	0.01	0.01	-0.01	0.11	0.00	0.01	-0.12
15	6	-0.01	0.00	0.00	0.05	-0.01	0.22	0.02	-0.03	0.08
16	1	0.04	0.02	0.00	-0.12	-0.03	0.18	-0.01	0.19	-0.20
17	78	0.01	-0.01	0.00	0.00	0.00	-0.06	0.00	0.00	-0.02
18	6	0.01	0.00	0.00	-0.04	-0.03	0.12	-0.01	0.03	0.17
19	1	-0.01	0.01	-0.01	0.01	-0.02	0.36	0.00	0.00	0.12
20	15	0.03	0.01	0.00	-0.01	0.00	-0.11	0.01	0.00	0.06
21	1	0.01	0.00	0.00	-0.17	-0.07	0.14	-0.09	0.13	0.18
22	1	0.02	0.00	0.00	-0.01	-0.02	0.15	0.02	-0.01	0.29
23	1	-0.09	0.08	0.03	-0.11	-0.08	-0.24	-0.05	0.04	0.08
24	1	-0.06	0.04	-0.01	0.12	0.12	-0.18	0.09	-0.06	0.08
25	6	-0.06	0.02	0.00	0.10	-0.01	0.19	0.00	-0.08	-0.13
26	1	-0.06	0.00	0.18	0.11	0.00	0.32	-0.01	-0.11	-0.08
27	1	0.05	-0.02	-0.03	0.22	-0.01	0.12	0.01	-0.19	-0.11
28	1	-0.09	0.01	0.00	0.07	-0.01	0.17	0.01	-0.06	-0.27

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1095.800035

Computed Cartesian coordinates, three lower frequencies PCM energy for **VI**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.310425	0.875762	0.848151
2	6	0	4.356706	1.423464	0.772651
3	7	0	3.374354	0.781051	-0.096974
4	1	0	4.564127	2.428470	0.394709
5	1	0	3.938482	1.523687	1.780137
6	6	0	3.055866	-0.581904	0.287541
7	1	0	3.709060	0.801525	-1.058255
8	1	0	2.794045	-0.592506	1.351641
9	1	0	3.912191	-1.273269	0.163196
10	6	0	1.002647	-2.090134	-0.044521
11	1	0	0.534371	-2.790399	-0.732705
12	1	0	1.042529	-2.401097	0.999136

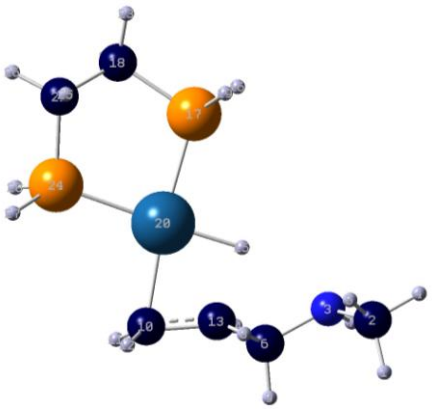
13	6	0	1.926903	-1.158991	-0.529709
14	1	0	2.059700	-1.106685	-1.612008
15	1	0	1.180853	0.845130	-0.466741
16	1	0	-1.115464	2.652317	-1.276627
17	15	0	-1.253263	1.775794	-0.185649
18	6	0	-3.066451	1.383793	-0.117935
19	1	0	-1.024853	2.652137	0.893345
20	78	0	-0.055127	-0.156600	-0.161716
21	6	0	-3.318796	0.159131	0.769657
22	1	0	-3.386932	1.189413	-1.148737
23	1	0	-3.632154	2.250538	0.240514
24	15	0	-2.108907	-1.196020	0.372290
25	1	0	-3.174421	0.411308	1.827227
26	1	0	-4.348561	-0.195590	0.657422
27	1	0	-2.246769	-2.092806	1.450379
28	1	0	-2.745927	-1.939232	-0.643866

	1	2	3
	A	A	A
Frequencies --	35.5301	47.5052	64.3087
Red. masses --	4.1099	4.1419	3.1642
Frc consts --	0.0031	0.0055	0.0077
IR Inten --	2.4078	7.8832	1.1415

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	-0.11	0.02	0.31	0.21	-0.32	-0.06	0.08	0.00	-0.09
2	6	-0.10	0.01	0.21	0.27	-0.20	0.01	0.11	0.04	-0.10
3	7	-0.01	0.00	0.10	0.14	-0.06	0.05	0.04	0.00	0.00
4	1	-0.07	0.01	0.22	0.37	-0.22	0.02	0.14	-0.01	-0.21
5	1	-0.21	0.01	0.16	0.35	-0.17	0.04	0.15	0.16	-0.10
6	6	-0.04	0.00	0.08	0.01	-0.02	0.06	-0.01	0.06	0.15
7	1	0.09	0.00	0.14	0.09	-0.09	0.04	0.01	-0.12	-0.01
8	1	-0.11	0.00	0.06	-0.04	0.01	0.05	-0.07	0.18	0.13
9	1	-0.03	0.00	0.14	-0.04	-0.10	0.11	-0.02	0.02	0.27
10	6	-0.01	-0.01	-0.05	-0.01	0.04	-0.02	0.01	0.01	0.15
11	1	0.02	0.01	-0.08	-0.01	0.06	-0.05	0.06	-0.04	0.17
12	1	-0.05	-0.03	-0.05	-0.03	0.01	-0.03	-0.05	0.09	0.18
13	6	0.01	0.00	0.01	0.01	0.04	0.02	0.02	-0.01	0.14
14	1	0.07	0.01	0.01	0.03	0.06	0.02	0.08	-0.09	0.14
15	1	-0.02	-0.01	-0.13	-0.05	0.06	-0.06	-0.01	0.00	-0.02
16	1	-0.11	-0.08	-0.15	-0.16	-0.04	-0.07	-0.07	0.00	0.01
17	15	0.00	-0.01	-0.07	-0.11	-0.02	-0.05	0.00	0.00	0.02
18	6	0.00	0.01	0.14	-0.09	-0.12	-0.04	-0.01	0.05	0.17
19	1	0.12	0.07	-0.16	-0.16	0.02	-0.07	0.11	-0.01	0.00
20	78	0.00	-0.01	-0.06	-0.01	0.04	-0.01	-0.01	-0.01	-0.02
21	6	0.10	0.05	0.22	-0.02	-0.10	0.01	0.04	-0.02	0.09
22	1	-0.11	-0.03	0.18	-0.08	-0.17	-0.03	-0.12	0.14	0.19
23	1	0.05	0.03	0.17	-0.14	-0.14	-0.07	0.06	0.03	0.30
24	15	0.03	0.02	0.12	0.05	-0.04	0.06	-0.03	-0.01	-0.13
25	1	0.22	0.08	0.19	-0.04	-0.05	0.00	0.14	-0.11	0.10
26	1	0.08	0.05	0.35	0.00	-0.16	0.03	0.02	0.02	0.15
27	1	0.14	0.05	0.16	0.13	0.00	0.10	-0.07	-0.18	-0.27
28	1	-0.08	0.01	0.21	0.08	-0.14	0.10	-0.07	0.18	-0.24

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1095.805258

Computed Cartesian coordinates, three lower frequencies PCM energy for **TS_{VI-VII}**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.389127	0.880338	1.015849
2	6	0	4.467301	1.460551	0.845850
3	7	0	3.536645	0.831129	-0.088087
4	1	0	4.745067	2.446250	0.462322
5	1	0	3.969983	1.605077	1.811104
6	6	0	3.128842	-0.504499	0.301572
7	1	0	3.955507	0.809945	-1.015751
8	1	0	2.811595	-0.481127	1.350172
9	1	0	3.937101	-1.257338	0.228292
10	6	0	1.069995	-2.007818	-0.100448
11	1	0	0.714994	-2.750124	-0.813547
12	1	0	1.177171	-2.370988	0.922150
13	6	0	1.992299	-1.010880	-0.561283
14	1	0	2.196721	-1.009078	-1.634345
15	1	0	1.335145	0.430684	-0.627892
16	1	0	-1.061494	2.613291	-1.417305
17	15	0	-1.188815	1.791067	-0.282236
18	6	0	-3.017954	1.499574	-0.129528
19	1	0	-0.889346	2.715893	0.738436
20	78	0	-0.119848	-0.245701	-0.170221
21	6	0	-3.296615	0.337500	0.833281
22	1	0	-3.386316	1.264617	-1.135541
23	1	0	-3.531029	2.408798	0.200726
24	15	0	-2.161776	-1.090044	0.475588
25	1	0	-3.107390	0.639855	1.870549
26	1	0	-4.343428	0.021920	0.772542
27	1	0	-2.274297	-1.918737	1.608250
28	1	0	-2.851855	-1.864400	-0.479127

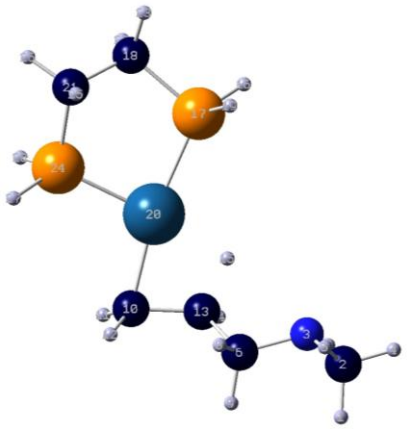
	1	2	3
	A	A	A
Frequencies --	-469.3757	36.7080	52.9970
Red. masses --	1.5125	3.9340	4.2328
Frc consts --	0.1963	0.0031	0.0070
IR Inten --	15.7524	2.6968	3.1326

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	-0.02	-0.02	-0.02	-0.19	0.12	0.29	-0.15	0.31	-0.03
2	6	-0.01	-0.01	-0.01	-0.20	0.08	0.17	-0.21	0.19	-0.09
3	7	-0.03	0.00	-0.01	-0.07	0.02	0.08	-0.11	0.04	-0.09
4	1	-0.01	-0.01	-0.01	-0.20	0.08	0.18	-0.30	0.20	-0.14
5	1	-0.01	-0.01	0.00	-0.31	0.07	0.11	-0.26	0.19	-0.12
6	6	-0.05	0.01	0.00	-0.05	0.01	0.05	0.00	0.02	-0.05
7	1	-0.05	0.00	-0.01	0.03	0.03	0.12	-0.08	0.05	-0.08
8	1	-0.01	-0.01	0.01	-0.10	-0.01	0.03	0.05	0.02	-0.04

9	1	-0.04	0.02	-0.02	-0.02	0.03	0.09	0.05	0.07	-0.08
10	6	0.04	-0.07	0.00	-0.01	-0.02	-0.02	0.01	-0.04	0.03
11	1	-0.09	-0.01	0.00	0.01	-0.02	-0.03	0.01	-0.06	0.05
12	1	-0.06	-0.05	0.02	-0.03	-0.02	-0.02	0.02	-0.02	0.04
13	6	0.00	-0.14	0.04	0.01	-0.03	-0.01	-0.01	-0.04	0.00
14	1	-0.17	0.13	0.02	0.06	-0.04	0.00	-0.04	-0.05	-0.01
15	1	-0.50	0.78	0.12	0.00	-0.04	-0.09	0.02	-0.05	0.03
16	1	0.06	-0.07	-0.02	-0.06	-0.07	-0.12	0.21	0.10	0.17
17	15	-0.01	-0.02	0.01	0.03	0.00	-0.06	0.11	0.02	0.10
18	6	0.00	0.00	0.00	0.04	0.05	0.14	0.09	0.11	-0.01
19	1	0.04	-0.03	0.00	0.16	0.05	-0.15	0.12	-0.07	0.18
20	78	0.01	0.02	0.00	0.00	-0.02	-0.05	0.01	-0.04	0.02
21	6	0.00	0.00	0.00	0.11	0.08	0.19	-0.01	0.07	-0.09
22	1	0.00	0.00	0.00	-0.07	0.04	0.18	0.13	0.19	-0.04
23	1	0.00	0.00	0.00	0.10	0.07	0.17	0.12	0.12	0.02
24	15	-0.02	-0.03	0.00	0.03	0.04	0.09	-0.06	0.03	-0.10
25	1	0.00	0.00	0.00	0.23	0.09	0.17	-0.05	0.00	-0.06
26	1	0.00	0.01	0.00	0.09	0.11	0.32	-0.02	0.12	-0.16
27	1	-0.09	-0.01	0.01	0.09	0.04	0.10	-0.18	-0.03	-0.15
28	1	-0.08	-0.01	0.03	-0.09	0.07	0.15	-0.04	0.12	-0.19

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1095.800775

Computed Cartesian coordinates, three lower frequencies PCM energy for **VII**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.580134	0.650933	1.054389
2	6	0	4.734826	1.335309	0.872183
3	7	0	3.755766	0.824027	-0.083906
4	1	0	5.131946	2.285216	0.503509
5	1	0	4.239409	1.529858	1.829837
6	6	0	3.206226	-0.465447	0.286226
7	1	0	4.188451	0.764483	-1.003632
8	1	0	2.853918	-0.404252	1.322866
9	1	0	3.934574	-1.296904	0.244279
10	6	0	1.093908	-1.892557	-0.153348
11	1	0	0.828445	-2.665147	-0.875286
12	1	0	1.275055	-2.292341	0.846377
13	6	0	2.035152	-0.844824	-0.616954
14	1	0	2.309421	-0.944636	-1.672566
15	1	0	1.482915	0.269289	-0.697672
16	1	0	-1.193540	2.642162	-1.423260
17	15	0	-1.260987	1.812757	-0.286885

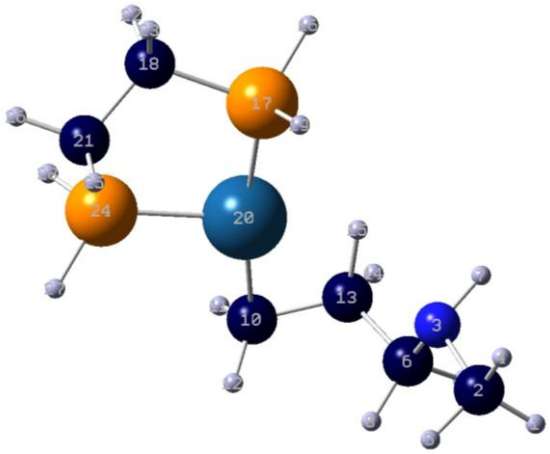
18	6	0	-3.079544	1.472354	-0.092044
19	1	0	-0.975005	2.754366	0.723242
20	78	0	-0.172860	-0.251917	-0.172791
21	6	0	-3.305537	0.302346	0.875601
22	1	0	-3.466212	1.229120	-1.089070
23	1	0	-3.610520	2.365050	0.253796
24	15	0	-2.142552	-1.092555	0.493654
25	1	0	-3.101982	0.608155	1.909194
26	1	0	-4.343258	-0.046150	0.837450
27	1	0	-2.185622	-1.925799	1.626934
28	1	0	-2.812506	-1.888176	-0.456839

	1	2	3
	A	A	A
Frequencies --	33.9778	50.5432	64.9154
Red. masses --	4.0501	4.2832	3.0936
Frc consts --	0.0028	0.0064	0.0077
IR Inten --	2.6399	1.9560	0.7863

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	0.20	-0.19	-0.22	-0.08	0.26	-0.12	-0.07	-0.04	0.02
2	6	0.23	-0.12	-0.14	-0.15	0.17	-0.12	-0.11	-0.06	0.10
3	7	0.11	-0.04	-0.06	-0.11	0.05	-0.10	-0.07	0.00	0.02
4	1	0.27	-0.15	-0.17	-0.26	0.20	-0.15	-0.16	0.01	0.22
5	1	0.33	-0.09	-0.10	-0.16	0.14	-0.12	-0.13	-0.22	0.11
6	6	0.05	0.00	-0.02	0.00	0.00	-0.07	0.00	-0.07	-0.14
7	1	0.03	-0.07	-0.10	-0.11	0.07	-0.10	-0.05	0.13	0.02
8	1	0.10	0.03	-0.01	0.05	-0.02	-0.05	0.04	-0.22	-0.12
9	1	0.01	-0.05	-0.04	0.06	0.05	-0.11	0.03	-0.04	-0.27
10	6	0.01	0.04	0.03	0.00	-0.05	0.01	-0.02	-0.02	-0.14
11	1	0.01	0.04	0.03	-0.01	-0.05	0.02	-0.09	0.04	-0.17
12	1	0.02	0.04	0.03	0.00	-0.04	0.01	0.04	-0.08	-0.17
13	6	0.00	0.05	0.02	-0.02	-0.05	-0.01	-0.03	-0.01	-0.13
14	1	-0.04	0.07	0.01	-0.06	-0.03	-0.03	-0.07	0.04	-0.14
15	1	0.01	0.05	0.09	-0.02	-0.03	0.01	-0.01	0.01	-0.06
16	1	0.01	0.05	0.07	0.25	0.13	0.19	0.06	-0.01	-0.01
17	15	-0.06	0.00	0.04	0.11	0.02	0.11	-0.01	0.00	-0.01
18	6	-0.06	-0.08	-0.13	0.08	0.09	-0.07	-0.01	-0.07	-0.16
19	1	-0.18	-0.03	0.10	0.07	-0.09	0.23	-0.13	0.01	0.01
20	78	-0.01	0.03	0.04	0.01	-0.03	0.04	0.01	0.02	0.02
21	6	-0.11	-0.10	-0.17	-0.05	0.05	-0.15	-0.04	0.00	-0.09
22	1	0.04	-0.08	-0.17	0.16	0.15	-0.12	0.10	-0.16	-0.18
23	1	-0.13	-0.10	-0.17	0.08	0.09	-0.08	-0.09	-0.07	-0.28
24	15	-0.01	-0.04	-0.07	-0.06	0.02	-0.10	0.05	0.01	0.12
25	1	-0.21	-0.10	-0.15	-0.15	-0.01	-0.12	-0.14	0.09	-0.10
26	1	-0.09	-0.14	-0.27	-0.06	0.08	-0.27	-0.02	-0.05	-0.14
27	1	-0.05	-0.03	-0.07	-0.18	-0.01	-0.12	0.10	0.17	0.24
28	1	0.09	-0.09	-0.11	-0.01	0.07	-0.17	0.10	-0.17	0.24

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1095.805369

Computed Cartesian coordinates, three lower frequencies PCM energy for **$TS_{VII-VIII}$**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.975715	1.570062	0.971984
2	6	0	3.908874	1.696432	1.218566
3	7	0	3.001296	1.095387	0.242757
4	1	0	3.695854	2.766673	1.293443
5	1	0	3.729534	1.248632	2.201921
6	6	0	3.243019	-0.323893	0.031338
7	1	0	3.098492	1.591671	-0.641926
8	1	0	3.314441	-0.794535	1.017705
9	1	0	4.192273	-0.533035	-0.491438
10	6	0	1.191462	-1.913555	-0.011572
11	1	0	0.878324	-2.813327	-0.543717
12	1	0	1.466513	-2.117304	1.024472
13	6	0	2.098939	-0.990898	-0.756800
14	1	0	2.383799	-1.384219	-1.738835
15	1	0	1.478827	-0.027274	-1.154093
16	1	0	-1.354538	2.285157	-1.889371
17	15	0	-1.246045	1.683177	-0.619828
18	6	0	-3.016374	1.388211	-0.127209
19	1	0	-0.857464	2.800173	0.148511
20	78	0	-0.099098	-0.317132	-0.229226
21	6	0	-3.086678	0.427663	1.068311
22	1	0	-3.521560	0.956016	-0.999375
23	1	0	-3.520891	2.330943	0.107368
24	15	0	-1.944991	-1.011840	0.814347
25	1	0	-2.760536	0.928247	1.988181
26	1	0	-4.111110	0.076502	1.232913
27	1	0	-1.832491	-1.616304	2.080459
28	1	0	-2.704563	-1.973329	0.118524

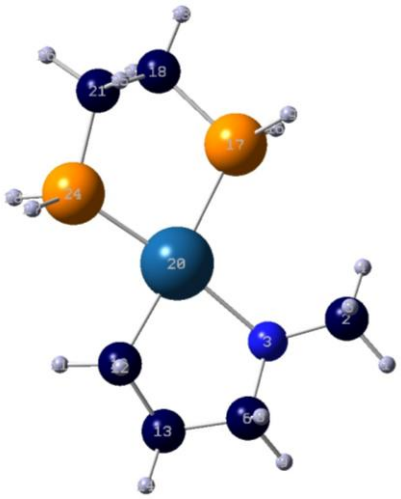
	1	2	3
	A	A	A
Frequencies --	-75.0788	38.2724	55.6786
Red. masses --	2.3919	3.8499	4.0033
Frc consts --	0.0079	0.0033	0.0073
IR Inten --	0.6585	2.7506	0.9151

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	0.14	-0.13	0.13	0.20	-0.14	-0.16	0.08	-0.17	0.26
2	6	0.12	0.06	-0.05	0.23	-0.14	-0.04	0.07	-0.09	0.18
3	7	0.17	0.08	-0.11	0.12	-0.06	0.02	0.09	0.00	0.10
4	1	0.27	0.10	-0.21	0.26	-0.14	0.06	0.14	-0.08	0.20
5	1	-0.10	0.21	-0.02	0.32	-0.20	-0.05	-0.04	-0.11	0.16
6	6	-0.04	0.01	0.14	0.07	-0.05	-0.09	0.01	-0.01	0.08
7	1	0.40	-0.06	-0.16	0.04	0.00	0.04	0.19	0.02	0.12

8	1	-0.27	0.14	0.22	0.16	-0.11	-0.13	-0.06	-0.03	0.07
9	1	0.01	-0.24	0.33	0.02	-0.03	-0.20	0.02	-0.06	0.12
10	6	0.00	-0.02	-0.07	0.00	0.04	0.02	0.00	0.02	-0.03
11	1	0.02	0.03	-0.16	-0.02	0.03	0.05	0.01	0.04	-0.07
12	1	-0.04	-0.11	-0.08	0.03	0.06	0.02	-0.02	-0.02	-0.04
13	6	-0.01	0.07	0.05	-0.01	0.02	-0.03	0.01	0.05	0.02
14	1	0.00	0.21	0.00	-0.09	0.01	-0.05	0.03	0.10	0.01
15	1	-0.02	0.14	0.17	0.00	0.05	0.04	0.02	0.09	0.06
16	1	0.03	0.01	0.03	-0.03	-0.02	-0.02	-0.22	-0.20	-0.18
17	15	0.01	0.00	0.03	-0.08	-0.01	-0.02	-0.09	-0.05	-0.12
18	6	0.00	0.01	0.01	-0.09	-0.13	-0.14	-0.04	-0.05	0.07
19	1	0.01	-0.01	0.04	-0.20	0.01	0.01	-0.06	0.05	-0.28
20	78	-0.01	-0.01	0.00	0.00	0.04	0.03	-0.01	0.01	-0.04
21	6	-0.02	-0.01	-0.01	-0.11	-0.10	-0.12	0.09	0.04	0.15
22	1	0.00	0.03	-0.01	0.01	-0.19	-0.17	-0.12	-0.12	0.15
23	1	0.00	0.01	0.02	-0.18	-0.16	-0.20	-0.03	-0.04	0.05
24	15	-0.04	-0.02	-0.03	0.00	-0.03	-0.01	0.06	0.03	0.11
25	1	-0.02	-0.03	0.00	-0.20	-0.05	-0.11	0.19	0.10	0.08
26	1	-0.03	0.00	-0.02	-0.10	-0.16	-0.18	0.11	0.05	0.28
27	1	-0.05	-0.04	-0.04	-0.01	0.03	0.03	0.19	0.09	0.13
28	1	-0.05	0.00	-0.05	0.10	-0.12	0.01	0.00	-0.01	0.23

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1095.799218

Computed Cartesian coordinates, three lower frequencies PCM energy for **VIII**



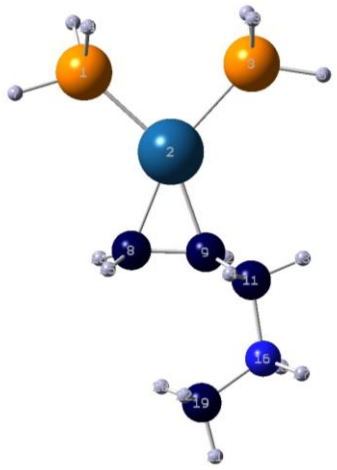
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.085807	2.698127	0.324730
2	6	0	2.084147	2.275336	0.467333
3	7	0	1.975785	0.959996	-0.203401
4	1	0	1.347152	2.965585	0.051127
5	1	0	1.898121	2.150755	1.536000
6	6	0	3.107471	0.053236	0.168904
7	1	0	2.052428	1.121729	-1.210693
8	1	0	3.148622	0.028478	1.263599
9	1	0	4.049845	0.477039	-0.201177
10	6	0	1.423677	-1.755413	0.119699
11	1	0	1.073583	-2.643686	-0.418862
12	1	0	1.474088	-2.017987	1.187110
13	6	0	2.801703	-1.321362	-0.386281
14	1	0	3.582692	-2.030722	-0.079949

15	1	0	2.820557	-1.291616	-1.484487
16	1	0	-1.453411	2.651494	-1.107350
17	15	0	-1.447681	1.635962	-0.125768
18	6	0	-3.118986	0.845457	-0.350422
19	1	0	-1.629920	2.444571	1.019132
20	78	0	0.136116	-0.124098	-0.026077
21	6	0	-3.186386	-0.478287	0.421135
22	1	0	-3.247638	0.672713	-1.425816
23	1	0	-3.917431	1.523021	-0.031658
24	15	0	-1.651661	-1.466592	0.106871
25	1	0	-3.231842	-0.295687	1.501686
26	1	0	-4.079157	-1.051234	0.148387
27	1	0	-1.664243	-2.482743	1.081460
28	1	0	-1.936456	-2.214501	-1.054189

		1			2			3		
		A			A			A		
Frequencies --		49.6627			60.2636			97.3392		
Red. masses --		3.2130			3.3442			2.8605		
Frc consts --		0.0047			0.0072			0.0160		
IR Inten --		1.1685			1.9144			1.4852		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	1	-0.03	0.04	-0.08	-0.06	-0.02	0.36	-0.11	0.06	0.00
2	6	-0.05	0.06	-0.12	-0.06	-0.05	0.25	-0.11	0.05	-0.04
3	7	0.00	-0.01	0.01	0.00	0.02	0.09	-0.04	0.02	0.00
4	1	-0.01	0.02	-0.26	-0.04	-0.01	0.29	-0.10	0.01	-0.11
5	1	-0.14	0.17	-0.12	-0.12	-0.19	0.22	-0.17	0.08	-0.04
6	6	-0.03	0.02	0.19	0.00	0.00	0.04	-0.04	0.05	0.09
7	1	0.09	-0.12	0.00	0.04	0.14	0.11	0.01	-0.02	0.00
8	1	-0.17	0.06	0.20	0.00	-0.05	0.04	-0.17	-0.01	0.09
9	1	0.01	0.02	0.30	0.00	0.03	0.06	-0.02	0.10	0.21
10	6	-0.01	-0.01	0.01	0.01	0.00	-0.03	0.02	-0.03	-0.20
11	1	0.05	0.01	-0.07	0.01	0.01	-0.06	0.06	0.08	-0.40
12	1	-0.13	-0.06	0.01	0.01	-0.03	-0.04	-0.03	-0.24	-0.25
13	6	0.06	0.00	0.19	0.00	0.03	-0.03	0.06	0.07	-0.03
14	1	0.03	0.02	0.32	0.01	0.02	-0.06	0.06	0.08	-0.02
15	1	0.21	-0.03	0.20	-0.01	0.08	-0.02	0.16	0.16	-0.03
16	1	-0.05	0.02	0.07	-0.03	-0.15	-0.29	0.15	0.05	0.08
17	15	0.01	0.01	0.05	0.01	0.00	-0.14	0.05	0.01	0.04
18	6	-0.02	0.04	0.18	-0.02	-0.01	0.07	0.06	0.05	-0.11
19	1	0.13	-0.01	0.08	0.08	0.18	-0.25	-0.02	-0.03	0.06
20	78	0.00	-0.01	-0.04	0.00	-0.01	-0.03	0.00	-0.02	0.00
21	6	0.03	0.01	0.13	0.04	0.05	0.18	-0.03	0.08	-0.06
22	1	-0.12	0.09	0.18	-0.12	-0.09	0.10	0.17	0.01	-0.11
23	1	0.02	0.04	0.28	0.02	0.02	0.10	0.04	0.07	-0.21
24	15	-0.01	0.00	-0.06	0.00	0.01	0.08	-0.03	0.01	0.12
25	1	0.13	-0.04	0.14	0.17	0.13	0.17	-0.11	0.13	-0.07
26	1	0.00	0.04	0.18	0.00	0.04	0.32	-0.02	0.09	-0.10
27	1	0.03	-0.08	-0.15	0.06	0.03	0.10	-0.07	0.16	0.27
28	1	-0.10	0.11	-0.11	-0.12	-0.01	0.11	-0.02	-0.16	0.22

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1095.857481

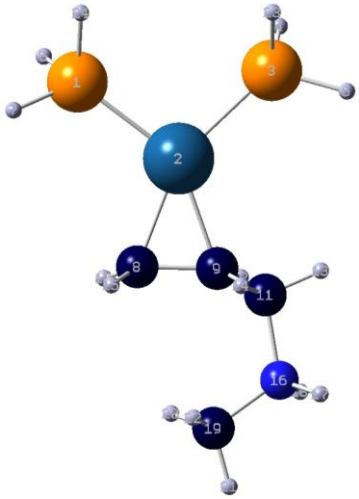
Computed Cartesian coordinates and PCM energy for **II(PH_3)** with a P-Pt-P angle fixed at 90°



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.377431	-1.340773	0.350592
2	78	0	-0.487740	-0.079526	-0.100571
3	15	0	-1.749034	1.871834	0.071635
4	1	0	-2.803748	2.043564	-0.853728
5	1	0	-3.445000	-1.294872	-0.574171
6	1	0	-1.199300	3.170944	-0.039700
7	1	0	-2.302775	-2.743375	0.496349
8	6	0	1.160480	-1.298613	-0.423762
9	6	0	1.543345	0.096382	-0.587941
10	1	0	1.085282	-1.928706	-1.310379
11	6	0	2.375761	0.806212	0.426572
12	1	0	1.671760	0.474393	-1.606978
13	1	0	2.212053	1.888284	0.427711
14	1	0	2.236878	0.420339	1.440159
15	1	0	1.480093	-1.842655	0.467980
16	7	0	3.895906	0.655677	0.140784
17	1	0	4.416046	1.304605	0.740327
18	1	0	4.057863	0.965859	-0.822681
19	6	0	4.446286	-0.722027	0.307839
20	1	0	3.894503	-1.393557	-0.349306
21	1	0	5.507276	-0.717484	0.050235
22	1	0	4.313157	-1.024259	1.347767
23	1	0	-2.493015	2.093550	1.253608
24	1	0	-3.116938	-1.060971	1.522182

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1018.410425

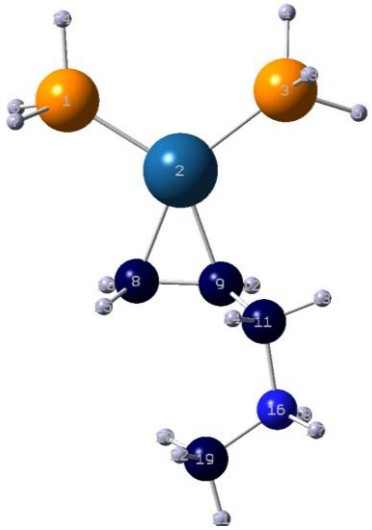
Computed Cartesian coordinates and PCM energy for **II(PH$_3$)** with a P-Pt-P angle fixed at 100°



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.310635	-1.454225	0.336010
2	78	0	-0.529502	-0.058589	-0.091191
3	15	0	-1.578926	1.995471	0.078989
4	1	0	-2.458422	2.374568	-0.960260
5	1	0	-3.076925	-1.885190	-0.769474
6	1	0	-0.835357	3.198231	0.133829
7	1	0	-2.052996	-2.718462	0.909386
8	6	0	1.104292	-1.306857	-0.445757
9	6	0	1.510844	0.080690	-0.592836
10	1	0	1.011441	-1.921504	-1.341349
11	6	0	2.356786	0.763249	0.428840
12	1	0	1.638449	0.470314	-1.607357
13	1	0	2.210273	1.847616	0.446387
14	1	0	2.213509	0.364899	1.436990
15	1	0	1.417090	-1.869253	0.436748
16	7	0	3.874685	0.594313	0.139255
17	1	0	4.404371	1.221626	0.753345
18	1	0	4.042978	0.922909	-0.816983
19	6	0	4.403407	-0.795029	0.277326
20	1	0	3.841765	-1.444209	-0.393807
21	1	0	5.464462	-0.801413	0.020062
22	1	0	4.265163	-1.116853	1.310703
23	1	0	-2.437586	2.268640	1.168763
24	1	0	-3.378427	-1.073190	1.180689

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1018.412559

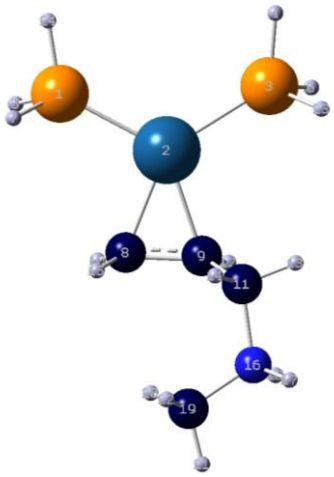
Computed Cartesian coordinates and PCM energy for **II(PH_3)** with a P-Pt-P angle fixed at 110°



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.238880	-1.567913	0.304815
2	78	0	-0.572993	-0.033987	-0.078394
3	15	0	-1.417246	2.102929	0.083645
4	1	0	-2.718163	2.431443	-0.361534
5	1	0	-2.401605	-2.563523	-0.682735
6	1	0	-0.735150	3.152899	-0.574819
7	1	0	-2.069879	-2.412191	1.423942
8	6	0	1.049289	-1.307108	-0.457388
9	6	0	1.474242	0.072633	-0.598866
10	1	0	0.934774	-1.915671	-1.354422
11	6	0	2.347446	0.730039	0.416702
12	1	0	1.591831	0.470913	-1.611060
13	1	0	2.231422	1.818016	0.436777
14	1	0	2.203370	0.334390	1.425736
15	1	0	1.363315	-1.876986	0.419749
16	7	0	3.858158	0.522017	0.111659
17	1	0	4.409078	1.147206	0.709059
18	1	0	4.021392	0.831717	-0.851824
19	6	0	4.359087	-0.875967	0.265677
20	1	0	3.778769	-1.523389	-0.391188
21	1	0	5.417381	-0.908215	-0.000910
22	1	0	4.223996	-1.179520	1.305001
23	1	0	-1.497414	2.706201	1.360104
24	1	0	-3.605288	-1.259276	0.497579

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1018.411095

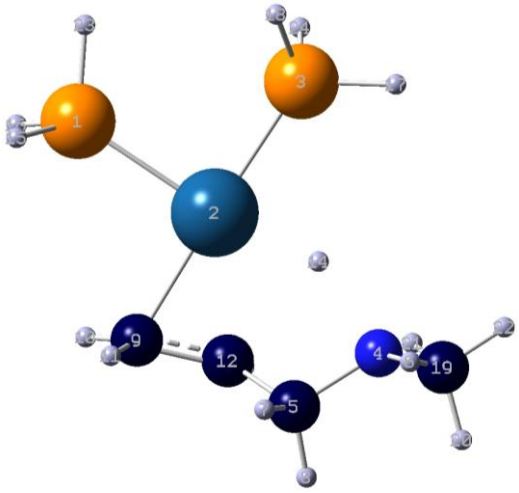
Computed Cartesian coordinates and PCM energy for **II(PH_3)** with a P-Pt-P angle fixed at 120°



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.174466	-1.655427	-0.294469
2	78	0	0.617685	-0.010352	0.065122
3	15	0	1.227866	2.201342	-0.080643
4	1	0	2.473682	2.702762	-0.525836
5	1	0	2.381071	-2.537100	0.788578
6	1	0	1.151648	2.936351	1.124184
7	1	0	1.829556	-2.610460	-1.275633
8	6	0	-0.986783	-1.303932	0.506681
9	6	0	-1.440982	0.065451	0.605556
10	1	0	-0.845753	-1.877070	1.422910
11	6	0	-2.327794	0.670657	-0.430813
12	1	0	-1.560003	0.494642	1.604423
13	1	0	-2.232662	1.759181	-0.489944
14	1	0	-2.174290	0.243654	-1.425534
15	1	0	-1.291361	-1.910250	-0.348875
16	7	0	-3.833509	0.444891	-0.118316
17	1	0	-4.395135	1.041572	-0.734718
18	1	0	-4.003437	0.780991	0.835142
19	6	0	-4.310361	-0.965707	-0.229937
20	1	0	-3.718747	-1.583564	0.445134
21	1	0	-5.367554	-1.007872	0.039582
22	1	0	-4.171801	-1.297470	-1.260126
23	1	0	0.412387	3.048265	-0.868779
24	1	0	3.528102	-1.477980	-0.664037

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1018.407615

Computed Cartesian coordinates, three lower frequencies PCM energy for **$TS_{II\text{-}VI}(PH_3)$** with a P-Pt-P angle fixed at 90°



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.634237	-0.687690	0.047076
2	78	0	-0.310361	-0.058485	-0.025507
3	15	0	-0.908182	2.157514	0.044141
4	7	0	2.812130	0.401918	0.580927
5	6	0	2.577172	-1.042689	0.514093
6	1	0	3.211377	0.667222	1.478497
7	1	0	2.325522	-1.397849	1.517883
8	1	0	3.472624	-1.583396	0.174298
9	6	0	0.330654	-2.140744	-0.108985
10	1	0	-0.196361	-2.674184	-0.897342
11	1	0	0.249584	-2.575403	0.887475
12	6	0	1.435341	-1.335620	-0.438789
13	1	0	1.658393	-1.207892	-1.499097
14	1	0	1.228191	0.617506	0.279086
15	1	0	-3.047264	-1.524628	1.103577
16	1	0	-3.188098	-1.400076	-1.036760
17	1	0	0.037443	3.172217	0.285484
18	1	0	-1.886582	2.522873	0.991607
19	6	0	3.588377	0.972238	-0.522376
20	1	0	4.565833	0.486237	-0.643372
21	1	0	3.027120	0.869570	-1.456741
22	1	0	3.745140	2.037749	-0.336228
23	1	0	-3.621437	0.313527	0.170131
24	1	0	-1.511244	2.658488	-1.127402

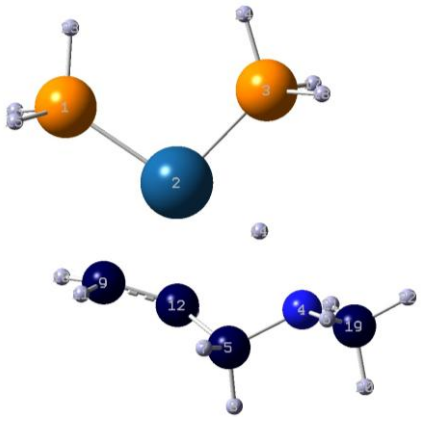
	1	2	3
	A	A	A
Frequencies --	-157.4906	36.8460	48.7861
Red. masses --	3.2889	1.1357	2.4125
Frc consts --	0.0481	0.0009	0.0034
IR Inten --	290.9877	0.2837	0.9955

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	15	0.00	0.06	0.03	0.00	0.00	0.04	0.01	-0.03	0.15
2	78	0.03	-0.02	0.00	0.00	0.00	-0.01	-0.01	0.00	-0.02
3	15	0.09	0.00	-0.01	0.00	0.00	-0.01	0.00	0.01	-0.07
4	7	-0.28	0.06	-0.04	0.00	-0.02	0.02	0.00	-0.02	0.06
5	6	-0.05	-0.01	-0.03	0.00	-0.01	-0.01	-0.02	-0.02	0.00
6	1	-0.50	0.19	0.03	-0.01	-0.04	0.03	-0.06	-0.06	0.10
7	1	-0.01	-0.04	-0.03	-0.01	-0.04	-0.02	-0.05	-0.05	-0.02
8	1	0.05	0.17	-0.02	0.00	-0.01	-0.02	-0.02	-0.01	0.00
9	6	-0.06	0.00	0.00	0.00	0.00	-0.05	0.00	0.01	-0.09

10	1	-0.05	-0.03	0.02	0.00	0.02	-0.06	0.01	0.05	-0.12
11	1	-0.04	0.00	0.00	0.00	-0.02	-0.06	-0.01	-0.04	-0.11
12	6	-0.04	-0.02	-0.03	0.00	0.01	-0.03	0.00	0.02	-0.04
13	1	-0.01	-0.10	-0.04	0.00	0.03	-0.02	0.03	0.07	-0.03
14	1	0.40	-0.05	0.17	0.00	-0.01	0.01	-0.02	0.00	-0.03
15	1	-0.02	0.02	-0.01	-0.04	0.45	0.39	0.18	-0.31	-0.01
16	1	0.03	0.08	0.01	0.09	-0.50	0.32	-0.16	0.26	0.05
17	1	0.01	0.10	-0.07	-0.02	-0.01	0.08	-0.03	-0.01	0.12
18	1	0.11	0.00	0.02	-0.08	0.00	-0.09	-0.17	0.01	-0.24
19	6	-0.16	0.12	0.06	0.01	0.01	0.05	0.09	0.00	0.14
20	1	-0.09	0.22	0.29	0.01	0.01	0.05	0.10	0.01	0.21
21	1	0.01	-0.04	-0.02	0.02	0.03	0.04	0.17	0.02	0.09
22	1	-0.33	0.15	0.02	0.01	0.01	0.07	0.07	0.00	0.18
23	1	-0.04	0.02	0.04	-0.04	0.02	-0.46	0.04	-0.05	0.57
24	1	0.01	-0.03	0.02	0.09	0.01	-0.05	0.22	0.03	-0.17

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1018.383717

Computed Cartesian coordinates, three lower frequencies PCM energy for **$TS_{II\text{-}VI}(PH_3)$** with a P-Pt-P angle fixed at 100°



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.650429	-0.645016	0.049044
2	78	0	-0.353697	-0.016575	-0.022963
3	15	0	-0.562466	2.257592	0.041003
4	7	0	2.801604	0.213327	0.579746
5	6	0	2.463570	-1.210804	0.506567
6	1	0	3.216696	0.445098	1.479689
7	1	0	2.187877	-1.551639	1.508967
8	1	0	3.318750	-1.811388	0.164195
9	6	0	0.151551	-2.151943	-0.117689
10	1	0	-0.408590	-2.649011	-0.906813
11	1	0	0.046531	-2.583003	0.878020
12	6	0	1.304216	-1.419367	-0.447039
13	1	0	1.533134	-1.301011	-1.507026
14	1	0	1.252848	0.542272	0.278822
15	1	0	-3.040687	-1.496732	1.102086
16	1	0	-3.175668	-1.372742	-1.038507
17	1	0	-0.112790	2.958235	-1.095378
18	1	0	0.122498	2.961033	1.050640
19	6	0	3.622969	0.729052	-0.518641
20	1	0	4.565941	0.177839	-0.631215
21	1	0	3.063097	0.662303	-1.457081
22	1	0	3.850386	1.781738	-0.332119

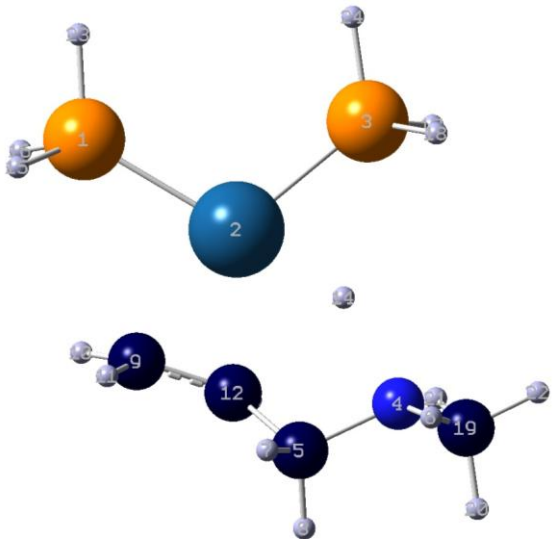
23	1	0	-3.661171	0.332184	0.167507
24	1	0	-1.842121	2.834102	0.181210

	1	2	3
	A	A	A
Frequencies --	-204.4253	49.7712	62.6671
Red. masses --	2.7881	2.8535	1.0801
Frc consts --	0.0686	0.0042	0.0025
IR Inten --	487.4481	2.1101	0.7102

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	15	0.01	0.04	0.03	0.01	-0.02	0.16	0.00	0.00	0.04
2	78	0.02	-0.02	0.00	0.00	0.01	-0.02	0.00	0.00	-0.01
3	15	0.07	-0.02	-0.01	-0.03	0.00	-0.06	0.01	0.00	0.00
4	7	-0.27	0.07	-0.05	0.00	-0.04	0.08	0.00	0.00	0.01
5	6	-0.05	-0.02	-0.03	-0.02	-0.03	-0.01	0.00	0.00	-0.01
6	1	-0.49	0.23	0.02	-0.08	-0.09	0.13	-0.01	-0.01	0.02
7	1	-0.02	-0.04	-0.03	-0.06	-0.08	-0.04	0.00	-0.01	-0.02
8	1	0.07	0.15	0.00	-0.02	-0.03	-0.01	0.00	0.00	-0.02
9	6	-0.05	0.01	0.00	0.00	0.01	-0.13	0.00	0.00	-0.02
10	1	-0.05	-0.02	0.01	0.01	0.07	-0.17	0.00	0.01	-0.03
11	1	-0.04	0.00	0.00	-0.02	-0.05	-0.16	0.01	-0.01	-0.03
12	6	-0.04	0.00	-0.03	0.01	0.03	-0.06	0.00	0.01	-0.01
13	1	0.00	-0.09	-0.03	0.04	0.08	-0.05	0.00	0.02	-0.01
14	1	0.52	-0.08	0.22	-0.02	-0.01	-0.02	0.00	0.00	0.00
15	1	-0.02	0.00	-0.01	0.13	0.07	0.27	-0.02	0.26	0.24
16	1	0.05	0.05	0.00	-0.08	-0.12	0.27	0.04	-0.28	0.20
17	1	-0.01	0.05	-0.01	-0.34	-0.07	-0.23	0.45	0.06	0.21
18	1	0.04	0.08	-0.04	0.22	0.09	-0.29	-0.36	-0.08	0.30
19	6	-0.12	0.09	0.04	0.10	0.00	0.18	0.01	0.01	0.02
20	1	-0.07	0.15	0.29	0.11	-0.01	0.24	0.01	0.02	0.03
21	1	0.04	-0.05	-0.03	0.19	0.04	0.12	0.02	0.02	0.02
22	1	-0.25	0.12	0.01	0.09	-0.01	0.24	0.00	0.01	0.04
23	1	-0.05	-0.01	0.02	0.01	-0.02	0.17	-0.01	0.02	-0.24
24	1	0.06	-0.04	0.03	-0.01	-0.01	0.24	-0.03	0.02	-0.45

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1018.385484

Computed Cartesian coordinates, three lower frequencies PCM energy for **$TS_{II\text{-}VI}(PH_3)$** with a P-Pt-P angle fixed at 110°



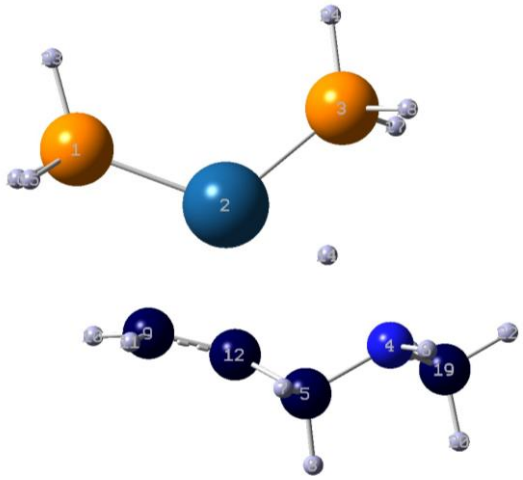
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.672340	-0.611218	0.033393
2	78	0	-0.389286	0.042712	-0.016224
3	15	0	-0.228063	2.313849	0.041683
4	7	0	2.795270	0.012915	0.568587
5	6	0	2.337467	-1.376999	0.502317
6	1	0	3.233283	0.209315	1.466111
7	1	0	2.036059	-1.689097	1.506647
8	1	0	3.137431	-2.050393	0.161083
9	6	0	-0.032924	-2.145551	-0.112732
10	1	0	-0.628844	-2.603554	-0.899350
11	1	0	-0.161603	-2.565837	0.884680
12	6	0	1.163703	-1.496357	-0.447814
13	1	0	1.394462	-1.389810	-1.508429
14	1	0	1.262597	0.458353	0.273421
15	1	0	-3.015519	-1.515479	1.058130
16	1	0	-3.146672	-1.335860	-1.078921
17	1	0	0.412076	2.905072	-1.064695
18	1	0	0.525458	2.873020	1.091439
19	6	0	3.657087	0.449918	-0.533491
20	1	0	4.547428	-0.183042	-0.644856
21	1	0	3.092963	0.429269	-1.471535
22	1	0	3.977824	1.478850	-0.351596
23	1	0	-3.739610	0.300798	0.173502
24	1	0	-1.375870	3.130890	0.113892

	1	2	3
	A	A	A
Frequencies --	-176.7704	49.5687	89.0287
Red. masses --	3.0132	3.7927	2.1742
Frc consts --	0.0555	0.0055	0.0102
IR Inten --	360.3334	2.3332	8.2522

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	15	0.01	0.04	0.03	0.01	-0.02	0.20	0.00	-0.01	-0.05
2	78	0.02	-0.02	0.00	0.00	0.01	-0.03	0.00	0.01	0.04
3	15	0.08	-0.03	-0.01	-0.04	0.01	-0.06	-0.02	0.01	-0.12
4	7	-0.27	0.08	-0.04	-0.01	-0.04	0.10	0.02	-0.07	0.03
5	6	-0.05	-0.02	-0.03	-0.03	-0.03	-0.01	0.02	-0.06	-0.10
6	1	-0.48	0.26	0.03	-0.10	-0.09	0.15	0.05	-0.17	0.03
7	1	-0.02	-0.05	-0.03	-0.09	-0.08	-0.04	0.07	-0.17	-0.12
8	1	0.07	0.15	-0.01	-0.03	-0.03	0.00	0.01	-0.03	-0.20
9	6	-0.06	0.01	0.00	0.00	0.01	-0.17	-0.01	0.00	-0.04
10	1	-0.06	-0.01	0.01	0.02	0.08	-0.22	-0.04	0.04	-0.03
11	1	-0.04	0.01	0.00	-0.02	-0.07	-0.20	0.03	-0.03	-0.05
12	6	-0.05	-0.01	-0.04	0.02	0.04	-0.07	-0.02	0.01	-0.06
13	1	-0.02	-0.09	-0.04	0.06	0.11	-0.06	-0.06	0.05	-0.07
14	1	0.46	-0.10	0.19	-0.02	0.00	-0.04	-0.03	-0.03	0.09
15	1	-0.01	0.00	-0.01	0.16	0.04	0.30	0.03	-0.32	-0.31
16	1	0.03	0.05	0.01	-0.12	-0.10	0.31	-0.03	0.32	-0.26
17	1	0.01	0.04	-0.02	-0.16	0.00	-0.13	-0.23	-0.09	-0.30
18	1	0.08	0.05	-0.05	0.06	0.04	-0.14	0.17	0.12	-0.31
19	6	-0.13	0.12	0.05	0.13	-0.02	0.21	-0.03	0.06	0.04
20	1	-0.06	0.19	0.29	0.14	-0.03	0.30	-0.03	0.08	-0.07
21	1	0.01	-0.04	-0.02	0.24	0.00	0.14	-0.07	0.16	0.06
22	1	-0.28	0.17	0.03	0.11	-0.03	0.27	-0.03	0.04	0.14
23	1	-0.03	-0.01	0.03	0.02	-0.03	0.28	0.00	-0.05	0.25
24	1	0.07	-0.05	0.04	-0.04	-0.01	0.04	-0.01	0.00	0.02

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1018.382788

Computed Cartesian coordinates, three lower frequencies PCM energy for **$TS_{II\text{-}VI}(PH_3)$** with a P-Pt-P angle fixed at 120°



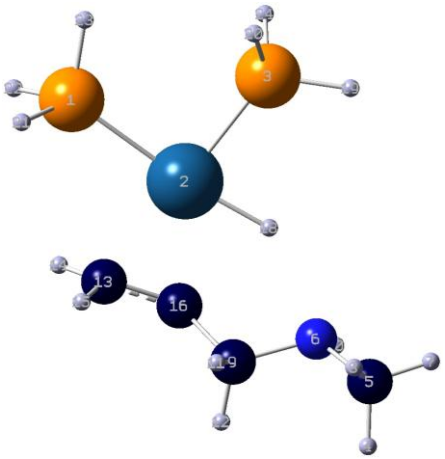
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.701126	-0.570315	-0.018011
2	78	0	0.423142	0.107658	0.007191
3	15	0	-0.106261	2.321787	-0.035972
4	7	0	-2.791088	-0.188266	-0.564212
5	6	0	-2.210282	-1.529155	-0.497415
6	1	0	-3.262980	-0.044749	-1.454364
7	1	0	-1.882601	-1.814047	-1.501684
8	1	0	-2.944634	-2.274380	-0.154954
9	6	0	0.199743	-2.127904	0.118137
10	1	0	0.825846	-2.540008	0.906652
11	1	0	0.350655	-2.544188	-0.877595
12	6	0	-1.031295	-1.555459	0.452030
13	1	0	-1.263855	-1.445596	1.511787
14	1	0	-1.239139	0.375265	-0.280157
15	1	0	3.004530	-1.505584	-1.026699
16	1	0	3.135823	-1.296237	1.109045
17	1	0	-0.923924	2.744467	1.029081
18	1	0	-0.882683	2.743634	-1.131548
19	6	0	-3.672997	0.173805	0.548585
20	1	0	-4.493552	-0.543635	0.685781
21	1	0	-3.094993	0.223554	1.477184
22	1	0	-4.100032	1.162356	0.361107
23	1	0	3.810212	0.289171	-0.167929
24	1	0	0.859881	3.350698	-0.015378

		1			2			3		
		A			A			A		
Frequencies --		-92.1615			42.8380			87.8279		
Red. masses --		3.6496			3.8474			3.5355		
Frc consts --		0.0183			0.0042			0.0161		
IR Inten --		103.4697			2.7846			10.5628		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	15	0.00	-0.04	0.05	0.01	0.02	0.20	0.00	0.03	-0.06
2	78	0.02	0.02	0.00	-0.01	-0.01	-0.04	0.00	-0.01	0.06

3	15	0.11	0.05	-0.03	-0.04	-0.02	-0.03	-0.02	-0.02	-0.17
4	7	-0.25	-0.09	0.00	0.00	0.04	0.09	0.04	0.12	0.05
5	6	-0.06	0.01	-0.05	-0.03	0.02	0.01	0.03	0.09	-0.15
6	1	-0.40	-0.21	0.07	-0.09	0.07	0.14	0.09	0.28	0.06
7	1	-0.02	0.10	-0.07	-0.11	0.04	-0.02	0.07	0.26	-0.18
8	1	0.07	-0.14	-0.08	-0.03	0.03	0.04	0.01	0.05	-0.29
9	6	-0.06	0.01	-0.02	0.01	-0.02	-0.18	0.00	-0.01	-0.08
10	1	-0.08	0.01	0.00	0.04	-0.09	-0.24	-0.04	-0.07	-0.09
11	1	-0.04	0.01	-0.01	-0.04	0.07	-0.22	0.05	0.07	-0.11
12	6	-0.06	0.02	-0.05	0.03	-0.04	-0.07	-0.01	-0.03	-0.10
13	1	-0.06	0.08	-0.06	0.09	-0.11	-0.05	-0.06	-0.13	-0.10
14	1	0.24	0.08	0.13	-0.02	-0.01	-0.07	-0.06	0.03	0.15
15	1	0.00	-0.01	0.03	0.15	-0.03	0.30	0.00	0.14	-0.15
16	1	-0.03	-0.06	0.05	-0.12	0.10	0.30	0.04	-0.07	-0.14
17	1	0.09	0.03	-0.04	-0.13	-0.04	-0.09	-0.02	0.15	-0.24
18	1	0.13	0.02	-0.06	0.04	-0.01	-0.09	-0.02	-0.19	-0.24
19	6	-0.16	-0.20	0.10	0.14	0.06	0.19	-0.01	-0.06	0.08
20	1	-0.03	-0.32	0.27	0.15	0.07	0.30	-0.03	-0.07	-0.11
21	1	-0.05	-0.03	0.02	0.26	0.06	0.12	-0.05	-0.26	0.12
22	1	-0.36	-0.28	0.10	0.13	0.06	0.24	0.04	-0.02	0.24
23	1	-0.01	-0.02	0.09	0.02	0.03	0.29	-0.03	0.07	0.00
24	1	0.13	0.03	-0.02	-0.06	0.00	0.06	-0.02	-0.01	-0.33

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1018.376021

Computed Cartesian coordinates and PCM energy for **VI(PH_3)** with a P-Pt-P angle fixed at 90°

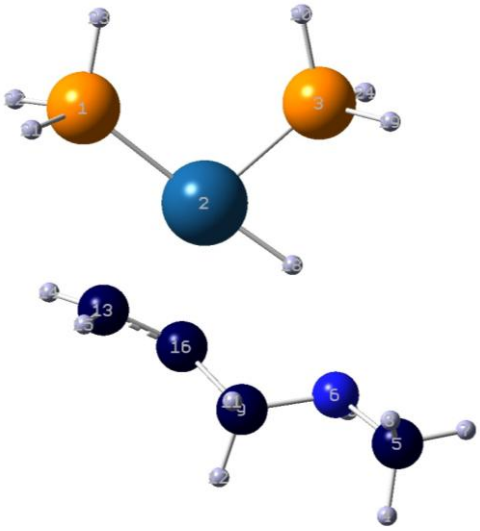


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.562735	-0.807859	0.452122
2	78	0	-0.365380	-0.025993	-0.099702
3	15	0	-1.130376	2.134085	-0.085345
4	1	0	5.035805	0.294195	0.689143
5	6	0	4.126584	0.915521	0.679866
6	7	0	3.068180	0.392085	-0.182089
7	1	0	4.396645	1.919502	0.341373
8	1	0	3.752187	0.994238	1.705887
9	6	0	2.641110	-0.958368	0.145795
10	1	0	3.364963	0.439239	-1.154992
11	1	0	2.471392	-1.016094	1.226545
12	1	0	3.401975	-1.720484	-0.103642
13	6	0	0.347820	-2.106501	-0.056224

14	1	0	-0.269994	-2.712416	-0.715827
15	1	0	0.402025	-2.433850	0.982001
16	6	0	1.384459	-1.337932	-0.598613
17	1	0	1.454531	-1.291415	-1.687268
18	1	0	1.061853	0.709356	-0.349553
19	1	0	-0.215159	3.198449	-0.147715
20	1	0	-1.896289	2.520151	1.032672
21	1	0	-2.724523	-1.525954	1.653716
22	1	0	-3.211979	-1.685223	-0.439626
23	1	0	-3.592616	0.140857	0.619914
24	1	0	-2.011591	2.482615	-1.127829

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1018.386233

Computed Cartesian coordinates and PCM energy for **VI(PH_3)** with a P-Pt-P angle fixed at 100°

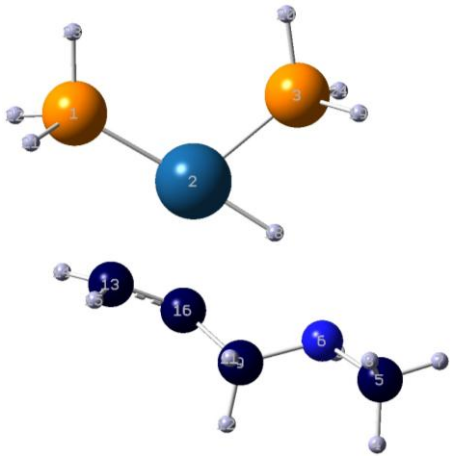


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.559474	-0.843637	0.438875
2	78	0	-0.411564	0.010580	-0.089722
3	15	0	-0.859144	2.248154	-0.070062
4	1	0	5.039536	0.013864	0.663342
5	6	0	4.173945	0.694635	0.676807
6	7	0	3.072993	0.260243	-0.182105
7	1	0	4.507538	1.684683	0.354235
8	1	0	3.816818	0.778194	1.708562
9	6	0	2.563737	-1.064974	0.129094
10	1	0	3.365800	0.301713	-1.156594
11	1	0	2.384829	-1.124539	1.208307
12	1	0	3.279311	-1.869008	-0.124649
13	6	0	0.228254	-2.110446	-0.102962
14	1	0	-0.407396	-2.677569	-0.779878
15	1	0	0.271857	-2.467658	0.925736
16	6	0	1.293348	-1.368725	-0.624988
17	1	0	1.364544	-1.293796	-1.711856
18	1	0	1.054855	0.679502	-0.349536
19	1	0	-0.085137	3.030950	0.804953
20	1	0	-2.154271	2.694152	0.260747
21	1	0	-2.663418	-1.678444	1.568856
22	1	0	-3.184807	-1.662225	-0.522623

23	1	0	-3.618674	0.046386	0.709384
24	1	0	-0.656820	2.926182	-1.285837

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1018.387901

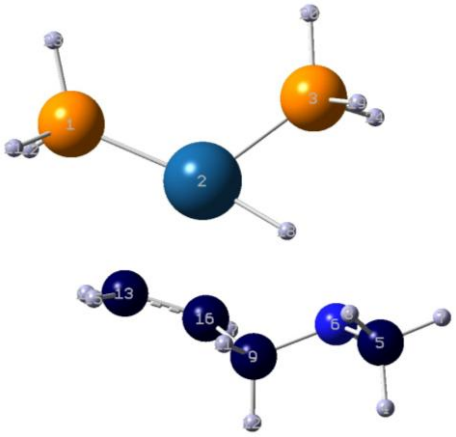
Computed Cartesian coordinates and PCM energy for **VI(PH_3)** with a P-Pt-P angle fixed at 110°



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.589660	-0.809648	0.423982
2	78	0	-0.443989	0.054021	-0.074725
3	15	0	-0.502577	2.332913	-0.079408
4	1	0	4.976564	-0.267807	0.656179
5	6	0	4.142577	0.449701	0.694327
6	7	0	3.024015	0.090930	-0.178239
7	1	0	4.519529	1.433996	0.403747
8	1	0	3.788618	0.513739	1.728381
9	6	0	2.457634	-1.222502	0.087165
10	1	0	3.318504	0.153321	-1.151311
11	1	0	2.288693	-1.316092	1.165418
12	1	0	3.132967	-2.045518	-0.209018
13	6	0	0.062968	-2.117848	-0.138407
14	1	0	-0.609933	-2.635039	-0.819345
15	1	0	0.100096	-2.499210	0.881768
16	6	0	1.164315	-1.432137	-0.659867
17	1	0	1.227780	-1.337783	-1.745666
18	1	0	1.091080	0.593747	-0.298467
19	1	0	0.382996	2.960165	0.814546
20	1	0	-1.690149	3.041251	0.194983
21	1	0	-2.653225	-1.693950	1.518412
22	1	0	-3.180855	-1.615295	-0.569189
23	1	0	-3.687532	0.019630	0.731760
24	1	0	-0.123540	2.932457	-1.293913

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1018.384265

Computed Cartesian coordinates and PCM energy for **VI(PH_3)** with a P-Pt-P angle fixed at 120°



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.650082	-0.677864	0.413358
2	78	0	-0.462534	0.107550	-0.057781
3	15	0	-0.043118	2.348049	-0.113981
4	1	0	4.843361	-0.565836	0.676793
5	6	0	4.026668	0.167481	0.744997
6	7	0	2.914414	-0.121751	-0.163360
7	1	0	4.428745	1.157227	0.513074
8	1	0	3.656520	0.181121	1.774866
9	6	0	2.305284	-1.434196	0.018226
10	1	0	3.221353	-0.009797	-1.128510
11	1	0	2.159045	-1.599390	1.090863
12	1	0	2.943897	-2.251018	-0.357787
13	6	0	-0.157301	-2.120624	-0.162937
14	1	0	-0.887385	-2.569509	-0.832979
15	1	0	-0.126457	-2.519590	0.850553
16	6	0	0.983020	-1.522336	-0.704660
17	1	0	1.029224	-1.415117	-1.790116
18	1	0	1.162599	0.449371	-0.202101
19	1	0	0.908046	2.795874	0.820163
20	1	0	-1.041806	3.330835	0.053859
21	1	0	-2.713655	-1.590459	1.484111
22	1	0	-3.245231	-1.457791	-0.597777
23	1	0	-3.751159	0.139473	0.744729
24	1	0	0.541607	2.793207	-1.313685

Total free energy in solution:
with all non electrostatic terms (a.u.) = -1018.376501