Table S1. B3LYP and CCSD(T)[a] Phosphine Dissociation Energies, Basis Set Superposition Errors (BSSE), and Corrected Energies (kcal/mol).

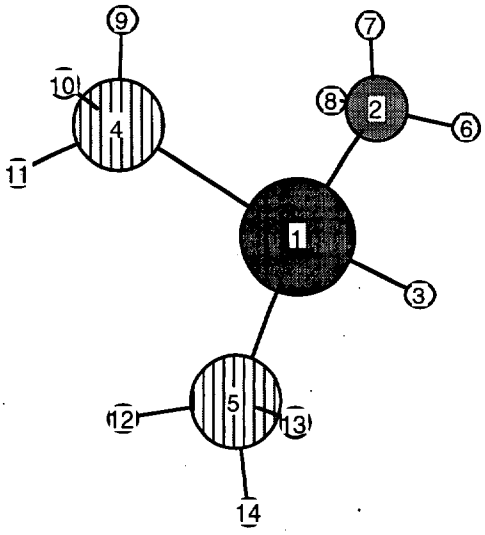
Phosphine Dissociation Reaction	Raw Energy for PH_3 Loss (ΔE)	BSSE Correction[b]	Corrected Energy for PH_3 Loss (ΔE_{corr})
1 ⟶ **4a** + PH_3	22.2[b] *27.6*	1.7 *7.5*	**20.5** ***20.1***
1 ⟶ **4b** + PH_3	27.4 *33.1*	1.7 *7.6*	**25.7** ***25.5***
13a ⟶ **7a** + PH_3	16.7 *22.3*	2.4 *8.6*	**14.3** ***13.7***
13b ⟶ **7a** + PH_3	13.9 *19.7*	2.5 *8.6*	**11.4** ***11.1***
13c ⟶ **7b** + PH_3	15.1 *22.0*	2.4 *8.2*	**12.7** ***13.8***
13c ⟶ **7c** + PH_3	17.4 *24.3*	2.2 *8.3*	**15.2** ***16.0***

[a]B3LYP energies are not italicized; CCSD(T) energies are italicized. [b]The correction for basis set superposition errors was calculated using the full counterpoise method.

Four-Coordinate Reactant Complex, (**1**)
$(PH_3)_2PtCH_3H$, B3LYP, C_1 Geometry

Zero Point Energy	.098855
Thermal correction to Enthalpy at 298K:	.109977

Nuclear Repulsion	321.557848
B3LYP	-846.634512
CCSD(T) single point	-844.672680



	X	Y	Z
Pt1	-.026065	-.336555	.000017
C2	-1.866746	-1.350839	.000178
H3	.570750	-1.808064	.000090
P4	-1.197059	1.746733	.000063
P5	2.214517	.388189	-.000238
H6	-1.750337	-2.435809	.000464
H7	-2.441121	-1.063812	-.891496
H8	-2.441309	-1.063373	.891590
H9	-2.616762	1.703399	-.001335
H10	-1.045715	2.682917	-1.060412
H11	-1.047773	2.681305	1.062247
H12	2.655890	1.743752	-.000787
H13	3.044007	-.054336	-1.064461
H14	3.044028	-.053482	1.064326

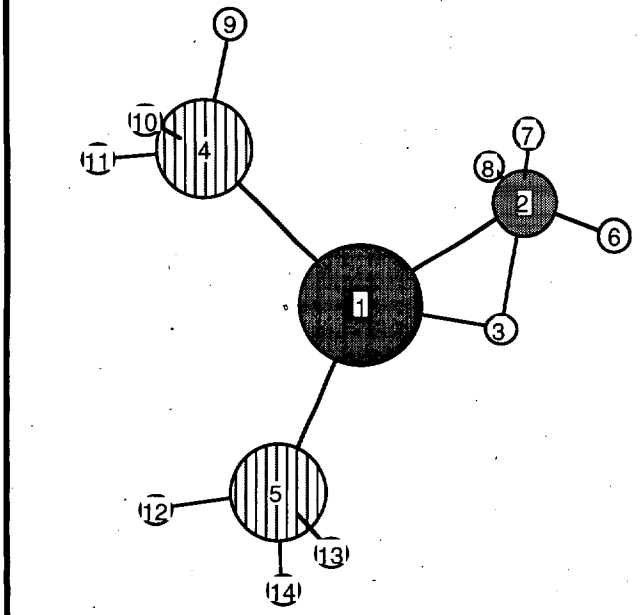
(1-2)	2.102	(1-3)	1.588	(1-4)	2.390	(1-5)	2.355	(2-6)	1.091	
(2-7)	1.099	(2-8)	1.099	(4-9)	1.420	(4-10)	1.423	(4-11)	1.423	
(5-12)	1.426	(5-13)	1.420	(5-14)	1.420					
(2-1-3)	83.2	(2-1-4)	89.5	(2-1-5)	169.1	(3-1-4)	172.7			
(3-1-5)	85.8	(4-1-5)	101.4	(1-2-6)	112.7	(1-2-7)	109.4			
(1-2-8)	109.4	(6-2-7)	108.4	(6-2-8)	108.4	(7-2-8)	108.5			
(1-4-9)	117.6	(1-4-10)	121.4	(1-4-11)	121.4	(9-4-10)	97.2			
(9-4-11)	97.2	(10-4-11)	96.5	(1-5-12)	126.0	(1-5-13)	117.4			
(1-5-14)	117.4	(12-5-13)	96.6	(12-5-14)	96.6	(13-5-14)	97.1			
(3-1-2-6)	0.0	(3-1-2-7)	-120.7	(3-1-2-8)	120.7					
(4-1-2-6)	180.0	(4-1-2-7)	59.3	(4-1-2-8)	-59.3					
(5-1-2-6)	0.0	(5-1-2-7)	-120.6	(5-1-2-8)	120.7					
(2-1-4-9)	-.1	(2-1-4-10)	-119.1	(2-1-4-11)	119.0					
(3-1-4-9)	-.1	(3-1-4-10)	-119.1	(3-1-4-11)	118.9					
(5-1-4-9)	179.9	(5-1-4-10)	60.9	(5-1-4-11)	-61.0					
(2-1-5-12)	180.0	(2-1-5-13)	57.6	(2-1-5-14)	-57.6					
(3-1-5-12)	180.0	(3-1-5-13)	57.6	(3-1-5-14)	-57.6					
(4-1-5-12)	0.0	(4-1-5-13)	-122.4	(4-1-5-14)	122.4					

Frequencies(cm-1): 16.8 46.4 60.0 100.0 119.7 169.6 257.6 281.9
332.6 473.7 475.2 503.7 534.8 629.4 781.4 825.1 850.7 1043.4
1064.0 1147.6 1150.4 1150.9 1154.8 1239.5 1457.8 1484.8 2158.1 2405.3
2427.7 2432.2 2445.8 2446.7 2447.2 3022.2 3094.1 3161.0

Four-Coordinate Transition State (**2**)
$(PH_3)_2PtCH_3H$, B3LYP, C_s Geometry

Zero Point Energy	.096367
Thermal correction to Enthalpy at 298K:	.107633

Nuclear Repulsion	316.019241
B3LYP	-846.605902
CCSD(T) single point	-844.638529



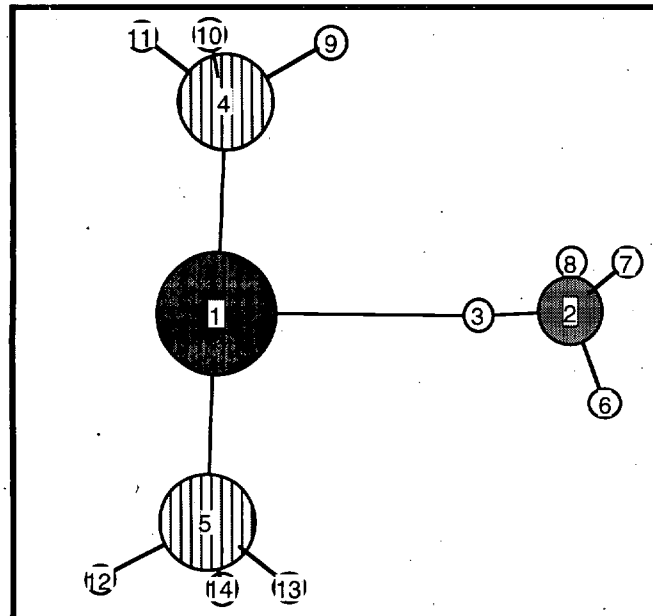
	X	Y	Z
Pt1	.000000	.486844	.000000
C2	-1.319944	2.313116	.000000
H3	.159499	2.104213	.000000
P4	-1.511479	-1.365555	.000000
P5	2.172880	-.303042	.000000
H6	-1.027887	3.368690	.000000
H7	-1.912967	2.133554	.900774
H8	-1.912967	2.133554	-.900774
H9	-2.925164	-1.173308	.000000
H10	-1.506203	-2.322065	1.055547
H11	-1.506203	-2.322065	-1.055547
H12	2.540200	-1.681771	.000000
H13	3.045172	.073135	1.059231
H14	3.045172	.073135	-1.059231

(1-2)	2.253	(1-3)	1.625	(1-4)	2.391	(1-5)	2.312	(2-6)	1.095
(2-7)	1.093	(4-9)	1.427	(4-10)	1.424	(5-12)	1.427	(5-13)	1.423
(2-1-3)	41.5	(2-1-4)	104.9	(2-1-5)	145.8	(3-1-4)	146.4		
(3-1-5)	104.3	(4-1-5)	109.2	(1-2-6)	128.7	(1-2-7)	100.6		
(6-2-7)	107.6	(7-2-8)	111.0	(1-4-9)	121.5	(1-4-10)	121.2		
(9-4-10)	95.4	(10-4-11)	95.6	(1-5-12)	124.9	(1-5-13)	119.1		
(12-5-13)	95.6	(13-5-14)	96.2						
(3-1-2-6)	0.0	(3-1-2-7)	-123.0	(4-1-2-6)	180.0				
(4-1-2-7)	57.0	(5-1-2-6)	0.0	(5-1-2-7)	-123.0				
(2-1-4-9)	0.0	(2-1-4-10)	-120.0	(3-1-4-9)	0.0				
(3-1-4-10)	-120.0	(5-1-4-9)	180.0	(5-1-4-10)	60.0				
(2-1-5-12)	180.0	(2-1-5-13)	58.4	(3-1-5-12)	180.0				
(3-1-5-13)	58.4	(4-1-5-12)	0.0	(4-1-5-13)	-121.6				

Frequencies(cm-1): -890.8 26.3 46.0 78.2 100.2 116.6 121.1 242.7
302.9 305.5 430.9 437.8 466.2 485.9 516.3 888.0 923.7 1042.5
1070.1 1149.4 1150.7 1158.6 1165.1 1243.1 1458.2 1479.5 2090.6 2389.5
2393.0 2409.2 2414.0 2420.9 2422.1 3056.9 3131.5 3167.2

Four-Coordinate Product Complex (**3**)
$(PH_3)_2Pt{\cdot}CH_4$, B3LYP, C_1 Geometry

Zero Point Energy	.100416	Nuclear Repulsion	287.189842
Thermal correction		B3LYP	-846.656732
to Enthalpy at 298K:	.113450	CCSD(T) single point	-844.682407



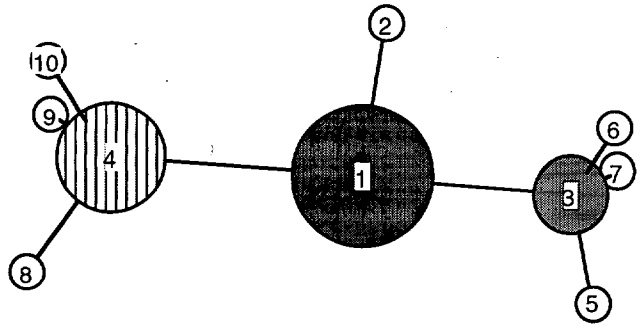
	X	Y	Z
Pt1	.003909	-.352078	.000005
C2	-.044982	4.050128	-.000110
H3	-.023008	2.955356	.016746
P4	-2.270398	-.383561	-.000057
P5	2.278391	-.339452	-.000039
H6	.941616	4.441109	.267494
H7	-.785297	4.412809	.719736
H8	-.312539	4.395203	-1.003601
H9	-2.995938	.704081	-.556531
H10	-2.975755	-.462765	1.230820
H11	-2.960541	-1.427060	-.673512
H12	2.988650	-1.378757	-.658912
H13	2.985158	-.387457	1.231633
H14	2.982742	.753964	-.572171

(1-3)	3.308	(1-4)	2.275	(1-5)	2.275	(2-3)	1.095	(2-6)	1.094
(2-7)	1.094	(2-8)	1.094	(4-9)	1.421	(4-10)	1.421	(4-11)	1.421
(5-12)	1.421	(5-13)	1.421	(5-14)	1.421				
(3-1-4)	90.3	(3-1-5)	90.1	(4-1-5)	179.5	(3-2-6)	109.6		
(3-2-7)	109.6	(3-2-8)	109.5	(6-2-7)	109.3	(6-2-8)	109.4		
(7-2-8)	109.5	(1-3-2)	178.6	(1-4-9)	120.0	(1-4-10)	119.8		
(1-4-11)	119.7	(9-4-10)	97.4	(9-4-11)	97.4	(10-4-11)	97.4		
(1-5-12)	119.7	(1-5-13)	119.8	(1-5-14)	120.0	(12-5-13)	97.4		
(12-5-14)	97.4	(13-5-14)	97.4						
(4-1-3-2)	-59.7	(5-1-3-2)	120.3	(3-1-4-9)	27.2				
(3-1-4-10)	-92.9	(3-1-4-11)	147.2	(5-1-4-9)	-152.8				
(5-1-4-10)	87.1	(5-1-4-11)	-32.8	(3-1-5-12)	-148.0				
(3-1-5-13)	92.1	(3-1-5-14)	-28.0	(4-1-5-12)	32.0				
(4-1-5-13)	-87.9	(4-1-5-14)	152.0	(6-2-3-1)	-135.6				
(7-2-3-1)	104.5	(8-2-3-1)	-15.6						

Frequencies(cm-1): 17.1 29.8 32.5 35.2 59.5 63.1 67.1 102.9
126.4 304.4 351.9 447.6 452.2 521.8 525.6 1029.8 1053.9 1144.6
1145.8 1146.2 1147.4 1332.9 1344.0 1347.2 1559.1 1560.6 2437.0 2438.0
2438.4 2439.7 2441.1 2443.3 3030.2 3146.7 3156.5 3157.8

Three-Coordinate Reactant Complex (**4a**), H-trans site open
$(PH_3)PtCH_3H$, B3LYP, C_1 Geometry

Zero Point Energy	.069700	Nuclear Repulsion	164.114619
Thermal correction to Enthalpy at 298K:	.078034	B3LYP	-503.459727
		CCSD(T) single point	-502.040257



	X	Y	Z
Pt1	-.544073	-.035950	.000010
H2	-.642430	1.486846	-.000184
C3	-2.598999	-.043901	.000004
P4	1.823505	-.022469	.000000
H5	-2.891805	-1.109491	.000115
H6	-3.023087	.430777	-.892396
H7	-3.023089	.430965	.892303
H8	2.588180	-1.223316	-.000171
H9	2.513503	.615740	1.065830
H10	2.513452	.616012	-1.065697

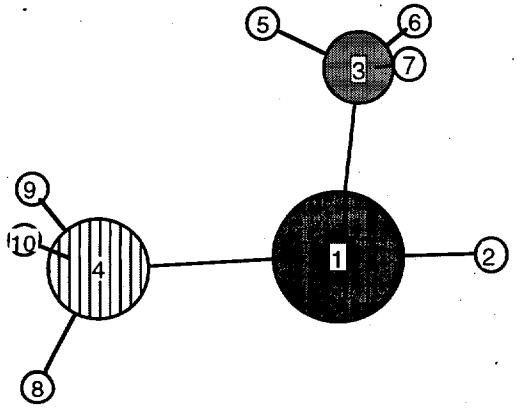
(1-2)	1.526	(1-3)	2.055	(1-4)	2.368	(3-5)	1.105	(3-6)	1.096

(3-7)	1.096	(4-8)	1.424	(4-9)	1.421	(4-10)	1.421					
(2-1-3)	86.5	(2-1-4)	93.4	(3-1-4)	179.9	(1-3-5)	105.6					
(1-3-6)	112.7	(1-3-7)	112.7	(5-3-6)	108.4	(5-3-7)	108.4					
(6-3-7)	109.0	(1-4-8)	122.2	(1-4-9)	119.2	(1-4-10)	119.2					
(8-4-9)	96.8	(8-4-10)	96.8	(9-4-10)	97.2							
(2-1-3-5)	180.0	(2-1-3-6)	61.9	(2-1-3-7)	-61.9							
(4-1-3-5)	179.8	(4-1-3-6)	61.7	(4-1-3-7)	-62.1							
(2-1-4-8)	180.0	(2-1-4-9)	59.3	(2-1-4-10)	-59.2							
(3-1-4-8)	-179.8	(3-1-4-9)	59.5	(3-1-4-10)	-59.0							

Frequencies(cm-1): 49.6 115.2 116.8 129.5 271.3 436.3 465.2 547.6
567.0 749.8 776.0 1050.8 1146.4 1151.9 1231.5 1431.7 1462.3 2389.3
2424.4 2441.7 2442.9 2981.8 3088.3 3127.9

Three-Coordinate Reactant Complex (**4b**), CH_3-trans site open
$(PH_3)PtCH_3H$, B3LYP, C1 Geometry

Zero Point Energy	.070836	Nuclear Repulsion	167.929292
Thermal correction		B3LYP	-503.451536
to Enthalpy at 298K:	.078979	CCSD(T) single point	-502.031418



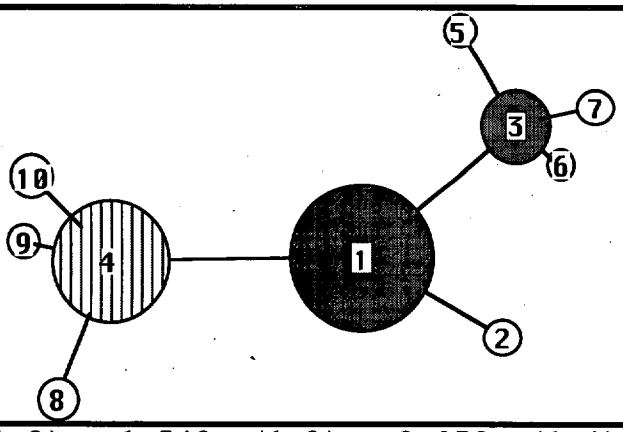
	X	Y	Z
Pt1	-.671687	-.714268	-.000230
H2	-2.136062	-1.318937	.000265
C3	-1.713824	1.044869	-.000161
P4	1.567446	.171352	.000124
H5	-1.015109	1.886406	-.043054
H6	-2.305913	1.080665	.919321
H7	-2.374301	1.047987	-.871963
H8	2.694438	-.695056	-.038052
H9	2.012515	.978137	1.082802
H10	1.986057	1.038130	-1.046067

(1-2)	1.584	(1-3)	2.045	(1-4)	2.408	(3-5)	1.095	(3-6)	1.094			
(3-7)	1.094	(4-8)	1.422	(4-9)	1.422	(4-10)	1.422					
(2-1-3)	81.8	(2-1-4)	179.1	(3-1-4)	99.1	(1-3-5)	109.6					
(1-3-6)	107.7	(1-3-7)	108.1	(5-3-6)	110.7	(5-3-7)	110.6					
(6-3-7)	110.1	(1-4-8)	120.9	(1-4-9)	120.0	(1-4-10)	119.9					
(8-4-9)	96.8	(8-4-10)	96.8	(9-4-10)	97.0							
(2-1-3-5)	-177.6	(2-1-3-6)	61.9	(2-1-3-7)	-57.0							
(4-1-3-5)	2.4	(4-1-3-6)	-118.1	(4-1-3-7)	123.0							
(2-1-4-8)	3.6	(2-1-4-9)	-116.7	(2-1-4-10)	123.7							
(3-1-4-8)	-178.2	(3-1-4-9)	61.5	(3-1-4-10)	-58.1							

Frequencies(cm-1): 12.0 44.6 100.0 242.5 317.7 376.4 563.3 620.1
816.2 829.9 844.7 1042.1 1143.1 1150.5 1250.9 1448.5 1460.8 2164.9
2431.7 2438.0 2441.4 3044.7 3149.6 3159.6

Transition state for isomeration of **4b** to **4a**
$(PH_3)PtCH_3H$, B3LYP, C1 Geometry

Zero Point Energy	.069850	Nuclear Repulsion	162.364790
Thermal correction		B3LYP	-503.444950
to Enthalpy at 298K:	.077493	CCSD(T) single point	-502.024114



	X	Y	Z
Pt1	-.256457	-.156957	.000001
H2	-1.411442	-1.188238	-.000024
C3	-2.059905	.833938	-.000001
P4	2.150374	.290164	.000001
H5	-1.750758	1.887338	-.000094
H6	-2.648151	.608616	.894555
H7	-2.648262	.608496	-.894453
H8	2.916529	-.903574	-.000096
H9	2.824795	.936901	1.069178
H10	2.824744	.937042	-1.069121

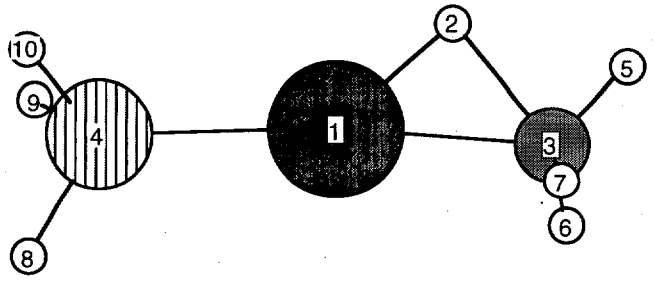
(1-2)	1.548	(1-3)	2.058	(1-4)	2.448	(2-3)	2.124	(3-5)	1.098
(3-6)	1.094	(3-7)	1.094	(4-8)	1.418	(4-9)	1.420	(4-10)	1.420
(2-1-3)	70.5	(2-1-4)	148.8	(3-1-4)	140.7	(1-2-3)	66.0		
(1-3-2)	43.4	(1-3-5)	102.4	(1-3-6)	111.8	(1-3-7)	111.8		
(2-3-5)	145.9	(2-3-6)	88.2	(2-3-7)	88.2	(5-3-6)	110.4		
(5-3-7)	110.4	(6-3-7)	109.7	(1-4-8)	112.2	(1-4-9)	123.4		
(1-4-10)	123.4	(8-4-9)	97.3	(8-4-10)	97.3	(9-4-10)	97.7		
(4-1-2-3)	180.0	(2-1-3-5)	180.0	(2-1-3-6)	61.7				
(2-1-3-7)	-61.7	(4-1-3-2)	180.0	(4-1-3-5)	0.0				
(4-1-3-6)	-118.3	(4-1-3-7)	118.3	(2-1-4-8)	0.0				
(2-1-4-9)	-115.6	(2-1-4-10)	115.6	(3-1-4-8)	180.0				
(3-1-4-9)	64.4	(3-1-4-10)	-64.4	(1-2-3-5)	0.0				
(1-2-3-6)	-125.1	(1-2-3-7)	125.1						

Frequencies(cm-1): -115.2 46.3 78.3 218.3 260.9 297.5 470.1 524.7
695.2 804.9 827.7 1019.2 1133.1 1154.4 1233.2 1443.0 1464.5 2299.8
2447.1 2452.8 2470.8 3030.2 3134.1 3154.4

Three-Coordinate Reductive Elimination Transition State (**5**)
$(PH_3)PtCH_3H$, B3LYP, C_1 Geometry

Zero Point Energy	.068844
Thermal correction to Enthalpy at 298K:	.076881

Nuclear Repulsion	165.051628
B3LYP	-503.448734
CCSD(T) single point	-502.024366



	X	Y	Z
Pt1	.484732	.022608	-.004294
H2	1.498980	-1.171280	-.016138
C3	2.616816	.043506	.006778
P4	-1.816514	.005523	.001926
H5	2.660952	1.121168	-.218574
H6	3.186876	-.489718	-.759103
H7	3.047426	-.147267	.993367
H8	-2.583365	1.205514	-.007063
H9	-2.494107	-.625869	1.077775
H10	-2.495121	-.643355	-1.062523

(1-2)	1.567	(1-3)	2.132	(1-4)	2.301	(2-3)	1.651	(3-5)	1.102
(3-6)	1.094	(3-7)	1.093	(4-8)	1.424	(4-9)	1.420	(4-10)	1.419
(2-1-3)	50.2	(2-1-4)	129.9	(3-1-4)	179.5	(1-2-3)	83.0		
(1-3-2)	46.8	(1-3-5)	92.8	(1-3-6)	120.9	(1-3-7)	113.4		
(2-3-5)	138.1	(2-3-6)	89.1	(2-3-7)	98.7	(5-3-6)	108.2		
(5-3-7)	109.8	(6-3-7)	110.0	(1-4-8)	122.2	(1-4-9)	118.9		
(1-4-10)	118.7	(8-4-9)	97.0	(8-4-10)	97.1	(9-4-10)	97.9		
(4-1-2-3)	-179.4	(2-1-3-5)	167.4	(2-1-3-6)	54.2				
(2-1-3-7)	-79.6	(4-1-3-2)	107.6	(4-1-3-5)	-85.1				
(4-1-3-6)	161.7	(4-1-3-7)	28.0	(2-1-4-8)	-179.0				
(2-1-4-9)	60.2	(2-1-4-10)	-58.4	(3-1-4-8)	73.8				

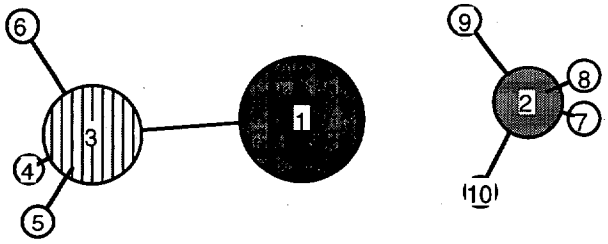
(3-1-4-9)	-47.0	(3-1-4-10)	-165.6	(1-2-3-5)	-19.1				
(1-2-3-6)	-135.9	(1-2-3-7)	114.0						

Frequencies(cm-1): -781.9 51.9 99.9 105.9 136.7 325.4 465.8 510.7
516.9 801.7 877.0 1049.9 1145.8 1148.0 1229.4 1438.8 1465.0 2234.7
2418.8 2449.9 2452.3 3009.7 3121.3 3163.4

Three-Coordinate Product Complex (**6**)
$(PH_3)Pt{\cdot}CH_4$, B3LYP, C_1 Geometry

Zero Point Energy	.073284
Thermal correction to Enthalpy at 298K:	.080708

Nuclear Repulsion	164.057009
B3LYP	-503.472276
CCSD(T) single point	-502.047103



	X	Y	Z
Pt1	.371579	-.000393	.002912
C2	2.801811	.000371	-.002998
P3	-1.812885	.000173	-.001559
H4	-2.511790	-.021215	1.236124
H5	-2.515780	1.081322	-.600723
H6	-2.516337	-1.059004	-.638178
H7	3.419970	-.001158	.897017
H8	3.403411	.001524	-.914049
H9	2.207055	-.946917	.003103
H10	2.207456	.947712	.005663

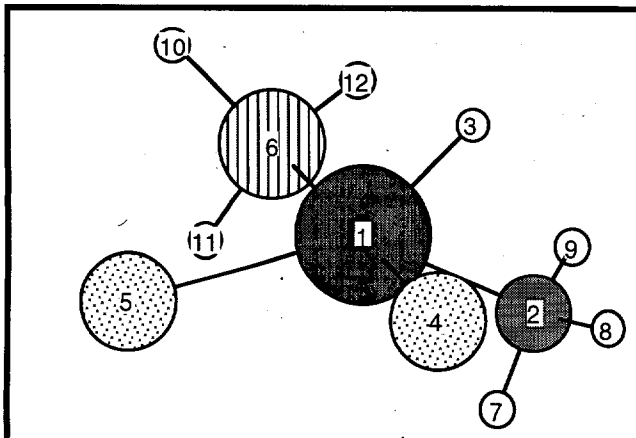
(1-2)	2.430	(1-3)	2.184	(1-9)	2.065	(1-10)	2.066	(2-7)	1.092
(2-8)	1.092	(2-9)	1.119	(2-10)	1.118	(3-4)	1.422	(3-5)	1.422
(3-6)	1.422								
(2-1-3)	179.7	(2-1-9)	27.3	(2-1-10)	27.3	(3-1-9)	152.7		
(3-1-10)	152.7	(9-1-10)	54.6	(1-2-7)	124.3	(1-2-8)	123.6		
(1-2-9)	57.9	(1-2-10)	57.9	(7-2-8)	112.1	(7-2-9)	107.2		
(7-2-10)	107.2	(8-2-9)	107.4	(8-2-10)	107.4	(9-2-10)	115.8		
(1-3-4)	119.3	(1-3-5)	119.7	(1-3-6)	119.7	(4-3-5)	97.8		
(4-3-6)	97.8	(5-3-6)	97.7	(1-9-2)	94.8	(1-10-2)	94.8		
(3-1-2-7)	172.8	(3-1-2-8)	-7.2	(3-1-2-9)	-97.6				
(3-1-2-10)	83.1	(9-1-2-7)	-89.6	(9-1-2-8)	90.3				
(9-1-2-10)	-179.3	(10-1-2-7)	89.7	(10-1-2-8)	-90.4				
(10-1-2-9)	179.3	(2-1-3-4)	-173.7	(2-1-3-5)	-53.8				
(2-1-3-6)	66.4	(9-1-3-4)	89.2	(9-1-3-5)	-150.8				
(9-1-3-6)	-30.7	(10-1-3-4)	-91.1	(10-1-3-5)	28.9				
(10-1-3-6)	149.0	(3-1-9-2)	179.4	(10-1-9-2)	-.4				
(3-1-10-2)	-179.4	(9-1-10-2)	0.4	(7-2-9-1)	120.2				
(8-2-9-1)	-119.2	(10-2-9-1)	0.7	(7-2-10-1)	-120.2				
(8-2-10-1)	119.2	(9-2-10-1)	-.7						

Frequencies(cm-1): -13.1 91.2 93.2 255.2 262.3 308.2 405.0 552.8
559.2 1055.4 1141.8 1146.0 1216.2 1361.9 1366.2 1491.9 1598.9 2423.7
2425.9 2433.1 2792.3 2870.8 3123.1 3193.8

Five-Coordinate Reactant Complex (**7a**), with chlorines mutually *cis*.
$(PH_3)Cl_2Pt(CH_3)H$, B3LYP, C_1 Geometry

Zero Point Energy	.076211
Thermal correction to Enthalpy at 298K:	.086974

Nuclear Repulsion	485.490875
B3LYP	-1423.899312
CCSD(T) single point	-1421.366969



	X	Y	Z
Pt1	.133746	-.283979	-.172234
C2	.541816	-2.171749	.666309
H3	.387288	-1.322865	-1.274915
Cl4	2.439003	.161984	-.203997
Cl5	-.499713	2.009056	.295135
P6	-2.163368	-.551518	-.203211
H7	.435817	-1.953465	1.733628
H8	1.568406	-2.448271	.429182
H9	-.161193	-2.944763	.348399
H10	-2.851718	.195998	-1.181795
H11	-2.850787	-.174935	.970580
H12	-2.703544	-1.844487	-.423894

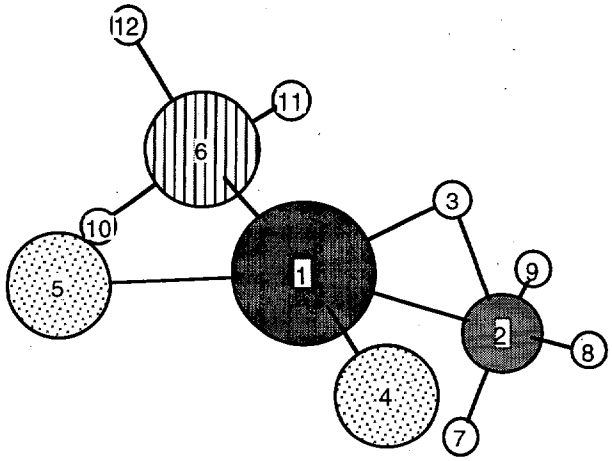
(1-2)	2.106	(1-3)	1.536	(1-4)	2.348	(1-5)	2.424	(1-6)	2.313
(2-7)	1.095	(2-8)	1.089	(2-9)	1.092	(6-10)	1.411	(6-11)	1.411
(6-12)	1.419								
(2-1-3)	69.4	(2-1-4)	89.2	(2-1-5)	145.3	(2-1-6)	95.4		
(3-1-4)	87.5	(3-1-5)	145.2	(3-1-6)	94.4	(4-1-5)	94.6		
(4-1-6)	175.4	(5-1-6)	81.5	(1-2-7)	101.0	(1-2-8)	108.9		
(1-2-9)	113.2	(7-2-8)	110.7	(7-2-9)	111.3	(8-2-9)	111.3		
(1-6-10)	115.6	(1-6-11)	116.2	(1-6-12)	119.1	(10-6-11)	101.4		
(10-6-12)	100.9	(11-6-12)	100.8						
(3-1-2-7)	-178.1	(3-1-2-8)	65.3	(3-1-2-9)	-59.0				
(4-1-2-7)	94.3	(4-1-2-8)	-22.3	(4-1-2-9)	-146.7				
(5-1-2-7)	-2.5	(5-1-2-8)	-119.1	(5-1-2-9)	116.5				
(6-1-2-7)	-85.4	(6-1-2-8)	158.0	(6-1-2-9)	33.6				
(2-1-6-10)	-153.8	(2-1-6-11)	87.5	(2-1-6-12)	-33.3				
(3-1-6-10)	-84.1	(3-1-6-11)	157.1	(3-1-6-12)	36.3				
(4-1-6-10)	30.0	(4-1-6-11)	-88.7	(4-1-6-12)	150.5				
(5-1-6-10)	61.1	(5-1-6-11)	-57.7	(5-1-6-12)	-178.5				

Frequencies(cm-1): 65.6 108.6 117.4 132.0 137.5 145.8 198.0 297.7
324.5 345.0 512.2 549.2 574.8 672.1 717.2 859.7 901.4 1030.3
1121.7 1132.1 1267.6 1451.0 1472.5 2382.4 2460.0 2509.4 2522.6 3063.1
3171.9 3209.2

Five-Coordinate Transition State (**8a**), with chlorines mutually *cis*.
$(PH_3)Cl_2Pt(CH_3)H$, B3LYP, C_1 Geometry

Zero Point Energy	.074714
Thermal correction to Enthalpy at 298K:	.085245

Nuclear Repulsion	485.645228
B3LYP	-1423.895742
CCSD(T) single point	-1421.361084



	X	Y	Z
Pt1	-.119231	.264568	-.109408
C2	-.689829	2.295725	.412287
H3	-.453143	1.506245	-.998045
Cl4	-2.414040	-.260619	-.135551
Cl5	.543536	-2.004604	.197476
P6	2.164856	.584671	-.126407
H7	-.693929	2.102477	1.488704
H8	-1.697152	2.553495	.084214
H9	.032656	3.075041	.160486
H10	2.865792	.163343	1.024477
H11	2.684184	1.896657	-.280132
H12	2.872449	-.095109	-1.140716

(1-2)	2.173	(1-3)	1.563	(1-4)	2.354	(1-5)	2.384	(1-6)	2.306
(2-3)	1.634	(2-7)	1.094	(2-8)	1.090	(2-9)	1.092	(6-10)	1.412

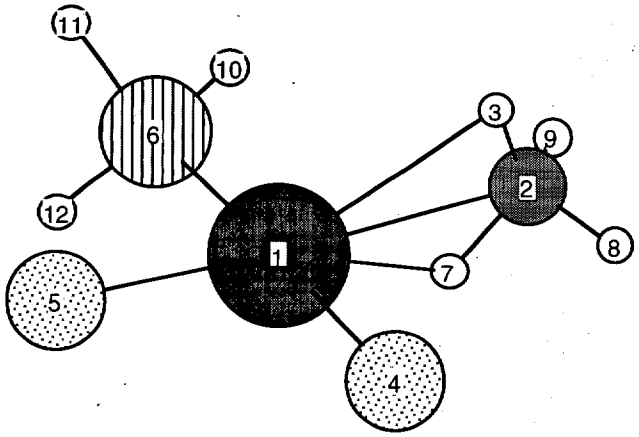
(6-11)	1.419	(6-12)	1.411				
(2-1-3)	48.5	(2-1-4)	87.4	(2-1-5)	158.7	(2-1-6)	97.6
(3-1-4)	87.9	(3-1-5)	152.7	(3-1-6)	95.6	(4-1-5)	93.4
(4-1-6)	175.0	(5-1-6)	81.8	(1-2-3)	45.8	(1-2-7)	94.1
(1-2-8)	113.0	(1-2-9)	116.0	(3-2-7)	139.9	(3-2-8)	89.3
(3-2-9)	92.9	(7-2-8)	109.5	(7-2-9)	110.8	(8-2-9)	111.9
(1-3-2)	85.6	(1-6-10)	116.4	(1-6-11)	119.4	(1-6-12)	115.8
(10-6-11)	100.5	(10-6-12)	101.1	(11-6-12)	100.6		
(3-1-2-7)	177.7	(3-1-2-8)	64.5	(3-1-2-9)	-66.7		
(4-1-2-3)	-89.4	(4-1-2-7)	88.3	(4-1-2-8)	-24.9		
(4-1-2-9)	-156.1	(5-1-2-3)	177.7	(5-1-2-7)	-4.6		
(5-1-2-8)	-117.8	(5-1-2-9)	111.0	(6-1-2-3)	90.7		
(6-1-2-7)	-91.5	(6-1-2-8)	155.2	(6-1-2-9)	24.1		
(4-1-3-2)	88.5	(5-1-3-2)	-178.2	(6-1-3-2)	-95.2		
(2-1-6-10)	100.0	(2-1-6-11)	-20.9	(2-1-6-12)	-141.3		
(3-1-6-10)	148.9	(3-1-6-11)	28.0	(3-1-6-12)	-92.5		
(4-1-6-10)	-78.2	(4-1-6-11)	160.9	(4-1-6-12)	40.5		
(5-1-6-10)	-58.5	(5-1-6-11)	-179.4	(5-1-6-12)	60.2		
(7-2-3-1)	-3.5	(8-2-3-1)	-123.9	(9-2-3-1)	124.2		

Frequencies(cm-1): -650.5 94.0 125.9 131.3 133.8 135.3 151.6 180.6
315.3 333.0 342.8 512.2 548.1 568.0 638.5 905.8 965.4 1032.5
1125.5 1132.2 1278.1 1455.6 1468.8 2299.1 2454.2 2506.5 2518.2 3068.4
3173.5 3201.7

Five-Coordinate Product Complex (**9a**), with chlorines mutually *cis*.
$(PH_3)Cl_2Pt\cdot CH_4$, B3LYP, C_1 Geometry

Zero Point Energy	.077055
Thermal correction to Enthalpy at 298K:	.088432

Nuclear Repulsion	479.666562
B3LYP	-1423.913403
CCSD(T) single point	-1421.376479



	X	Y	Z
Pt1	.095363	.189781	-.042027
C2	1.015829	2.543727	.120195
H3	.934257	2.166255	1.143319
Cl4	2.344246	-.484316	-.045211
Cl5	-.671663	-1.996489	.070495
P6	-2.133898	.718407	-.039662
H7	.689963	1.855345	-.728330
H8	2.071534	2.709524	-.102346
H9	.403659	3.441112	.001719
H10	-2.539984	2.077313	-.103956
H11	-2.884610	.290689	1.079117
H12	-2.911764	.178921	-1.089107

(1-2)	2.533	(1-3)	2.453	(1-4)	2.348	(1-5)	2.320	(1-6)	2.291
(1-7)	1.897	(2-3)	1.094	(2-7)	1.140	(2-8)	1.092	(2-9)	1.093
(6-10)	1.420	(6-11)	1.414	(6-12)	1.413				
(2-1-3)	25.3	(2-1-4)	85.3	(2-1-5)	173.2	(2-1-6)	98.0		
(2-1-7)	24.9	(3-1-4)	84.5	(3-1-5)	148.1	(3-1-6)	98.4		
(3-1-7)	50.2	(4-1-5)	92.6	(4-1-6)	176.7	(4-1-7)	87.2		
(5-1-6)	84.0	(5-1-7)	161.6	(6-1-7)	95.9	(1-2-3)	73.3		
(1-2-7)	44.5	(1-2-8)	118.7	(1-2-9)	123.6	(3-2-7)	117.8		
(3-2-8)	108.4	(3-2-9)	110.1	(7-2-8)	102.5	(7-2-9)	104.8		
(8-2-9)	113.3	(1-3-2)	81.5	(1-6-10)	119.9	(1-6-11)	116.6		
(1-6-12)	116.5	(10-6-11)	100.0	(10-6-12)	100.0	(11-6-12)	100.4		
(1-7-2)	110.5								
(3-1-2-7)	-179.6	(3-1-2-8)	102.2	(3-1-2-9)	-103.3				
(4-1-2-3)	-87.0	(4-1-2-7)	93.4	(4-1-2-8)	15.2				

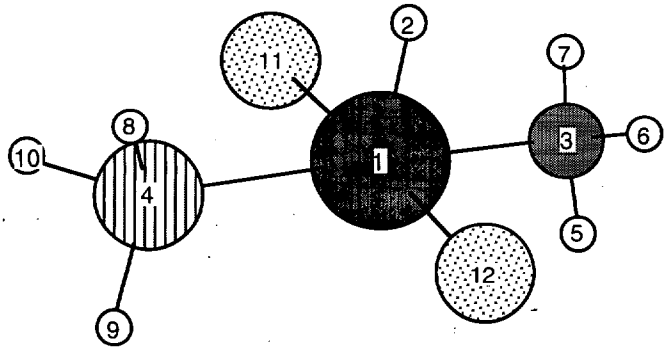
(4-1-2-9)	169.7	(5-1-2-3)	-14.1	(5-1-2-7)	166.3
(5-1-2-8)	88.1	(5-1-2-9)	-117.4	(6-1-2-3)	92.8
(6-1-2-7)	-86.8	(6-1-2-8)	-165.0	(6-1-2-9)	-10.5
(7-1-2-3)	179.6	(7-1-2-8)	-78.2	(7-1-2-9)	76.3
(4-1-3-2)	90.7	(5-1-3-2)	176.9	(6-1-3-2)	-90.9
(7-1-3-2)	-.2	(2-1-6-10)	6.7	(2-1-6-11)	-114.1
(2-1-6-12)	127.6	(3-1-6-10)	32.3	(3-1-6-11)	-88.5
(3-1-6-12)	153.1	(4-1-6-10)	-176.7	(4-1-6-11)	62.5
(4-1-6-12)	-55.8	(5-1-6-10)	-179.8	(5-1-6-11)	59.4
(5-1-6-12)	-58.9	(7-1-6-10)	-18.3	(7-1-6-11)	-139.1
(7-1-6-12)	102.5	(3-1-7-2)	0.2	(4-1-7-2)	-84.9
(5-1-7-2)	-175.0	(6-1-7-2)	96.3	(7-2-3-1)	0.3
(8-2-3-1)	-115.3	(9-2-3-1)	120.3	(3-2-7-1)	-.5
(8-2-7-1)	118.4	(9-2-7-1)	-123.2		

Frequencies(cm-1): 84.5 112.7 116.2 122.8 132.4 137.6 166.4 209.1
325.1 339.3 350.0 353.8 455.8 555.0 564.2 1039.2 1130.5 1132.7
1185.7 1309.3 1409.7 1512.5 1619.7 2451.3 2492.8 2499.6 2570.8 3079.1
3164.3 3201.1

Five-Coordinate Reactant Complex (**7b**), with chlorines mutually *trans*.
H-trans site empty, $(PH_3)Cl_2Pt(CH_3)H$, B3LYP, C_1 Geometry

Zero Point Energy	.073942
Thermal correction to Enthalpy at 298K:	.085536

Nuclear Repulsion	476.841803
B3LYP	-1423.898994
CCSD(T) single point	-1421.365142



	X	Y	Z
Pt1	.052222	-.342466	.027953
H2	.072504	-.495570	1.534367
C3	.257112	-2.406687	-.008226
P4	-.264798	2.162686	-.001329
H5	.265412	-2.653107	-1.077851
H6	-.601936	-2.868988	.480147
H7	1.202219	-2.693315	.454837
H8	-1.130274	2.705958	.978918
H9	-.849387	2.765850	-1.143617
H10	.844417	3.028726	.162462
Cl11	2.395736	-.112475	-.053791
Cl12	-2.296540	-.571369	-.053452

(1-2)	1.514	(1-3)	2.075	(1-4)	2.525	(1-11)	2.356	(1-12)	2.361
(3-5)	1.098	(3-6)	1.091	(3-7)	1.091	(4-8)	1.416	(4-9)	1.418
(4-10)	1.417								
(2-1-3)	85.1	(2-1-4)	96.5	(2-1-11)	91.8	(2-1-12)	92.2		
(3-1-4)	177.7	(3-1-11)	89.9	(3-1-12)	90.1	(4-1-11)	91.6		
(4-1-12)	88.3	(11-1-12)	176.0	(1-3-5)	104.0	(1-3-6)	109.6		
(1-3-7)	109.9	(5-3-6)	110.3	(5-3-7)	110.4	(6-3-7)	112.4		
(1-4-8)	116.7	(1-4-9)	118.9	(1-4-10)	120.4	(8-4-9)	98.2		
(8-4-10)	99.4	(9-4-10)	99.0						
(2-1-3-5)	179.3	(2-1-3-6)	61.4	(2-1-3-7)	-62.6				
(4-1-3-5)	42.0	(4-1-3-6)	-75.9	(4-1-3-7)	160.1				
(11-1-3-5)	-88.9	(11-1-3-6)	153.2	(11-1-3-7)	29.2				
(12-1-3-5)	87.2	(12-1-3-6)	-30.8	(12-1-3-7)	-154.7				
(2-1-4-8)	-38.7	(2-1-4-9)	-156.1	(2-1-4-10)	81.9				
(3-1-4-8)	98.5	(3-1-4-9)	-18.9	(3-1-4-10)	-141.0				
(11-1-4-8)	-130.7	(11-1-4-9)	112.0	(11-1-4-10)	-10.1				
(12-1-4-8)	53.3	(12-1-4-9)	-64.1	(12-1-4-10)	173.9				

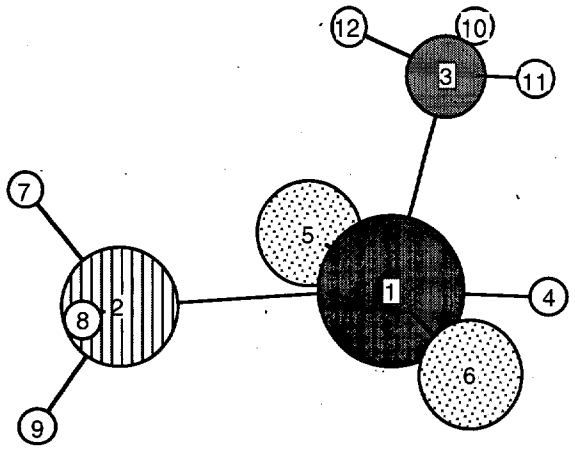
Frequencies(cm-1): 35.3 88.4 95.1 105.7 130.2 136.3 206.6 219.1
325.7 349.0 383.6 413.9 429.8 491.9 558.5 836.2 888.3 1011.6
1136.8 1139.6 1259.2 1442.5 1456.7 2459.4 2473.9 2480.3 2489.1 3047.9

3160.5 3205.7

Five-Coordinate Reactant Complex (**7c**), with chlorines mutually *trans*.
CH_3-trans site empty, $(PH_3)Cl_2Pt(CH_3)H$, B3LYP, C_1 Geometry

Zero Point Energy	.075007
Thermal correction to Enthalpy at 298K:	.086603

Nuclear Repulsion	477.465962
B3LYP	-1423.895476
CCSD(T) single point	-1421.361394



	X	Y	Z
Pt1	-.034049	-.469801	-.282834
P2	.117874	2.040373	.244827
C3	-.056963	-1.339354	1.601444
H4	-.094220	-1.951407	-.715979
Cl5	2.320157	-.550947	-.423329
Cl6	-2.384590	-.385883	-.412620
H7	1.057866	2.474708	1.212536
H8	-1.016537	2.765470	.688243
H9	.514259	2.897577	-.812444
H10	.818224	-1.985010	1.662117
H11	-.996823	-1.883625	1.684587
H12	-.000851	-.504663	2.302024

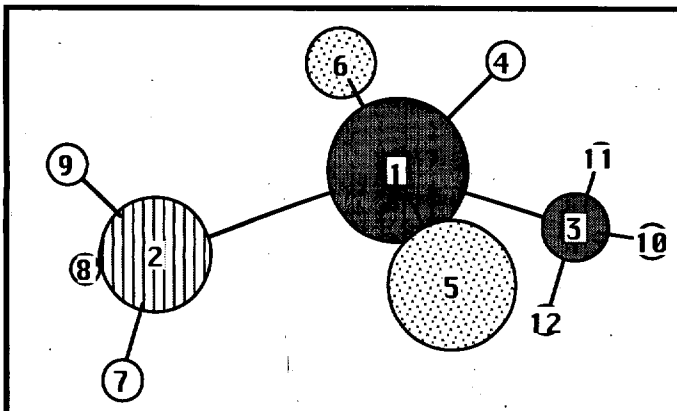
(1-2)	2.570	(1-3)	2.075	(1-4)	1.545	(1-5)	2.360	(1-6)	2.356
(2-7)	1.417	(2-8)	1.417	(2-9)	1.418	(3-10)	1.089	(3-11)	1.089
(3-12)	1.091								
(2-1-3)	102.9	(2-1-4)	175.4	(2-1-5)	89.2	(2-1-6)	92.0		
(3-1-4)	81.5	(3-1-5)	92.9	(3-1-6)	93.1	(4-1-5)	89.4		
(4-1-6)	88.8	(5-1-6)	173.4	(1-2-7)	118.6	(1-2-8)	121.1		
(1-2-9)	117.0	(7-2-8)	99.2	(7-2-9)	98.0	(8-2-9)	98.5		
(1-3-10)	106.9	(1-3-11)	106.7	(1-3-12)	105.2	(10-3-11)	113.1		
(10-3-12)	112.1	(11-3-12)	112.2						
(3-1-2-7)	46.3	(3-1-2-8)	-76.6	(3-1-2-9)	163.4				
(4-1-2-7)	-119.0	(4-1-2-8)	118.1	(4-1-2-9)	-2.0				
(5-1-2-7)	-46.5	(5-1-2-8)	-169.4	(5-1-2-9)	70.6				
(6-1-2-7)	139.9	(6-1-2-8)	17.1	(6-1-2-9)	-103.0				
(2-1-3-10)	-119.2	(2-1-3-11)	119.5	(2-1-3-12)	0.1				
(4-1-3-10)	59.6	(4-1-3-11)	-61.7	(4-1-3-12)	178.9				
(5-1-3-10)	-29.3	(5-1-3-11)	-150.6	(5-1-3-12)	90.0				
(6-1-3-10)	148.0	(6-1-3-11)	26.7	(6-1-3-12)	-92.7				

Frequencies(cm-1): 34.6 66.3 80.0 89.3 118.0 123.0 147.4 187.2
325.6 338.5 348.9 399.5 544.7 812.2 821.5 861.4 879.7 1012.0
1137.7 1140.2 1261.2 1445.5 1455.5 2345.6 2458.6 2479.5 2482.5 3085.9
3211.2 3230.8

Transition State for isomerization of **7c** to **7b**.
$(PH_3)Cl_2Pt(CH_3)H$, B3LYP, C_1 Geometry

Zero Point Energy	.074371
Thermal correction to Enthalpy at 298K:	.085134

Nuclear Repulsion	475.155964
B3LYP	-1423.891992
CCSD(T) single point	-1421.357758



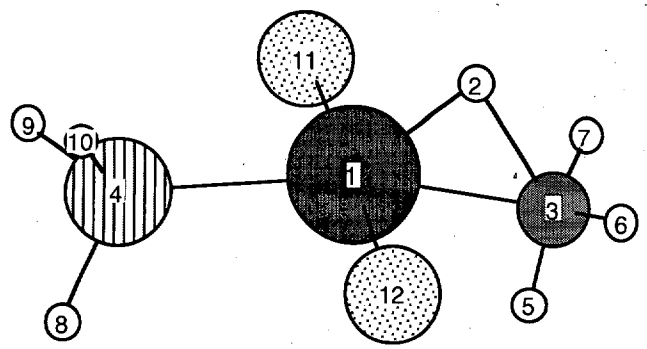
	X	Y	Z
Pt1	.000004	-.219942	-.107513
P2	-.000032	2.311499	.317113
C3	.000024	-2.031326	.937779
H4	.000017	-1.398241	-1.087090
Cl5	2.359371	-.177931	-.157970
Cl6	-2.359366	-.177981	-.157971
H7	1.087153	2.935027	.975566
H8	-1.087213	2.934982	.975616
H9	-.000076	3.079381	-.872921
H10	.909918	-2.584961	.708129
H11	-.909857	-2.584983	.708127
H12	.000018	-1.659766	1.966186

(1-2)	2.567	(1-3)	2.091	(1-4)	1.532	(1-5)	2.360	(1-6)	2.360
(2-7)	1.416	(2-8)	1.416	(2-9)	1.416	(3-4)	2.122	(3-10)	1.090
(3-11)	1.090	(3-12)	1.093						
(2-1-3)	140.5	(2-1-4)	149.8	(2-1-5)	89.2	(2-1-6)	89.2		
(3-1-4)	69.7	(3-1-5)	91.5	(3-1-6)	91.5	(4-1-5)	90.0		
(4-1-6)	90.0	(5-1-6)	176.8	(1-2-7)	120.7	(1-2-8)	120.7		
(1-2-9)	113.3	(7-2-8)	100.3	(7-2-9)	98.7	(8-2-9)	98.7		
(1-3-4)	42.7	(1-3-10)	109.6	(1-3-11)	109.6	(1-3-12)	100.1		
(4-3-10)	87.2	(4-3-11)	87.2	(4-3-12)	142.8	(10-3-11)	113.3		
(10-3-12)	111.8	(11-3-12)	111.8	(1-4-3)	67.6				
(3-1-2-7)	63.3	(3-1-2-8)	-63.3	(3-1-2-9)	180.0				
(4-1-2-7)	-116.7	(4-1-2-8)	116.7	(4-1-2-9)	0.0				
(5-1-2-7)	-28.1	(5-1-2-8)	-154.7	(5-1-2-9)	88.6				
(6-1-2-7)	154.7	(6-1-2-8)	28.1	(6-1-2-9)	-88.6				
(2-1-3-4)	180.0	(2-1-3-10)	-117.6	(2-1-3-11)	117.6				
(2-1-3-12)	0.0	(4-1-3-10)	62.4	(4-1-3-11)	-62.4				
(4-1-3-12)	180.0	(5-1-3-4)	-89.4	(5-1-3-10)	-27.0				
(5-1-3-11)	-151.9	(5-1-3-12)	90.6	(6-1-3-4)	89.4				
(6-1-3-10)	151.9	(6-1-3-11)	27.0	(6-1-3-12)	-90.6				
(2-1-4-3)	180.0	(5-1-4-3)	91.6	(6-1-4-3)	-91.6				
(10-3-4-1)	-123.3	(11-3-4-1)	123.3	(12-3-4-1)	0.0				

Frequencies(cm-1): -75.7 50.5 105.8 112.6 120.6 125.3 172.1 177.8
324.3 338.3 347.8 415.2 503.4 650.7 661.3 854.5 897.9 1001.5
1133.6 1137.7 1254.9 1447.6 1456.3 2399.3 2470.5 2492.5 2496.7 3074.1
3195.9 3226.2

Five-Coordinate Transition State (**8b**), with chlorines mutually *trans*.
$(PH_3)Cl_2Pt(CH_3)H$, B3LYP, C_1 Geometry

Zero Point Energy	.073320	Nuclear Repulsion	479.524151
Thermal correction to Enthalpy at 298K:	.084485	B3LYP	-1423.893209
		CCSD(T) single point	-1421.357320



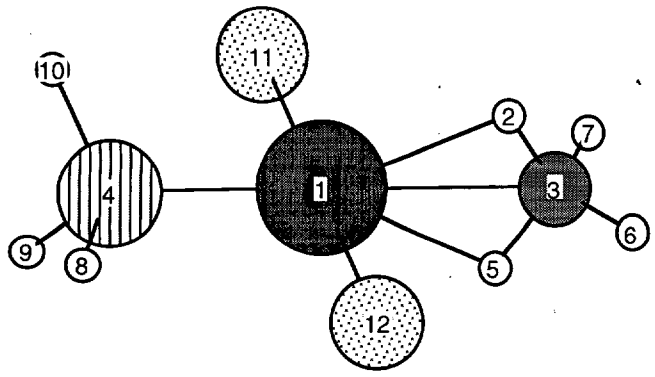
	X	Y	Z
Pt1	-.041413	-.318069	-.063312
H2	-.128339	-1.347932	-1.214868
C3	-.206059	-2.430826	.193879
P4	.209007	2.098278	.061760
H5	-.188447	-2.398159	1.288740
H6	.658081	-2.977374	-.184976
H7	-1.156354	-2.829429	-.161699
H8	.678749	2.654450	1.276530
H9	-.919317	2.918934	-.167878
H10	1.145580	2.665487	-.831060
Cl11	-2.394994	-.111493	-.027048
Cl12	2.321861	-.467916	-.029120

(1-2)	1.547	(1-3)	2.135	(1-4)	2.433	(1-11)	2.363	(1-12)	2.368
(2-3)	1.779	(3-5)	1.095	(3-6)	1.090	(3-7)	1.090	(4-8)	1.416
(4-9)	1.414	(4-10)	1.413						
(2-1-3)	55.0	(2-1-4)	134.8	(2-1-11)	90.8	(2-1-12)	91.4		
(3-1-4)	170.0	(3-1-11)	90.4	(3-1-12)	90.7	(4-1-11)	90.9		
(4-1-12)	87.7	(11-1-12)	177.8	(1-2-3)	79.5	(1-3-2)	45.5		
(1-3-5)	95.1	(1-3-6)	113.1	(1-3-7)	112.9	(2-3-5)	140.6		
(2-3-6)	89.7	(2-3-7)	90.1	(5-3-6)	110.5	(5-3-7)	110.5		
(6-3-7)	113.2	(1-4-8)	117.9	(1-4-9)	119.1	(1-4-10)	115.8		
(8-4-9)	100.1	(8-4-10)	99.5	(9-4-10)	101.1				
(4-1-2-3)	178.0	(11-1-2-3)	-90.0	(12-1-2-3)	89.9				
(2-1-3-5)	179.5	(2-1-3-6)	64.7	(2-1-3-7)	-65.6				
(4-1-3-2)	-171.8	(4-1-3-5)	7.7	(4-1-3-6)	-107.2				
(4-1-3-7)	122.5	(11-1-3-2)	90.6	(11-1-3-5)	-89.8				
(11-1-3-6)	155.3	(11-1-3-7)	25.0	(12-1-3-2)	-91.2				
(12-1-3-5)	88.3	(12-1-3-6)	-26.5	(12-1-3-7)	-156.8				
(2-1-4-8)	-159.8	(2-1-4-9)	78.6	(2-1-4-10)	-42.3				
(3-1-4-8)	10.7	(3-1-4-9)	-110.8	(3-1-4-10)	128.3				
(11-1-4-8)	108.2	(11-1-4-9)	-13.3	(11-1-4-10)	-134.3				
(12-1-4-8)	-70.2	(12-1-4-9)	168.3	(12-1-4-10)	47.4				
(1-2-3-5)	-.8	(1-2-3-6)	-123.8	(1-2-3-7)	123.0				

Frequencies(cm-1): -628.5 32.9 75.5 105.7 115.1 126.3 132.0 181.0
273.9 322.8 347.0 439.9 470.6 525.2 533.6 863.2 932.3 1006.4
1130.0 1134.0 1255.2 1451.7 1452.9 2338.8 2475.3 2497.6 2511.7 3063.1
3174.5 3215.7

Five-Coordinate Product Complex (**9b**), with chlorines mutually *trans*.
$(PH_3)Cl_2Pt{\cdot}CH_4$, B3LYP, C_1 Geometry

Zero Point Energy	.076993	Nuclear Repulsion	479.694438
Thermal correction		B3LYP	-1423.930352
to Enthalpy at 298K:	.088886	CCSD(T) single point	-1421.393424



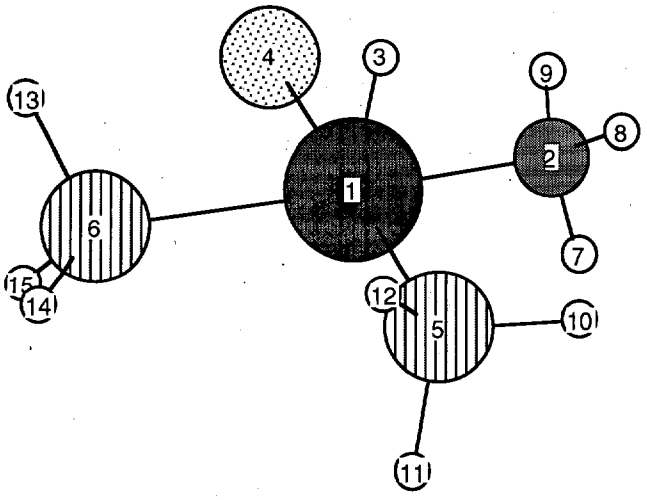
	X	Y	Z
Pt1	-.041915	.194888	-.000002
H2	-.286717	2.155318	-.940216
C3	-.355656	2.738041	.000007
P4	.293375	-1.990345	.000004
H5	-.286751	2.155311	.940228
H6	-1.334951	3.220368	-.000009
H7	.480564	3.439763	.000024
H8	-.867209	-2.793086	-.000054
H9	1.024073	-2.501668	1.094629
H10	1.024182	-2.501661	-1.094552
Cl11	2.307427	.469119	-.000003
Cl12	-2.381862	-.072378	-.000003

(1-2)	2.188	(1-3)	2.562	(1-4)	2.211	(1-5)	2.188	(1-11)	2.365
(1-12)	2.355	(2-3)	1.108	(3-5)	1.108	(3-6)	1.092	(3-7)	1.092
(4-8)	1.411	(4-9)	1.412	(4-10)	1.412				
(2-1-3)	25.5	(2-1-4)	154.5	(2-1-5)	50.9	(2-1-11)	90.4		
(2-1-12)	89.5	(3-1-4)	178.3	(3-1-5)	25.5	(3-1-11)	90.4		
(3-1-12)	89.5	(4-1-5)	154.5	(4-1-11)	87.9	(4-1-12)	92.2		
(5-1-11)	90.4	(5-1-12)	89.5	(11-1-12)	179.9	(1-2-3)	96.5		
(1-3-2)	58.0	(1-3-5)	58.0	(1-3-6)	123.3	(1-3-7)	123.0		
(2-3-5)	116.1	(2-3-6)	106.7	(2-3-7)	106.9	(5-3-6)	106.7		
(5-3-7)	106.9	(6-3-7)	113.8	(1-4-8)	115.9	(1-4-9)	115.9		
(1-4-10)	115.9	(8-4-9)	102.7	(8-4-10)	102.7	(9-4-10)	101.7		
(1-5-3)	96.5								
(4-1-2-3)	-176.1	(5-1-2-3)	0.2	(11-1-2-3)	-90.0				
(12-1-2-3)	89.9	(2-1-3-5)	179.6	(2-1-3-6)	89.8				
(2-1-3-7)	-90.2	(4-1-3-2)	90.2	(4-1-3-5)	-90.2				
(4-1-3-6)	180.0	(4-1-3-7)	0.0	(5-1-3-2)	-179.6				
(5-1-3-6)	-89.8	(5-1-3-7)	90.2	(11-1-3-2)	90.2				
(11-1-3-5)	-90.2	(11-1-3-6)	180.0	(11-1-3-7)	0.0				
(12-1-3-2)	-89.8	(12-1-3-5)	89.8	(12-1-3-6)	0.0				
(12-1-3-7)	180.0	(2-1-4-8)	-93.4	(2-1-4-9)	146.1				
(2-1-4-10)	27.1	(3-1-4-8)	180.0	(3-1-4-9)	59.5				
(3-1-4-10)	-59.5	(5-1-4-8)	93.4	(5-1-4-9)	-27.1				
(5-1-4-10)	-146.1	(11-1-4-8)	180.0	(11-1-4-9)	59.5				
(11-1-4-10)	-59.5	(12-1-4-8)	0.0	(12-1-4-9)	-120.5				
(12-1-4-10)	120.5	(2-1-5-3)	-.2	(4-1-5-3)	176.1				
(11-1-5-3)	90.0	(12-1-5-3)	-89.9	(1-2-3-5)	-.3				
(1-2-3-6)	-119.2	(1-2-3-7)	118.7	(2-3-5-1)	0.3				
(6-3-5-1)	119.2	(7-3-5-1)	-118.7						

Frequencies(cm-1): 55.8 75.5 102.3 103.7 112.5 129.7 172.0 200.6
203.7 279.7 323.9 346.3 400.2 601.1 620.1 1017.9 1121.5 1122.9
1223.5 1346.7 1371.2 1527.1 1570.7 2495.8 2510.4 2522.8 2911.1 2992.7
3127.4 3207.2

Five-Coordinate Cation Reactant Complex (**10a**), with PH_3 mutually *cis*.
H-trans site empty, $(PH_3)_2ClPt(CH_3)H^+$, B3LYP, C_1 Geometry

Zero Point Energy	.101478	Nuclear Repulsion	499.481996
Thermal correction		B3LYP	-1306.592752
to Enthalpy at 298K:	.114192	CCSD(T) single point	-1304.085691



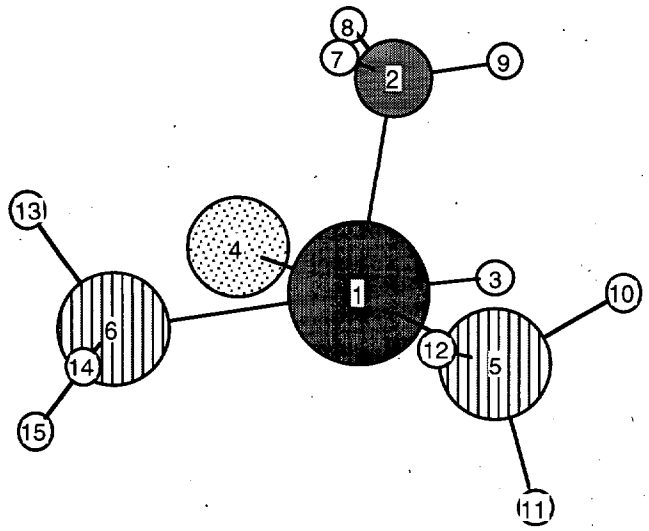
	X	Y	Z
Pt1	-.123687	-.293438	.020233
C2	-.737441	-2.308395	-.061212
H3	-.277608	-.517561	1.518744
C14	2.089125	-1.034601	-.020646
P5	-2.367814	.385315	-.021651
P6	.957308	2.002027	-.021198
H7	-.909382	-2.478733	-1.132007
H8	-1.644824	-2.503920	.513756
H9	.090079	-2.920690	.294905
H10	-3.318478	-.582950	.368371
H11	-2.851318	.781392	-1.290505
H12	-2.724137	1.492651	.779791
H13	1.848541	2.186563	1.057904
H14	.258420	3.235234	.003064
H15	1.822189	2.218355	-1.117235

(1-2)	2.108	(1-3)	1.523	(1-4)	2.334	(1-5)	2.345	(1-6)	2.538
(2-7)	1.098	(2-8)	1.092	(2-9)	1.089	(5-10)	1.412	(5-11)	1.414
(5-12)	1.413	(6-13)	1.412	(6-14)	1.418	(6-15)	1.413		
(2-1-3)	82.4	(2-1-4)	88.4	(2-1-5)	89.8	(2-1-6)	171.1		
(3-1-4)	93.8	(3-1-5)	87.9	(3-1-6)	101.1	(4-1-5)	177.4		
(4-1-6)	83.3	(5-1-6)	98.4	(1-2-7)	103.4	(1-2-8)	113.1		
(1-2-9)	107.7	(7-2-8)	110.8	(7-2-9)	110.5	(8-2-9)	111.0		
(1-5-10)	116.2	(1-5-11)	115.1	(1-5-12)	117.3	(10-5-11)	102.1		
(10-5-12)	102.2	(11-5-12)	101.7	(1-6-13)	112.0	(1-6-14)	125.2		
(1-6-15)	114.3	(13-6-14)	100.6	(13-6-15)	100.7	(14-6-15)	100.5		
(3-1-2-7)	170.7	(3-1-2-8)	50.8	(3-1-2-9)	-72.3				
(4-1-2-7)	-95.2	(4-1-2-8)	144.8	(4-1-2-9)	21.8				
(5-1-2-7)	82.8	(5-1-2-8)	-37.1	(5-1-2-9)	-160.2				
(6-1-2-7)	-75.4	(6-1-2-8)	164.6	(6-1-2-9)	41.6				
(2-1-5-10)	20.7	(2-1-5-11)	-98.5	(2-1-5-12)	141.9				
(3-1-5-10)	-61.7	(3-1-5-11)	179.0	(3-1-5-12)	59.4				
(4-1-5-10)	68.6	(4-1-5-11)	-50.6	(4-1-5-12)	-170.2				
(6-1-5-10)	-162.6	(6-1-5-11)	78.1	(6-1-5-12)	-41.5				
(2-1-6-13)	-77.1	(2-1-6-14)	161.0	(2-1-6-15)	36.7				
(3-1-6-13)	35.5	(3-1-6-14)	-86.5	(3-1-6-15)	149.3				
(4-1-6-13)	-57.1	(4-1-6-14)	-179.0	(4-1-6-15)	56.7				
(5-1-6-13)	125.0	(5-1-6-14)	3.0	(5-1-6-15)	-121.3				

Frequencies(cm-1):	25.7	82.1	87.9	100.0	112.8	129.3	138.9	215.9
231.9	309.6	358.2	385.7	438.9	455.7	505.5	527.4	574.0	603.4
834.2	894.4	999.6	1025.3	1114.8	1118.9	1122.4	1125.3	1273.6	1432.9
1465.6	2423.8	2466.0	2485.4	2504.2	2509.9	2517.8	2519.4	3048.2	3164.0

Five-Coordinate Cation Reactant Complex (**10b**), with PH_3 mutually *cis*.
CH_3-trans site empty, $(PH_3)_2ClPt(CH_3)H^+$, B3LYP, C_1 Geometry

Zero Point Energy	.102667	Nuclear Repulsion	500.430915
Thermal correction		B3LYP	-1306.591870
to Enthalpy at 298K:	.115176	CCSD(T) single point	-1304.084617



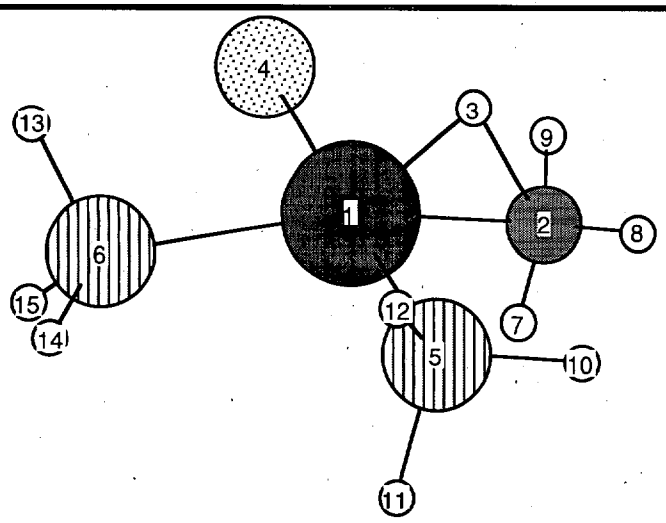
	X	Y	Z
Pt1	-.070490	-.238746	-.140519
C2	-.249243	-.950020	1.843534
H3	-.402188	-1.726647	-.467059
Cl4	2.179250	-.826197	-.327221
P5	-2.374442	.167143	-.257898
P6	.821573	2.124264	.227966
H7	-.509311	-.070808	2.434917
H8	.743166	-1.338432	2.067603
H9	-1.011332	-1.727349	1.876477
H10	-3.211015	-.833670	.282298
H11	-2.870775	.283239	-1.576299
H12	-2.894981	1.332671	.349455
H13	1.741971	2.206193	1.296643
H14	.031173	3.273402	.482089
H15	1.622747	2.597958	-.835125

(1-2)	2.115	(1-3)	1.559	(1-4)	2.333	(1-5)	2.342	(1-6)	2.553
(2-7)	1.091	(2-8)	1.089	(2-9)	1.089	(5-10)	1.412	(5-11)	1.414
(5-12)	1.414	(6-13)	1.413	(6-14)	1.418	(6-15)	1.413		
(2-1-3)	81.8	(2-1-4)	94.1	(2-1-5)	91.3	(2-1-6)	101.9		
(3-1-4)	87.0	(3-1-5)	86.9	(3-1-6)	171.2	(4-1-5)	171.2		
(4-1-6)	84.7	(5-1-6)	101.0	(1-2-7)	104.9	(1-2-8)	103.6		
(1-2-9)	109.1	(7-2-8)	113.1	(7-2-9)	113.1	(8-2-9)	112.1		
(1-5-10)	116.2	(1-5-11)	114.0	(1-5-12)	118.9	(10-5-11)	101.9		
(10-5-12)	101.6	(11-5-12)	101.8	(1-6-13)	113.0	(1-6-14)	125.6		
(1-6-15)	113.6	(13-6-14)	100.4	(13-6-15)	100.4	(14-6-15)	100.3		
(3-1-2-7)	-155.3	(3-1-2-8)	85.8	(3-1-2-9)	-33.8				
(4-1-2-7)	118.4	(4-1-2-8)	-.6	(4-1-2-9)	-120.2				
(5-1-2-7)	-68.6	(5-1-2-8)	172.5	(5-1-2-9)	52.9				
(6-1-2-7)	32.9	(6-1-2-8)	-86.0	(6-1-2-9)	154.4				
(2-1-5-10)	-42.9	(2-1-5-11)	-161.0	(2-1-5-12)	79.0				
(3-1-5-10)	38.8	(3-1-5-11)	-79.3	(3-1-5-12)	160.7				
(4-1-5-10)	85.0	(4-1-5-11)	-33.1	(4-1-5-12)	-153.2				
(6-1-5-10)	-145.3	(6-1-5-11)	96.7	(6-1-5-12)	-23.4				
(2-1-6-13)	37.5	(2-1-6-14)	-85.5	(2-1-6-15)	151.0				
(3-1-6-13)	-76.3	(3-1-6-14)	160.7	(3-1-6-15)	37.2				
(4-1-6-13)	-55.7	(4-1-6-14)	-178.6	(4-1-6-15)	57.8				
(5-1-6-13)	131.1	(5-1-6-14)	8.1	(5-1-6-15)	-115.4				

Frequencies(cm-1):	58.3	74.4	84.5	103.4	112.4	124.7	136.7	159.9
213.0	309.4	357.6	394.0	442.1	499.7	541.5	566.1	789.6	843.7
855.5	878.1	1001.0	1027.1	1115.5	1121.0	1126.0	1126.6	1270.5	1439.1
1461.4	2284.1	2467.4	2486.9	2502.5	2507.3	2514.0	2517.0	3090.4	3224.0

Five-Coordinate Cation Transition State (**11**), with PH_3 mutually *cis*.
$(PH_3)_2ClPt(CH_3)H^+$, B3LYP, C_1 Geometry

Zero Point Energy	.101160	Nuclear Repulsion	500.932952
Thermal correction to Enthalpy at 298K:	.113261	B3LYP	-1306.591267
		CCSD(T) single point	-1304.082740



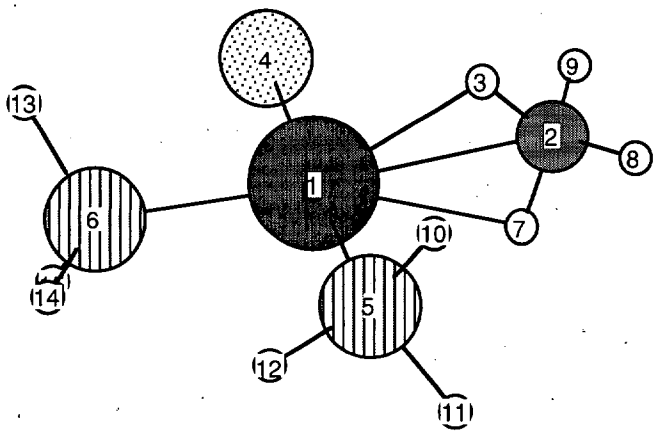
	X	Y	Z
Pt1	.120533	-.294028	-.071030
C2	.592976	-2.351055	.330751
H3	.397674	-1.242503	-1.259585
C14	-2.147021	-.890481	-.104728
P5	2.378399	.316838	-.070606
P6	-.846718	1.994105	.119494
H7	.602461	-2.271435	1.423397
H8	1.555860	-2.685960	-.056784
H9	-.227482	-2.979846	-.011299
H10	3.306628	-.726542	-.281489
H11	2.872398	.902893	1.117941
H12	2.781452	1.262168	-1.040467
H13	-1.694664	2.282782	-.969462
H14	-.076941	3.180439	.202364
H15	-1.720699	2.150860	1.216450

(1-2)	2.148	(1-3)	1.546	(1-4)	2.345	(1-5)	2.339	(1-6)	2.491
(2-3)	1.948	(2-7)	1.096	(2-8)	1.091	(2-9)	1.089	(5-10)	1.412
(5-11)	1.414	(5-12)	1.413	(6-13)	1.410	(6-14)	1.417	(6-15)	1.411
(2-1-3)	61.1	(2-1-4)	88.4	(2-1-5)	92.2	(2-1-6)	161.9		
(3-1-4)	90.4	(3-1-5)	89.3	(3-1-6)	133.8	(4-1-5)	179.1		
(4-1-6)	81.9	(5-1-6)	97.8	(1-2-3)	44.0	(1-2-7)	96.8		
(1-2-8)	114.9	(1-2-9)	109.2	(3-2-7)	140.7	(3-2-8)	88.5		
(3-2-9)	89.8	(7-2-8)	111.7	(7-2-9)	111.2	(8-2-9)	112.1		
(1-3-2)	74.9	(1-5-10)	116.2	(1-5-11)	116.5	(1-5-12)	116.7		
(10-5-11)	101.7	(10-5-12)	101.8	(11-5-12)	101.5	(1-6-13)	111.2		
(1-6-14)	124.2	(1-6-15)	113.7	(13-6-14)	101.6	(13-6-15)	101.8		
(14-6-15)	101.4								
(3-1-2-7)	176.1	(3-1-2-8)	58.4	(3-1-2-9)	-68.6				
(4-1-2-3)	91.3	(4-1-2-7)	-92.6	(4-1-2-8)	149.7				
(4-1-2-9)	22.7	(5-1-2-3)	-88.0	(5-1-2-7)	88.2				
(5-1-2-8)	-29.6	(5-1-2-9)	-156.5	(6-1-2-3)	148.7				
(6-1-2-7)	-35.2	(6-1-2-8)	-152.9	(6-1-2-9)	80.1				
(4-1-3-2)	-88.0	(5-1-3-2)	92.9	(6-1-3-2)	-167.1				
(2-1-5-10)	20.4	(2-1-5-11)	-99.4	(2-1-5-12)	140.6				
(3-1-5-10)	-40.7	(3-1-5-11)	-160.4	(3-1-5-12)	79.5				
(4-1-5-10)	-106.7	(4-1-5-11)	133.5	(4-1-5-12)	13.5				
(6-1-5-10)	-174.8	(6-1-5-11)	65.4	(6-1-5-12)	-54.7				
(2-1-6-13)	-116.2	(2-1-6-14)	122.1	(2-1-6-15)	-2.0				
(3-1-6-13)	24.7	(3-1-6-14)	-96.9	(3-1-6-15)	139.0				
(4-1-6-13)	-58.0	(4-1-6-14)	-179.6	(4-1-6-15)	56.3				
(5-1-6-13)	121.2	(5-1-6-14)	-.5	(5-1-6-15)	-124.5				
(7-2-3-1)	-6.1	(8-2-3-1)	-129.4	(9-2-3-1)	118.5				

Frequencies(cm-1):	-332.0	63.2	71.3	106.1	117.1	122.0	140.1	143.8
208.3	273.2	312.1	354.0	448.1	490.5	514.7	534.2	566.6	644.7
856.7	923.1	993.8	1028.3	1111.9	1121.0	1122.3	1124.5	1269.2	1436.2
1464.1	2335.5	2474.5	2486.0	2506.5	2515.2	2515.2	2532.2	3064.1	3185.1

Five-Coordinate Cation Product Complex (**12**), with PH_3 mutually *trans*.
$[(PH_3)_2ClPt{\cdot}CH_4]^+$, B3LYP, C_1 Geometry

Zero Point Energy	.104353	Nuclear Repulsion	502.568417
Thermal correction		B3LYP	-1306.630031
to Enthalpy at 298K:	.117186	CCSD(T) single point	-1304.119168



	X	Y	Z
Pt1	-.090313	.192864	-.018142
C2	-.610196	2.681614	.053938
H3	-.500166	2.049611	-.865412
C14	2.188106	.743675	-.023594
P5	-2.349447	-.377499	-.016102
P6	.774958	-1.895818	.028206
H7	-.502919	2.189358	1.037056
H8	-1.601992	3.135723	.000246
H9	.199372	3.410905	-.020694
H10	-3.128797	.148574	-1.072695
H11	-3.099710	.027719	1.112557
H12	-2.689028	-1.747663	-.087424
H13	1.592722	-2.199148	-1.077508
H14	-.150851	-2.964122	.047430
H15	1.587693	-2.154931	1.148907

(1-2)	2.543	(1-3)	2.082	(1-4)	2.344	(1-5)	2.330	(1-6)	2.261
(1-7)	2.296	(2-3)	1.121	(2-7)	1.105	(2-8)	1.092	(2-9)	1.092
(5-10)	1.414	(5-11)	1.415	(5-12)	1.413	(6-13)	1.408	(6-14)	1.414
(6-15)	1.408								

(2-1-3)	25.6	(2-1-4)	88.2	(2-1-5)	92.4	(2-1-6)	168.9
(2-1-7)	25.7	(3-1-4)	88.9	(3-1-5)	91.6	(3-1-6)	155.2
(3-1-7)	51.4	(4-1-5)	179.4	(4-1-6)	81.1	(4-1-7)	88.4
(5-1-6)	98.3	(5-1-7)	92.2	(6-1-7)	149.6	(1-2-3)	53.5
(1-2-7)	64.5	(1-2-8)	126.2	(1-2-9)	120.0	(3-2-7)	118.0
(3-2-8)	106.5	(3-2-9)	104.3	(7-2-8)	108.5	(7-2-9)	106.6
(8-2-9)	113.1	(1-3-2)	100.9	(1-5-10)	116.3	(1-5-11)	116.4
(1-5-12)	118.0	(10-5-11)	101.4	(10-5-12)	101.0	(11-5-12)	101.0
(1-6-13)	113.9	(1-6-14)	116.6	(1-6-15)	114.0	(13-6-14)	103.2
(13-6-15)	104.5	(14-6-15)	103.2	(1-7-2)	89.8		

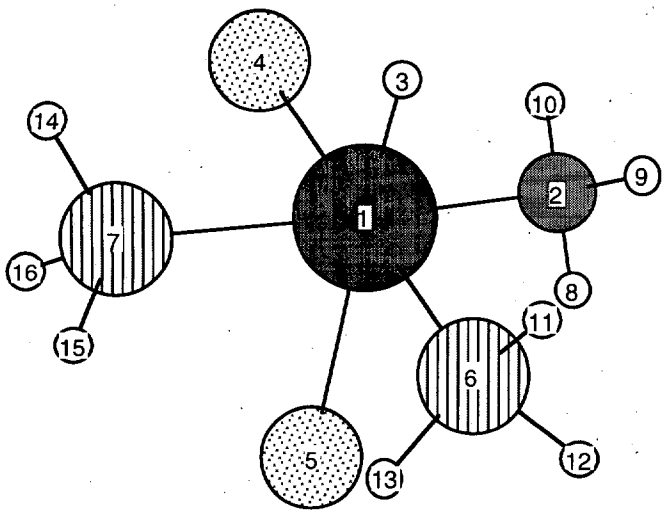
(3-1-2-7)	178.9	(3-1-2-8)	83.9	(3-1-2-9)	-85.9
(4-1-2-3)	91.2	(4-1-2-7)	-89.9	(4-1-2-8)	175.1
(4-1-2-9)	5.3	(5-1-2-3)	-88.7	(5-1-2-7)	90.1
(5-1-2-8)	-4.8	(5-1-2-9)	-174.6	(6-1-2-3)	106.0
(6-1-2-7)	-75.2	(6-1-2-8)	-170.1	(6-1-2-9)	20.1
(7-1-2-3)	-178.9	(7-1-2-8)	-94.9	(7-1-2-9)	95.2
(4-1-3-2)	-88.2	(5-1-3-2)	92.2	(6-1-3-2)	-153.9
(7-1-3-2)	0.6	(2-1-5-10)	58.1	(2-1-5-11)	-61.3
(2-1-5-12)	178.3	(3-1-5-10)	32.4	(3-1-5-11)	-87.0
(3-1-5-12)	152.7	(4-1-5-10)	-115.4	(4-1-5-11)	125.2
(4-1-5-12)	4.9	(6-1-5-10)	-124.7	(6-1-5-11)	115.9
(6-1-5-12)	-4.5	(7-1-5-10)	83.8	(7-1-5-11)	-35.5
(7-1-5-12)	-155.9	(2-1-6-13)	-74.9	(2-1-6-14)	165.1
(2-1-6-15)	44.9	(3-1-6-13)	7.5	(3-1-6-14)	-112.6
(3-1-6-15)	127.2	(4-1-6-13)	-59.9	(4-1-6-14)	180.0
(4-1-6-15)	59.9	(5-1-6-13)	120.0	(5-1-6-14)	-.1
(5-1-6-15)	-120.2	(7-1-6-13)	-131.0	(7-1-6-14)	109.0
(7-1-6-15)	-11.2	(3-1-7-2)	-.6	(4-1-7-2)	89.3
(5-1-7-2)	-90.9	(6-1-7-2)	158.5	(7-2-3-1)	-1.1
(8-2-3-1)	-123.2	(9-2-3-1)	116.9	(3-2-7-1)	1.0
(8-2-7-1)	122.1	(9-2-7-1)	-115.8		

Frequencies(cm-1):	38.0	56.3	103.0	113.0	133.7	144.3	148.9	181.5
214.3	276.3	312.7	315.8	351.1	377.1	537.7	560.2	602.2	631.7
1008.3	1038.3	1105.1	1115.8	1122.6	1124.6	1184.4	1338.5	1391.5	1519.5
1558.2	2482.0	2490.6	2499.3	2504.7	2532.0	2547.7	2809.9	3004.0	3125.4

Six-Coordinate Reactant Complex (**13a**), chlorines *cis*.
H is *trans* to Cl, $(PH_3)_2Cl_2Pt(CH_3)H$, B3LYP, C_1 Geometry

Zero Point Energy	.104495
Thermal correction to Enthalpy at 298K:	.118274

Nuclear Repulsion	728.470880
B3LYP	-1767.065204
CCSD(T) single point	-1763.990947



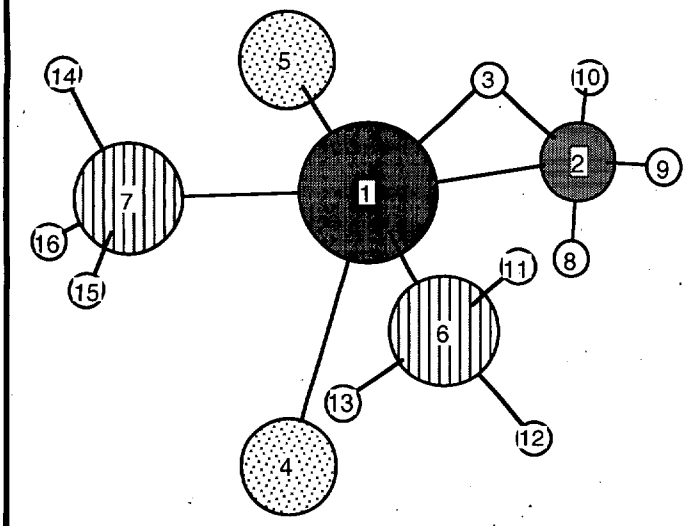
	X	Y	Z
Pt1	-.005517	-.307520	-.427952
C2	.626591	-2.319103	-.329483
H3	-.291828	-.595281	-1.928436
Cl4	-2.262528	-1.029771	-.035753
Cl5	.674712	.208755	1.958863
P6	2.201099	.269858	-.723277
P7	-1.055318	1.938482	-.397185
H8	1.046619	-2.446074	.671150
H9	1.357676	-2.568155	-1.104928
H10	-.273057	-2.921918	-.453829
H11	2.753782	.222722	-2.029352
H12	3.115217	-.535736	-.014715
H13	2.588147	1.565680	-.320813
H14	-1.994396	2.279232	-1.401747
H15	-.312427	3.150405	-.378731
H16	-1.843829	2.131270	.755509

(1-2)	2.111	(1-3)	1.554	(1-4)	2.402	(1-5)	2.535	(1-6)	2.300
(1-7)	2.479	(2-8)	1.093	(2-9)	1.094	(2-10)	1.090	(6-11)	1.419
(6-12)	1.409	(6-13)	1.411	(7-14)	1.417	(7-15)	1.422	(7-16)	1.410
(2-1-3)	85.6	(2-1-4)	89.3	(2-1-5)	94.0	(2-1-6)	87.6		
(2-1-7)	171.7	(3-1-4)	85.9	(3-1-5)	174.9	(3-1-6)	95.7		
(3-1-7)	95.8	(4-1-5)	99.2	(4-1-6)	176.3	(4-1-7)	82.7		
(5-1-6)	79.2	(5-1-7)	85.3	(6-1-7)	100.4	(1-2-8)	105.6		
(1-2-9)	112.6	(1-2-10)	105.9	(8-2-9)	111.4	(8-2-10)	110.9		
(9-2-10)	110.2	(1-6-11)	118.9	(1-6-12)	114.5	(1-6-13)	117.2		
(11-6-12)	101.0	(11-6-13)	100.7	(12-6-13)	101.7	(1-7-14)	119.3		
(1-7-15)	123.4	(1-7-16)	111.8	(14-7-15)	98.7	(14-7-16)	100.1		
(15-7-16)	99.5								
(3-1-2-8)	173.3	(3-1-2-9)	51.5	(3-1-2-10)	-69.0				
(4-1-2-8)	-100.8	(4-1-2-9)	137.4	(4-1-2-10)	17.0				
(5-1-2-8)	-1.6	(5-1-2-9)	-123.4	(5-1-2-10)	116.1				
(6-1-2-8)	77.4	(6-1-2-9)	-44.5	(6-1-2-10)	-164.9				
(7-1-2-8)	-86.3	(7-1-2-9)	151.9	(7-1-2-10)	31.5				
(2-1-6-11)	84.4	(2-1-6-12)	-35.0	(2-1-6-13)	-154.0				
(3-1-6-11)	-.9	(3-1-6-12)	-120.4	(3-1-6-13)	120.6				
(4-1-6-11)	115.2	(4-1-6-12)	-4.3	(4-1-6-13)	-123.3				
(5-1-6-11)	179.0	(5-1-6-12)	59.5	(5-1-6-13)	-59.5				
(7-1-6-11)	-98.0	(7-1-6-12)	142.6	(7-1-6-13)	23.6				
(2-1-7-14)	-79.1	(2-1-7-15)	155.6	(2-1-7-16)	37.1				
(3-1-7-14)	20.6	(3-1-7-15)	-104.7	(3-1-7-16)	136.8				
(4-1-7-14)	-64.5	(4-1-7-15)	170.2	(4-1-7-16)	51.7				
(5-1-7-14)	-164.4	(5-1-7-15)	70.3	(5-1-7-16)	-48.2				
(6-1-7-14)	117.5	(6-1-7-15)	-7.8	(6-1-7-16)	-126.3				

Frequencies(cm-1): 70.5 97.1 105.6 111.3 125.8 133.0 145.7 157.9
167.5 216.1 232.9 272.3 319.5 339.5 459.9 462.9 531.7 585.9
596.7 755.4 805.6 875.0 881.1 1012.8 1039.0 1117.2 1129.0 1133.1
1136.7 1256.5 1458.2 1477.4 2301.5 2437.1 2453.5 2474.9 2510.4 2526.3
2527.8 3059.6 3166.4 3201.2

Six-Coordinate Transition State (**14**), chlorines *cis*.
H is *trans* to Cl, $(PH_3)_2Cl_2Pt(CH_3)H$, B3LYP, C_1 Geometry

Zero Point Energy .102570	Nuclear Repulsion 723.134615
Thermal correction	B3LYP -1767.034042
to Enthalpy at 298K: .116203	CCSD(T) single point -1763.951627



	X	Y	Z
Pt1	-.180709	-.277133	-.171125
C2	-.516972	-2.387063	.443121
H3	-.752615	-1.623018	-.824526
C14	-2.432332	.206526	.480117
C15	1.487819	.954248	1.699254
P6	2.035321	-.670037	-.660436
P7	-.153768	2.023470	-.817895
H8	-.200738	-2.162884	1.465941
H9	.124139	-3.155466	.005447
H10	-1.563413	-2.697283	.457879
H11	2.302619	-1.468818	-1.811618
H12	2.757417	-1.388276	.311946
H13	2.871645	.430709	-.923180
H14	-.953379	2.444996	-1.912241
H15	1.069511	2.650791	-1.154494
H16	-.624641	2.873350	.199523

(1-2)	2.223	(1-3)	1.602	(1-4)	2.393	(1-5)	2.793	(1-6)	2.303
(1-7)	2.390	(2-3)	1.499	(2-8)	1.094	(2-9)	1.092	(2-10)	1.092
(5-6)	2.917	(5-7)	3.190	(6-11)	1.426	(6-12)	1.408	(6-13)	1.407
(7-14)	1.419	(7-15)	1.415	(7-16)	1.407				
(2-1-3)	42.4	(2-1-4)	88.5	(2-1-5)	108.9	(2-1-6)	92.4		
(2-1-7)	171.9	(3-1-4)	86.8	(3-1-5)	149.0	(3-1-6)	96.5		
(3-1-7)	134.6	(4-1-5)	106.9	(4-1-6)	175.9	(4-1-7)	83.7		
(5-1-6)	69.1	(5-1-7)	75.5	(6-1-7)	95.5	(1-2-3)	46.1		
(1-2-8)	91.2	(1-2-9)	117.9	(1-2-10)	114.7	(3-2-8)	137.0		
(3-2-9)	96.4	(3-2-10)	90.3	(8-2-9)	110.4	(8-2-10)	108.8		
(9-2-10)	111.6	(1-3-2)	91.6	(1-5-6)	47.5	(1-5-7)	46.5		
(6-5-7)	69.2	(1-6-5)	63.4	(1-6-11)	116.6	(1-6-12)	115.7		
(1-6-13)	118.6	(5-6-11)	179.8	(5-6-12)	79.7	(5-6-13)	80.0		
(11-6-12)	100.1	(11-6-13)	100.1	(12-6-13)	102.9	(1-7-5)	58.0		
(1-7-14)	119.2	(1-7-15)	120.1	(1-7-16)	112.5	(5-7-14)	176.3		
(5-7-15)	83.8	(5-7-16)	78.7	(14-7-15)	99.9	(14-7-16)	100.9		
(15-7-16)	101.2								
(3-1-2-8)	-175.6	(3-1-2-9)	70.5	(3-1-2-10)	-64.2				
(4-1-2-3)	86.9	(4-1-2-8)	-88.7	(4-1-2-9)	157.4				
(4-1-2-10)	22.7	(5-1-2-3)	-165.7	(5-1-2-8)	18.7				
(5-1-2-9)	-95.2	(5-1-2-10)	130.1	(6-1-2-3)	-97.0				
(6-1-2-8)	87.4	(6-1-2-9)	-26.6	(6-1-2-10)	-161.2				
(7-1-2-3)	72.2	(7-1-2-8)	-103.4	(7-1-2-9)	142.6				
(7-1-2-10)	8.0	(4-1-3-2)	-91.3	(5-1-3-2)	27.0				
(6-1-3-2)	86.4	(7-1-3-2)	-169.2	(2-1-5-6)	85.2				
(2-1-5-7)	-172.9	(3-1-5-6)	66.4	(3-1-5-7)	168.2				
(4-1-5-6)	179.6	(4-1-5-7)	-78.6	(6-1-5-7)	101.8				
(7-1-5-6)	-101.8	(2-1-6-5)	-109.3	(2-1-6-11)	70.4				
(2-1-6-12)	-46.8	(2-1-6-13)	-169.8	(3-1-6-5)	-151.6				
(3-1-6-11)	28.1	(3-1-6-12)	-89.2	(3-1-6-13)	147.9				
(4-1-6-5)	-5.8	(4-1-6-11)	174.0	(4-1-6-12)	56.7				
(4-1-6-13)	-66.3	(5-1-6-11)	179.8	(5-1-6-12)	62.5				
(5-1-6-13)	-60.5	(7-1-6-5)	72.2	(7-1-6-11)	-108.0				
(7-1-6-12)	134.7	(7-1-6-13)	11.7	(2-1-7-5)	124.2				
(2-1-7-14)	-53.0	(2-1-7-15)	-176.5	(2-1-7-16)	64.7				
(3-1-7-5)	-171.5	(3-1-7-14)	11.3	(3-1-7-15)	-112.1				
(3-1-7-16)	129.1	(4-1-7-5)	109.3	(4-1-7-14)	-67.9				

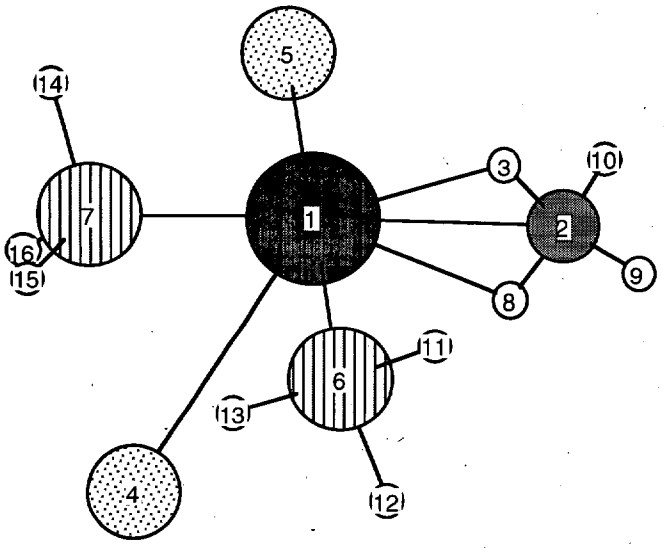
(4-1-7-15)	168.7	(4-1-7-16)	49.9	(5-1-7-14)	-177.2
(5-1-7-15)	59.3	(5-1-7-16)	-59.4	(6-1-7-5)	-66.7
(6-1-7-14)	116.1	(6-1-7-15)	-7.4	(6-1-7-16)	-126.1
(8-2-3-1)	6.5	(9-2-3-1)	-123.1	(10-2-3-1)	125.1
(1-5-6-11)	-86.0	(1-5-6-12)	-125.7	(1-5-6-13)	129.1
(7-5-6-1)	-49.4	(7-5-6-11)	-135.4	(7-5-6-12)	-175.1
(7-5-6-13)	79.7	(1-5-7-14)	41.1	(1-5-7-15)	-131.5
(1-5-7-16)	125.8	(6-5-7-1)	50.6	(6-5-7-14)	91.7
(6-5-7-15)	-80.9	(6-5-7-16)	176.3		

Frequencies(cm-1): -948.2 56.0 83.1 95.8 117.1 124.9 128.4 138.2
170.3 197.2 212.3 258.7 284.0 323.3 339.5 485.5 522.8 527.8
587.8 594.3 639.5 900.8 999.9 1011.3 1040.9 1092.6 1113.2 1130.7
1138.8 1263.5 1455.8 1473.9 2145.0 2398.0 2449.0 2481.2 2524.0 2543.9
2547.4 3068.1 3168.4 3190.4

Six-Coordinate Product Complex (**15**), chlorines *cis*.
$(PH_3)_2Cl_2Pt(CH_3)H$, B3LYP, C_1 Geometry

Zero Point Energy	.106144
Thermal correction to Enthalpy at 298K:	.120476

Nuclear Repulsion	704.725442
B3LYP	-1767.057310
CCSD(T) single point	-1763.967706



	X	Y	Z
Pt1	.402035	.136467	-.120479
C2	1.993608	2.065290	.739123
H3	1.838674	1.629404	-.279757
Cl4	2.145902	-1.380279	.361134
Cl5	-2.739166	-.405526	1.039998
P6	-1.319352	1.632578	-.554648
P7	-.870887	-1.674686	-.593201
H8	1.379579	1.627983	1.537348
H9	1.778543	3.133921	.661734
H10	3.041376	1.865429	.972999
H11	-.874402	2.747259	-1.332614
H12	-1.900867	2.310464	.531103
H13	-2.422431	1.232996	-1.328583
H14	-.070387	-2.447993	-1.481533
H15	-2.044050	-1.544990	-1.350883
H16	-1.107300	-2.600347	.431297

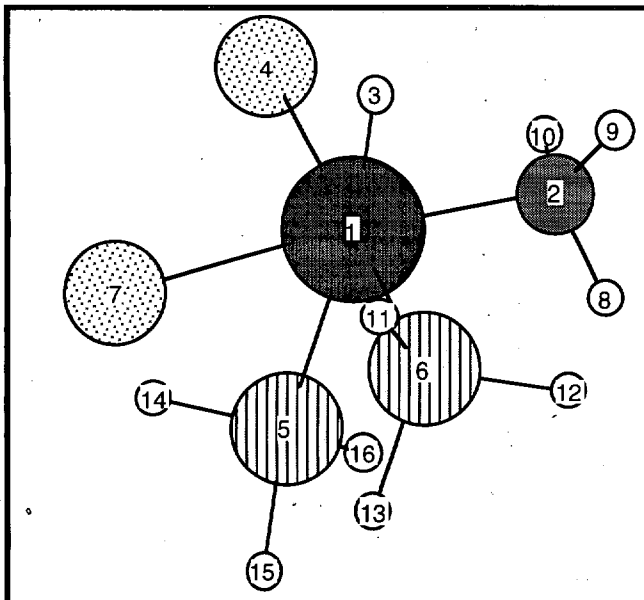
(1-2)	2.644	(1-3)	2.078	(1-4)	2.361	(1-5)	3.392	(1-6)	2.322
(1-7)	2.264	(1-8)	2.435	(2-3)	1.119	(2-8)	1.098	(2-9)	1.093
(2-10)	1.092	(5-6)	2.952	(5-7)	2.787	(6-11)	1.430	(6-12)	1.406
(6-13)	1.405	(7-14)	1.424	(7-15)	1.403	(7-16)	1.401		
(2-1-3)	23.8	(2-1-4)	87.6	(2-1-5)	124.2	(2-1-6)	92.1		
(2-1-7)	171.9	(2-1-8)	24.5	(3-1-4)	88.1	(3-1-5)	141.4		
(3-1-6)	92.0	(3-1-7)	161.4	(3-1-8)	48.3	(4-1-5)	120.8		
(4-1-6)	179.0	(4-1-7)	86.8	(4-1-8)	87.6	(5-1-6)	58.7		
(5-1-7)	54.8	(5-1-8)	103.7	(6-1-7)	93.4	(6-1-8)	91.7		
(7-1-8)	149.1	(1-2-3)	48.4	(1-2-8)	67.0	(1-2-9)	124.9		
(1-2-10)	120.9	(3-2-8)	115.4	(3-2-9)	106.8	(3-2-10)	104.9		
(8-2-9)	109.3	(8-2-10)	107.9	(9-2-10)	112.5	(1-3-2)	107.8		
(1-5-6)	42.2	(1-5-7)	41.5	(6-5-7)	71.1	(1-6-5)	79.1		
(1-6-11)	111.9	(1-6-12)	118.2	(1-6-13)	120.1	(5-6-11)	169.0		
(5-6-12)	73.5	(5-6-13)	74.0	(11-6-12)	100.0	(11-6-13)	99.6		
(12-6-13)	103.8	(1-7-5)	83.7	(1-7-14)	104.4	(1-7-15)	120.6		
(1-7-16)	118.1	(5-7-14)	171.7	(5-7-15)	73.4	(5-7-16)	76.1		
(14-7-15)	100.6	(14-7-16)	101.1	(15-7-16)	108.4	(1-8-2)	88.5		
(3-1-2-8)	179.7	(3-1-2-9)	81.6	(3-1-2-10)	-82.5				

(4-1-2-3)	90.7	(4-1-2-8)	-89.5	(4-1-2-9)	172.3
(4-1-2-10)	8.3	(5-1-2-3)	-143.1	(5-1-2-8)	36.7
(5-1-2-9)	-61.5	(5-1-2-10)	134.5	(6-1-2-3)	-90.2
(6-1-2-8)	89.5	(6-1-2-9)	-8.7	(6-1-2-10)	-172.7
(7-1-2-3)	136.8	(7-1-2-8)	-43.4	(7-1-2-9)	-141.6
(7-1-2-10)	54.4	(8-1-2-3)	-179.7	(8-1-2-9)	-98.2
(8-1-2-10)	97.8	(4-1-3-2)	-88.3	(5-1-3-2)	52.7
(6-1-3-2)	90.7	(7-1-3-2)	-162.4	(8-1-3-2)	0.1
(2-1-5-6)	68.8	(2-1-5-7)	-170.2	(3-1-5-6)	46.0
(3-1-5-7)	167.0	(4-1-5-6)	179.0	(4-1-5-7)	-60.0
(6-1-5-7)	121.0	(7-1-5-6)	-121.0	(8-1-5-6)	83.6
(8-1-5-7)	-155.4	(2-1-6-5)	-129.5	(2-1-6-11)	50.3
(2-1-6-12)	-65.1	(2-1-6-13)	166.4	(3-1-6-5)	-153.3
(3-1-6-11)	26.5	(3-1-6-12)	-88.8	(3-1-6-13)	142.6
(4-1-6-5)	-57.3	(4-1-6-11)	122.5	(4-1-6-12)	7.2
(4-1-6-13)	-121.4	(5-1-6-11)	179.8	(5-1-6-12)	64.5
(5-1-6-13)	-64.1	(7-1-6-5)	44.5	(7-1-6-11)	-135.7
(7-1-6-12)	109.0	(7-1-6-13)	-19.6	(8-1-6-5)	-105.0
(8-1-6-11)	74.8	(8-1-6-12)	-40.5	(8-1-6-13)	-169.1
(2-1-7-5)	85.7	(2-1-7-14)	-96.0	(2-1-7-15)	152.1
(2-1-7-16)	15.2	(3-1-7-5)	-153.9	(3-1-7-14)	24.3
(3-1-7-15)	-87.5	(3-1-7-16)	135.6	(4-1-7-5)	131.8
(4-1-7-14)	-49.9	(4-1-7-15)	-161.7	(4-1-7-16)	61.3
(5-1-7-14)	178.3	(5-1-7-15)	66.4	(5-1-7-16)	-70.5
(6-1-7-5)	-47.2	(6-1-7-14)	131.1	(6-1-7-15)	19.2
(6-1-7-16)	-117.7	(8-1-7-5)	52.0	(8-1-7-14)	-129.8
(8-1-7-15)	118.4	(8-1-7-16)	-18.6	(3-1-8-2)	-.1
(4-1-8-2)	89.4	(5-1-8-2)	-149.5	(6-1-8-2)	-91.3
(7-1-8-2)	169.1	(8-2-3-1)	-.3	(9-2-3-1)	-122.0
(10-2-3-1)	118.4	(3-2-8-1)	0.2	(9-2-8-1)	120.6
(10-2-8-1)	-116.7	(1-5-6-11)	-179.0	(1-5-6-12)	-124.0
(1-5-6-13)	125.9	(7-5-6-1)	-36.9	(7-5-6-11)	144.1
(7-5-6-12)	-160.9	(7-5-6-13)	89.0	(1-5-7-14)	-168.2
(1-5-7-15)	-124.6	(1-5-7-16)	121.0	(6-5-7-1)	37.5
(6-5-7-14)	-130.7	(6-5-7-15)	-87.1	(6-5-7-16)	158.5

Frequencies(cm-1):	44.3	59.4	91.1	103.5	115.2	125.9	141.4	164.7
171.6	208.0	277.6	293.6	305.5	318.7	336.6	378.8	387.6	558.4
573.6	604.2	631.2	990.7	1030.0	1053.8	1073.4	1133.6	1147.0	1231.2
1332.8	1384.3	1526.1	1573.9	2370.2	2411.8	2537.6	2550.4	2559.0	2588.3
2812.8	3060.8	3138.3	3195.3						

Six-Coordinate Reactant Complex (**13b**), chlorines *cis*.
H is *trans* to PH_3, $(PH_3)_2Cl_2Pt(CH_3)H$, B3LYP, C_1 Geometry

Zero Point Energy	.104131	Nuclear Repulsion	725.699357
Thermal correction		B3LYP	-1767.060735
to Enthalpy at 298K:	.118135	CCSD(T) single point	-1763.986771



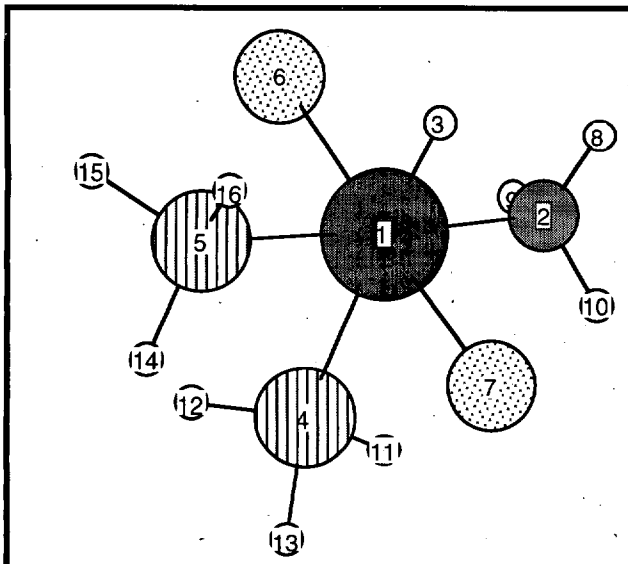
	X	Y	Z
Pt1	.018740	.373612	-.359160
C2	.614319	2.380616	-.105309
H3	-.220231	.742791	-1.851519
Cl4	2.273922	-.161115	-.962918
P5	.700373	-.417182	1.922245
P6	-2.224173	.780141	-.041442
Cl7	-.941509	-1.953312	-.605982
H8	.189899	2.773731	.824953
H9	.275050	2.984156	-.950462
H10	1.704422	2.387808	-.062444
H11	-3.051054	.431399	-1.127141
H12	-2.645960	2.113763	.205025
H13	-2.859320	.101984	1.020858
H14	1.397836	-1.640320	1.847409
H15	-.225272	-.741108	2.950683
H16	1.617356	.337947	2.698645

(1-2)	2.109	(1-3)	1.556	(1-4)	2.395	(1-5)	2.509	(1-6)	2.301
(1-7)	2.529	(2-8)	1.095	(2-9)	1.093	(2-10)	1.091	(5-14)	1.410
(5-15)	1.421	(5-16)	1.419	(6-11)	1.409	(6-12)	1.420	(6-13)	1.411
(2-1-3)	86.2	(2-1-4)	88.7	(2-1-5)	96.5	(2-1-6)	95.2		
(2-1-7)	174.0	(3-1-4)	87.5	(3-1-5)	171.4	(3-1-6)	86.6		
(3-1-7)	93.8	(4-1-5)	84.4	(4-1-6)	172.7	(4-1-7)	97.3		
(5-1-6)	101.2	(5-1-7)	84.4	(6-1-7)	78.8	(1-2-8)	109.5		
(1-2-9)	110.2	(1-2-10)	107.0	(8-2-9)	109.8	(8-2-10)	110.6		
(9-2-10)	109.7	(1-5-14)	111.1	(1-5-15)	123.6	(1-5-16)	120.4		
(14-5-15)	99.4	(14-5-16)	99.8	(15-5-16)	98.4	(1-6-11)	115.0		
(1-6-12)	118.6	(1-6-13)	117.2	(11-6-12)	101.1	(11-6-13)	101.4		
(12-6-13)	100.8								
(3-1-2-8)	137.4	(3-1-2-9)	16.6	(3-1-2-10)	-102.7				
(4-1-2-8)	-135.0	(4-1-2-9)	104.1	(4-1-2-10)	-15.1				
(5-1-2-8)	-50.8	(5-1-2-9)	-171.6	(5-1-2-10)	69.1				
(6-1-2-8)	51.2	(6-1-2-9)	-69.7	(6-1-2-10)	171.1				
(7-1-2-8)	47.5	(7-1-2-9)	-73.3	(7-1-2-10)	167.5				
(2-1-5-14)	-134.6	(2-1-5-15)	107.6	(2-1-5-16)	-18.7				
(3-1-5-14)	-26.8	(3-1-5-15)	-144.5	(3-1-5-16)	89.2				
(4-1-5-14)	-46.6	(4-1-5-15)	-164.3	(4-1-5-16)	69.4				
(6-1-5-14)	128.7	(6-1-5-15)	11.0	(6-1-5-16)	-115.3				
(7-1-5-14)	51.3	(7-1-5-15)	-66.4	(7-1-5-16)	167.3				
(2-1-6-11)	120.3	(2-1-6-12)	0.6	(2-1-6-13)	-120.7				
(3-1-6-11)	34.5	(3-1-6-12)	-85.2	(3-1-6-13)	153.5				
(4-1-6-11)	-1.4	(4-1-6-12)	-121.1	(4-1-6-13)	117.5				
(5-1-6-11)	-141.9	(5-1-6-12)	98.4	(5-1-6-13)	-23.0				
(7-1-6-11)	-60.1	(7-1-6-12)	-179.7	(7-1-6-13)	58.9				

Frequencies(cm-1): 63.0 75.1 90.2 106.6 107.2 126.2 134.5 154.0
179.3 207.6 216.1 271.9 322.2 339.4 431.8 441.4 533.1 584.8
589.8 767.1 832.3 869.0 873.5 1011.5 1039.4 1122.4 1128.1 1131.6
1135.5 1266.8 1460.2 1479.6 2300.0 2439.0 2443.7 2461.4 2512.3 2526.7
2535.7 3055.4 3155.2 3187.9

Six-Coordinate Reactant Complex (**13c**), chlorines *trans*.
$(PH_3)_2Cl_2Pt(CH_3)H$, B3LYP, C_1 Geometry

Zero Point Energy	.102734	Nuclear Repulsion	716.105737
Thermal correction to Enthalpy at 298K:	.117547	B3LYP	-1767.062470
		CCSD(T) single point	-1763.988572



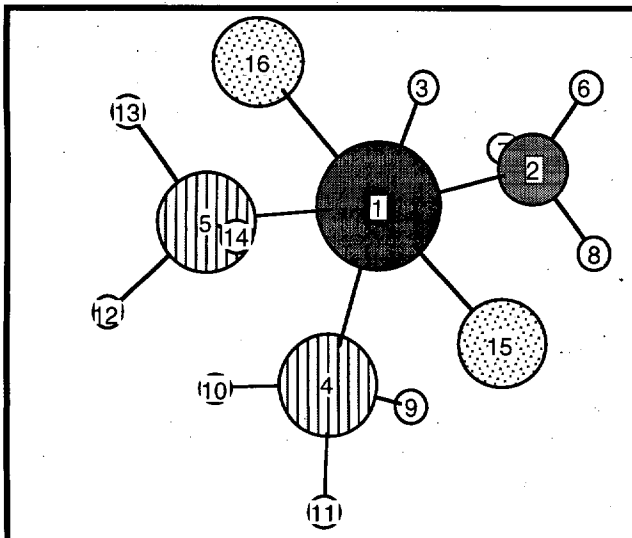
	X	Y	Z
Pt1	-.011437	-.054885	-.288466
C2	-.281872	-1.970085	-1.114832
H3	.059707	.407997	-1.765433
P4	-.179871	-1.018075	2.040552
P5	.379839	2.307599	.408791
Cl6	-2.383966	.274459	-.353633
Cl7	2.366504	-.376763	-.332224
H8	-.319928	-1.885532	-2.201441
H9	-1.227418	-2.366610	-.738731
H10	.572816	-2.579830	-.813984
H11	-.477589	-2.402769	2.098457
H12	-1.172435	-.559504	2.943653
H13	.935304	-1.009885	2.916889
H14	1.218342	2.623728	1.508762
H15	-.719299	3.146806	.720787
H16	1.011159	3.123494	-.560214

(1-2)	2.103	(1-3)	1.549	(1-4)	2.526	(1-5)	2.494	(1-6)	2.396
(1-7)	2.400	(2-8)	1.091	(2-9)	1.092	(2-10)	1.092	(4-11)	1.418
(4-12)	1.418	(4-13)	1.418	(5-14)	1.419	(5-15)	1.418	(5-16)	1.415
(2-1-3)	84.5	(2-1-4)	90.4	(2-1-5)	173.0	(2-1-6)	89.3		
(2-1-7)	89.9	(3-1-4)	174.8	(3-1-5)	88.6	(3-1-6)	88.8		
(3-1-7)	88.7	(4-1-5)	96.5	(4-1-6)	90.7	(4-1-7)	91.8		
(5-1-6)	91.9	(5-1-7)	88.7	(6-1-7)	177.4	(1-2-8)	109.0		
(1-2-9)	107.9	(1-2-10)	107.4	(8-2-9)	109.9	(8-2-10)	110.2		
(9-2-10)	112.3	(1-4-11)	115.1	(1-4-12)	120.7	(1-4-13)	121.0		
(11-4-12)	98.2	(11-4-13)	98.4	(12-4-13)	98.9	(1-5-14)	121.4		
(1-5-15)	120.0	(1-5-16)	115.1	(14-5-15)	99.0	(14-5-16)	98.0		
(15-5-16)	98.9								
(3-1-2-8)	-3.0	(3-1-2-9)	-122.3	(3-1-2-10)	116.4				
(4-1-2-8)	176.5	(4-1-2-9)	57.2	(4-1-2-10)	-64.1				
(5-1-2-8)	-13.6	(5-1-2-9)	-132.9	(5-1-2-10)	105.8				
(6-1-2-8)	85.9	(6-1-2-9)	-33.5	(6-1-2-10)	-154.8				
(7-1-2-8)	-91.7	(7-1-2-9)	149.0	(7-1-2-10)	27.7				
(2-1-4-11)	-4.2	(2-1-4-12)	-121.7	(2-1-4-13)	113.8				
(3-1-4-11)	1.5	(3-1-4-12)	-116.0	(3-1-4-13)	119.5				
(5-1-4-11)	177.1	(5-1-4-12)	59.6	(5-1-4-13)	-65.0				
(6-1-4-11)	85.1	(6-1-4-12)	-32.4	(6-1-4-13)	-156.9				
(7-1-4-11)	-94.1	(7-1-4-12)	148.4	(7-1-4-13)	23.9				
(2-1-5-14)	-129.9	(2-1-5-15)	105.9	(2-1-5-16)	-12.1				
(3-1-5-14)	-140.4	(3-1-5-15)	95.3	(3-1-5-16)	-22.7				
(4-1-5-14)	40.0	(4-1-5-15)	-84.3	(4-1-5-16)	157.7				
(6-1-5-14)	130.9	(6-1-5-15)	6.6	(6-1-5-16)	-111.4				
(7-1-5-14)	-51.7	(7-1-5-15)	-175.9	(7-1-5-16)	66.1				

Frequencies(cm-1):	35.9	44.2	45.7	85.9	90.2	97.3	110.3	128.6
162.8	202.6	211.3	221.7	310.0	332.8	405.3	410.7	437.6	441.1
537.7	805.3	825.7	876.3	880.8	1011.4	1026.1	1137.5	1140.3	1142.8
1145.1	1255.8	1452.5	1474.3	2331.0	2453.6	2455.3	2474.9	2476.3	2476.9
2488.8	3072.3	3187.6	3192.7						

Four-coordinate reactant complex, plus two chlorine atoms (**1+2Cl**)
$(PH_3)_2Cl_2Pt(CH_3)H$, B3LYP partial optimization, C_1 Geometry

Zero Point Energy	NA	Nuclear Repulsion	729.189460
Thermal correction		B3LYP	-1767.056431
to Enthalpy at 298K:	NA	CCSD(T) single point	-1763.983452



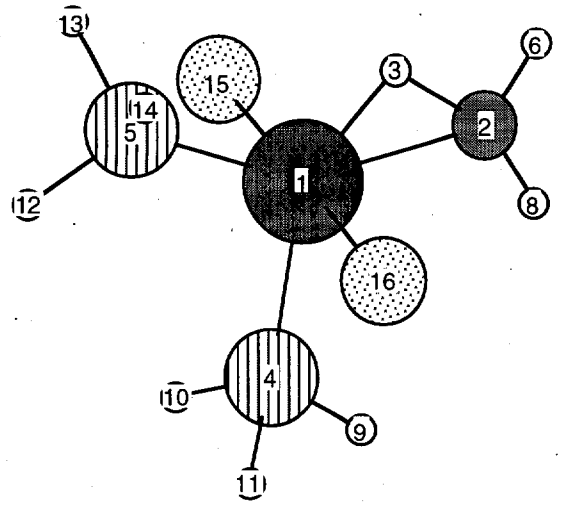
	X	Y	Z
Pt1	.000060	-.019761	-.251358
C2	.001027	-1.866691	-1.254219
H3	.000091	.567925	-1.726536
P4	.000979	-1.177826	1.839145
P5	-.001831	2.225267	.459491
H6	.001533	-1.757006	-2.339889
H7	-.890538	-2.439553	-.963847
H8	.892548	-2.439186	-.962990
H9	.000365	-2.597770	1.804608
H10	-1.059481	-1.021273	2.774490
H11	1.063179	-1.022162	2.772657
H12	-.002928	2.675030	1.812293
H13	-1.066527	3.051286	.011641
H14	1.062259	3.052741	.012882
Cl15	-2.404946	-.032089	-.310045
Cl16	2.405030	-.029099	-.310168

(1-2)	2.102	(1-3)	1.588	(1-4)	2.390	(1-5)	2.355	(1-15)	2.406
(1-16)	2.406	(2-6)	1.091	(2-7)	1.099	(2-8)	1.099	(4-9)	1.420
(4-10)	1.423	(4-11)	1.423	(5-12)	1.426	(5-13)	1.420	(5-14)	1.420
(2-1-3)	83.2	(2-1-4)	89.5	(2-1-5)	169.1	(2-1-15)	89.1		
(2-1-16)	89.1	(3-1-4)	172.7	(3-1-5)	85.8	(3-1-15)	88.8		
(3-1-16)	88.8	(4-1-5)	101.4	(4-1-15)	91.1	(4-1-16)	91.1		
(5-1-15)	90.7	(5-1-16)	90.7	(15-1-16)	177.2	(1-2-6)	112.7		
(1-2-7)	109.4	(1-2-8)	109.4	(6-2-7)	108.4	(6-2-8)	108.4		
(7-2-8)	108.5	(1-4-9)	117.6	(1-4-10)	121.4	(1-4-11)	121.4		
(9-4-10)	97.2	(9-4-11)	97.2	(10-4-11)	96.5	(1-5-12)	126.0		
(1-5-13)	117.4	(1-5-14)	117.4	(12-5-13)	96.6	(12-5-14)	96.6		
(13-5-14)	97.1								
(3-1-2-6)	0.0	(3-1-2-7)	-120.7	(3-1-2-8)	120.7				
(4-1-2-6)	180.0	(4-1-2-7)	59.4	(4-1-2-8)	-59.3				
(5-1-2-6)	0.1	(5-1-2-7)	-120.5	(5-1-2-8)	120.8				
(15-1-2-6)	88.9	(15-1-2-7)	-31.7	(15-1-2-8)	-150.4				
(16-1-2-6)	-88.9	(16-1-2-7)	150.5	(16-1-2-8)	31.8				
(2-1-4-9)	-.1	(2-1-4-10)	-119.1	(2-1-4-11)	119.0				
(3-1-4-9)	-.2	(3-1-4-10)	-119.3	(3-1-4-11)	118.8				
(5-1-4-9)	179.9	(5-1-4-10)	60.9	(5-1-4-11)	-61.0				
(15-1-4-9)	89.0	(15-1-4-10)	-30.0	(15-1-4-11)	-151.9				
(16-1-4-9)	-89.2	(16-1-4-10)	151.8	(16-1-4-11)	29.9				
(2-1-5-12)	179.9	(2-1-5-13)	57.5	(2-1-5-14)	-57.7				
(3-1-5-12)	180.0	(3-1-5-13)	57.6	(3-1-5-14)	-57.6				
(4-1-5-12)	0.0	(4-1-5-13)	-122.4	(4-1-5-14)	122.4				
(15-1-5-12)	91.2	(15-1-5-13)	-31.2	(15-1-5-14)	-146.4				
(16-1-5-12)	-91.3	(16-1-5-13)	146.3	(16-1-5-14)	31.1				

Frequencies(cm-1): NA

Four-coordinate transition state, plus two chlorine atoms (**2+2Cl**)
$(PH_3)_2Cl_2Pt(CH_3)H$, B3LYP partial optimization, C_s Geometry

Zero Point Energy	NA	Nuclear Repulsion	723.961538
Thermal correction		B3LYP	-1767.029994
to Enthalpy at 298K:	NA	CCSD(T) single point	-1763.952341



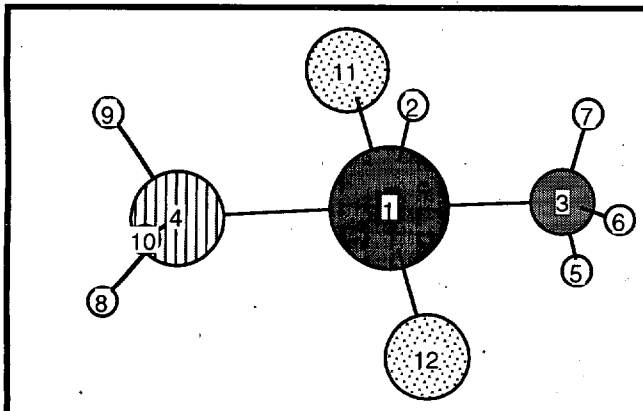
	X	Y	Z
Pt1	.000000	.313753	.000000
C2	-1.309422	2.147584	.000000
H3	.168796	1.930177	.000000
P4	-1.522104	-1.529925	.000000
P5	2.168302	-.488614	.000000
H6	-1.011301	3.201461	.000000
H7	-1.903468	1.971435	.900775
H8	-1.903468	1.971435	-.900775
H9	-2.934661	-1.329553	.000000
H10	-1.522328	-2.486449	1.055547
H11	-1.522328	-2.486449	-1.055547
H12	2.527689	-1.869432	.000000
H13	3.042743	-.117458	1.059231
H14	3.042743	-.117458	-1.059231
Cl15	.005269	.325803	2.403843
Cl16	.005269	.325803	-2.403843

(1-2)	2.253	(1-3)	1.625	(1-4)	2.391	(1-5)	2.312	(1-15)	2.404
(2-3)	1.494	(2-6)	1.095	(2-7)	1.093	(4-9)	1.427	(4-10)	1.424
(5-12)	1.427	(5-13)	1.423						
(2-1-3)	41.5	(2-1-4)	104.9	(2-1-5)	145.8	(2-1-15)	89.8		
(3-1-4)	146.4	(3-1-5)	104.3	(3-1-15)	89.7	(4-1-5)	109.2		
(4-1-15)	90.3	(5-1-15)	90.0	(15-1-16)	179.4	(1-2-3)	46.1		
(1-2-6)	128.7	(1-2-7)	100.6	(3-2-6)	82.6	(3-2-7)	120.9		
(6-2-7)	107.6	(7-2-8)	111.0	(1-3-2)	92.4	(1-4-9)	121.5		
(1-4-10)	121.2	(9-4-10)	95.4	(10-4-11)	95.6	(1-5-12)	124.9		
(1-5-13)	119.1	(12-5-13)	95.6	(13-5-14)	96.2				
(3-1-2-6)	0.0	(3-1-2-7)	-123.0	(4-1-2-3)	180.0				
(4-1-2-6)	180.0	(4-1-2-7)	57.0	(5-1-2-3)	0.0				
(5-1-2-6)	0.0	(5-1-2-7)	-123.0	(15-1-2-3)	89.7				
(15-1-2-6)	89.7	(15-1-2-7)	-33.3	(15-1-2-8)	-147.2				
(4-1-3-2)	0.0	(5-1-3-2)	180.0	(15-1-3-2)	-90.1				
(2-1-4-9)	0.0	(2-1-4-10)	-120.0	(3-1-4-9)	0.0				
(3-1-4-10)	-120.0	(5-1-4-9)	180.0	(5-1-4-10)	60.0				
(15-1-4-9)	89.9	(15-1-4-10)	-30.1	(15-1-4-11)	-150.1				
(2-1-5-12)	180.0	(2-1-5-13)	58.4	(3-1-5-12)	180.0				
(3-1-5-13)	58.4	(4-1-5-12)	0.0	(4-1-5-13)	-121.6				
(15-1-5-12)	90.3	(15-1-5-13)	-31.3	(15-1-5-14)	-148.1				
(6-2-3-1)	180.0	(7-2-3-1)	73.9						

Frequencies(cm-1): NA

Three-coordinate reactant complex, plus two chlorine atoms (**4a+2Cl**)
$(PH_3)Cl_2Pt(CH_3)H$, B3LYP partial optimization, C_1 Geometry

Zero Point Energy	NA	Nuclear Repulsion	484.099529
Thermal correction		B3LYP	-1423.894937
to Enthalpy at 298K:	NA	CCSD(T) single point	-1421.361540



	X	Y	Z
Pt1	.000052	-.305335	.019172
C2	.000345	-2.360329	.031656
H3	-.001075	-.389135	1.542842
P4	-.000265	2.062275	.010485
H5	.001218	-2.663814	-1.030939
H6	-.892314	-2.779817	.509934
H7	.892374	-2.779545	.511343
H8	.000878	2.816500	-1.196981
H9	1.064729	2.758059	.643816
H10	-1.066708	2.757814	.641649
Cl11	2.361120	-.323175	-.068036
Cl12	-2.361010	-.323659	-.068079

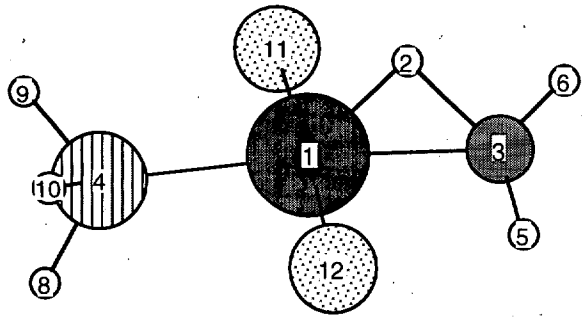
(1-2)	2.055	(1-3)	1.526	(1-4)	2.368	(1-11)	2.363	(1-12)	2.363
(2-5)	1.105	(2-6)	1.096	(2-7)	1.096	(4-8)	1.424	(4-9)	1.421
(4-10)	1.421								
(2-1-3)	86.5	(2-1-4)	179.9	(2-1-11)	89.6	(2-1-12)	89.6		
(3-1-4)	93.4	(3-1-11)	92.1	(3-1-12)	92.0	(4-1-11)	90.4		
(4-1-12)	90.4	(11-1-12)	175.7	(1-2-5)	105.6	(1-2-6)	112.7		
(1-2-7)	112.7	(5-2-6)	108.4	(5-2-7)	108.4	(6-2-7)	109.0		
(1-4-8)	122.2	(1-4-9)	119.2	(1-4-10)	119.2	(8-4-9)	96.8		
(8-4-10)	96.8	(9-4-10)	97.2						
(3-1-2-5)	180.0	(3-1-2-6)	61.9	(3-1-2-7)	-61.9				
(4-1-2-5)	-179.8	(4-1-2-6)	62.1	(4-1-2-7)	-61.7				
(11-1-2-5)	-87.8	(11-1-2-6)	154.1	(11-1-2-7)	30.3				
(12-1-2-5)	87.9	(12-1-2-6)	-30.2	(12-1-2-7)	-154.0				
(2-1-4-8)	179.7	(2-1-4-9)	59.0	(2-1-4-10)	-59.5				
(3-1-4-8)	180.0	(3-1-4-9)	59.2	(3-1-4-10)	-59.2				
(11-1-4-8)	87.8	(11-1-4-9)	-33.0	(11-1-4-10)	-151.4				
(12-1-4-8)	-87.9	(12-1-4-9)	151.3	(12-1-4-10)	32.8				

Frequencies(cm-1): NA

Three-coordinate transition state, plus two chlorine atoms (**5+2Cl**)
$(PH_3)Cl_2Pt(CH_3)H$, B3LYP partial optimization, C_1 Geometry

Zero Point Energy	NA
Thermal correction to Enthalpy at 298K:	NA

Nuclear Repulsion	485.338360
B3LYP	-1423.890038
CCSD(T) single point	-1421.352779



	X	Y	Z
Pt1	.003431	-.163471	-.004943
C2	.021090	-2.295578	.007276
H3	.050081	-1.172421	-1.202462
P4	-.033897	2.137530	-.012982
H5	.228025	-2.341187	1.088360
H6	.803925	-2.852936	-.514635
H7	-.956029	-2.738733	-.202561
H8	-.056444	2.899365	1.190022
H9	-1.107643	2.803110	-.660524
H10	1.032419	2.833256	-.640308
Cl11	2.371953	-.120697	.043708
Cl12	-2.364897	-.171607	.043278

(1-2)	2.132	(1-3)	1.567	(1-4)	2.301	(1-11)	2.369	(1-12)	2.369
(2-3)	1.651	(2-5)	1.102	(2-6)	1.094	(2-7)	1.093	(4-8)	1.424
(4-9)	1.420	(4-10)	1.419						
(2-1-3)	50.2	(2-1-4)	179.5	(2-1-11)	90.6	(2-1-12)	90.3		
(3-1-4)	129.9	(3-1-11)	89.9	(3-1-12)	92.5	(4-1-11)	89.9		
(4-1-12)	89.3	(11-1-12)	177.5	(1-2-3)	46.8	(1-2-5)	92.8		

(1-2-6)	120.9	(1-2-7)	113.4	(3-2-5)	138.1	(3-2-6)	89.1
(3-2-7)	98.7	(5-2-6)	108.2	(5-2-7)	109.8	(6-2-7)	110.0
(1-3-2)	83.0	(1-4-8)	122.2	(1-4-9)	118.9	(1-4-10)	118.6
(8-4-9)	97.0	(8-4-10)	97.1	(9-4-10)	97.9		
(3-1-2-5)	167.4	(3-1-2-6)	54.2	(3-1-2-7)	-79.6		
(4-1-2-3)	107.6	(4-1-2-5)	-85.1	(4-1-2-6)	161.7		
(4-1-2-7)	28.0	(11-1-2-3)	-89.4	(11-1-2-5)	78.0		
(11-1-2-6)	-35.2	(11-1-2-7)	-169.0	(12-1-2-3)	93.0		
(12-1-2-5)	-99.7	(12-1-2-6)	147.2	(12-1-2-7)	13.4		
(4-1-3-2)	-179.4	(11-1-3-2)	90.8	(12-1-3-2)	-88.3		
(2-1-4-8)	73.8	(2-1-4-9)	-47.0	(2-1-4-10)	-165.6		
(3-1-4-8)	-179.0	(3-1-4-9)	60.2	(3-1-4-10)	-58.4		
(11-1-4-8)	-89.3	(11-1-4-9)	149.9	(11-1-4-10)	31.3		
(12-1-4-8)	88.3	(12-1-4-9)	-32.4	(12-1-4-10)	-151.1		
(5-2-3-1)	-19.1	(6-2-3-1)	-135.9	(7-2-3-1)	114.0		

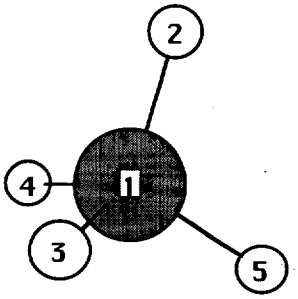
Frequencies(cm-1): NA

Methane

CH_4, B3LYP, T_d Geometry

Zero Point Energy	.044799
Thermal correction to Enthalpy at 298K:	.048612

Nuclear Repulsion	13.386558
B3LYP	-40.527104
CCSD(T) single point	-40.392670



	X	Y	Z
C1	.000000	.000000	.000000
H2	.631607	.631607	.631607
H3	-.631607	-.631607	.631607
H4	-.631607	.631607	-.631607
H5	.631607	-.631607	-.631607

(1-2) 1.094 (2-1-3) 109.5

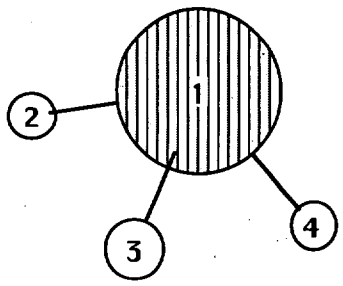
Frequencies(cm-1): 1338.7 1338.7 1338.7 1557.8 1557.8 3040.9 3164.0 3164.0 3164.0

Phosphine

PH_3, B3LYP, C_{3v} Geometry

Zero Point Energy	.024123
Thermal correction to Enthalpy at 298K:	.027969

Nuclear Repulsion	17.441697
B3LYP	-343.139346
CCSD(T) single point	-342.588453



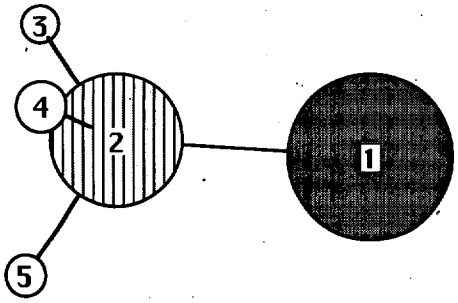
	X	Y	Z
P1	.000000	.000000	.130223
H2	.000000	1.195366	-.651113
H3	-1.035217	-.597683	-.651113
H4	1.035217	-.597683	-.651113

(1-2) 1.428 (2-1-3) 92.9

Frequencies(cm-1): 1049.9 1162.3 1162.3 2397.4 2408.4 2408.4

$PtPH_3$
B3LYP, C_{3v} Geometry

Zero Point Energy	.027705	Nuclear Repulsion	93.221513
Thermal correction to Enthalpy at 298K:	.032207	B3LYP	-462.926493
		CCSD(T) single point	-461.632519



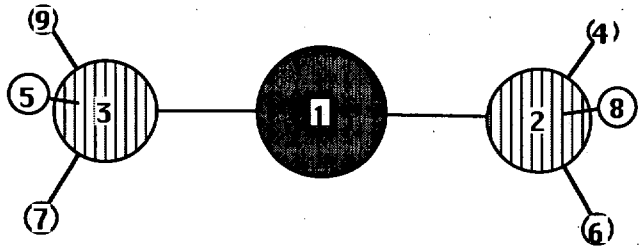
	X	Y	Z
Pt1	.000000	.000000	1.131519
P2	.000000	.000000	-1.017237
H3	.000000	1.244360	-1.702929
H4	-1.077647	-.622180	-1.702929
H5	1.077647	-.622180	-1.702929

(1-2) 2.149 (2-3) 1.421 (1-2-3) 118.9 (3-2-4) 98.7

Frequencies(cm-1): 430.8 557.8 557.8 1042.5 1135.8 1135.8 2431.5 2431.5 2437.6

$Pt(PH_3)_2$
B3LYP, C_s Geometry

Zero Point Energy	.054895	Nuclear Repulsion	214.317179
Thermal correction to Enthalpy at 298K:	.062955	B3LYP	-806.128975
		CCSD(T) single point	-804.287906



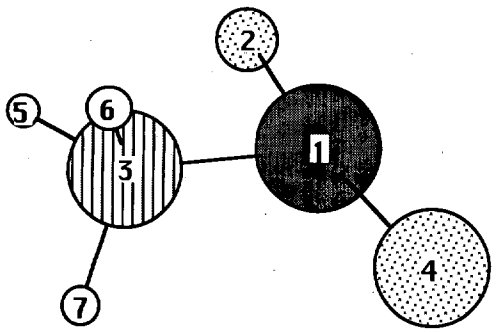
	X	Y	Z
Pt1	-.000024	.016742	.000000
P2	-.000024	-.006216	2.271817
P3	-.000024	-.006216	-2.271817
H4	.338173	1.166014	3.000359
H5	-1.195323	-.319069	-2.973037
H6	.857716	-.904376	2.961850
H7	.857716	-.904376	-2.961850
H8	-1.195323	-.319069	2.973037
H9	.338173	1.166014	-3.000359

(1-2) 2.272 (2-4) 1.421 (2-6) 1.421 (2-8) 1.421
(2-1-3) 178.8 (1-2-4) 120.3 (1-2-6) 119.5 (1-2-8) 119.7
(4-2-6) 97.4 (4-2-8) 97.4 (6-2-8) 97.4
(3-1-2-4) 164.0 (3-1-2-6) 43.9 (3-1-2-8) -75.7

Frequencies(cm-1): 61.2 63.7 64.8 306.6 354.0 446.4 450.4 520.8 525.2 1028.6 1052.7 1145.2 1145.8 1146.3 1146.9 2437.5 2438.6 2438.9 2439.7 2439.9 2442.7

$PtCl_2PH_3$, trans.
B3LYP, C_s Geometry

Zero Point Energy	.030680	Nuclear Repulsion	359.968827
Thermal correction to Enthalpy at 298K:	.038933	B3LYP	-1383.394035
		CCSD(T) single point	-1380.985793



	X	Y	Z
Pt1	.000000	.506067	.000000
Cl2	-2.302004	.814800	.000000
P3	-.032700	-1.675751	.000000
Cl4	2.337925	.530705	.000000
H5	-1.317692	-2.258402	.000000
H6	.598770	-2.294055	1.100673
H7	.598770	-2.294055	-1.100673

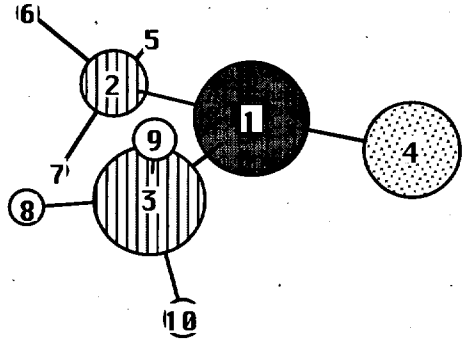
(1-2)	2.323	(1-3)	2.182	(1-4)	2.338	(3-5)	1.411	(3-6)	1.412
(2-1-3)	96.8	(2-1-4)	171.8	(3-1-4)	91.5	(1-3-5)	115.2		
(1-3-6)	115.5	(5-3-6)	103.1	(6-3-7)	102.5				
(2-1-3-5)	0.0	(2-1-3-6)	-120.2	(4-1-3-5)	180.0				
(4-1-3-6)	59.8								

Frequencies(cm-1): 49.4 70.1 104.8 106.9 334.6 359.0 425.4 608.9
621.6 1018.1 1117.3 1118.3 2497.9 2514.9 2519.9

$PtCl(PH_3)_2^+$, cis.
B3LYP, C_1 Geometry

Zero Point Energy	.057838
Thermal correction to Enthalpy at 298K:	.067293

Nuclear Repulsion	380.934817
B3LYP	-1266.084538
CCSD(T) single point	-1263.702887



	X	Y	Z
Pt1	-.067052	-.520703	.000002
P2	-2.394885	-.391431	-.000001
P3	.460781	1.650583	.000000
Cl4	2.205990	-.880400	-.000001
H5	-3.033501	-1.654206	-.000056
H6	-3.025890	.242436	-1.094879
H7	-3.025899	.242348	1.094924
H8	-.638395	2.535454	.000029
H9	1.220146	2.043085	-1.120086
H10	1.220198	2.043077	1.120053

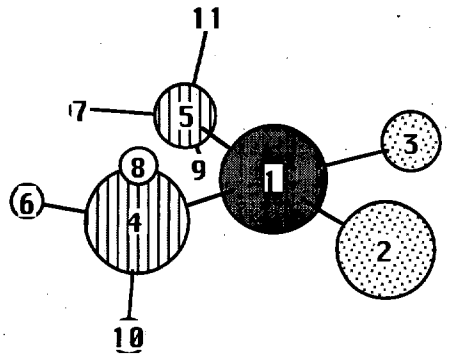
(1-2)	2.331	(1-3)	2.235	(1-4)	2.301	(2-5)	1.415	(2-6)	1.414
(2-7)	1.414	(3-8)	1.411	(3-9)	1.409	(3-10)	1.409		
(2-1-3)	100.5	(2-1-4)	174.2	(3-1-4)	85.3	(1-2-5)	113.6		
(1-2-6)	118.1	(1-2-7)	118.1	(5-2-6)	101.5	(5-2-7)	101.5		
(6-2-7)	101.5	(1-3-8)	115.2	(1-3-9)	113.5	(1-3-10)	113.5		
(8-3-9)	104.2	(8-3-10)	104.2	(9-3-10)	105.3				
(3-1-2-5)	180.0	(3-1-2-6)	61.4	(3-1-2-7)	-61.4				
(4-1-2-5)	0.0	(4-1-2-6)	-118.6	(4-1-2-7)	118.6				
(2-1-3-8)	0.0	(2-1-3-9)	-119.9	(2-1-3-10)	119.9				
(4-1-3-8)	180.0	(4-1-3-9)	60.1	(4-1-3-10)	-60.1				

Frequencies(cm-1): 45.5 87.4 101.0 108.3 122.0 310.1 370.1 390.0
530.6 543.9 603.2 628.7 996.8 1032.0 1100.7 1109.4 1113.4 1125.6
2480.3 2500.8 2503.7 2505.4 2533.6 2545.2

$PtCl_2(PH_3)_2$, cis.
B3LYP, C_{2v} Geometry

Zero Point Energy	.059243
Thermal correction to Enthalpy at 298K:	.070222

Nuclear Repulsion	575.399617
B3LYP	-1726.583735
CCSD(T) single point	-1723.631353



	X	Y	Z
Pt1	.000000	.000000	.015666
Cl2	.000000	1.748463	-1.602121
Cl3	.000000	-1.748463	-1.602121
P4	.000000	1.780102	1.440136
P5	.000000	-1.780102	1.440136
H6	.000000	1.575254	2.846331
H7	.000000	-1.575254	2.846331
H8	-1.088478	2.672555	1.323352
H9	1.088478	-2.672555	1.323352
H10	1.088478	2.672555	1.323352
H11	-1.088478	-2.672555	1.323352

(1-2)	2.382	(1-4)	2.280	(4-6)	1.421	(4-8)	1.412	(4-10)	1.412
(5-11)	1.412								
(2-1-3)	94.4	(2-1-4)	81.4	(2-1-5)	175.9	(4-1-5)	102.7		
(1-4-6)	120.4	(1-4-8)	116.2	(1-4-10)	116.2	(6-4-8)	100.0		
(6-4-10)	100.0	(8-4-10)	100.8	(1-5-11)	116.2	(7-5-11)	100.0		
(9-5-11)	100.8								
(2-1-4-6)	180.0	(2-1-4-8)	59.2	(2-1-4-10)	-59.2				
(5-1-4-6)	0.0	(5-1-4-8)	-120.8	(5-1-4-10)	120.8				
(2-1-5-11)	-59.2	(4-1-5-11)	120.8						

Frequencies(cm-1):	84.0	108.0	126.6	129.6	132.5	138.7	141.0	312.9	
335.6	345.2	346.1	563.2	568.6	589.3	591.5	1031.2	1052.8	1123.9
1127.9	1134.5	1135.0	2437.3	2440.5	2497.6	2498.2	2506.5	2506.6	