Accurate Prediction of ^{195}Pt NMR Chemical Shifts for a Series of Pt(II) and Pt(IV) Antitumor Agents by a Non-Relativistic DFT Computational Protocol

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Gaussian 09, Revision A.02, Frisch, M. J.; Schlegel, H. B.; Scusseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millan, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda. R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian, Inc., Wallingford CT, 2009

Table S1. The structural and ^{195}Pt NMR parameters of the $[PtCl_6]^{2-}$ and $[PtCl_4]^{2-}$ reference compounds calculated at various levels of theory along with the percent deviations from the experimental data.

Functional	$[PtCl_6]^{2-}$			$[PtCl_4]^{2-}$		
	Pt-Cl (Å)	σ (ppm)	Dev(%)	Pt-Cl (Å)	δ (ppm)	Dev(%)
SVWN	2.363	46.0	-103	2.370	521	-68
HSE2PBE	2.402	-1626	0	2.424	1254	-23
X3LYP	2.430	-2144	32	2.455	1605	-1
O3LYP	2.426	-1033	-37	2.450	1309	-20
M05-2X	2.402	-4941	204	2.438	6171	279
PW91PW91	2.428	-595	-63	2.439	631	-61
CAM-B3LYP	2.401	-2574	58	2.430	1772	9
B3PW91	2.409	-1592	-2	2.430	1430	-12
PBE0	**2.396**	**-1611**	**-1**	**2.419**	**1684**	**3**
mPW1PW91	**2.400**	**-1689**	**4**	**2.423**	**1659**	**2**
mPW3PBE	2.405	-1514	-7	2.425	1433	-12
PBEh1PBE	2.401	-1400	-14	2.424	1268	-22
M06-2X	2.408	-5584	243	2.456	6137	277
M06-L	2.429	-1000	-39	2.464	21	-99
M06	2.414	-2048	26	2.443	572	-65
B3LYP	**2.435**	**-1756**	**8**	**2.459**	**1518**	**-7**
BP86	2.435	-1051	-35	2.445	619	-62
HCTH407	2.445	-1191	-27	2.462	933	-43
tHCTH	2.428	-731	-55	2.440	515	-68
wB97XD	2.405	-2797	72	2.438	1563	-4
BMK	2.408	-3594	121	2.459	2592	59
VSXC	2.443	-1976	21	2.477	510	-69
BB95	2.434	-1074	-34	2.446	409	-75
TPSS	2.427	-426	-74	2.443	355	-78
LC-wPBE	2.374	-2716	67	2.438	2095	29
B97-2	**2.411**	**-1678**	**3**	**2.435**	**1599**	**-2**
SC	-	-2063	27		1782	9
Expt	2.316	-1628		2.315	1628	
aiMD	2.385±0.021			2.346±0.026		
EXAFS	2.330			2.304		
ADF-COSMO	2.375			2.348		

Table S2. The changes of the isotropic shielding tensor elements (σ^{iso}) observed along the diabatic (unrelaxed) rotation around the Pt-N bond computed at the PBE0/SARC-ZORA(Pt) ∪ 6-31+G(d)(E) level.

Compound	Torsional barrier	δ (^{195}Pt)$_{max}$(φ°)	δ (^{195}Pt)$_{min}$(φ°)	$\Delta[\delta(^{195}Pt)]$
cis-$(CH_3NH_2)_2PtCl_2$	1.2	-1041 (150)	-1097 (50)	56
cis-$(C_2H_5NH_2)_2PtCl_2$	3.6	-1099 (130)	-1155 (50)	56
cis-$(n\text{-}C_3H_7NH_2)_2PtCl_2$	7.8	-953 (100)	-1117 (300)	164
cis-$(n\text{-}C_4H_9NH_2)_2PtCl_2$	7.3	-943 (100)	-1117 (300)	174
cis-$(n\text{-}C_5H_{11}NH_2)_2PtCl_2$	7.6	-956 (100)	-1100 (320)	144
cis-$(n\text{-}C_6H_{13}NH_2)_2PtCl_2$	7.7	-987 (80)	-1149 (290)	162
cis-$(n\text{-}C_7H_{15}NH_2)_2PtCl_2$	7.8	-1010 (90)	-1171 (280)	161
cis-$(n\text{-}C_8H_{17}NH_2)_2PtCl_2$	7.4	-987 (80)	-1149 (290)	162
cis-$(i\text{-}PrNH_2)_2PtCl_2$	-	-1166 (140)	-1221 (0)	55
cis-$(i\text{-}BuNH_2)_2PtCl_2$	5.8	-1021 (120)	-1155 (0)	134
cis-$(i\text{-}AmNH_2)_2PtCl_2$	7.8	-973 (250)	-1125 (70)	152
cis-$(c\text{-}C_3H_5NH_2)_2PtCl_2$	12.4	-1224 (160)	-1280 (70)	56
cis-$(c\text{-}C_4H_7NH_2)_2PtCl_2$	-	-944 (120)	-1048 (10)	104
cis-$(c\text{-}C_5H_9NH_2)_2PtCl_2$	-	-1022 (190)	-1949 (130)	924
cis-$(c\text{-}C_6H_{11}NH_2)_2PtCl_2$	-	-1103 (70)	-1245 (0)	142
cis-$(c\text{-}C_7H_{13}NH_2)_2PtCl_2$	-	-1181 (30)	-1230 (0)	49
cis-$(c\text{-}C_8H_{15}NH_2)_2PtCl_2$	-	-1103 (30)	-1551 (80)	448
cis-$(1\text{-Adamantamine})_2PtCl_2$	-	-1195 (0)	-1902 (240)	707
cis-$(C_5H_5N)_2PtCl_2$	5.7	-1387 (80)	-1668 (0)	281
cis-$(C_5H_{10}NH)_2PtCl_2$	13.7	-937 (90)	-1216 (0)	279
cis-$[(CH_3)_2NH]_2PtCl_2$	9.3	-1043 (90)	-1298 (180)	255
cis-$(c\text{-}C_3H_5NH_2)(NH_3)PtCl_2$	7.3	-1042 (110)	-1250 (0)	208
cis-$(c\text{-}C_4H_7NH_2)(NH_3)PtCl_2$	-	-1098 (10)	-2107 (120)	1009
cis-$(c\text{-}C_5H_9NH_2)(NH_3)PtCl_2$	16.9	-1190 (10)	-1332 (60)	142
cis-$(c\text{-}C_6H_{11}NH_2)(NH_3)PtCl_2$	-	-1256 (0)	-1808 (130)	552
cis-$(Thiazole)_2PtCl_2$	7.1	-1402 (60)	-1889 (140)	487

Table S3. Selected structural parameters (bond lengths in Å, bond angles in degrees) for *cis*-bis(amine) Pt(II) anticancer agents with carboxylato- and acetylacetonato- leaving ligands calculated at the GIAO-PBE0/SARC-ZORA(Pt) ∪ 6-31+G(d)(E) level in solution.

Compound	R_{Pt-O}	R_{Pt-N}	<N-Pt-N	<O-Pt-O	Solvent
Carboplatin[a]	2.077 (2.075)[b]	2.129 (2.120)	93.3 (91.3)	90.9 (90.4)	DMF
	2.082 (2.092)	2.121 (2.108)	91.7 (89.9)	90.2 (89.5)	water[c]
	2.025[d]	*2.021*	*95.3*	*90.5*	*solid state*
Oxaliplatin[e]	2.089 (2.082)	2.126(2.118)	80.6 (80.9)	80.7(80.9)	DMF
	2.102 (2.107)	2.113 (2.101)	80.8 (81.0)	80.3 (80.2)	water[c]
	2.021; 2.031	*2.011; 2.028*	*83.8*	*82.8*	*solid state*
cis-$(NH_3)_2Pt(OOCCH_3)_2$	2.115 (2.110)	2.110 (2.100)	89.1 (88.3)	82.0(82.8)	DMF
	2.126 (2.120)	2.105 (2.097)	88.2 (87.9)	83.0 (81.1)	water[c]
cis-$(NH_3)_2Pt(OOCC_6H_5)_2$	2.116 (2.112)	2.107 (2.097)	89.1 (88.1)	82.0 (82.8)	DMF
	(2.120)	(2.094)	(88.0)	(81.0)	water[c]
$(C_5H_{10}NH)_2Pt(OOCCOO)$	2.087; 2.102	2.148	95.1	81.1	DMF
	(2.087; 2.093)	(2.140)	(93.9)	(81.2)	DMF
	2.098	2.138; 2.155	94.7	80.9	water[c]
	(2.109; 2.120)	(2.125)	(92.6)	(80.2)	water
(1,4-DACH)Pt(OOCCOO)	2.085 (2.081)	2.139 (2.130)	97.8 (97.6)	81.6(81.6)	DMF
	2.099 (2.105)	2.127(2.117)	97.4 (97.4)	81.0 (80.8)	water[c]
(1,4-DACH)Pt(CBDCA)[f]	2.086 (2.084)	2.135 (2.127)	98.1 (98.1)	91.4 (90.9)	DMF
	2.095 (2.102)	2.124 (2.117)	98.0 (97.9)	90.7 (89.7)	water[c]
(1,4-DACH)Pt($OOCCH_2COO$)	2.091 (2.087)	2.133 (2.126)	98.1 (98.0)	92.4 (91.6)	DMF
	2.099 (2.105)	2.123 (2.115)	98.0 (97.9)	91.2 (90.6)	water[c]

[a] Carboplatin = c*is*-diammine(1,1-cyclobutanedicarboxylato)platinum(II). [b] Figures in parentheses are the structural parameters calculated in solution employing the SMD model. [c] Employing Gaussian03 package for calculations in aqueous solution. [d] Figures in italics are the experimentally determined structural parameters using X-Ray crystallography. [e] Oxaliplatin = (DACH)(oxalato)platinum(II). [f] CBDCA = 1,1-cyclobutanedicarboxylate.

Table S4. Selected structural parameters (bond lengths in Å, bond angles in degrees) for a series of diacetylbis(amine)platinum(II) complexes calculated at the GIAO-PBE0/SARC-ZORA(Pt)∪6-31+G(d)(E) level in solution.

Compound]	Pt-C	Pt-N	<C-Pt-C	<N-Pt-N	Solvent
$Pt(OCMe)_2(H_2NEt)_2$	2.070	2.302	94.6	95.0	$CHCl_3$
$Pt(OCMe)_2(H_2N^iPr)_2$	2.069; 2.071	2.310; 2.318	94.1	95.9	$CHCl_3$
	1.976; 1.985	2.176	89.1	88.0	Solid state
$Pt(OCMe)_2(H_2NCH_2Ph)_2$	2.071	2.301	94.8	95.1	$CHCl_3$
	1.979	2.164	91.8	92.7	Solid state
$Pt(OCMe)_2(H_2NCH_2CH_2Ph)_2$	2.070	2.302	94.8	94.6	$CHCl_3$
$Pt(OCMe)_2(H_2NCH_2CH=CH_2)$	2.070	2.304	94.9	94.9	$CHCl_3$
$Pt(OCMe)_2(H_2NCy)_2$	2.070	2.325	93.7	95.7	$CHCl_3$
$Pt(OCMe)_2(HNMe_2)_2$	2.059; 2.087	2.330; 2.334	91.8	91.5	CH_2Cl_2
$Pt(OCMe)_2(HNEt_2)_2$	2.060; 2.090	2.354; 2.355	91.3	91.0	CH_2Cl_2
$Pt(OCMe)_2(H_2NCH_2CH_2NH_2)$	2.062; 2.071	2.299; 2.316	91.8	76.8	$CHCl_3$
$Pt(OCMe)_2(Me_2NCH_2CH_2NH_2)$	2.054; 2.082	2.308; 2.396	91.5	77.0	$CHCl_3$
$Pt(OCMe)_2(MeNHCH_2CH_2NHMe$		2.314; 2.333	91.8	78.0	$CHCl_3$
)	2.062; 2.073				
$Pt(OCMe)_2(Me_2NCH_2CH_2NMe_2)$	2.073	2.347; 2.348	85.3	79.4	CH_2Cl_2

[a] Figures in parentheses are the structural parameters calculated in solution employing the SMD model.

Table S5. Selected structural parameters (bond lengths in Á, bond angles in degrees) for octahedral Pt(IV) anticancer agents calculated at the GIAO-PBE0/SARC-ZORA(Pt) ∪ 6-31+G(d)(E) level in solution.

Compound]	Pt-O	Pt-Cl	Pt-N	<O-Pt-O	<Cl-Pt-Cl	<N-Pt-N	Solvent
cct-$[Pt(NH_3)_2Cl_2(OOCH)_2]$	2.059 (2.063)[a]	2.359 (2.367)	2.129 (2.116)	176.6 (175.8)	94.3 (95.1)	94.3 (93.1)	DMSO
cct-		2.360 (2.369)	2.125 (2.117)	170.7 (171.0)	91.4 (91.3)	97.2 (96.9)	DMSO
$[Pt(NH_3)(Cha)Cl_2(OOCCH_3)_2]$(Satraplatin)	2.063 (2.064)						
	2.01; 2.06	2.308; 2.312	2.067; 2.073	174.7	90.39	94.3	Solid state
cct-$[Pt(NH_3)_2Cl_2(OOCCH_3)_2]$	2.064	2.359; 2.385	2.100; 2.121	171.0	91.7	92.8	water
	(2.065; 2.067)	(2.369; 2.390)	(2.097; 2.109)	170.7	91.8	91.8	water
	2.030	2.318	2.049	176.7	91.23	90.7	Solid state
cct-$[Pt(NH_3)_2Cl_2(OOCCF_3)_2]$	2.061 (2.061)	2.353 (2.363)	2.116 (2.110)	171.2 (170.7)	91.6 (91.7)	93.1 (92.3)	water
cct-$[Pt(NH_3)_2Cl_2(OOCCHCl_2)_2]$ (Mitaplatin)	2.052 (2.052)	2.356 (2.363)	2.117 (2.108)	173.8 (174.1)	94.4 (94.8)	93.3 (91.0)	DMSO
$Pt(en)Cl_2(OOCCH_3)_2$	2.063 (2.063)	2.366 (2.375)	2.099 (2.096)	171.4 (171.7)	92.2 (92.4)	82.3 (82.2)	DMSO
$Pt(en)Cl_2(OOCCF_3)_2$	2.061 (2.061)	2.360 (2.371)	2.114 (2.11)	171.7 (171.3)	91.9 (91.9)	82.2 (82.2)	water
$Pt(1,2\text{-DACH})Cl_2(OOCCH_3)_2$	2.063 (2.063)	2.366 (2.375)	2.103 (2.100)	172.0 (172.2)	91.8 (91.7)	81.5 (81.4)	acetone
	2.036	2.331	2.01	167.9	94.1	84.0	Solid state
$Pt(1,4\text{-DACH})(OOCCH_3)_2Cl_2$	2.064 (2.066)	2.376 (2.384)	2.133 (2.129)	168.1 (168.2)	97.8 (98.1)	97.0 (96.8)	acetone
	2.007; 2.010	2.315; 2.322	2.037; 2.067	174.2	91.9	97.4	Solid state
cct-$\{Pt(NH_3)_2Cl_2[OOCNH(^tBu)]_2\}$	2.055 (2.052)	2.371 (2.376)	2.107 (2.102)	173.9 (174.1)	95.3 (95.5)	91.7 (90.7)	DMSO
	2.0062; 2.0117	2.3145; 2.3326	2.037; 2.037	174.06	92.57	90.0	Solid state
cct-$\{Pt(NH_3)_2Cl_2[OOCNH(c\text{-pentyl})]_2\}$	2.050 (2.050)	2.362 (2.370)	2.104 (2.096)	171.3 (171.7)	94.8 (95.6)	93.1 (91.5)	DMSO
	1.9970; 2.0088	2.3170; 2.3324	2.0423; 2.038	174.22	91.99	90.02	Solid state
cct-$\{Pt(NH_3)_2Cl_2[OOCNH(c\text{-hexyl})]_2\}$	2.049 (2.050)	2.362 (2.370)	2.103 (2.096)	171.5 (171.5)	94.9 (95.2)	93.0 (91.2)	DMSO
	2.001; 2.026	2.3075; 2.3170	2.041; 2.042	174.17	91.48	93.17	Solid state
cct-$[Pt(NH_3)_2Cl_2(OOCNHPh)_2]$	2.056 (2.056)	2.374 (2.378)	2.105 (2.102)	173.8 (173.7)	93.4 (93.0)	90.1 (90.3)	DMSO
	1.993; 1.995	2.3202; 3.3272	1.993; 1.995	174.94	92.68	92.21	
$Pt(1,2\text{-DACH})(OH)_2(oxalate)$	2.042 (2.044)	2.053 (2.056)[b]	2.085 (2.082)	174.5 (174.9)	81.8 (81.7)[c]	81.2 (81.2)	DMF
cct-$[Pt(NH_3)_2Cl_2(OH)_2]$ (Oxoplatin)	2.046 (2.051)	2.367 (2.373)	2.104 (2.101)	172.2 (173.9)	92.1 (92.2)	92.5 (91.2)	water
	2.008	2.317	2.056	176.9	90.48	94.3	Solid state
cct-$[Pt(iPrNH_2)_2Cl_2(OH)_2]$ (Iproplatin)	2.042 (2.047)	2.382 (2.388)	2.119 (2.113)	174.3 (176.8)	93.1 (93.3)	94.6 (92.5)	water
$Pt(hpip)Cl_2(OH)_2$	2.047 (2.053)	2.383 (2.390)	2.133 (2.131)	178.8 (179.2)	91.9 (91.6)	73.8 (73.7)	water
$Pt(mhpip)Cl_2(OH)_2$	2.047	2.387	2.122; 2.167	178.7	90.2	74.7	water
	(2.053)	(2.389; 2.395)	(2.121; 2.167)	(178.9)	(90.0)	(74.7)	water
$Pt(dmhpip)Cl_2(OH)_2$	2.046; 2.049	2.389	2.163	178.7	87.3	75.5	water
	(2.053)	(2.397)	(2.163)	(170.3)	(87.4)	(75.5)	water
$Pt(1,4\text{-DACH})(OH)_2Cl_2$	2.043 (2.048)	2.385 (2.389)	2.111 (2.122)	174.5 (176.9)	93.0 (92.5)	98.0 (97.9)	water
	2.043 (2.044)	2.385 (2.393)	2.111 (2.106)	174.6 (174.6)	93.0 (92.8)	98.1 (97.9)	DMF

[a] Figures in parentheses are the structural parameters calculated in solution employing the SMD model.

Table S6 Cartesian Coordinates and energies of antitumour agents (in Hartrees)

***cis*-$(NH_3)_2PtCl_2$** (DMF)

```
Pt,0,0.,0.,0.149007493
Cl,0,0.0241350672,1.7574695274,-1.4847976822
N,0,-0.0134432292,-1.5398176075,1.6299584327
Cl,0,-0.0241350672,-1.7574695274,-1.4847976822
N,0,0.0134432292,1.5398176075,1.6299584327
H,0,-0.7980144193,-1.4701828722,2.2753765455
H,0,0.8403748279,-1.5529070235,2.1849257384
H,0,-0.0836484936,-2.4397386096,1.1559832194
H,0,0.7980144193,1.4701828722,2.2753765455
H,0,-0.8403748279,1.5529070235,2.1849257384
H,0,0.0836484936,2.4397386096,1.1559832194

Sum of electronic and zero-point Energies=          -18347.973183
Sum of electronic and thermal Energies=             -18347.963814
Sum of electronic and thermal Enthalpies=           -18347.962870
Sum of electronic and thermal Free Energies=        -18348.008856
```

***trans*-$(NH_3)_2PtCl_2$** (DMF)

```
Pt,0,0.,0.,0.0032282075
Cl,0,0.,0.,-2.4118895839
N,0,0.,-2.1193018823,0.0025074443
Cl,0,0.,0.,2.4197401204
N,0,0.,2.1193018823,0.0025074443
H,0,-0.8203027348,-2.489958261,0.4784639321
H,0,0.8203027348,-2.489958261,0.4784639321
H,0,0.,-2.4817664948,-0.9497746859
H,0,0.8203027348,2.489958261,0.4784639321
H,0,-0.8203027348,2.489958261,0.4784639321
H,0,0.,2.4817664948,-0.9497746859

Sum of electronic and zero-point Energies=          -18347.978195
Sum of electronic and thermal Energies=             -18347.968759
Sum of electronic and thermal Enthalpies=           -18347.967814
Sum of electronic and thermal Free Energies=        -18348.014041
```

***cis*-$(CH_3NH_2)_2PtCl_2$** (DMF)

```
Pt,0,0.0135955385,-0.0714416681,-0.0826305323
Cl,0,1.7506278262,-1.6561209182,0.4123910774
N,0,-1.5350473753,1.3368490363,-0.5534681968
Cl,0,-1.7586380662,-1.6406180441,0.3303314639
N,0,1.5932808033,1.3200567111,-0.4908417389
```

C,0,-2.1886538017,1.9559065683,0.6141818771
C,0,2.0738492488,2.0966820953,0.6659107375
H,0,-1.2004988019,2.0636888947,-1.1840560491
H,0,-2.225448796,0.8043577002,-1.0818106
H,0,1.340496788,1.9505160404,-1.2502707433
H,0,2.3555171541,0.7450108476,-0.8489039207
H,0,-2.9995864685,2.6218536757,0.2995223701
H,0,-1.4518819192,2.5279943261,1.180923753
H,0,-2.5922672338,1.1655699747,1.2489249748
H,0,2.9072460032,2.7474470789,0.3794719385
H,0,2.4048810374,1.4034124103,1.4408747265
H,0,1.259553063,2.7080042708,1.0588658623

Sum of electronic and zero-point Energies= -18426.423652
Sum of electronic and thermal Energies= -18426.411699
Sum of electronic and thermal Enthalpies= -18426.410755
Sum of electronic and thermal Free Energies= -18426.464117

cis-$(C_2H_5NH_2)_2PtCl_2$ (DMF)

Pt,0,-0.0050357849,-0.410889578,-0.0957540112
Cl,0,1.8605855935,-1.8628665088,0.3468591473
N,0,-1.659875568,0.8824331112,-0.5267301523
Cl,0,-1.6509193255,-2.0882453673,0.4144787615
N,0,1.4528545493,1.0787008323,-0.6025099441
C,0,-2.0530143703,1.8219809308,0.5452859762
C,0,-3.2886702047,2.6320728536,0.1888911986
C,0,2.0523827409,1.8007721541,0.5411601896
C,0,3.1087660918,2.8051500154,0.1112264966
H,0,-1.5061956477,1.3936189974,-1.3959214619
H,0,-2.4323622938,0.2409573167,-0.7129075963
H,0,1.0772061252,1.7478777425,-1.2742243682
H,0,2.1862624784,0.5698035409,-1.0971014404
H,0,-1.2006573742,2.4796817301,0.7379524447
H,0,-2.2213209216,1.2268013987,1.4470365209
H,0,-3.5420362539,3.3045760326,1.0155240622
H,0,-4.1517952937,1.9816095489,0.0069443462
H,0,-3.1212668908,3.2441740194,-0.7047932984
H,0,2.4767192703,1.0431497095,1.2052603387
H,0,1.2409789528,2.2968215768,1.0812853423
H,0,3.5285821948,3.3007312226,0.9933244249
H,0,2.6847856242,3.5787212043,-0.5395680776
H,0,3.9307563078,2.3146605163,-0.4228438991

Sum of electronic and zero-point Energies= -18504.904499
Sum of electronic and thermal Energies= -18504.889934
Sum of electronic and thermal Enthalpies= -18504.888990
Sum of electronic and thermal Free Energies= -18504.948856

cis-(*n*-$C_3H_7NH_2)_2PtCl_2$ (DMF)

```
Pt,0,0.0109824574,-0.5700456724,-0.1423066507
Cl,0,1.7423368218,-2.194995895,0.2319216769
N,0,-1.5248034695,0.8796789573,-0.5168108876
Cl,0,-1.7704029308,-2.1287790557,0.2761579581
N,0,1.5896680224,0.8230019486,-0.5566148633
C,0,-2.1174760509,1.4928575278,0.6924595574
C,0,-3.1980734421,2.5260702287,0.3911356924
C,0,2.0123261393,1.6618047434,0.5854460861
C,0,3.1587747404,2.6139607043,0.2602544308
C,0,-4.4238554691,1.9632635655,-0.320778291
C,0,4.4605658842,1.9192495833,-0.1250641397
H,0,-1.1942971388,1.6099803877,-1.1477097411
H,0,-2.2443576975,0.3699395355,-1.0290543364
H,0,1.3579681426,1.413252125,-1.355784265
H,0,2.3662448139,0.2330715034,-0.8564361954
H,0,-1.3029688014,1.9522499521,1.2599907385
H,0,-2.5205579221,0.6731628986,1.295213286
H,0,-3.4997041043,2.9603151971,1.3530739958
H,0,-2.7638557384,3.3489958002,-0.1936242985
H,0,2.2944520115,0.9793191111,1.3936186532
H,0,1.1368058919,2.2260398514,0.9194419736
H,0,3.3224009044,3.231213555,1.1530283941
H,0,2.8462853705,3.3033086115,-0.5364089967
H,0,-5.1954886244,2.7333361727,-0.4266205582
H,0,-4.8593533278,1.1283191652,0.2417730845
H,0,-4.1898917955,1.6039621558,-1.330176354
H,0,5.2645010082,2.651620119,-0.2550019789
H,0,4.3737260828,1.3685073386,-1.0693865013
H,0,4.7756692214,1.2108068843,0.6508965303

Sum of electronic and zero-point Energies=          -18583.375561
Sum of electronic and thermal Energies=             -18583.358428
Sum of electronic and thermal Enthalpies=           -18583.357484
Sum of electronic and thermal Free Energies=        -18583.424226
```

cis-(*n*-$C_4H_9NH_2)_2PtCl_2$ (DMF)

```
Pt,0,0.0170460375,-0.8777703454,-0.1138410822
Cl,0,1.7779847957,-2.4915408325,0.1887153956
N,0,-1.5436435988,0.556000187,-0.4245585678
Cl,0,-1.7346447325,-2.463428141,0.3275385176
N,0,1.573902687,0.5355947901,-0.5375885217
C,0,-2.0980330068,1.1836964494,0.795243195
C,0,-3.1786569836,2.2210848173,0.5083732236
C,0,1.9621893594,1.4140862473,0.5872927181
C,0,3.120988829,2.3525104668,0.2676860932
```

C,0,-4.4375723876,1.669337024,-0.157141276
C,0,4.45074089,1.6540254532,-0.00768657
C,0,5.5984792136,2.6426633063,-0.1815234815
C,0,-5.5174097065,2.7332390352,-0.3221807883
H,0,-1.2448885491,1.2791806672,-1.0792451618
H,0,-2.2779892907,0.0329472747,-0.9010302394
H,0,1.347660663,1.0988607215,-1.357391997
H,0,2.3645359016,-0.0508772877,-0.80619225
H,0,-1.2665059842,1.6452081217,1.3354265716
H,0,-2.4883971066,0.3731701252,1.4183505416
H,0,-3.4496494055,2.6781783726,1.4701704101
H,0,-2.7554262359,3.0299319875,-0.1056070519
H,0,2.2150182005,0.7616445721,1.4292308434
H,0,1.0777813108,1.9913100393,0.871817579
H,0,3.2382020131,3.0216351108,1.1314342585
H,0,2.8509852195,2.9952357075,-0.5831494984
H,0,-4.8284488734,0.8354410258,0.4428651072
H,0,-4.196366905,1.2543195066,-1.1458079693
H,0,4.3761585165,1.033831626,-0.9118352913
H,0,4.6770373979,0.9687507042,0.8214652444
H,0,6.5428822966,2.124966725,-0.3834176111
H,0,5.7349751115,3.2492337657,0.7222902545
H,0,5.4069702741,3.3277534331,-1.0166310318
H,0,-6.4106886774,2.3226037173,-0.8060382707
H,0,-5.1579628432,3.5679682692,-0.9366852006
H,0,-5.8198924305,3.1416803571,0.6499179077

Sum of electronic and zero-point Energies= -18661.848804
Sum of electronic and thermal Energies= -18661.829018
Sum of electronic and thermal Enthalpies= -18661.828074
Sum of electronic and thermal Free Energies= -18661.901114

***cis*-(*n*-$C_5H_{11}NH_2)_2PtCl_2$** (DMF)

Pt,0,-0.0035809205,-0.728069298,0.0788010637
Cl,0,1.7808322992,-2.2159918402,0.7013118829
N,0,-1.5794102136,0.5977492879,-0.5212024537
Cl,0,-1.7348636739,-2.3029893708,0.6274289931
N,0,1.5345934969,0.6709334555,-0.4445288009
C,0,-2.084120938,1.5017249991,0.5346096387
C,0,-3.2038066352,2.4271921954,0.065393197
C,0,2.0863904042,1.451182719,0.6848955461
C,0,3.1829012744,2.429963668,0.2730894781
C,0,-4.4744377191,1.7362645148,-0.433719382
C,0,4.4271128485,1.8054448095,-0.3621267607
C,0,-5.1792285769,0.8641249242,0.6032804515
C,0,5.1705081227,0.8128910277,0.5294504652
C,0,6.4658211759,0.3183502986,-0.1052912847
C,0,-6.4985776695,0.2995547836,0.0877111745

H,0,-1.3110322099,1.138241818,-1.3437764306
H,0,-2.3269339642,-0.0253778793,-0.8273339315
H,0,1.2268703664,1.3041950283,-1.1828198879
H,0,2.2714087933,0.098319323,-0.8560606604
H,0,-1.2373104748,2.0962111344,0.8898942187
H,0,-2.4080542685,0.8689884382,1.3657170412
H,0,-3.4555250996,3.0795267663,0.91300174
H,0,-2.8135344414,3.0864500723,-0.7226038837
H,0,2.4487314092,0.7283066873,1.4207854234
H,0,1.2561056532,1.9954480306,1.1442943398
H,0,3.4761632206,2.9800264773,1.1779616775
H,0,2.7566902919,3.1751659253,-0.4131799688
H,0,-5.1701290798,2.5168948296,-0.7715518588
H,0,-4.2568043232,1.1353268164,-1.3296874694
H,0,5.1116623059,2.6213787052,-0.6326093814
H,0,4.1677919583,1.3179596839,-1.3142843363
H,0,-5.3607232758,1.4584066054,1.5104508648
H,0,-4.5283089813,0.0327065504,0.9069634407
H,0,4.52874723,-0.0502205461,0.7541517752
H,0,5.3909579076,1.2907257593,1.4949655729
H,0,6.9823711933,-0.3977988417,0.5439741484
H,0,7.1533309607,1.1511332522,-0.2995550325
H,0,6.2702010962,-0.1805725867,-1.0628750887
H,0,-6.9875465568,-0.3283242871,0.8412977927
H,0,-6.3412664309,-0.3152327294,-0.8074933129
H,0,-7.1943155554,1.1044477924,-0.1806220014

cis-(*n*-$C_6H_{13}NH_2$)$_2PtCl_2$ (DMF)

Pt,0,0.0408302748,-1.3383101321,-0.1553895198
Cl,0,1.6898612901,-3.0934304696,-0.1094202968
N,0,-1.4193868234,0.23365767,-0.2213013268
Cl,0,-1.8285588954,-2.8531655191,-0.0497250237
N,0,1.7028144618,0.0046334834,-0.3166110678
C,0,-1.9858836188,0.6403443805,1.0835966138
C,0,-3.0278161112,1.7488595254,0.9721838344
C,0,1.9568648793,0.9298281858,0.8075406632
C,0,3.1898119312,1.8049712181,0.6039948804
C,0,-4.2928244865,1.3576650398,0.2116664702
C,0,4.5078821386,1.0324270213,0.5737423885
C,0,5.7493515424,1.9249757953,0.5296746877
C,0,-5.3402908364,2.4676058885,0.1939594071
C,0,5.901304346,2.7422510772,-0.7516878779
C,0,-6.6077907831,2.0901931367,-0.5674845795
C,0,7.1998895608,3.5408712974,-0.7868413484
C,0,-7.6459943717,3.2065218841,-0.5864884659
H,0,-1.0579736528,1.0525160638,-0.7109988587
H,0,-2.1621461876,-0.1399686446,-0.8116828967
H,0,1.6322969862,0.529511478,-1.1889188215
H,0,2.4964361585,-0.6270150594,-0.432661644

H,0,-1.1544134157,0.9629456124,1.7170516346
H,0,-2.4170833175,-0.2580941357,1.5355885564
H,0,-3.2969990813,2.0440632837,1.9956564216
H,0,-2.5694707084,2.6349825896,0.5086032198
H,0,2.0563763031,0.3206419635,1.7117507256
H,0,1.0687043511,1.5570036097,0.9278255372
H,0,3.2147415249,2.5282526683,1.4310628775
H,0,3.0618163606,2.3926103877,-0.3152908746
H,0,-4.724932084,0.4545020166,0.6677246306
H,0,-4.0485842366,1.0932955249,-0.8279063567
H,0,4.535110617,0.3558001927,-0.2932922212
H,0,4.5603984858,0.3931903086,1.4667132967
H,0,6.6396119841,1.2911129358,0.6493931333
H,0,5.7388092028,2.6040420621,1.3957986592
H,0,-4.903150282,3.372266841,-0.2550551387
H,0,-5.6036185293,2.7349843533,1.2283757024
H,0,5.0523246548,3.4300188424,-0.8626049786
H,0,5.8632428679,2.0639500848,-1.6167410925
H,0,-7.045495897,1.1882789478,-0.1160811895
H,0,-6.3420856453,1.8181213857,-1.599164481
H,0,7.2911491744,4.1188959026,-1.7138391881
H,0,8.0725075483,2.8790534246,-0.7181982258
H,0,7.2522907633,4.2460028812,0.0523739993
H,0,-8.5452108935,2.9091575339,-1.1385444016
H,0,-7.2453755131,4.1101533919,-1.0630713622
H,0,-7.9537000369,3.4774110702,0.4313658985

Sum of electronic and zero-point Energies= -18818.794830
Sum of electronic and thermal Energies= -18818.769603
Sum of electronic and thermal Enthalpies= -18818.768659
Sum of electronic and thermal Free Energies= -18818.856269

***cis*-(*n*-$C_7H_{13}NH_2)_2PtCl_2$ (DMF)**

Pt,0,0.0723507946,-1.5931578893,-0.2352041571
Cl,0,1.7171058072,-3.3525193293,-0.228321609
N,0,-1.3848753521,-0.0194036926,-0.2760777579
Cl,0,-1.8016383339,-3.1058957995,-0.2641839043
N,0,1.743971872,-0.2486578409,-0.236250595
C,0,-1.9904392553,0.3298449373,1.0279696971
C,0,-3.0232215497,1.4486338328,0.9360060619
C,0,1.9024973943,0.6591897833,0.9188265768
C,0,3.1602211073,1.5196583598,0.8444538812
C,0,-4.2667133639,1.1007673202,0.121057158
C,0,4.4651248334,0.7294113723,0.9311854399
C,0,5.717238751,1.6051677697,1.0054346391
C,0,-5.3037960365,2.2211603366,0.1157410284
C,0,5.9951943562,2.4244312691,-0.2530255643
C,0,-6.5492398692,1.8750451799,-0.6971435184
C,0,7.3060433468,3.2033770558,-0.1828818611

C,0,7.584533193,4.0171558984,-1.4417785452
C,0,-7.5695666252,3.0090214829,-0.8090235823
C,0,-8.204751594,3.4143686212,0.517970812
H,0,-1.0100791023,0.819570978,-0.7193446628
H,0,-2.1094986639,-0.3667941969,-0.9038718148
H,0,1.7506170863,0.2885690232,-1.1038521795
H,0,2.5427908865,-0.8818961354,-0.2936230718
H,0,-1.1780001978,0.6178248765,1.7015404661
H,0,-2.4395066656,-0.586150628,1.4238953036
H,0,-3.321486745,1.69903841,1.9633418887
H,0,-2.5465588307,2.3518306943,0.5269955671
H,0,1.9081724782,0.0384502286,1.8206611394
H,0,1.0157706546,1.2983071375,0.9627796479
H,0,3.1151264143,2.233752937,1.6786219891
H,0,3.1282688963,2.1186937176,-0.0757962248
H,0,-4.7206747034,0.1842994101,0.5266681531
H,0,-3.9919848483,0.8753541334,-0.920098702
H,0,4.5629133681,0.0560515292,0.0666748603
H,0,4.4268923747,0.0858669366,1.8218133122
H,0,6.5836388332,0.9579438333,1.2027040319
H,0,5.636134609,2.28017469,1.8708472005
H,0,-4.8470049858,3.1355199639,-0.2930720273
H,0,-5.5823781962,2.4531295727,1.1530728408
H,0,5.1724683251,3.1306262847,-0.4348245461
H,0,6.020817555,1.7512527222,-1.1240058604
H,0,-7.036499108,0.9922389252,-0.2555811094
H,0,-6.2381387992,1.5780914064,-1.7093707468
H,0,8.1342491092,2.5014935187,-0.0081055499
H,0,7.282643916,3.8721510557,0.6897022526
H,0,8.5310330223,4.5651195297,-1.3656225415
H,0,6.7882749925,4.7502843704,-1.6227174555
H,0,7.6446336193,3.3688687054,-2.325186723
H,0,-8.3621581141,2.7000006308,-1.5041591681
H,0,-7.0863877899,3.8844675853,-1.2671748299
H,0,-8.974770355,4.1804473952,0.3687483855
H,0,-7.4664359416,3.8236491249,1.2171340202
H,0,-8.6815025699,2.5532839664,1.004179955

Sum of electronic and zero-point Energies= -18897.266770
Sum of electronic and thermal Energies= -18897.238936
Sum of electronic and thermal Enthalpies= -18897.237992
Sum of electronic and thermal Free Energies= -18897.332531

cis-(*n*-$C_8H_{13}NH_2)_2PtCl_2$ (DMF)

Pt,0,0.0414849561,-1.905184476,-0.1452147945
Cl,0,1.6472871556,-3.6989338898,-0.0956339065
N,0,-1.3725799351,-0.2948021443,-0.2276756118
Cl,0,-1.862154104,-3.3804064291,-0.1401301905
N,0,1.7340810348,-0.5915359991,-0.1700221884

C,0,-2.0014318698,0.0743865568,1.0598646263
C,0,-3.0234411101,1.199789869,0.9351843772
C,0,2.0277055562,0.1370472177,1.0824557426
C,0,3.284977398,0.9976180419,1.0072968203
C,0,-4.2556538249,0.8492707432,0.1043439387
C,0,4.5749830813,0.2039349352,0.802751599
C,0,5.8473907804,1.0374745648,0.9632749465
C,0,-5.2899398067,1.9718652959,0.0755866692
C,0,6.0230492916,2.1403841049,-0.0783494454
C,0,-6.5224196554,1.6233284578,-0.7562122738
C,0,7.3486563477,2.8839959464,0.05948604
C,0,7.5375339682,3.9912254163,-0.973642538
C,0,-7.5386455559,2.7577672771,-0.8944005145
C,0,-8.2152851313,3.172897186,0.4104182576
C,0,-9.2828488197,4.242224716,0.2042749433
C,0,8.8655813838,4.7255448918,-0.8256395097
H,0,-0.9626820006,0.5332682591,-0.6604624346
H,0,-2.090019336,-0.6218564818,-0.8743054804
H,0,1.6646425633,0.0651733684,-0.9476632518
H,0,2.5102533714,-1.214834738,-0.3958371697
H,0,-1.199667826,0.3635369445,1.7455011807
H,0,-2.466196028,-0.8330702498,1.4571590466
H,0,-3.3373133572,1.4655966127,1.9539837732
H,0,-2.5335429428,2.0940901052,0.5225120799
H,0,2.1183317512,-0.6120813943,1.8756127014
H,0,1.159339129,0.7604235587,1.3144994782
H,0,3.3497916907,1.5551233698,1.9523688144
H,0,3.1602344374,1.748382243,0.2151445432
H,0,-4.7180379842,-0.062954638,0.510023203
H,0,-3.9663260921,0.6152715805,-0.9309975388
H,0,4.5835078468,-0.2592911931,-0.1950900328
H,0,4.5993270303,-0.6221394416,1.5281941937
H,0,6.7144295531,0.3634779283,0.9136073174
H,0,5.8622256341,1.4815509279,1.970106444
H,0,-4.8247865011,2.8830898058,-0.3307616063
H,0,-5.5848865523,2.2101483084,1.1069069996
H,0,5.1992331486,2.8644506824,-0.0035178845
H,0,5.9559550559,1.7003981775,-1.0853968074
H,0,-7.0183660041,0.7434832619,-0.3186390873
H,0,-6.1937433138,1.319551853,-1.7607960068
H,0,8.1786987315,2.1658297404,-0.0238656468
H,0,7.4192220871,3.3161322347,1.069485713
H,0,6.7092266406,4.709578066,-0.8894034206
H,0,7.4667605732,3.5597377633,-1.9826290633
H,0,-8.3159909364,2.4498175677,-1.6090681254
H,0,-7.0450654794,3.6348409049,-1.3409050008
H,0,-7.464673037,3.544635325,1.1206148267
H,0,-8.6683155773,2.2862246442,0.8780848395
H,0,-9.7560919889,4.5270109169,1.1513469097
H,0,-10.0723288398,3.8874639722,-0.4704783164

H,0,-8.8521081105,5.1491687812,-0.238952022
H,0,8.9757567152,5.5144175978,-1.5790067264
H,0,9.7123226223,4.0365524954,-0.9377585829
H,0,8.9492781849,5.1943808573,0.1630431534

Sum of electronic and zero-point Energies= -18975.740169
Sum of electronic and thermal Energies= -18975.709613
Sum of electronic and thermal Enthalpies= -18975.708669
Sum of electronic and thermal Free Energies= -18975.810309

cis-(*i*-$PrNH_2)_2PtCl_2$ (DMF)

Pt,0,0.0792977142,-0.6131741059,-0.2121089049
Cl,0,2.111402409,-1.867778905,0.1235614013
N,0,-1.7620203809,0.4212168544,-0.6369352438
Cl,0,-1.3309231243,-2.475465454,0.3820080078
N,0,1.3577142836,1.0167817935,-0.7899963422
C,0,-2.1836101288,1.6428656687,0.0945562012
C,0,-3.5346374732,2.1222573327,-0.4260187532
C,0,1.6001423034,2.1543543017,0.1374893315
C,0,2.5048175522,3.1859022809,-0.5283100435
C,0,-2.2111386629,1.3729834166,1.5893543322
C,0,2.1769996956,1.6538616866,1.4510425349
H,0,-1.7795895225,0.6092658163,-1.6396747361
H,0,-2.4574767329,-0.313160163,-0.483909193
H,0,1.0366245734,1.3799689414,-1.6877411413
H,0,2.248782278,0.5528626961,-0.9806833005
H,0,-1.4319774165,2.4081750768,-0.1256745604
H,0,-3.8195180864,3.0547413261,0.0727414068
H,0,-4.3163063202,1.3785990779,-0.2271195408
H,0,-3.5042720209,2.312900518,-1.504761628
H,0,0.6225710131,2.6095515976,0.326247672
H,0,2.6373674115,4.0493957009,0.1322112384
H,0,2.0791116406,3.5464337576,-1.471805049
H,0,3.495272604,2.7617910104,-0.7345510451
H,0,-2.5059683173,2.2807698882,2.1255256513
H,0,-1.2297026844,1.0576168555,1.958354943
H,0,-2.9377422817,0.5872654063,1.8305784998
H,0,2.3329108343,2.4997210041,2.1285249958
H,0,3.1443724699,1.1619439912,1.2934576878
H,0,1.5053403703,0.9396786284,1.9384955779

Sum of electronic and zero-point Energies= -18583.383253
Sum of electronic and thermal Energies= -18583.366367
Sum of electronic and thermal Enthalpies= -18583.365423
Sum of electronic and thermal Free Energies= -18583.429810

cis-(*i*-$BuNH_2)_2PtCl_2$ (DMF)

Pt,0,0.2736139685,-1.0304253171,0.0181643866

```
Cl,0,-0.1378934574,-2.4096707007,1.9482564126
N,0,0.6759746924,0.1852080911,-1.708033326
Cl,0,-0.2645176768,-2.7716009822,-1.5536078849
N,0,0.7616638225,0.5170842419,1.4222471395
C,0,0.0088727454,1.4942960725,-1.8361555892
C,0,0.3472795402,2.2416000959,-3.1293785529
C,0,-0.3686700903,1.3256834423,1.9226138414
C,0,0.0460344603,2.4259481242,2.9032170702
C,0,-0.2396511847,3.6504254462,-3.0610322812
C,0,-0.1484181088,1.5045848809,-4.3721007896
C,0,0.6903643588,1.8622760545,4.168594504
C,0,-1.174608485,3.2783574156,3.245212027
H,0,1.6868457377,0.3026669388,-1.7832418205
H,0,0.4070121672,-0.4272596786,-2.4791180464
H,0,1.4906430102,1.1262048222,1.0499827635
H,0,1.1874594573,0.0116161634,2.199044575
H,0,0.3058162373,2.1027837938,-0.9763613306
H,0,-1.0710854249,1.3233265542,-1.7656060986
H,0,1.4431559428,2.3300800251,-3.1868114228
H,0,-1.0730355527,0.6334644625,2.3964512453
H,0,-0.8712450224,1.7662352772,1.0559256819
H,0,0.7797313298,3.0696162723,2.3933808267
H,0,0.018201522,4.2198952655,-3.9608774629
H,0,0.1386814088,4.2026756857,-2.1926408818
H,0,-1.334415508,3.6153688983,-2.9898725062
H,0,0.0954709785,2.0731554588,-5.2765893164
H,0,-1.2384308982,1.3777851816,-4.3397823654
H,0,0.305307681,0.5129081715,-4.4857668886
H,0,0.9473598772,2.6722349881,4.8605696851
H,0,1.6163735719,1.3123712843,3.9619450514
H,0,0.0006536654,1.1840588481,4.6879372775
H,0,-0.8959593252,4.1006950593,3.9136139569
H,0,-1.940460484,2.6787605201,3.7538372182
H,0,-1.6269939568,3.7130251426,2.3460019013

Sum of electronic and zero-point Energies=          -18661.852628
Sum of electronic and thermal Energies=             -18661.832563
Sum of electronic and thermal Enthalpies=           -18661.831619
Sum of electronic and thermal Free Energies=        -18661.905548
```

cis-(*i*-AmNH$_2$)$_2$PtCl$_2$ (DMF)

```
Pt,0,-0.0001167031,-1.2206449195,0.0005233767
Cl,0,1.4719114019,-2.8561120178,-0.980155094
Cl,0,-1.4721995426,-2.8556299674,0.9819323985
N,0,-1.3051215709,0.2503105411,0.8435628858
C,0,-2.2725277389,0.8645954415,-0.0909336231
C,0,-3.212664745,1.8424541306,0.6038487433
C,0,-4.1561035731,2.5823741269,-0.3528728558
C,0,-5.1089401027,1.634281738,-1.0805893789
```

C,0,-4.9413028063,3.6483305639,0.4096033325
N,0,1.3049778328,0.2499024696,-0.8430914047
C,0,2.272415676,0.8644664347,0.0911868132
C,0,3.2126378453,1.8420002159,-0.6039369104
C,0,4.1561627442,2.5821420823,0.3525296683
C,0,5.1089826302,1.6342062989,1.0804732289
C,0,4.9413871074,3.6478356117,-0.4102874174
H,0,-0.7731904309,0.9781046272,1.3210522511
H,0,-1.8133667241,-0.251413494,1.5736177046
H,0,-2.8207148177,0.0446309786,-0.56176438
H,0,-1.703655157,1.374745983,-0.875385232
H,0,-2.6102129451,2.5832539544,1.1491116938
H,0,-3.808881073,1.3038470894,1.3557951441
H,0,-3.5360606494,3.092243037,-1.1065503798
H,0,-5.7946000922,2.196369904,-1.7257629696
H,0,-5.7160723529,1.0680930994,-0.3614574118
H,0,-4.5798255977,0.9141136994,-1.7146650802
H,0,-5.5920328229,4.2157604949,-0.2663004749
H,0,-4.2719957787,4.3587086626,0.9097724915
H,0,-5.5773329813,3.1878963158,1.1772877173
H,0,0.7730990108,0.9775538929,-1.320855775
H,0,1.8131919435,-0.2521324777,-1.5729538707
H,0,2.8205309795,0.0446362654,0.5623343826
H,0,1.7035619116,1.3749505574,0.8754351804
H,0,2.6102486304,2.5826781574,-1.1494338914
H,0,3.8087914669,1.3030884291,-1.3557149833
H,0,3.5361852485,3.0922639162,1.1060899248
H,0,5.7947000684,2.196442425,1.7254566519
H,0,5.7160540397,1.0677835478,0.3614742497
H,0,4.5798622579,0.9142444414,1.7147775773
H,0,5.5921869799,4.2154149133,0.265423698
H,0,4.2720974014,4.3581146943,-0.9106202012
H,0,5.5773490292,3.1871471355,-1.1778757803

Sum of electronic and zero-point Energies= -18740.325219
Sum of electronic and thermal Energies= -18740.302596
Sum of electronic and thermal Enthalpies= -18740.301652
Sum of electronic and thermal Free Energies= -18740.382366

cis-(*c*-$C_3H_5NH_2)_2PtCl_2$ (DMF)

Pt,0,-0.439311421,-0.1515428788,-0.3069996775
Cl,0,-2.5444420046,0.8653627666,0.2738130361
Cl,0,-1.1555370129,-2.3717508645,0.3040347371
N,0,1.4337232866,-1.0563493014,-0.8468196099
N,0,0.1479663208,1.821803573,-0.9307649955
C,0,2.4762175923,-1.0340839394,0.1716486098
C,0,3.5953423249,-2.0342402265,0.1203875083
C,0,2.5290947276,-2.128345959,1.1840893396
C,0,1.17668069,2.5075875332,-0.161578322

C,0,1.1447911022,4.0025877623,-0.022374065
C,0,0.8157006246,3.1141072405,1.1527713482
H,0,1.7908368021,-0.658095877,-1.7155444491
H,0,1.181789092,-2.022548042,-1.0614922665
H,0,-0.7331426576,2.3367306075,-0.8724197567
H,0,0.4037013572,1.816088974,-1.9185430293
H,0,2.7125057467,-0.0271758879,0.4987588834
H,0,4.5889492127,-1.6940586274,0.398740767
H,0,3.573377757,-2.7737632389,-0.6768091306
H,0,1.796308641,-2.926062856,1.0930831738
H,0,2.781162727,-1.8590882285,2.2057123014
H,0,2.1482161831,2.0351115744,-0.2608962471
H,0,0.3231117246,4.5368559175,-0.4935402341
H,0,2.0947761874,4.5298151086,-0.0322855734
H,0,1.5321813054,3.0297662281,1.9647828774
H,0,-0.226334409,3.0546151515,1.4585787246

Sum of electronic and zero-point Energies= -18580.948330
Sum of electronic and thermal Energies= -18580.933423
Sum of electronic and thermal Enthalpies= -18580.932479
Sum of electronic and thermal Free Energies= -18580.993809

cis-(*c*-$C_4H_7NH_2)_2PtCl_2$ (DMF)

Pt,0,0.562327,-0.095312,-0.181494
Cl,0,2.638111,-0.342386,1.010181
Cl,0,0.599999,2.302899,-0.067288
N,0,0.588759,-2.227229,-0.399996
H,0,1.331717,-2.596155,0.192889
N,0,-1.279363,0.088365,-1.265313
C,0,-2.569563,-0.005467,-0.555195
C,0,-2.844817,0.951901,0.611153
C,0,-3.633192,-0.19964,1.274677
C,0,-2.835475,-1.185145,0.390559
H,0,-0.274863,-2.699266,-0.139698
H,0,0.805942,-2.498436,-1.3576
H,0,-1.271854,-0.583902,-2.033039
H,0,-1.218322,1.0089,-1.704237
H,0,-3.372469,0.065878,-1.300324
H,0,-3.362446,1.889936,0.388773
H,0,-1.920964,1.165761,1.159335
H,0,-4.693836,-0.17774,1.003958
H,0,-3.543406,-0.312768,2.358323
H,0,-1.91546,-1.487221,0.903212
H,0,-3.340882,-2.067213,-0.014259

Sum of electronic and zero-point Energies= -18503.703292
Sum of electronic and thermal Energies= -18503.690493
Sum of electronic and thermal Enthalpies= -18503.689549

Sum of electronic and thermal Free Energies= -18503.744596

cis-(*c*-$C_5H_9NH_2)_2PtCl_2$ (DMF)

Pt,0,0.1709003451,-0.7760393602,-0.0033932008
Cl,0,1.6916814574,-2.3407744917,1.0131367484
Cl,0,-0.8636393819,-2.4513293143,-1.3896925517
N,0,1.0678625742,0.7300468006,1.2533637266
C,0,2.1203045361,1.6321814134,0.7320172521
C,0,3.3942437726,0.9119099222,0.3025269516
C,0,4.1471998249,1.9677225817,-0.5282288385
C,0,3.0746579375,2.9911919079,-0.9879347593
C,0,1.732553012,2.4140794094,-0.5172362211
N,0,-1.247944497,0.5829129422,-0.8688025886
C,0,-2.6041628899,0.5529331036,-0.2861119477
C,0,-2.6544169203,1.0554870798,1.1543698818
C,0,-4.143452134,1.3721178453,1.3943924726
C,0,-4.784505617,1.5053483723,-0.0126974165
C,0,-3.6163171574,1.4470769844,-1.0041369452
H,0,0.3233430299,1.2900184153,1.6682107036
H,0,1.4599179888,0.1853305527,2.0232206699
H,0,2.3624817483,2.3443154072,1.5354192311
H,0,3.1185427838,0.0498234401,-0.3177441947
H,0,3.9755987379,0.5346812374,1.1508211304
H,0,4.661914345,1.5052389912,-1.3763553343
H,0,4.9149760804,2.4626327367,0.07631496
H,0,3.0865223828,3.1546399674,-2.0699858806
H,0,3.2498587908,3.9648151383,-0.5161177353
H,0,0.9737054043,3.1842033883,-0.3354166975
H,0,1.3443959787,1.7099014076,-1.2662794485
H,0,-0.8994988751,1.5420804585,-0.869182014
H,0,-1.2996320988,0.3016052049,-1.848598113
H,0,-2.9351906016,-0.4907352428,-0.3327411341
H,0,-2.0591733473,1.9771611549,1.2304414142
H,0,-2.2438200787,0.332246748,1.8670916589
H,0,-4.2581436321,2.2881016542,1.9825038738
H,0,-4.6246461549,0.5692074844,1.9626436459
H,0,-5.3676023077,2.4251193553,-0.1226341327
H,0,-5.4689857688,0.6693316571,-0.197189211
H,0,-3.9010248835,1.0639244871,-1.9901825317
H,0,-3.1787483843,2.4460451598,-1.1446944241

Sum of electronic and zero-point Energies= -18737.965051
Sum of electronic and thermal Energies= -18737.946168
Sum of electronic and thermal Enthalpies= -18737.945224
Sum of electronic and thermal Free Energies= -18738.016971

cis-(*c*-$C_6H_{11}NH_2)_2PtCl_2$ (DMF)

Pt,0,0.0014290173,-0.8465874666,0.0388014144
Cl,0,-0.9854568515,-2.4967181752,1.4936811422
Cl,0,1.0001798883,-2.5218399486,-1.3800220242
N,0,0.9980663648,0.601989496,-1.2170668088
C,0,2.2898059659,1.2108790074,-0.7972418959
C,0,3.3685009417,0.1509293048,-0.613352687
C,0,4.6994022846,0.7981515603,-0.2276244602
C,0,4.5590261384,1.6648358117,1.0226715373
C,0,3.4568976488,2.7079877568,0.8483355629
C,0,2.1300951523,2.0511515763,0.4640280513
N,0,-1.0194949728,0.6168649195,1.2564799857
C,0,-2.3067616357,1.2130123403,0.8066223155
C,0,-3.3657871049,0.1420189365,0.5768856419
C,0,-4.696087753,0.7812485152,0.1755722862
C,0,-4.539849779,1.6739943434,-1.0545413677
C,0,-3.45001479,2.7230301523,-0.8407353613
C,0,-2.1261006432,2.0700437872,-0.4401138078
H,0,0.347839317,1.3488340796,-1.4594172213
H,0,1.1545130628,0.0791363502,-2.08056778
H,0,2.5979494259,1.8787474392,-1.6171786134
H,0,3.4798878496,-0.4371265121,-1.5328279552
H,0,3.0496270009,-0.5471505053,0.1730758026
H,0,5.0592318294,1.4182992478,-1.0620712136
H,0,5.4538268802,0.0177351783,-0.0701572297
H,0,5.5125002274,2.1564030378,1.2533457446
H,0,4.317303467,1.0235332479,1.8833685221
H,0,3.7488669956,3.42336871,0.0655879456
H,0,3.3255363859,3.2874942772,1.7701299615
H,0,1.8056362415,1.3972803907,1.2870325877
H,0,1.3596902057,2.8204340189,0.3170001979
H,0,-0.3771933919,1.369494722,1.5026874988
H,0,-1.1894881829,0.1024120223,2.1224986225
H,0,-2.647298141,1.8666992222,1.6252032547
H,0,-3.4887041533,-0.4685467034,1.4799043832
H,0,-3.0201542516,-0.5325915756,-0.2193653131
H,0,-5.0806330609,1.3803296792,1.0143430132
H,0,-5.437841928,-0.0042557512,-0.0134878191
H,0,-5.4931104267,2.1621169549,-1.2932664624
H,0,-4.2770100415,1.0517961829,-1.9230236757
H,0,-3.7629917042,3.4229037628,-0.0521535381
H,0,-3.3052153263,3.3187592204,-1.7500570329
H,0,-1.7841120688,1.4276631925,-1.2649520602
H,0,-1.3624890839,2.8410731933,-0.2698461442

Sum of electronic and zero-point Energies= -18816.453851
Sum of electronic and thermal Energies= -18816.433900
Sum of electronic and thermal Enthalpies= -18816.432956
Sum of electronic and thermal Free Energies= -18816.504414

cis-(*c*-$C_7H_{13}NH_2)_2PtCl_2$ (DMF)

```
Pt,0,0.0071273171,-1.8116694884,-1.5500201953
Cl,0,-1.8104931626,-3.4002954374,-1.5741439201
Cl,0,1.6922683398,-3.5249747778,-1.3589556419
N,0,-1.5051067224,-0.3045281931,-1.802892262
C,0,-1.8893755895,0.6017866316,-0.6860142442
C,0,-2.5094719114,-0.1998915794,0.4553527172
C,0,-2.5950549186,0.5573743374,1.8087925476
C,0,-2.140511498,2.0205143076,1.8027470431
C,0,-3.0554443167,2.9756999816,1.0199740421
C,0,-3.7343285717,2.3549770728,-0.1999678109
C,0,-2.8104189438,1.7091823594,-1.232464948
N,0,1.6564393038,-0.437349029,-1.7144065838
C,0,1.9374799756,0.5828952467,-0.6728767011
C,0,3.2031503684,1.3666683083,-1.0388006244
C,0,3.4142900506,2.684180439,-0.2433425721
C,0,2.3872425954,2.9848810299,0.8529489633
C,0,2.4552352827,2.0467390445,2.0679508753
C,0,2.8584707579,0.6092173231,1.7426266842
C,0,2.0115581355,-0.1107694302,0.6944507879
H,0,-2.326077014,-0.8431030076,-2.0892324589
H,0,-1.2515954974,0.2609968526,-2.6138273965
H,0,-0.9530430146,1.0463444827,-0.340532997
H,0,-1.9156524922,-1.1106099125,0.590706835
H,0,-3.5074640352,-0.5364398626,0.1427943445
H,0,-1.9832869885,0.0212167533,2.5443319793
H,0,-3.6245402053,0.5087090767,2.1869718332
H,0,-1.1137454505,2.0833181622,1.4203546627
H,0,-2.0770250546,2.3645487222,2.8432308569
H,0,-2.4815538091,3.8625514091,0.7176978402
H,0,-3.8489676845,3.3395920098,1.6869121254
H,0,-4.3265019361,3.1266679656,-0.7088679032
H,0,-4.4593356051,1.6037162218,0.1404595578
H,0,-3.4450271427,1.2702071029,-2.0165465601
H,0,-2.1949511171,2.4748555703,-1.7248339604
H,0,2.4574879819,-1.0693308707,-1.7869327024
H,0,1.5820340781,0.0202623533,-2.6234237428
H,0,1.0861876344,1.2684651397,-0.7022552284
H,0,3.1544680823,1.6043288462,-2.1092628548
H,0,4.0695707321,0.7025851427,-0.9175749318
H,0,3.4056591007,3.5216955179,-0.9509439641
H,0,4.4173367846,2.681104757,0.2027501204
H,0,1.3778586598,2.973652086,0.4221873461
H,0,2.5399148042,4.017203856,1.1933518786
H,0,1.4870763095,2.0546270564,2.5875866775
H,0,3.1887758538,2.4408142962,2.7846613177
H,0,2.8331558495,0.0158568219,2.6657815892
H,0,3.9072475281,0.5996723001,1.4165392078
H,0,2.4397985862,-1.1116509872,0.5444922663
```

H,0,0.9918354697,-0.2722282489,1.0691730548

Sum of electronic and zero-point Energies= -18894.896674
Sum of electronic and thermal Energies= -18894.873918
Sum of electronic and thermal Enthalpies= -18894.872974
Sum of electronic and thermal Free Energies= -18894.951421

cis-(*c*-$C_8H_{15}NH_2)_2PtCl_2$ (DMF)

Pt,0,-0.0182286947,-1.6674934458,-0.1848944942
Cl,0,1.7642820714,-3.1100963323,0.5622208006
Cl,0,-1.7023293345,-3.1367169757,0.7149036578
N,0,1.5239216501,-0.4442231843,-1.0607027063
C,0,2.5224478175,0.2227265605,-0.1699605699
C,0,3.6839913846,0.7102220564,-1.0443306638
C,0,4.9241110054,1.2755247394,-0.3278489019
C,0,4.7352515228,2.1930432684,0.8848007694
C,0,3.991885268,3.5240664514,0.6763709846
C,0,2.7816406563,3.541333758,-0.2633707136
C,0,1.5672507017,2.674352387,0.1099466543
C,0,1.8157893012,1.2770606398,0.6910832495
N,0,-1.596769897,-0.4383995167,-1.0078207473
C,0,-2.7202083101,0.0404691136,-0.1501600658
C,0,-2.145347465,0.8947853781,0.9820969213
C,0,-3.1338653088,1.622676608,1.9012085093
C,0,-4.1070204011,2.6511071758,1.3048396425
C,0,-3.5637849169,3.6665700824,0.293610842
C,0,-2.9015510772,3.146886091,-0.992596713
C,0,-3.5744185218,1.9911281106,-1.7448972355
C,0,-3.8260437266,0.6593692551,-1.0162948056
H,0,2.0200775718,-1.1027317577,-1.6625903457
H,0,1.1326020915,0.251225597,-1.697809874
H,0,2.880020045,-0.5731682517,0.4918036966
H,0,3.2932414641,1.431545535,-1.770114767
H,0,4.0282372653,-0.1455566593,-1.6426389326
H,0,5.5292001765,1.7930757232,-1.0855691151
H,0,5.5341799615,0.4266492506,0.0098369855
H,0,5.7395863688,2.4343425038,1.2598866684
H,0,4.2714474264,1.617763358,1.6928119691
H,0,4.7071264259,4.25651705,0.2761825396
H,0,3.6947800317,3.9090430203,1.6629949601
H,0,3.1235625674,3.3041842075,-1.2762754202
H,0,2.4290007452,4.5804168539,-0.3241298919
H,0,0.9075714738,2.6118143523,-0.7687286759
H,0,0.9821991371,3.2127288895,0.8687644784
H,0,2.3637574131,1.3811248586,1.6305437967
H,0,0.8460096017,0.851100356,0.9796539567
H,0,-1.1884209282,0.3639553415,-1.487809749
H,0,-1.9853644801,-1.0237633838,-1.7484527214
H,0,-3.1414250881,-0.867649754,0.2934321174

H,0,-1.4305786684,1.6180242744,0.5770410729
H,0,-1.5497511498,0.2218607343,1.6132648598
H,0,-2.5208488334,2.129171769,2.6595713736
H,0,-3.7254320319,0.8767483404,2.4514186885
H,0,-4.5192650729,3.2225983914,2.1484581571
H,0,-4.9729974486,2.1441880033,0.8677042712
H,0,-2.8427412952,4.3275276608,0.7967737093
H,0,-4.4082507975,4.3112542638,0.0105720345
H,0,-1.8558563733,2.8899182758,-0.7947299328
H,0,-2.8473788558,3.9918068575,-1.693510171
H,0,-2.9690032893,1.7966619294,-2.6420160756
H,0,-4.5477930464,2.3313554168,-2.1262181186
H,0,-4.7134624935,0.736543467,-0.3830949248
H,0,-4.0969516397,-0.0864336957,-1.7784910344

Sum of electronic and zero-point Energies= -18973.351610
Sum of electronic and thermal Energies= -18973.326737
Sum of electronic and thermal Enthalpies= -18973.325792
Sum of electronic and thermal Free Energies= -18973.409468

cis-(1-Adamantamine)$_2$PtCl$_2$ (DMF)

Pt,0,0.0004283001,-1.3519135555,-0.0317041561
Cl,0,1.2251813823,-3.001425514,-1.295759451
Cl,0,-1.2225392694,-3.0360395019,1.1876650616
C,0,2.4078168578,0.7282499528,-0.4569047167
C,0,2.0651324268,1.4226794193,0.8642966892
C,0,3.3290918914,2.0610202574,1.4589039262
C,0,2.9858898728,1.7638321144,-1.436363086
C,0,4.7201467081,0.2710385173,0.3952160539
C,0,5.2926294849,1.2992672271,-0.5881062732
C,0,4.2524140843,2.3962047479,-0.8442293973
C,0,3.8977369333,3.0909815465,0.4756488828
C,0,4.3716853034,0.9663475787,1.7169586845
C,0,3.4532363925,-0.3599244801,-0.1986099135
N,0,1.187032725,0.1261075812,-1.0656418472
C,0,-2.4091665295,0.7135016862,0.4490718722
C,0,-2.067222103,1.4436728244,-0.8529102932
C,0,-3.3319043189,2.0962794984,-1.4302403845
C,0,-2.9885316138,1.7216484378,1.4559993567
C,0,-4.7208843253,0.2766408814,-0.4152877905
C,0,-5.2946623345,1.2773336607,0.595313531
C,0,-4.2557793299,2.3682184672,0.8809888057
C,0,-3.9018576268,3.0987094688,-0.4196686213
C,0,-4.3731617733,1.0077035523,-1.7177923502
C,0,-3.4532770126,-0.3685687429,0.1614743369
N,0,-1.1877194386,0.0966152594,1.0414980382
H,0,1.6600246599,0.6849308731,1.5708993124
H,0,1.3015826012,2.1975283959,0.6985035697
H,0,3.0650900461,2.5542185402,2.4033179153

H,0,2.2348810209,2.5419481438,-1.6375729018
H,0,3.2170234377,1.275545648,-2.3939542653
H,0,5.4584601576,-0.5209674153,0.5758034213
H,0,5.5649551338,0.8085949385,-1.5332093335
H,0,6.2106603781,1.7414873058,-0.1770903692
H,0,4.6506728119,3.1299471398,-1.557096629
H,0,4.7924176,3.5628911748,0.9044408008
H,0,3.1645205516,3.890290023,0.2972806099
H,0,3.9811962659,0.2346398368,2.4381810853
H,0,5.2754167655,1.4069458498,2.1600802085
H,0,3.6905640857,-0.8770723788,-1.1386852668
H,0,3.038906298,-1.1115128812,0.485437619
H,0,1.467681996,-0.3677362832,-1.9159165958
H,0,0.5738106506,0.8799616153,-1.3785575676
H,0,-1.6611562628,0.7257262253,-1.5790871166
H,0,-1.3046334607,2.2146984016,-0.6661950411
H,0,-3.0684272194,2.6150433716,-2.3610061418
H,0,-2.238481427,2.4949731766,1.6781623196
H,0,-3.2191463557,1.2074877921,2.4000768795
H,0,-5.4582361944,-0.5110962732,-0.6172113621
H,0,-5.566465924,0.7610602187,1.5268312003
H,0,-6.2131905142,1.7293808423,0.1962728146
H,0,-4.6549671564,3.0820147441,1.6133224144
H,0,-4.797080565,3.5809200278,-0.8356784073
H,0,-3.1696135647,3.8938054313,-0.2197763932
H,0,-3.9817328129,0.2961524162,-2.4584124466
H,0,-5.2773899608,1.4589864202,-2.1489867698
H,0,-3.6900600292,-0.9110932022,1.087278416
H,0,-3.0379840772,-1.1010062856,-0.542472415
H,0,-1.4678279368,-0.4201344844,1.8782293674
H,0,-0.5753166862,0.8424887663,1.3744921104

Sum of electronic and zero-point Energies= -19125.670385
Sum of electronic and thermal Energies= -19125.647245
Sum of electronic and thermal Enthalpies= -19125.646300
Sum of electronic and thermal Free Energies= -19125.724096

cis-(2-Adamantamine)$_2$PtCl$_2$ (DMF)

Pt,0,-1.2559580386,-1.5764646913,0.
Cl,0,-1.0997072784,-3.2799363139,1.6967508337
Cl,0,-1.0997072784,-3.2799363139,-1.6967508337
C,0,0.6969758237,-0.1386596025,2.6496633857
C,0,-0.8259778539,-0.1335834463,2.8184229513
C,0,-1.2328348167,1.0041239592,3.7735485945
C,0,1.2064612761,1.2228225019,2.1564779032
C,0,0.9169551059,0.6534418652,5.0246551595
C,0,1.4289416586,2.0103856474,4.5242597117
C,0,0.8141453545,2.3211726107,3.1531650905
C,0,-0.7145261372,2.3620961242,3.2771478208

C,0,-0.6117467177,0.6999543217,5.1454706043
C,0,1.31492632,-0.4389386679,4.0234548778
N,0,-1.5338865799,-0.0512386386,1.515784098
C,0,-1.2328348167,1.0041239592,-3.7735485945
C,0,-0.8259778539,-0.1335834463,-2.8184229513
C,0,0.6969758237,-0.1386596025,-2.6496633857
C,0,-0.7145261372,2.3620961242,-3.2771478208
C,0,0.9169551059,0.6534418652,-5.0246551595
C,0,1.4289416586,2.0103856474,-4.5242597117
C,0,0.8141453545,2.3211726107,-3.1531650905
C,0,1.2064612761,1.2228225019,-2.1564779032
C,0,1.31492632,-0.4389386679,-4.0234548778
C,0,-0.6117467177,0.6999543217,-5.1454706043
N,0,-1.5338865799,-0.0512386386,-1.515784098
H,0,0.969551959,-0.9281954118,1.9377318989
H,0,-1.133168831,-1.090969098,3.2496012093
H,0,-2.328379994,1.0287449332,3.8639276588
H,0,0.8127777039,1.4587888968,1.1569207471
H,0,2.298920459,1.1800756636,2.0476404019
H,0,1.3554832384,0.4299388628,6.0064254797
H,0,2.5255644707,1.9944535016,4.4488662411
H,0,1.1659835275,2.80089891,5.2415115677
H,0,1.1802625824,3.2923971705,2.7944923655
H,0,-1.0176532518,3.1436508856,3.9872611198
H,0,-1.1673114051,2.6385137514,2.3132900037
H,0,-0.9923953441,-0.2578415777,5.5270979117
H,0,-0.9124491866,1.4754696373,5.8633697108
H,0,2.4086363104,-0.4866514111,3.9308236926
H,0,0.9781634722,-1.4229307274,4.3788644831
H,0,-1.3539988407,0.8622654114,1.1016337247
H,0,-2.5385820113,-0.0656250304,1.6973118514
H,0,-2.328379994,1.0287449332,-3.8639276588
H,0,-1.133168831,-1.090969098,-3.2496012093
H,0,0.969551959,-0.9281954118,-1.9377318989
H,0,-1.1673114051,2.6385137514,-2.3132900037
H,0,-1.0176532518,3.1436508856,-3.9872611198
H,0,1.3554832384,0.4299388628,-6.0064254797
H,0,1.1659835275,2.80089891,-5.2415115677
H,0,2.5255644707,1.9944535016,-4.4488662411
H,0,1.1802625824,3.2923971705,-2.7944923655
H,0,2.298920459,1.1800756636,-2.0476404019
H,0,0.8127777039,1.4587888968,-1.1569207471
H,0,0.9781634722,-1.4229307274,-4.3788644831
H,0,2.4086363104,-0.4866514111,-3.9308236926
H,0,-0.9124491866,1.4754696373,-5.8633697108
H,0,-0.9923953441,-0.2578415777,-5.5270979117
H,0,-2.5385820113,-0.0656250304,-1.6973118514
H,0,-1.3539988407,0.8622654114,-1.1016337247

Sum of electronic and zero-point Energies= -19125.656382
Sum of electronic and thermal Energies= -19125.634647
Sum of electronic and thermal Enthalpies= -19125.633702
Sum of electronic and thermal Free Energies= -19125.708455

cis-$(C_5H_5N)_2PtCl_2$ (DMF)

Pt,0,-0.0000263399,-0.778880214,-0.0001334005
Cl,0,1.7402001681,-2.4352221088,-0.0161065204
Cl,0,-1.7377650967,-2.4380385417,0.0155636808
C,0,1.9037902877,1.2685610847,-1.1691728509
C,0,2.0472187608,1.1386368654,1.1394752888
C,0,2.8870615155,2.2481172662,-1.2153735785
H,0,1.428017789,0.8984899092,-2.0711991773
C,0,3.0347841875,2.1143107358,1.1732764753
H,0,1.6841959946,0.6658568525,2.0458255805
C,0,3.4636966205,2.6803686636,-0.0241911084
H,0,3.1887120593,2.6572454349,-2.1739151879
H,0,3.4546933021,2.4163938305,2.1270160727
H,0,4.2353448148,3.4445750025,-0.0291181705
C,0,-1.9054049073,1.2668676366,1.1693528959
C,0,-2.0486468232,1.1375938638,-1.1393366064
C,0,-2.8883552036,2.2467385749,1.2157177643
H,0,-1.4298119723,0.8964417425,2.071328277
C,0,-3.0358872683,2.1136080117,-1.1729765192
H,0,-1.6856725399,0.6649692078,-2.0457876599
C,0,-3.4646859036,2.6795437873,0.0245890128
H,0,-3.1899452995,2.6557317351,2.1743366104
H,0,-3.4555877338,2.4161022672,-2.1266782191
H,0,-4.2359948276,3.4440928768,0.0296308119
N,0,1.4938976618,0.7279470971,-0.0117440992
N,0,-1.495529246,0.7264484185,0.0118206279

Sum of electronic and zero-point Energies= -18730.876636
Sum of electronic and thermal Energies= -18730.861054
Sum of electronic and thermal Enthalpies= -18730.860110
Sum of electronic and thermal Free Energies= -18730.924117

cis-$(C_5H_{10}NH)_2PtCl_2$ (DMF)

Pt,0,0.0003578056,-0.8505118134,0.0026703793
Cl,0,1.5276189055,-2.7214989742,-0.0166356847
Cl,0,-1.9318843714,-2.3057060445,-0.0122192111
C,0,1.9591446107,1.2042231975,-1.2137263344
C,0,2.0095413176,1.1438518301,1.2410921347
H,0,2.4782975985,-0.3761867807,-0.0342942023
C,0,3.3335384944,1.8654930958,-1.2506600234
H,0,1.1742991398,1.9705703838,-1.2142987759
H,0,1.7987660109,0.5627720957,-2.0845895912
C,0,3.3857367588,1.8016685492,1.2548790126

H,0,1.2277472363,1.9099357496,1.3096993825
H,0,1.8816950787,0.4607423309,2.085199505
C,0,3.5909778912,2.6735565708,0.0187085863
H,0,3.392343125,2.501407422,-2.1420060932
H,0,4.1037701712,1.0891549955,-1.3626343918
H,0,3.4829801496,2.3911253227,2.1743606173
H,0,4.1582413013,1.0205260176,1.2948192514
H,0,4.606458666,3.0863580738,0.0079442311
H,0,2.900739681,3.5287913249,0.0547999456
C,0,-2.0832522525,1.0221928986,-1.2253691785
C,0,-2.166830682,0.9486696357,1.226188189
H,0,-0.6655007348,1.6841780355,0.0733786941
C,0,-2.9052299532,2.3064704576,-1.2404307553
H,0,-2.7292709013,0.1408730607,-1.2883064218
H,0,-1.3828380875,0.9858719204,-2.0652566922
C,0,-2.989182,2.2322239952,1.2615339921
H,0,-2.8148174336,0.0676474148,1.192232237
H,0,-1.5254014825,0.859833237,2.1079535541
C,0,-3.8109396025,2.3940777723,-0.0147325351
H,0,-3.4913648588,2.3347514782,-2.1669421489
H,0,-2.2287713423,3.1733027065,-1.2672212583
H,0,-3.6363751414,2.206945781,2.1465954018
H,0,-2.3177434392,3.094533104,1.3849520826
H,0,-4.3493935019,3.3490931381,-0.0045474667
H,0,-4.5698229201,1.6000097496,-0.0637817423
N,0,1.7801172382,0.3719079794,-0.0018951931
N,0,-1.2961524754,0.8827442886,0.0254405035

Sum of electronic and zero-point Energies= -18737.964573
Sum of electronic and thermal Energies= -18737.946878
Sum of electronic and thermal Enthalpies= -18737.945934
Sum of electronic and thermal Free Energies= -18738.012160

cis-$[(CH_3)_2NH]_2PtCl_2$ (DMF)

Pt,0,0.0173349391,-0.2624642343,0.0135128005
Cl,0,-1.9981310849,-1.5921815607,0.0296229372
N,0,1.8779093882,0.8412574494,-0.0039025011
Cl,0,1.4251852294,-2.2198122269,0.0465502235
N,0,-1.1892977071,1.5404296493,-0.0182626314
C,0,2.1043065903,1.6645777617,-1.2015726049
C,0,-2.0138513441,1.6539824259,-1.2354598962
C,0,2.1631302366,1.5767379427,1.2379293973
H,0,2.5197440198,0.047364269,-0.04757889
H,0,-0.5228407384,2.3103264366,-0.0361506507
C,0,-2.0057025028,1.701191012,1.1991023901
H,0,3.1339262632,2.0435652217,-1.2154960415
H,0,1.4252764238,2.521143525,-1.2027957927
H,0,1.9240353396,1.0635548237,-2.0946586096
H,0,-2.554784178,2.6088357441,-1.2392262109

H,0,-2.7277006732,0.8290384731,-1.2540041638
H,0,-1.3724950397,1.5947388833,-2.1171728017
H,0,2.054623141,0.9032706496,2.0899822006
H,0,1.4628672793,2.4084432157,1.3489676995
H,0,3.1832518754,1.9809215389,1.2171393492
H,0,-1.3587009388,1.6745740856,2.0783781673
H,0,-2.7200652694,0.8782544988,1.2540132897
H,0,-2.5456212492,2.6561504157,1.1706823396

Sum of electronic and zero-point Energies= -18504.878880
Sum of electronic and thermal Energies= -18504.864516
Sum of electronic and thermal Enthalpies= -18504.863572
Sum of electronic and thermal Free Energies= -18504.921231

cis-$(CH_3NH_2)(NH_3)PtCl_2$ (DMF)

Pt,0,0.4226597026,-0.0630237222,-0.0764701408
Cl,0,2.6410060882,-0.8620841921,0.3843837968
Cl,0,1.0476574423,2.2568212212,0.0393038988
N,0,-1.5553552065,0.6354104924,-0.4799733996
N,0,-0.1520580149,-2.1243760145,-0.2150061037
C,0,-2.6199645164,0.2229535659,0.4496213412
H,0,-2.7430118546,-0.8608487991,0.4094114665
H,0,-3.5711478179,0.6967372883,0.1839346385
H,0,-0.6748204556,-2.3500360846,-1.0590868163
H,0,-1.8093596889,0.3837949912,-1.4344139059
H,0,-1.4638085255,1.6518431074,-0.4729532816
H,0,0.6989568342,-2.6859474899,-0.2214965501
H,0,-0.7063417278,-2.4307118871,0.5824100627
H,0,-2.3420122593,0.513067523,1.4641349936

Sum of electronic and zero-point Energies= -18387.198481
Sum of electronic and thermal Energies= -18387.187964
Sum of electronic and thermal Enthalpies= -18387.187019
Sum of electronic and thermal Free Energies= -18387.236557

cis-(*i*-$PrNH_2)(NH_3)PtCl_2$ (DMF)

Pt,0,0.0361222309,-0.6685484985,-0.1666880424
Cl,0,2.1156715044,-1.7691726852,0.3328768245
N,0,-1.8055042142,0.3239268843,-0.6440095808
Cl,0,-1.311800577,-2.4775885036,0.668259544
N,0,1.2264259899,0.9401807509,-0.9389505001
C,0,-2.1614933248,1.5742113028,0.0783291306
C,0,-3.4577863648,2.1522281918,-0.478766707
H,0,1.1667380377,1.7830061222,-0.3706052696
C,0,-2.2527205458,1.305161104,1.5715725381
H,0,-1.8213318897,0.4967424994,-1.6494381935
H,0,-2.5246453284,-0.3821175869,-0.4709053661
H,0,2.2005282014,0.6389375699,-0.9316785667

H,0,0.9924621334,1.197534359,-1.8958711913
H,0,-1.3469582877,2.281482822,-0.1144071408
H,0,-3.6920338377,3.0964457222,0.0242966607
H,0,-4.2956691907,1.4637873405,-0.3140863032
H,0,-3.3798856457,2.3540871263,-1.5531609389
H,0,-2.510095697,2.2296236313,2.0984183687
H,0,-1.3043096053,0.9328943728,1.9728237427
H,0,-3.0326135891,0.5646774746,1.7884909913

Sum of electronic and zero-point Energies= -18465.679089
Sum of electronic and thermal Energies= -18465.665983
Sum of electronic and thermal Enthalpies= -18465.665039
Sum of electronic and thermal Free Energies= -18465.720529

cis-(*c*-$C_3H_5NH_2$)(NH_3)$PtCl_2$ (DMF)

Pt,0,0.4176856116,-0.0692106692,-0.0827416769
Cl,0,2.6533133194,-0.8406429273,0.3468386819
Cl,0,1.0005449396,2.2575473402,0.0848243931
N,0,-1.5778225538,0.6050392382,-0.4888016488
N,0,-0.1314248997,-2.1328886712,-0.2429617796
C,0,-2.6015087694,0.2591844359,0.488252183
C,0,-3.4505816046,-0.9518047432,0.2720137419
C,0,-4.0527186637,0.4266206249,0.1485448495
H,0,-0.4388522956,-2.3894261859,-1.1790165306
H,0,-1.8521042631,0.2916592827,-1.4202568343
H,0,-1.4863975324,1.6212321065,-0.5467640355
H,0,0.6865047224,-2.7004611937,-0.0235272779
H,0,-0.8717188805,-2.3931372717,0.4060712127
H,0,-2.2867366929,0.4890339605,1.5010773767
H,0,-3.6999401608,-1.5588640311,1.1375786661
H,0,-3.314660052,-1.5124224495,-0.6505138934
H,0,-4.3002303916,0.7736580452,-0.8519694792
H,0,-4.7151248331,0.7833631088,0.9320730513

Sum of electronic and zero-point Energies= -18464.461991
Sum of electronic and thermal Energies= -18464.449789
Sum of electronic and thermal Enthalpies= -18464.448845
Sum of electronic and thermal Free Energies= -18464.503876

cis-(*c*-$C_4H_7NH_2$)(NH_3)$PtCl_2$ (DMF)

Pt,0,0.562327,-0.095312,-0.181494
Cl,0,2.638111,-0.342386,1.010181
Cl,0,0.599999,2.302899,-0.067288
N,0,0.588759,-2.227229,-0.399996
H,0,1.331717,-2.596155,0.192889
N,0,-1.279363,0.088365,-1.265313
C,0,-2.569563,-0.005467,-0.555195
C,0,-2.844817,0.951901,0.611153

C,0,-3.633192,-0.19964,1.274677
C,0,-2.835475,-1.185145,0.390559
H,0,-0.274863,-2.699266,-0.139698
H,0,0.805942,-2.498436,-1.3576
H,0,-1.271854,-0.583902,-2.033039
H,0,-1.218322,1.0089,-1.704237
H,0,-3.372469,0.065878,-1.300324
H,0,-3.362446,1.889936,0.388773
H,0,-1.920964,1.165761,1.159335
H,0,-4.693836,-0.17774,1.003958
H,0,-3.543406,-0.312768,2.358323
H,0,-1.91546,-1.487221,0.903212
H,0,-3.340882,-2.067213,-0.014259

Sum of electronic and zero-point Energies= -18503.703292
Sum of electronic and thermal Energies= -18503.690493
Sum of electronic and thermal Enthalpies= -18503.689549
Sum of electronic and thermal Free Energies= -18503.744596

***cis*-(*c*-$C_5H_9NH_2$)(NH_3)$PtCl_2$ (DMF)**

Pt,0,-0.7784882628,-0.1107102904,-0.1444248984
Cl,0,-0.943518291,2.2834974016,-0.0367831202
Cl,0,-2.8108632411,-0.4523691565,1.0938453001
N,0,0.9948306546,0.1837096927,-1.3318680473
C,0,2.3495672778,0.1036880133,-0.7404247795
C,0,2.6135558082,1.1514094733,0.3376294839
C,0,3.8457021546,0.6114354615,1.0958279363
C,0,3.9798599946,-0.8769038863,0.6841833906
C,0,2.667284976,-1.2068542482,-0.0324368703
N,0,-0.6898889596,-2.2466558846,-0.3257713686
H,0,-0.767612784,-2.5548509491,-1.2933022917
H,0,0.9426712452,-0.4485703217,-2.130442822
H,0,0.8628161031,1.1212957405,-1.7147120089
H,0,3.0669245348,0.2404387575,-1.5638044363
H,0,1.73721657,1.1999342346,0.9957273971
H,0,2.7670337751,2.1533872018,-0.0769961936
H,0,3.7101565052,0.7171759219,2.1770452614
H,0,4.7502845053,1.1704538897,0.8344212042
H,0,4.1612004313,-1.5377425807,1.5375381329
H,0,4.8209957955,-1.0067374379,-0.0074619596
H,0,2.7420470518,-2.066195279,-0.7085772818
H,0,1.8820748391,-1.4080433164,0.709259192
H,0,0.1517761049,-2.6685994613,0.0607771702
H,0,-1.4867537888,-2.6323069763,0.1802486096

Sum of electronic and zero-point Energies= -18542.967832
Sum of electronic and thermal Energies= -18542.953940
Sum of electronic and thermal Enthalpies= -18542.952996

Sum of electronic and thermal Free Energies= -18543.011012

cis-(*c*-$C_6H_{11}NH_2$)(NH_3)$PtCl_2$ (DMF)

Pt,0,0.9798350163,-0.1126990457,-0.1632621625
Cl,0,1.1928246782,2.2805040674,-0.1068370902
Cl,0,2.9123245949,-0.4559224718,1.2340090231
N,0,0.8803044088,-2.2507127785,-0.3158069282
H,0,1.0399573192,-2.5731477069,-1.2685868064
N,0,-0.7421178182,0.1786317748,-1.4252762632
C,0,-2.1203875036,0.1414399395,-0.8699804246
C,0,-2.3255400932,1.2343806612,0.1707957025
C,0,-3.7636390779,1.2156348326,0.6907415632
C,0,-4.1418121993,-0.1569712096,1.2454183574
C,0,-3.8973139591,-1.2575713392,0.2140553993
C,0,-2.4543080772,-1.2278006478,-0.2921860454
H,0,0.0015933248,-2.6561530581,-0.0007757814
H,0,1.6236422124,-2.6379600091,0.2647930214
H,0,-0.6807910963,-0.4790697552,-2.202924563
H,0,-0.5801280748,1.1022089917,-1.830251096
H,0,-2.8003192749,0.3339010692,-1.7149529026
H,0,-2.0854087706,2.2156554274,-0.2573147558
H,0,-1.6229418378,1.0677335675,0.9994316733
H,0,-4.449826261,1.479822443,-0.127596052
H,0,-3.8849607868,1.9866190591,1.4613752141
H,0,-5.1923911224,-0.1615181579,1.5620240845
H,0,-3.5400069873,-0.3633125497,2.1429877883
H,0,-4.5834498509,-1.1244353244,-0.6352242492
H,0,-4.1165370318,-2.2425535104,0.6435028631
H,0,-1.7761326121,-1.4296870975,0.5500038686
H,0,-2.2988691194,-2.0107171717,-1.0470634384

Sum of electronic and zero-point Energies= -18582.213915
Sum of electronic and thermal Energies= -18582.199319
Sum of electronic and thermal Enthalpies= -18582.198375
Sum of electronic and thermal Free Energies= -18582.257208

cis-(Quinoline)(NH_3)$PtCl_2$ (DMF)

Pt,0,1.5370870957,-2.2321407227,-0.355553642
Cl,0,3.275793769,-3.8888603724,-0.4487308767
Cl,0,-0.2041399839,-3.8768791317,-0.224882275
H,0,2.1600778127,-1.2542946413,-2.8785345467
C,0,3.55321719,-0.3510847511,0.743367002
C,0,4.4080236186,0.9572397448,-1.515582251
C,0,4.5243506325,0.6567007242,0.8710658308
H,0,3.1968832024,-0.8846276201,1.6189936627
C,0,4.9473253994,1.3126555091,-0.2583487808
H,0,4.9145553277,0.8948334649,1.85460274

H,0,5.6934461206,2.1010670772,-0.2012557731
H,0,-0.9101376728,-1.2053612135,-0.280327094
H,0,0.0481917481,-0.2075701934,0.6074438318
H,0,0.0322325498,-0.0832524992,-1.0292563423
N,0,3.0230082339,-0.7053125704,-0.4180018839
N,0,-0.0009649258,-0.7449734644,-0.2560765047
C,0,3.4298138791,-0.0813750167,-1.5707780355
C,0,3.3064251098,0.1863548079,-3.9711628093
C,0,4.2681399165,1.2208471755,-3.92138246
H,0,2.8880156322,-0.1102218823,-4.9288766946
C,0,4.8092894746,1.5964479976,-2.7156405576
H,0,4.5786580133,1.7133448229,-4.8382672291
H,0,5.5533152594,2.3870831763,-2.6604740381
C,0,2.8927925974,-0.4544204212,-2.8251412731

Sum of electronic and zero-point Energies= -18692.846848
Sum of electronic and thermal Energies= -18692.831993
Sum of electronic and thermal Enthalpies= -18692.831049
Sum of electronic and thermal Free Energies= -18692.891019

$(H_2NCH_2CH_2NH_2)PtCl_2$ (DMF)

Pt,0,-0.1353400696,0.0000230251,-0.0000242332
Cl,0,-1.7230523,1.7027111161,0.0540658379
N,0,1.3910289082,-1.3642983703,-0.046566981
Cl,0,-1.7231259834,-1.7025944679,-0.0539801927
N,0,1.3910955409,1.364261705,0.0467092293
C,0,2.6609493164,-0.6853276397,0.3214214852
H,0,1.4600143539,-1.7573304177,-0.9867080291
H,0,1.2135643876,-2.1539956267,0.5745700418
H,0,1.2136836824,2.1539824621,-0.5744130371
C,0,2.6609949246,0.6852354181,-0.3212353916
H,0,1.4600635109,1.7572612972,0.9868648917
H,0,3.5247609123,1.2742621048,0.0013042801
H,0,2.6844705234,0.6007266109,-1.411130162
H,0,3.524693122,-1.2743963915,-0.0010954175
H,0,2.6843991704,-0.6008208252,1.411317678

Sum of electronic and zero-point Energies= -1229.766867
Sum of electronic and thermal Energies= -1229.757873
Sum of electronic and thermal Enthalpies= -1229.756929
Sum of electronic and thermal Free Energies= -1229.802954

$[H_2NCH_2CH_2NH(CH_2CH_2OH)]PtCl_2$ (DMF)

Pt,0,-0.1480021796,0.0483948473,-0.2081918463
Cl,0,-1.9985223703,-1.3588675636,-0.8279208505
N,0,1.6257375853,1.1204277984,0.3697137073
Cl,0,-1.5156688277,2.0017624556,0.1090854171
N,0,1.2271971968,-1.549185618,-0.4831147051

C,0,2.7687930812,0.3027860971,-0.1220434002
C,0,1.6521642627,1.4315232895,1.8138314251
H,0,1.6049164188,1.9999981556,-0.1470109089
H,0,0.8791391353,-2.428801796,-0.1048906148
C,0,2.5116524759,-1.1654251166,0.1451216237
H,0,1.3438444656,-1.6938326689,-1.4859156997
H,0,3.3366981867,-1.7727147205,-0.2433747322
H,0,2.427081412,-1.361179152,1.2170423492
H,0,3.7107258397,0.6151209813,0.3416333399
H,0,2.8519481273,0.4808922272,-1.1985098531
C,0,2.7259752752,2.4401200128,2.2014783762
O,0,2.5628928575,2.665814791,3.5904356033
H,0,1.7888952007,0.5006674505,2.3712992051
H,0,0.6725974683,1.8387760863,2.0779729526
H,0,2.5845384002,3.3711969843,1.6331326194
H,0,3.7329654781,2.0583617686,1.9882465997
H,0,3.2371305103,3.2944636902,3.8830793921

Sum of electronic and zero-point Energies= -18578.852582
Sum of electronic and thermal Energies= -18578.839142
Sum of electronic and thermal Enthalpies= -18578.838198
Sum of electronic and thermal Free Energies= -18578.895075

[MeHNCH$_2$CH$_2$NHMe]PtCl$_2$ (DMF)

Pt,0,-0.158391473,0.0002877319,-0.0003133016
Cl,0,-1.801461674,-1.7528501945,-0.1330602721
N,0,1.4429756824,1.4171549538,0.1430201216
Cl,0,-1.801652832,1.7533202732,0.1323263489
N,0,1.4429079116,-1.4164937401,-0.1436561035
C,0,2.6697408608,0.7004535115,-0.2876127617
C,0,1.5641630287,2.0346043698,1.4757797409
H,0,1.2480852532,2.160364382,-0.5264815195
H,0,1.2478274289,-2.159837168,0.5256576088
C,0,2.6695552663,-0.6998901243,0.287448912
C,0,1.5644075089,-2.0337106415,-1.4764880933
H,0,3.5654131941,-1.2475134346,-0.0313757792
H,0,2.667978552,-0.6687799042,1.3806758236
H,0,3.5655206334,1.2479456548,0.0316505634
H,0,2.66868473,0.6694193923,-1.3808402437
H,0,1.7363696367,1.2631545373,2.2284864359
H,0,0.6318403816,2.5519713743,1.7072063081
H,0,2.3978603592,2.7473074028,1.4901725079
H,0,1.7365388162,-1.2621327149,-2.2290783769
H,0,0.632228261,-2.5512545198,-1.7080947514
H,0,2.398258074,-2.7462396418,-1.4908701684

Sum of electronic and zero-point Energies= -18503.710003
Sum of electronic and thermal Energies= -18503.697858
Sum of electronic and thermal Enthalpies= -18503.696914

Sum of electronic and thermal Free Energies= -18503.749586

(1,2-DACH)$PtCl_2$ (DMF)

Pt,0,0.944889003,-0.0000128152,-0.0001168786
Cl,0,2.5807580117,1.7673518359,0.0457812777
N,0,-0.665511635,-1.3831449839,-0.014125471
Cl,0,2.5811792792,-1.7671070763,-0.0453152395
N,0,-0.6655129632,1.3830438876,0.0134490583
C,0,-1.9367728945,-0.6842825237,-0.3367982573
H,0,-0.7169010889,-1.8013367531,0.9157135281
H,0,-0.5006202959,-2.1526703611,-0.6624375253
H,0,-0.5005383714,2.1526623971,0.6616206873
C,0,-1.936694363,0.6841857547,0.3363907395
H,0,-0.7169605365,1.8010194302,-0.9164796331
C,0,-3.1680354794,1.515290712,-0.0657261828
H,0,-1.9230181532,0.5303814508,1.4220508331
C,0,-4.3840699676,0.6406671772,-0.4124220222
C,0,-4.383745483,-0.6406666881,0.4133440059
C,0,-3.1680791832,-1.515328054,0.0655652024
H,0,-1.9232682324,-0.5304512121,-1.4224581169
H,0,-2.9123238821,2.1443646468,-0.9282746329
H,0,-3.4114643107,2.1969083219,0.7571180043
H,0,-2.9120805075,-2.1448885223,0.9276742831
H,0,-3.4121529834,-2.1965037675,-0.7574572317
H,0,-4.3683625682,0.3816481737,-1.4797632338
H,0,-5.3039257999,1.2115586918,-0.2450774993
H,0,-5.3037684355,-1.2115193517,0.246767725
H,0,-4.3671191595,-0.3816703709,1.4806765795

Sum of electronic and zero-point Energies= -18581.026847
Sum of electronic and thermal Energies= -18581.013695
Sum of electronic and thermal Enthalpies= -18581.012751
Sum of electronic and thermal Free Energies= -18581.069488

(1,4-DACH)$PtCl_2$ (DMF)

Pt,0,-0.0645689149,0.714858323,-0.0120060868
C,0,0.5267282468,-2.1527836699,-1.3372737422
N,0,-0.3575667454,-0.6918979176,1.5838012517
H,0,0.9565718284,-2.5590422391,-2.2611851824
N,0,0.3032854277,-0.7040877417,-1.5813718807
H,0,0.3850067184,-0.5162674079,2.2614666513
H,0,-1.205918783,-0.3364337128,2.0248166174
H,0,-0.5689251416,-3.9389114236,-1.0254953666
H,0,-1.4697595566,-2.7403699083,-1.9304865614
C,0,-0.7944236885,-2.8664119657,-1.0750474934
C,0,-1.4903730493,-2.4249211935,0.2166127795
H,0,-2.1968147647,-3.204674865,0.5207582962
C,0,1.5249547519,-2.3491914543,-0.182492238

C,0,-0.5043916545,-2.1547519626,1.3669755337
H,0,-2.0895956928,-1.523355375,0.0391323575
C,0,0.852523324,-2.8027582468,1.11738784
H,0,2.0756238579,-1.4141020219,-0.0219467092
H,0,2.2717979109,-3.0960263952,-0.4723912845
H,0,-0.9127126442,-2.5656034891,2.2985796215
H,0,1.5199212665,-2.625756313,1.9700192775
H,0,0.6835912193,-3.8863449623,1.0876655548
H,0,1.1320112137,-0.3126658881,-2.0292006545
H,0,-0.4470727887,-0.5803854015,-2.2619250019
Cl,0,-0.4531615364,2.3636761572,1.7014879055
Cl,0,0.236869195,2.3489090746,-1.7561814851

Sum of electronic and zero-point Energies= -18581.025288
Sum of electronic and thermal Energies= -18581.012749
Sum of electronic and thermal Enthalpies= -18581.011805
Sum of electronic and thermal Free Energies= -18581.065970

(1,2-DACH)PtCl(Gua) (DMF)

Pt,0,0.7780156707,0.1618012337,-1.105770499
H,0,5.138609362,1.3940941886,2.3229904542
N,0,-0.8133511612,-1.2092034423,-0.9333563474
Cl,0,2.1470780569,-1.4149881161,-2.3058736203
N,0,-0.6255587377,1.415771834,-0.0947645988
C,0,-2.0701909097,-0.5086459144,-0.5561420171
H,0,-0.5563751821,-1.8863286489,-0.2130654209
H,0,-0.9431073824,-1.7466386827,-1.7907581663
H,0,-0.1994863709,1.9650860382,0.650937593
C,0,-1.7406868093,0.5929511865,0.4443382689
H,0,-0.9832263158,2.0889901849,-0.7737178976
C,0,-2.9772622256,1.4466462628,0.774554678
H,0,-1.3504008364,0.1243246921,1.3557038333
C,0,-4.2904432141,0.6553653295,0.6541749391
C,0,-4.0748812493,-0.8127453284,1.0030681434
C,0,-3.1267551094,-1.4820437796,-0.0053358264
H,0,-2.4342263472,-0.0358530956,-1.4761448332
H,0,-3.008492874,2.3114931702,0.0989856367
H,0,-2.863614935,1.8457760303,1.7887049265
H,0,-2.621198477,-2.3299177388,0.4748487504
H,0,-3.6946977557,-1.8926034096,-0.8477549408
H,0,-4.6802106145,0.7289453042,-0.3700645397
H,0,-5.0473907366,1.1032065887,1.3071434598
H,0,-5.0279978277,-1.3523507334,1.0205642367
H,0,-3.6574450482,-0.8855347993,2.0163232798
N,0,4.8472391022,1.7858295395,1.4332929688
C,0,5.5766154473,2.8046644631,0.8773519367
N,0,5.2499461412,3.3848980702,-0.2610140243
C,0,4.1361051552,2.8734744949,-0.8088769855
C,0,3.3327773463,1.8446268577,-0.3313229222

C,0,3.6763369356,1.2145073084,0.9052662963
N,0,3.5572542228,3.2688068932,-1.9821609092
C,0,2.4578551664,2.5001681513,-2.1896401292
N,0,2.2933090917,1.6334786337,-1.2142434156
O,0,3.104514963,0.3088735251,1.5051258215
N,0,6.6482155246,3.24847503,1.5660205918
H,0,3.8894047031,4.0028669981,-2.595172598
H,0,1.8196166669,2.6032417405,-3.0546900241
H,0,7.2654664857,3.880431047,1.0752536519
H,0,7.0771400782,2.6769588926,2.2797202488

Sum of electronic and zero-point Energies= -18662.704507
Sum of electronic and thermal Energies= -18662.684458
Sum of electronic and thermal Enthalpies= -18662.683514
Sum of electronic and thermal Free Energies= -18662.755259

cis-(Thiazole)$_2$PtCl$_2$ (DMF)

Pt,0,0.0008489461,-0.8565203995,-0.0004224706
Cl,0,-1.7371650086,-2.5171005859,0.0100933935
Cl,0,1.7407364967,-2.5151292694,-0.0119237245
N,0,-1.4836040274,0.6220520256,0.0074954932
C,0,-1.6389678731,1.4889649373,0.9516275018
C,0,-2.4427990222,0.7522426872,-1.0886294698
S,0,-2.8991876278,2.6433611923,0.703921941
H,0,-1.0292451599,1.5160337409,1.8475621685
C,0,-3.2623856331,1.9607056147,-0.8034364261
H,0,-3.036051793,-0.1808529747,-1.1436136314
H,0,-1.902065931,0.8096091448,-2.0487707016
H,0,-4.0709372781,2.3393701809,-1.4133246446
N,0,1.4837938533,0.6235320673,-0.0075981728
C,0,2.4429430457,0.7540736653,1.0885239854
C,0,1.6382689855,1.4910753625,-0.9513109967
C,0,3.2610909411,1.9636896741,0.8040866195
H,0,3.0372888998,-0.1783941953,1.1427117912
S,0,2.897232128,2.646696183,-0.702979376
H,0,1.0285611636,1.5179294602,-1.8472631258
H,0,4.0692465471,2.3428831255,1.4141692305
H,0,1.9022963475,0.8100793631,2.0487806153

Sum of electronic and zero-point Energies= -19373.371741
Sum of electronic and thermal Energies= -19373.355390
Sum of electronic and thermal Enthalpies= -19373.354445
Sum of electronic and thermal Free Energies= -19373.419732

cis-(NH$_3$)$_2$Pt(CH$_3$)Cl (DMF)

Pt,0,-0.0102538158,0.0965610565,0.0521179637
C,0,0.0032500648,1.6146181492,-1.3589997965
N,0,-0.024744566,-1.5671455735,1.6194834145

```
Cl,0,-0.0849951457,-1.6151013475,-1.6844477355
N,0,0.056931403,1.6634247295,1.5627613004
H,0,-0.8313751111,-1.5432622982,2.239500157
H,0,0.8012517982,-1.5826594333,2.2137289368
H,0,-0.0540476792,-2.459954405,1.1306155178
H,0,0.8842226111,1.5836589031,2.1503943179
H,0,-0.7506052448,1.6244899243,2.1811790205
H,0,0.0724927591,2.5949860569,1.1529320685
H,0,-0.0271557003,1.1955195968,-2.3697964237
H,0,0.9173077137,2.2121800924,-1.23853965
H,0,-0.8723790872,2.2599845487,-1.2045290913

Sum of electronic and zero-point Energies=          -17927.708452
Sum of electronic and thermal Energies=             -17927.697808
Sum of electronic and thermal Enthalpies=           -17927.696863
Sum of electronic and thermal Free Energies=        -17927.746236
```

cis-$(NH_3)_2PtBr_2$ (DMF)

```
Pt,0,-0.0000854384,-0.0243183985,0.5283149598
Br,0,-0.0140201394,1.8271035419,-1.1719896822
Br,0,0.0133708488,-1.8443380057,-1.2055973235
N,0,0.0230988697,-1.5790162822,2.0140234335
N,0,-0.0228608214,1.5028397692,2.0422905752
H,0,-0.7591750686,-1.5220278381,2.6634120787
H,0,0.8799217133,-1.5739994039,2.5643458625
H,0,-0.0325167169,-2.4818350145,1.5439182983
H,0,0.7589771198,1.4334731199,2.6909942752
H,0,-0.8800402095,1.4878889597,2.5918817737
H,0,0.0333298426,2.4142295524,1.5891057487

Sum of electronic and zero-point Energies=          -22570.081327
Sum of electronic and thermal Energies=             -22570.071412
Sum of electronic and thermal Enthalpies=           -22570.070468
Sum of electronic and thermal Free Energies=        -22570.120296
```

cis-$(NH_3)_2PtI_2$ (DMF)

```
Pt,0,0.,0.,0.7905912286
I,0,-0.0107295848,1.9653120493,-1.0627397188
I,0,0.0107295848,-1.9653120493,-1.0627397188
N,0,0.0009188415,-1.5338212426,2.3308322125
N,0,-0.0009188415,1.5338212426,2.3308322125
H,0,-0.8791293134,-1.5482285695,2.8431829092
H,0,0.7483175699,-1.4020019267,3.0098424005
H,0,0.1244391858,-2.4566664673,1.9170480822
H,0,0.8791293134,1.5482285695,2.8431829092
H,0,-0.7483175699,1.4020019267,3.0098424005
H,0,-0.1244391858,2.4566664673,1.9170480822
```

Sum of electronic and zero-point Energies= -31266.138828
Sum of electronic and thermal Energies= -31266.129256
Sum of electronic and thermal Enthalpies= -31266.128312
Sum of electronic and thermal Free Energies= -31266.177877

cis-$(C_5H_5N)_2PtI_2$ (DMF)

Pt,0,0.0007561884,-0.8336020783,-0.0003183585
I,0,1.9583037236,-2.6943308033,-0.1197654308
I,0,-1.9544681467,-2.696784098,0.1187122824
C,0,1.9142296753,1.2543660468,-1.1847854104
C,0,2.0133398995,1.1694568001,1.1264502762
C,0,2.8541697489,2.2764029881,-1.2280236006
H,0,1.475509647,0.8486873299,-2.0903880169
C,0,2.9560197735,2.1886705859,1.1652327396
H,0,1.6522055491,0.6961474981,2.0335948193
C,0,3.3853374445,2.7535216301,-0.0327507275
H,0,3.1585770564,2.6830329062,-2.1868388613
H,0,3.3413331638,2.5247830039,2.1223030832
H,0,4.1224820237,3.5511355518,-0.034665987
C,0,-1.9152141492,1.2516258367,1.1848866774
C,0,-2.0140166239,1.1676732126,-1.1263987864
C,0,-2.8562190609,2.2726679428,1.22850437
H,0,-1.4761601381,0.8459836794,2.0903438486
C,0,-2.9577409508,2.1859330583,-1.164802404
H,0,-1.6523097753,0.6951491505,-2.0337249099
C,0,-3.387754305,2.7497940622,0.0333995658
H,0,-3.161142364,2.6785350314,2.1874788656
H,0,-3.3433082889,2.5220928057,-2.1217538653
H,0,-4.1257094182,3.5466573758,0.0356060684
N,0,1.5033377828,0.7154900546,-0.0279537776
N,0,-1.5036450953,0.7137143086,0.0278463696

Sum of electronic and zero-point Energies= -31649.043842
Sum of electronic and thermal Energies= -31649.027422
Sum of electronic and thermal Enthalpies= -31649.026478
Sum of electronic and thermal Free Energies= -31649.095318

cis-$(EtNH_2)_2Pt(OCMe)_2$ ($CHCl_3$)
(PCM)

Pt	7.47155	13.76472	4.11711
O	5.25217	12.54845	5.49516
O	9.69231	12.55727	2.73355
N	6.31325	15.31603	5.3624
N	8.62646	15.32305	2.87754
H	5.99867	16.09927	4.79159
H	8.94027	16.10434	3.45143
H	5.47743	14.77573	5.59394
H	9.46297	14.78514	2.64295
C	6.43759	12.35812	5.22979

C	8.50739	12.36388	2.99894
C	7.14011	11.1805	5.87883
C	7.80661	11.18732	2.34612
H	6.41969	10.46365	6.29315
H	8.52809	10.4732	1.92894
H	7.75334	11.58032	6.69847
H	7.1923	11.58895	1.52817
H	7.82861	10.68177	5.19117
H	7.11931	10.68495	3.03233
C	6.94135	15.8245	6.59214
C	7.99643	15.83574	1.65054
H	7.86554	16.33941	6.30658
H	7.07165	16.3479	1.93911
H	7.23609	14.95562	7.18978
H	7.70258	14.96894	1.04946
C	6.04798	16.74961	7.40547
C	8.88755	16.76581	0.84039
H	9.80398	16.25483	0.52218
H	5.7599	17.63498	6.82534
H	6.56858	17.09385	8.3067
H	5.1321	16.23576	7.72064
H	9.17468	17.64914	1.42406
H	8.36557	17.11305	-0.05889

***cis*-(^{i}PrNH$_2$)$_2$Pt(OCMe)$_2$ (CHCl$_3$)**

(PCM)

C	10.86424	13.26092	19.89852
C	11.53881	11.98737	20.36973
C	9.05482	11.61393	18.1097
C	10.15585	11.48277	17.07442
C	6.6704	15.40681	17.31671
C	6.35623	13.91882	17.27707
C	4.90726	13.65495	16.87913
C	9.05274	14.25796	22.84214
C	8.20281	15.18996	21.99296
C	6.73938	14.77553	21.99633
N	6.68607	13.30696	18.58114
N	8.71271	15.20584	20.60569
O	11.48224	14.31973	19.993
O	8.17265	10.75853	18.13836
Pt	8.8813	13.29645	19.30145
H	12.61453	12.13858	20.52594
H	11.07533	11.70462	21.32493
H	11.36377	11.15515	19.68189
H	9.93472	12.19995	16.2716
H	11.13316	11.76119	17.47865
H	10.18669	10.47195	16.6478
H	6.05788	15.91508	18.07409
H	7.72763	15.57679	17.55018
H	6.45344	15.87156	16.34901

H	7.01783	13.43947	16.54508
H	4.6939	12.58003	16.85092
H	4.69461	14.06716	15.88599
H	4.21648	14.12293	17.59303
H	8.99031	13.23121	22.46134
H	10.10616	14.56074	22.83802
H	8.70168	14.26571	23.8799
H	8.27747	16.20615	22.41109
H	6.32951	14.82917	23.01069
H	6.13381	15.43095	21.35735
H	6.63488	13.74298	21.6407
H	6.05212	13.67455	19.29038
H	6.51594	12.30064	18.53533
H	8.2092	15.91477	20.07452
H	9.69483	15.48945	20.59753

***cis*-$(PhCH_2NH_2)_2Pt(OCMe)_2$ ($CHCl_3$)**

(PCM)

Pt	7.4714	13.70809	4.1126
O	5.30087	12.49883	5.57563
O	9.64191	12.4991	2.64931
N	6.31541	15.26138	5.35499
N	8.62733	15.26148	2.87025
H	5.99432	16.04458	4.78769
H	8.94848	16.04465	3.43754
H	5.48278	14.71765	5.59118
H	9.4599	14.71769	2.634
C	6.47489	12.30595	5.26633
C	8.46796	12.30603	2.95879
C	7.20327	11.13312	5.89395
C	7.7397	11.13304	2.33135
H	6.50083	10.42443	6.35071
H	8.4422	10.42455	1.87435
H	7.85873	11.53865	6.67724
H	7.08387	11.5384	1.54828
H	7.85455	10.6237	5.17842
H	7.08879	10.62341	3.04707
C	6.94261	15.77661	6.58783
C	8.00009	15.77675	1.63745
H	7.87615	16.27468	6.30594
H	7.0666	16.2749	1.9194
H	7.21048	14.90944	7.19974
H	7.7321	14.9096	1.02557
C	6.06062	16.72228	7.36571
C	8.88209	16.72235	0.85951
C	9.86509	16.22803	-0.00614
C	10.70998	17.0974	-0.69336
C	10.58074	18.47695	-0.52599
C	9.60126	18.98072	0.32918
C	8.75813	18.10691	1.01558

C	5.07757	16.22806	8.23135
H	9.9669	15.153	-0.14599
H	11.4663	16.69835	-1.36467
H	11.23693	19.15586	-1.06465
H	9.48947	20.05445	0.45833
H	7.98939	18.5058	1.67571
C	4.2327	17.0975	8.9185
C	4.36202	18.47703	8.75108
C	5.34156	18.98071	7.89592
C	6.18467	18.10684	7.20959
H	4.9757	15.15304	8.37123
H	3.47633	16.69852	9.5898
H	3.70585	19.156	9.28968
H	5.45341	20.05443	7.76673
H	6.95345	18.50566	6.54947

***cis*-($PhCH_2CH_2NH_2)_2Pt(OCMe)_2$ ($CHCl_3$)**
(PCM)

Pt	7.4703	13.5311	4.11306
O	5.28433	12.3314	5.55717
O	9.65618	12.33073	2.6694
C	6.45888	12.13055	5.25315
C	8.48142	12.1304	2.97294
C	7.1724	10.94924	5.8822
C	7.7675	10.94966	2.34328
H	6.45903	10.23201	6.30755
H	7.80053	11.34552	6.69228
H	7.84747	10.45231	5.18039
H	8.48065	10.23196	1.91835
H	7.14029	11.3465	1.53275
H	7.09153	10.45316	3.04452
N	6.3048	15.09273	5.33892
C	6.93876	15.67168	6.52905
C	6.01733	16.59565	7.33458
C	6.71009	17.16192	8.54686
C	7.39218	18.38227	8.48009
C	8.07061	18.88599	9.58951
C	8.07757	18.17309	10.78822
C	7.40087	16.95578	10.86827
C	6.72401	16.45676	9.75624
H	5.95246	15.83738	4.73931
H	5.49529	14.52857	5.60607
H	7.83145	16.22152	6.20943
H	7.28314	14.84541	7.15993
H	5.12785	16.02915	7.63998
H	5.67146	17.41113	6.68503
H	7.38638	18.94817	7.54988
H	8.59025	19.83853	9.51856
H	8.60286	18.56532	11.65537

H	7.3959	16.39503	11.79984
H	6.19354	15.50874	9.82861
N	8.63615	15.09251	2.88729
C	8.00239	15.67124	1.69695
C	8.92398	16.595	0.89135
C	8.2314	17.16105	-0.32115
C	7.54932	18.38142	-0.25471
C	6.87106	18.88495	-1.36432
C	6.86428	18.17182	-2.56291
C	7.54097	16.9545	-2.64263
C	8.21765	16.45566	-1.53039
H	8.98831	15.83728	3.48685
H	9.44577	14.5284	2.62037
H	7.10968	16.22119	2.01633
H	7.65806	14.84485	1.06618
H	9.81347	16.02839	0.58618
H	9.26979	17.4106	1.54077
H	7.55499	18.9475	0.67539
H	6.35141	19.83751	-1.29363
H	6.33912	18.5639	-3.4302
H	7.54609	16.39358	-3.5741
H	8.74809	15.50761	-1.6025

***cis*-$(CH_2{=}CHCH_2NH_2)_2Pt(OCMe)_2$ ($CHCl_3$)**
(PCM)

Pt	7.4717	13.76314	4.11364
O	5.21453	12.56144	5.43602
O	9.7273	12.56715	2.784
N	6.28371	15.31987	5.32716
N	8.65889	15.32112	2.90033
H	5.98705	16.10792	4.75333
H	8.95679	16.10963	3.47286
H	5.44148	14.78078	5.53752
H	9.50035	14.78093	2.68955
C	6.40532	12.36305	5.20366
C	8.53867	12.36343	3.02323
C	7.08585	11.1877	5.87804
C	7.86144	11.18148	2.35729
H	6.35216	10.48769	6.29764
H	8.59703	10.48531	1.93471
H	7.70066	11.59151	6.69438
H	7.23766	11.5783	1.54437
H	7.77167	10.66806	5.20321
H	7.18435	10.65914	3.03884
C	6.89072	15.82599	6.57201
C	8.05046	15.82582	1.6556
H	7.85067	16.29133	6.32333
H	7.09132	16.29254	1.90495
H	7.10726	14.95362	7.19981

H	7.83207	14.95252	1.02971
C	6.01768	16.79881	7.30773
C	8.92317	16.79628	0.91635
H	9.89842	16.42029	0.60139
H	9.24317	18.72558	0.0997
C	8.57848	18.05597	0.64002
H	5.04202	16.42415	7.62293
H	7.61158	18.45946	0.93824
H	5.69692	18.73145	8.11633
C	6.36223	18.05953	7.57958
H	7.32917	18.46194	7.28001

***cis*-$(CyNH_2)_2Pt(OCMe)_2$ ($CHCl_3$)
(PCM)

Pt	7.39084	12.63144	2.12915
O	5.07496	11.42947	3.34029
O	9.64277	11.3691	0.86011
C	6.27085	11.2194	3.14782
C	8.43655	11.21481	1.04045
C	6.90267	10.00375	3.79892
C	7.74214	10.07001	0.32757
H	6.14171	9.28265	4.12371
H	7.45114	10.35893	4.68244
H	7.63763	9.52231	3.14809
H	8.46391	9.32543	-0.03187
H	7.21824	10.49893	-0.53796
H	6.97878	9.59759	0.95176
N	6.21531	14.19246	3.38864
C	6.72984	14.75593	4.65198
C	7.01137	13.6477	5.66116
C	7.55481	14.22088	6.96993
C	8.80304	15.06925	6.7305
C	8.53746	16.16534	5.69917
C	7.98853	15.57915	4.39844
H	5.92973	14.95689	2.7785
H	5.37144	13.64545	3.5722
H	5.96588	15.42444	5.08452
H	7.7466	12.95735	5.2214
H	6.09834	13.06624	5.84625
H	7.77566	13.40455	7.66883
H	6.78019	14.83968	7.44744
H	9.6157	14.42198	6.36814
H	9.14938	15.51146	7.67337
H	9.45558	16.73042	5.49528
H	7.81219	16.884	6.10938
H	7.77685	16.38177	3.67755
H	8.7444	14.92041	3.94444
N	8.65351	14.18755	0.95073
C	6.96266	15.7204	0.01381

C	6.44987	16.40142	-1.25508
C	6.12593	15.37556	-2.34055
C	7.32557	14.47233	-2.62367
C	7.8335	13.8041	-1.34608
C	8.1741	14.84225	-0.28209
H	8.97919	14.90302	1.59896
H	9.46642	13.60483	0.73943
H	6.17037	15.08264	0.43446
H	7.21718	16.47241	0.77432
H	7.21482	17.09852	-1.6288
H	5.56415	17.00562	-1.02208
H	5.8067	15.88364	-3.2595
H	5.27779	14.75693	-2.01095
H	8.13442	15.07052	-3.06965
H	7.06118	13.70609	-3.36299
H	8.71315	13.18283	-1.5611
H	7.06003	13.13433	-0.94146
H	8.97509	15.48823	-0.68052

***cis*-$(Me_2NH)_2Pt(OCMe)_2$ (CH_2Cl_2)**

(PCM)

Pt	9.00692	13.26258	19.34054
C	10.93258	13.15253	20.13723
C	11.78098	11.90061	20.08212
C	9.33887	11.62124	18.14205
C	10.05003	11.8513	16.81851
H	5.58478	13.6689	16.86257
C	6.63855	13.52608	17.14402
H	7.00403	12.61689	16.65882
H	8.25321	14.02756	22.43597
C	7.90356	14.91629	21.904
H	6.85938	14.75583	21.61429
N	6.79856	13.39619	18.5959
N	8.72266	15.12532	20.71135
O	11.38134	14.12579	20.74653
O	8.92194	10.50071	18.4091
H	12.6977	12.0155	20.67365
H	11.19967	11.04577	20.44639
H	12.04454	11.67614	19.04171
H	9.50556	12.6058	16.23724
H	11.04931	12.2641	16.99757
H	10.12649	10.92225	16.23864
H	7.22485	14.3752	16.78303
H	9.05825	16.51856	19.17932
H	8.44181	17.23958	20.69264
H	7.35493	16.31469	19.63839
H	7.94045	15.77973	22.58578
H	6.04652	12.28634	20.21578
H	6.40229	11.34324	18.75783

H	4.94078	12.36914	18.81427
H	6.45151	14.25596	19.01614
C	5.99336	12.28844	19.12385
C	8.37954	16.36811	20.02321
H	9.70816	15.1646	20.98585

***cis*-$(Et_2NH)_2Pt(OCMe)_2$ (CH_2Cl_2)**
(PCM)

Pt	9.31366	13.45017	19.18197
C	11.17173	13.42388	20.13866
C	12.17286	12.2995	19.9815
C	9.88261	11.91528	17.93058
C	10.64635	12.27535	16.66623
C	7.57954	14.84771	16.34931
C	6.9806	13.54892	16.85559
H	5.92177	13.50339	16.56536
H	8.1582	13.62761	21.98758
C	7.8341	14.64864	21.7569
H	6.82262	14.57206	21.33636
N	7.12577	13.40916	18.31461
N	8.72449	15.15275	20.69795
O	11.44579	14.33035	20.92685
O	9.56661	10.74705	18.11975
H	13.03675	12.4424	20.64235
H	11.68443	11.34308	20.20161
H	12.5132	12.24345	18.94088
H	9.98808	12.85911	16.0097
H	11.50161	12.91845	16.89883
H	10.97824	11.3751	16.13282
H	7.47722	12.68698	16.39525
H	8.10508	17.16867	20.96189
H	7.36784	16.31142	19.61141
C	9.36658	17.03846	19.23095
C	7.8061	15.47013	23.04192
H	6.69599	12.16913	19.92476
H	6.94799	11.33606	18.39994
C	4.95041	12.14411	18.66307
H	6.68248	14.22238	18.74328
C	6.46157	12.20501	18.85502
C	8.31262	16.45293	20.15344
H	9.67308	15.23705	21.07835
H	7.45941	14.91742	15.26272
H	8.64768	14.91477	16.58334
H	7.07839	15.71632	16.79451
H	9.02069	17.99447	18.82292
H	9.58318	16.36324	18.39643
H	10.30325	17.22151	19.77045
H	7.18533	14.96364	23.78989
H	7.39065	16.47224	22.89469

H	8.81458	15.57425	23.46005
H	4.55092	11.27571	19.19898
H	4.66131	12.04099	17.61238
H	4.46063	13.03852	19.06859

***cis*-($H_2NCH_2CH_2NH_2$)Pt($OCMe)_2$ ($CHCl_3$)**
(PCM)

Pt	6.19932	10.57467	6.10419
O	3.8975	8.97357	6.88882
O	8.10095	9.42012	4.32409
C	5.09144	9.14889	7.09934
C	7.02367	9.15054	4.84685
C	5.76806	8.36896	8.21435
C	6.33368	7.85376	4.48115
H	5.07071	7.66883	8.69306
H	6.87754	7.32435	3.68884
H	6.15737	9.07157	8.96235
H	5.30414	8.0587	4.1661
H	6.63452	7.82662	7.81815
H	6.26423	7.21329	5.36903
N	7.30218	12.32301	5.09871
N	5.5343	12.4084	7.35339
C	7.27426	13.48603	5.99541
H	6.86225	12.54478	4.20799
H	8.25149	12.02868	4.88323
H	4.53922	12.39832	7.56385
C	5.89044	13.62994	6.60937
H	6.01298	12.39375	8.25197
H	5.85752	14.52466	7.24519
H	5.14725	13.76119	5.81504
H	7.54705	14.41814	5.48264
H	8.01365	13.31633	6.7862

***cis*-($Me_2NCH_2CH_2NH_2$)Pt($OCMe)_2$ ($CHCl_3$)**
(PCM)

Pt	6.09268	10.49549	6.15688
O	3.58036	9.15685	6.77607
O	7.43034	9.40614	3.87138
C	4.77296	9.19417	7.04224
C	6.59651	9.08412	4.71121
C	5.30956	8.34623	8.18407
C	5.94705	7.72065	4.59475
H	4.54276	7.65578	8.55864
H	6.33904	7.16903	3.73136
H	5.62754	9.01096	8.99816
H	4.86136	7.84126	4.5023
H	6.19933	7.79193	7.86695
H	6.12097	7.14476	5.51146

N	7.52572	12.26163	5.40377
N	5.56619	12.23466	7.58069
C	7.42904	13.31364	6.42817
C	7.03261	12.73694	4.10763
C	8.92072	11.83727	5.25943
H	4.56684	12.2679	7.76745
C	6.0191	13.49064	6.96298
H	6.01893	12.1043	8.48363
H	6.00712	14.32831	7.67329
H	5.32087	13.73719	6.1575
H	7.80501	14.27324	6.03506
H	8.08508	13.0274	7.2595
H	8.96672	11.03587	4.51949
H	9.28901	11.45591	6.21636
H	9.56167	12.67594	4.93881
H	7.09748	11.91819	3.38765
H	7.63089	13.59025	3.74488
H	5.9872	13.04649	4.18517

cis-(MeHNCH$_2$CH$_2$NHMe)Pt(OCMe)$_2$ ($CHCl_3$)
(PCM)

Pt	6.3277	10.5769	6.34268
O	4.52833	9.75456	8.39174
O	8.29218	8.62816	5.42752
C	5.47363	9.31237	7.74517
C	7.12824	8.98665	5.30333
C	5.99318	7.92611	8.05958
C	6.25131	8.30904	4.26282
H	5.4745	7.49495	8.92484
H	6.79413	7.50914	3.7423
H	7.07262	7.96873	8.24447
H	5.90685	9.05535	3.53536
H	5.85384	7.27626	7.18689
H	5.35168	7.90412	4.74122
N	7.04484	12.26661	4.90239
N	5.5291	12.4762	7.39549
C	6.8861	13.53361	5.63286
H	6.35196	12.24711	4.15503
C	8.37318	12.14158	4.29616
H	4.56315	12.24011	7.60911
C	5.57404	13.55578	6.40113
C	6.20552	12.80805	8.65144
H	5.44218	14.54284	6.87095
H	4.73929	13.40941	5.70546
H	6.93342	14.39643	4.95072
H	7.73241	13.62339	6.32339
H	6.06529	11.98361	9.35396
H	5.80998	13.73357	9.09643
H	7.27821	12.93286	8.48041

H	8.41576	11.23065	3.69517
H	9.12392	12.06148	5.08702
H	8.61805	13.00524	3.66036

***cis*-($Me_2NCH_2CH_2NMe_2$)$Pt(OCMe)_2$** (CH_2Cl_2)
(PCM)

Pt	6.05916	10.43869	6.18883
O	3.76655	8.88022	7.13784
O	7.81963	8.29957	5.23462
C	4.97102	9.05318	7.28104
C	6.71286	8.80552	5.09256
C	5.70974	8.28544	8.36079
C	5.78772	8.28011	4.01129
H	5.02037	7.68345	8.96713
H	6.27955	7.51016	3.40255
H	6.2688	8.9772	9.00254
H	5.44599	9.10323	3.37205
H	6.4535	7.63383	7.88557
H	4.89064	7.86288	4.48538
N	7.26742	12.09064	5.03956
N	5.36533	12.3618	7.34256
C	7.17699	13.28239	5.90335
C	6.6576	12.344	3.72918
C	8.67578	11.72672	4.85109
C	3.91155	12.4092	7.53138
C	5.78772	13.48141	6.48076
C	6.02208	12.43049	8.65294
H	5.76106	14.42903	7.04409
H	5.05447	13.57221	5.67323
H	7.46931	14.18518	5.34165
H	7.90596	13.16184	6.71089
H	5.69167	11.58896	9.26675
H	5.76943	13.36975	9.17246
H	7.10687	12.3656	8.54454
H	8.74291	10.83857	4.21896
H	9.12859	11.49483	5.81849
H	9.23782	12.54794	4.37707
H	6.7379	11.44461	3.11375
H	7.1651	13.17494	3.21154
H	5.59842	12.58733	3.83722
H	3.59696	11.57499	8.16227
H	3.41154	12.31583	6.56394
H	3.60377	13.35478	8.00693

***cct*-[$Pt(NH_3)_2Cl_2(OOCH)_2$]** (DMSO)
(PCM)

Pt	0.10204	-0.16273	-0.10496
O	0.33427	1.87509	-0.28055

N	-1.95726	0.35076	0.04576
Cl	0.08659	-0.20284	2.25319
N	0.13498	-0.06236	-2.23175
Cl	2.39351	-0.69423	-0.27725
O	-0.23464	-2.20087	0.00445
C	1.19317	2.62604	0.36349
C	-1.0626	-2.83179	-0.7789
O	-1.24489	-4.03627	-0.70777
O	2.02881	2.30933	1.18306
H	-2.29329	0.09355	0.97476
H	-2.57771	-0.07228	-0.64357
H	-2.02102	1.36639	-0.04571
H	0.85553	-0.68311	-2.60149
H	0.39415	0.89864	-2.4631
H	-0.74319	-0.2716	-2.70524
H	1.05353	3.67615	0.04245
H	-1.60594	-2.22379	-1.52477

***cct*-[Pt(NH$_3$)(Cha)Cl$_2$(OCOCH$_3$)$_2$]** (water)
(PCM)

Pt	0.08357	0.25647	-0.01363
C	2.95758	-0.65415	-0.04633
C	4.39234	-0.27591	0.23634
C	0.13952	-1.38741	-2.74045
Cl	0.09612	2.13571	1.4795
Cl	-0.01477	-1.25422	1.79704
O	2.63771	-1.80791	-0.3357
N	0.0672	-1.45867	-1.26674
N	0.19835	1.71347	-1.557
C	0.50052	-2.77784	-3.28071
O	-1.96526	0.48719	-0.09116
O	2.14523	0.36002	0.07577
C	-2.82831	-0.49205	-0.17463
O	-2.55832	-1.67894	-0.35142
C	-4.25028	-0.01123	-0.00765
C	-1.16443	-0.89376	-3.35813
C	-1.05801	-0.8564	-4.88303
C	0.60218	-2.74968	-4.80689
C	-0.68167	-2.22545	-5.44583
H	4.59826	0.75959	-0.04252
H	5.06397	-0.95542	-0.29245
H	4.56886	-0.37908	1.31336
H	0.96479	-0.71086	-2.99985
H	0.90101	-1.94203	-0.89584
H	-0.8023	-1.91841	-0.95544
H	0.65523	1.39898	-2.41183
H	-0.73677	2.05057	-1.78711
H	0.73133	2.50147	-1.18734
H	-0.27626	-3.49175	-2.97124

H	1.44764	-3.11239	-2.83993
H	-4.93753	-0.72322	-0.46897
H	-4.38869	0.9847	-0.43432
H	-4.4718	0.04741	1.06435
H	-1.43732	0.09527	-2.97223
H	-1.97298	-1.57623	-3.06228
H	-2.01027	-0.51533	-5.3061
H	-0.29941	-0.11646	-5.17832
H	0.83097	-3.75835	-5.17152
H	1.44646	-2.10914	-5.10052
H	-0.5647	-2.16743	-6.53503
H	-1.5002	-2.93428	-5.25222

***cct*-[Pt(NH$_3$)$_2$Cl$_2$(OCOCH$_3$)$_2$]** (water)
(PCM)

Pt	0.00352	0.19972	-0.17191
Cl	0.02672	2.38849	0.77605
Cl	0.02622	-0.80017	1.96509
C	2.89423	-0.65669	-0.15571
C	4.33029	-0.19553	-0.06845
O	2.59323	-1.84998	-0.13987
N	-0.01625	-1.72824	-1.00507
N	-0.01386	1.13441	-2.07627
O	-2.05406	0.37044	-0.17112
O	2.06161	0.34834	-0.22604
C	-2.89509	-0.62652	-0.10221
O	-2.60516	-1.82294	-0.08225
C	-4.33392	-0.16479	-0.0804
H	4.55654	0.03733	0.97842
H	-0.02767	-1.73173	-2.02348
H	0.85058	-2.16977	-0.66734
H	-0.8799	-2.16051	-0.6476
H	0.81155	0.89786	-2.62674
H	-0.84912	0.90114	-2.61302
H	-0.01061	2.14364	-1.92078
H	-4.90676	-0.80532	0.59499
H	-4.7484	-0.2789	-1.08846
H	-4.42492	0.88033	0.2197
H	4.4959	0.70928	-0.65748
H	4.9951	-0.99494	-0.40152

***cct*-[Pt(NH$_3$)$_2$Cl$_2$(OCOCF$_3$)$_2$]** (water)
(PCM)

Pt	0.0194	0.15518	-0.11841
C	2.88385	-0.69388	-0.15377
C	4.3489	-0.18356	-0.03642
H	0.00344	-1.58299	-2.17219
H	0.83858	1.12434	-2.48193

Cl	0.03147	2.20908	1.06263
Cl	0.02737	-1.07521	1.88714
O	2.66605	-1.88654	-0.25602
F	4.6377	0.66856	-1.03108
N	0.0087	-1.68735	-1.15836
N	0.01237	1.29952	-1.90932
H	0.85898	-2.18668	-0.87524
H	-0.84111	-2.18208	-0.86591
H	-0.82118	1.12878	-2.47254
H	0.01651	2.28578	-1.64315
O	-2.03493	0.31928	-0.10221
F	5.21369	-1.1958	-0.09393
O	2.07462	0.3084	-0.12533
F	4.53533	0.4591	1.12561
C	-2.84974	-0.67868	-0.12163
O	-2.63945	-1.87245	-0.22655
C	-4.3106	-0.16062	0.01274
F	-5.18148	-1.16805	-0.03683
F	-4.60589	0.69486	-0.97707
F	-4.48049	0.48091	1.17797

***cct*-[Pt(NH$_3$)$_2$Cl$_2$(OCOCHCl$_2$)$_2$]** (DMSO)
(PCM)

Pt	-0.16228	-0.03608	-0.29691
O	0.74961	1.76143	-0.68406
N	-1.96518	1.06093	-0.53852
Cl	-0.41556	0.35381	2.02427
N	0.08481	-0.32779	-2.37895
Cl	1.80922	-1.30379	-0.05511
O	-1.27885	-1.74303	0.0671
C	1.7424	2.28054	-0.01555
C	-1.42341	-2.7218	-0.76303
C	2.0071	3.69594	-0.58842
Cl	3.71972	4.11885	-0.47672
O	2.37797	1.82294	0.90505
Cl	0.98698	4.85241	0.30964
C	-2.1845	-3.87296	-0.07113
O	-1.03913	-2.81794	-1.91877
Cl	-3.35978	-4.60542	-1.17258
Cl	-0.98539	-5.06171	0.49733
H	-2.37603	1.19873	0.38613
H	-2.65316	0.58796	-1.12454
H	-1.7651	1.98011	-0.93518
H	-0.27348	-1.27103	-2.58588
H	1.08007	-0.28354	-2.59529
H	-0.40065	0.36927	-2.94214
H	1.71486	3.7582	-1.63458
H	-2.72224	-3.51298	0.80326

[Pt(en)Cl_2($OCOCH_3$)$_2$] (DMSO)
(PCM)

C	18.93229	-0.83354	-0.61573
C	19.7889	0.19796	-1.30888
C	15.58711	-1.95422	1.37994
C	16.08385	-0.61994	1.89606
H	15.1648	-2.55203	2.1927
H	15.29125	-0.07569	2.41882
Cl	20.29103	-1.80961	3.35545
Cl	19.67217	-4.05415	0.84121
O	18.11216	-1.51513	-1.23506
H	20.03205	1.02983	-0.64456
N	16.71552	-2.71026	0.80091
N	17.21869	-0.87472	2.81684
Pt	18.44208	-2.35896	1.94168
H	14.81094	-1.8116	0.62083
H	16.45514	0.00582	1.08103
H	16.98743	-2.40266	-0.14819
H	16.5592	-3.72499	0.86075
H	16.90078	-1.23793	3.71796
H	17.75825	-0.02802	3.00131
O	17.82621	-3.63322	3.44257
H	19.2807	0.5591	-2.20529
O	19.17997	-0.90913	0.66326
H	20.72782	-0.28182	-1.60897
C	17.12375	-4.72065	3.25074
O	16.61864	-5.07492	2.1864
C	16.9991	-5.54618	4.5089
H	16.10956	-6.17653	4.45039
H	16.96333	-4.91568	5.39999
H	17.88195	-6.1912	4.58692

[Pt(en)Cl_2($OCOCF_3$)$_2$] (water)
(PCM)

C	18.93326	-0.93511	-0.67292
C	19.80697	0.16414	-1.34124
C	15.57125	-1.99498	1.35452
C	16.08948	-0.66919	1.87048
H	15.15743	-2.59559	2.16898
H	15.3101	-0.12512	2.4125
Cl	20.3064	-1.90679	3.25207
Cl	19.64117	-4.12271	0.75499
O	18.15801	-1.58667	-1.35022
F	19.60333	1.35523	-0.76048
N	16.6851	-2.75625	0.74568
N	17.23904	-0.93251	2.77145
Pt	18.443	-2.42477	1.87271
H	14.7834	-1.84045	0.61065

H	16.44745	-0.03655	1.055
H	16.91598	-2.45534	-0.21066
H	16.50757	-3.76596	0.76667
H	16.93563	-1.29093	3.67974
H	17.78582	-0.0879	2.94702
O	17.84748	-3.7112	3.36855
F	19.5219	0.28035	-2.63763
O	19.18026	-0.98328	0.58964
F	21.10877	-0.13598	-1.22489
C	17.15183	-4.77787	3.16265
O	16.61789	-5.18661	2.14901
C	17.02687	-5.58567	4.48569
F	16.29622	-6.68552	4.30733
F	16.44217	-4.84601	5.43967
F	18.23596	-5.95527	4.93152

$[Pt(en)Cl_2(OCOCF_3)_2]$ (MeOH)
(PCM)

C	18.99617	-0.93445	-0.62463
C	19.82218	0.17543	-1.33425
C	15.58841	-2.05046	1.28754
C	16.05379	-0.70272	1.79785
H	15.16153	-2.64757	2.09799
H	15.24091	-0.16946	2.30004
Cl	20.24221	-1.8187	3.36116
Cl	19.72249	-4.089	0.87796
O	18.25227	-1.61018	-1.31701
F	20.68151	0.80061	-0.52877
N	16.74178	-2.79261	0.73216
N	17.17554	-0.92045	2.7449
Pt	18.44741	-2.40142	1.91961
H	14.82326	-1.92899	0.51427
H	16.42528	-0.07554	0.98403
H	17.00301	-2.49818	-0.21874
H	16.58821	-3.80602	0.76198
H	16.8471	-1.26749	3.64881
H	17.69619	-0.06003	2.92284
O	17.82285	-3.67791	3.41184
F	18.9862	1.09396	-1.84308
O	19.20794	-0.96427	0.64216
F	20.51397	-0.35881	-2.34877
C	17.15998	-4.76373	3.19728
O	16.6721	-5.19944	2.1718
C	17.00397	-5.55389	4.52774
F	16.31144	-6.6763	4.33867
F	16.35944	-4.81513	5.44369
F	18.20265	-5.88173	5.02938

cct-[Pt(1,2-DACH)Cl_2($OCOCH_3$)$_2$] (acetone)
(PCM)

Pt	-0.58561	0.23401	0.2351
C	-1.98606	-2.24048	-0.75574
C	-3.00599	-3.30896	-0.44536
C	1.80109	-1.07537	-0.99541
C	1.54115	-1.78518	0.33653
C	2.80332	-2.43415	0.90607
C	4.00094	-1.4864	0.9364
C	4.2397	-0.85966	-0.43495
C	2.99356	-0.12525	-0.92783
Cl	-1.72369	0.81827	2.25637
Cl	-2.23674	1.29314	-1.08792
O	-1.52199	-2.09851	-1.8892
H	-2.91437	-3.66449	0.58315
N	0.56116	-0.37343	-1.41938
N	0.93824	-0.79249	1.27199
H	2.00936	-1.84829	-1.74636
H	0.76977	-2.54755	0.19459
H	3.03555	-3.29711	0.26844
H	2.58482	-2.83619	1.90262
H	3.84818	-0.69302	1.68289
H	4.88767	-2.0405	1.26424
H	5.08177	-0.1599	-0.39464
H	4.51372	-1.64353	-1.15542
H	2.77507	0.71592	-0.2565
H	3.16381	0.30627	-1.92062
H	-0.09397	-0.99259	-1.92544
H	0.74923	0.49823	-1.93551
H	1.61346	-0.09992	1.60248
H	0.54928	-1.25102	2.09792
O	0.48046	1.98492	0.46746
H	-2.90069	-4.13749	-1.14868
O	-1.68799	-1.51661	0.28883
H	-4.00503	-2.87367	-0.5648
C	0.90563	2.71425	-0.534
O	0.92386	2.37253	-1.71509
C	1.38449	4.07346	-0.08447
H	2.07918	4.48342	-0.82011
H	1.85365	4.02642	0.90093
H	0.51557	4.73782	-0.01136

cct-[Pt(1,4-DACH)Cl_2($OCOCH_3$)$_2$] (acetone)
(PCM)

Pt	-0.04486	-0.36719	-0.03987
O	-2.07595	-0.67042	0.16546
N	-0.37634	1.26135	1.29781
N	-0.45953	0.69072	-1.84552

Cl	0.43766	-1.52459	1.97854
Cl	0.29718	-2.17685	-1.54137
O	1.87316	0.343	-0.31615
C	-0.61335	2.67268	0.87457
C	-1.00121	2.07981	-1.91028
C	-2.01333	2.87718	0.31157
C	0.4773	3.15398	-0.08984
C	0.05138	3.12454	-1.56486
C	-2.26562	2.22345	-1.0548
C	3.00125	-0.33378	-0.24655
C	4.17879	0.56082	-0.58701
O	3.13061	-1.51308	0.03154
C	-2.70095	-1.80378	0.41114
C	-4.19301	-1.56686	0.55431
O	-2.19609	-2.90634	0.53063
H	0.44936	1.22548	1.89757
H	-1.15791	0.93322	1.86941
H	-1.09916	0.05867	-2.32941
H	0.428	0.63909	-2.35038
H	-0.54028	3.24369	1.80886
H	-1.26903	2.20915	-2.96661
H	-2.13803	3.96374	0.2268
H	-2.76711	2.54435	1.03508
H	1.38121	2.55621	0.05644
H	0.73761	4.1832	0.17766
H	-0.39437	4.08917	-1.83713
H	0.93024	3.00748	-2.21009
H	-2.98269	2.83808	-1.60855
H	-2.7307	1.24215	-0.92625
H	5.11061	0.05868	-0.3197
H	4.10742	1.521	-0.06851
H	4.17763	0.76366	-1.66374
H	-4.71949	-2.52316	0.54077
H	-4.568	-0.92033	-0.24396
H	-4.38808	-1.06435	1.50822

***cct*-$Pt(NH_3)_2Cl_2(OCONH^tBu)_2$ (DMSO) (PCM)**

Pt	0.83561	-0.00368	-1.0648
O	1.02328	2.04578	-0.94977
Cl	-1.44295	0.29536	-0.48265
N	1.20787	-0.21446	0.99846
Cl	0.51078	0.308	-3.39492
N	2.88061	-0.23038	-1.52043
O	0.81017	-2.0582	-1.03502
C	2.03967	2.5742	-0.29129
C	-0.04309	-2.8304	-1.69064
N	2.02939	3.92319	-0.33556
C	2.99926	4.83324	0.29845

O	2.91385	1.91254	0.30635
N	0.22023	-4.16921	-1.55574
O	-0.98005	-2.44213	-2.38687
C	2.53742	6.24692	-0.05513
C	4.40261	4.59395	-0.26468
C	2.98633	4.65222	1.81863
C	1.08514	-4.87433	-0.59514
C	0.91484	-6.36302	-0.90726
C	0.64035	-4.60314	0.84581
C	2.55457	-4.4937	-0.78856
H	1.94818	0.45643	1.23765
H	1.49612	-1.16914	1.21034
H	0.35936	-0.0023	1.52338
H	3.17923	-1.19137	-1.35684
H	3.39704	0.42547	-0.92239
H	3.03601	-0.00202	-2.50251
H	1.26628	4.33769	-0.85308
H	-0.51519	-4.72862	-1.96768
H	3.21827	6.98089	0.3871
H	1.53009	6.44244	0.33218
H	2.53136	6.40081	-1.14103
H	5.10894	5.30363	0.18099
H	4.41021	4.73795	-1.35123
H	4.74441	3.57923	-0.04286
H	3.68032	5.36099	2.28468
H	3.2905	3.63856	2.09381
H	1.98338	4.83933	2.21918
H	1.52779	-6.96152	-0.22595
H	1.22589	-6.58575	-1.93467
H	-0.12923	-6.67679	-0.78308
H	1.2731	-5.15311	1.5521
H	-0.39804	-4.92132	0.99432
H	0.71037	-3.53722	1.08264
H	3.18597	-5.12063	-0.14877
H	2.73276	-3.44907	-0.52242
H	2.85797	-4.64715	-1.83029

cct-Pt(NH$_3$)$_2$Cl$_2$[OCONH(c-pentyl)]$_2$ (DMSO)
(PCM)

Pt	-0.04384	-0.27352	-0.61885
O	0.74336	1.58234	-0.99264
N	-1.85822	0.78779	-0.53752
Cl	-0.08293	-0.19392	1.74156
N	-0.0826	-0.40171	-2.73203
Cl	2.0187	-1.4525	-0.7448
O	-0.89006	-2.15155	-0.55169
C	1.69658	2.19466	-0.30531
C	-2.11534	-2.40365	-0.13094
N	1.84455	3.50131	-0.68573

O	2.38518	1.70422	0.58775
C	1.24222	4.13355	-1.84107
C	1.15111	5.6569	-1.68314
C	1.9929	3.9656	-3.16726
C	1.03171	6.20788	-3.12044
C	1.33306	5.01507	-4.06161
N	-2.27773	-3.71077	0.18447
C	-3.5533	-4.33022	0.46915
O	-3.04074	-1.57714	-0.03871
C	-4.07383	-5.25495	-0.64079
C	-3.53052	-5.24377	1.69647
C	-5.10932	-6.15938	0.05515
C	-4.84646	-6.01682	1.57832
H	-2.57475	0.05267	-0.37058
H	-2.04766	1.31794	-1.38633
H	-1.81971	1.43477	0.24863
H	-0.96	-0.77663	-3.09147
H	0.67321	-1.02416	-3.02134
H	0.08733	0.51924	-3.13751
H	2.67424	3.93691	-0.30271
H	0.23567	3.71537	-1.95011
H	2.07377	6.02063	-1.21035
H	0.32014	5.95307	-1.03436
H	1.93174	2.94636	-3.56464
H	3.0548	4.20236	-3.00763
H	1.7441	7.02441	-3.28013
H	0.03472	6.61838	-3.31303
H	1.95814	5.29928	-4.91468
H	0.39736	4.61236	-4.47022
H	-1.47188	-4.3083	0.05213
H	-4.26137	-3.51219	0.63581
H	-3.23317	-5.85182	-1.01968
H	-4.48427	-4.69589	-1.4886
H	-3.43138	-4.68788	2.63506
H	-2.6722	-5.92677	1.61981
H	-5.0058	-7.1983	-0.27523
H	-6.13169	-5.85184	-0.19009
H	-4.80635	-6.98456	2.08886
H	-5.65421	-5.442	2.04745

cct-Pt(NH$_3$)$_2$Cl$_2$[OCONH(c-hexyl)]$_2$ (DMSO) (PCM)

Pt	-0.07968	-0.3116	-0.79098
O	0.69925	1.55853	-1.09986
N	-1.88582	0.74983	-0.60188
Cl	-0.04087	-0.33583	1.57096
N	-0.19015	-0.34586	-2.90518
Cl	1.97483	-1.48533	-1.04125
O	-0.9208	-2.19254	-0.78153

C	1.69326	2.1216	-0.42736
C	-2.15571	-2.46466	-0.40294
N	1.8481	3.4428	-0.75038
O	2.40819	1.57644	0.41161
C	1.22544	4.13678	-1.86772
C	1.12937	5.62939	-1.55261
C	1.97155	3.90628	-3.18623
C	1.3235	4.67487	-4.33755
C	0.48748	6.40247	-2.70456
N	-2.35277	-3.79479	-0.25349
C	1.22607	6.16635	-4.02114
C	-3.62209	-4.40179	0.10916
O	-3.06661	-1.63478	-0.22661
C	-3.9238	-5.59321	-0.80072
C	-3.6445	-4.81503	1.58373
C	-5.24737	-6.25886	-0.42375
C	-4.97004	-5.47899	1.9559
C	-5.26929	-6.67032	1.04749
H	-2.60208	0.00805	-0.46511
H	-2.08971	1.33316	-1.41157
H	-1.82549	1.34563	0.22245
H	-1.08183	-0.69966	-3.25071
H	0.55078	-0.95976	-3.2465
H	-0.02739	0.59052	-3.27668
H	2.70196	3.84334	-0.38231
H	0.20991	3.73435	-1.9632
H	2.1421	6.02266	-1.37092
H	0.56027	5.77151	-0.62522
H	2.004	2.83133	-3.40481
H	3.01313	4.23973	-3.06057
H	1.89273	4.51466	-5.26203
H	0.31378	4.2757	-4.51829
H	0.46386	7.47303	-2.46483
H	-0.55977	6.08293	-2.81452
H	-1.54171	-4.39009	-0.35701
H	0.72203	6.69748	-4.83882
H	2.24017	6.58761	-3.94844
H	-4.3825	-3.62897	-0.05187
H	-3.10819	-6.32755	-0.7107
H	-3.94073	-5.26008	-1.84614
H	-3.46018	-3.93367	2.21093
H	-2.81666	-5.5173	1.76521
H	-5.42126	-7.12946	-1.06863
H	-6.07247	-5.55656	-0.61568
H	-4.94709	-5.79334	3.00701
H	-5.78249	-4.74201	1.86686
H	-6.24216	-7.10916	1.30365
H	-4.51491	-7.45359	1.21648

cct-Pt(NH$_3$)$_2$Cl$_2$(OCONHPh)$_2$ (DMSO)
(PCM)

Pt	0.67311	-1.21827	0.06264
Cl	2.73087	-0.0361	0.1142
Cl	-0.62591	0.76709	-0.01119
O	0.76814	-1.14174	-1.98927
O	0.6296	-1.07981	2.11304
N	1.77495	-3.01085	0.12683
N	-1.12151	-2.31777	0.01878
C	0.53839	-2.21407	-2.71356
C	0.35079	-2.13012	2.85222
N	0.65371	-1.9387	-4.04463
O	0.2535	-3.3343	-2.26138
C	0.49093	-2.79138	-5.14732
C	0.67432	-2.22344	-6.41706
C	0.16217	-4.14901	-5.04326
C	0.02273	-4.91276	-6.20214
C	0.20424	-4.3516	-7.46481
N	0.37679	-1.81471	4.17914
C	0.53173	-2.99839	-7.56279
C	0.13918	-2.63389	5.29357
O	0.09587	-3.26376	2.41585
C	0.23803	-2.02791	6.5551
C	-0.18407	-3.99417	5.20858
C	-0.40205	-4.72274	6.37796
C	0.01773	-2.76807	7.71147
C	-0.30464	-4.12375	7.6325
H	1.5381	-3.54609	-0.71514
H	1.48142	-3.52074	0.96668
H	2.77564	-2.81833	0.15765
H	-1.92646	-1.69317	-0.01773
H	-1.15017	-2.89104	0.8685
H	-1.09359	-2.91639	-0.81331
H	0.89144	-0.97817	-4.25522
H	0.92985	-1.16928	-6.50442
H	0.01895	-4.595	-4.06763
H	-0.23271	-5.96537	-6.10715
H	0.09265	-4.95771	-8.35961
H	0.60073	-0.84801	4.3762
H	0.67826	-2.53824	-8.53662
H	0.48886	-0.9715	6.62765
H	-0.26231	-4.46941	4.23941
H	-0.65225	-5.77784	6.29776
H	0.09944	-2.27874	8.67866
H	-0.4769	-4.70269	8.53563

Pt(1,2-DACH)$_2$(OH)$_2$(oxalate)$_2$ (DMF)
(PCM) 6-31G(d,p)(E)

Pt	0	-0.43283	-0.04052	0.11348
C	0	-3.03919	0.89396	-0.4486
C	0	-3.18333	-0.62413	-0.16972
C	0	2.37958	-0.9418	0.53567
C	0	2.34718	0.54364	0.89864
C	0	3.70347	1.21005	0.66917
C	0	4.26135	0.93952	-0.72776
C	0	4.30122	-0.55738	-1.02772
C	0	2.92254	-1.19803	-0.8662
O	0	-1.82308	1.37936	-0.37182
O	0	-2.07601	-1.26115	0.12324
O	0	-4.01063	1.56772	-0.72223
O	0	-4.27068	-1.16089	-0.22277
N	0	0.9967	-1.47163	0.67862
N	0	1.26241	1.18266	0.10449
H	0	3.0169	-1.45374	1.26661
H	0	2.04097	0.65034	1.94352
H	0	4.39286	0.81179	1.42339
H	0	3.6178	2.28463	0.8638
H	0	3.65837	1.45331	-1.4893
H	0	5.26494	1.36986	-0.80274
H	0	4.66835	-0.73341	-2.04348
H	0	5.01152	-1.04472	-0.34647
H	0	2.21965	-0.80547	-1.61219
H	0	2.98399	-2.27995	-1.03016
H	0	0.76249	-1.61098	1.66339
H	0	0.88281	-2.35836	0.18928
H	0	1.49939	1.26123	-0.88623
H	0	1.05408	2.11653	0.45462
O	0	-0.07904	-0.30351	-1.87403
H	0	-0.66642	0.33292	-2.30235
O	0	-0.6249	0.22711	2.12261
H	0	-1.43662	-0.23873	2.36087

$Pt(NH_3)_2Cl_2(OH)_2$ (water)
(PCM) 6-31G(d,p)(E)

Pt	0	0.46988	-0.05956	0.04109
O	0	0.48987	-0.29268	-1.98382
N	0	1.852	1.50376	-0.20439
O	0	0.74942	0.18336	2.04554
N	0	1.97174	-1.52807	0.08985
H	0	2.46814	1.35912	-1.00065
H	0	2.39303	1.6064	0.65157
H	0	1.31331	2.35491	-0.35387
H	0	1.51501	-2.41199	0.30682
H	0	2.67906	-1.34006	0.79619
H	0	2.39768	-1.59877	-0.83183
H	0	-0.37312	-0.66344	-2.20512
H	0	-0.09791	0.49783	2.3837

Cl	0	-1.22985	1.59332	-0.00709
Cl	0	-1.09586	-1.81979	0.31219

Pt(^{i}PrNH$_2$)$_2$Cl$_2$(OH)$_2$ (water)
(PCM) 6-31G(d,p)(E)

Pt	0	-0.17734	0.31731	-0.20533
O	0	1.83349	0.67308	-0.19148
N	0	0.25532	-0.69004	1.61184
O	0	-2.14406	-0.23004	-0.16345
N	0	0.04096	-1.40937	-1.41321
H	0	0.68307	0.076	2.13324
H	0	1.00721	-1.35342	1.42251
C	0	-0.81738	-1.31701	2.42703
C	0	1.35265	-2.09667	-1.56314
H	0	-0.29722	-1.09002	-2.32284
H	0	-0.67671	-2.03399	-1.04598
H	0	1.90912	1.60735	0.04082
H	0	0.54016	-2.30768	3.80736
Cl	0	-0.50412	2.24904	1.15152
Cl	0	-0.58354	1.51106	-2.2255
C	0	-0.28075	-1.5829	3.82958
C	0	-1.3282	-2.57871	1.75404
H	0	-1.62189	-0.57732	2.47173
C	0	2.20064	-1.35742	-2.58295
C	0	1.11813	-3.55536	-1.93601
H	0	1.84865	-2.04748	-0.58817
H	0	-1.07952	-1.99488	4.45235
H	0	0.07762	-0.66496	4.30555
H	0	-2.56891	0.37469	-0.78532
H	0	-2.06465	-3.06219	2.40113
H	0	-0.51566	-3.29505	1.58529
H	0	-1.82102	-2.34116	0.8089
H	0	3.17687	-1.84248	-2.66398
H	0	2.34725	-0.3214	-2.27155
H	0	1.7292	-1.38437	-3.57212
H	0	2.08041	-4.06774	-2.02008
H	0	0.6047	-3.63583	-2.89981
H	0	0.52461	-4.07605	-1.17777

Pt(hpip)$_2$Cl$_2$(OH)$_2$ (water)
(PCM) 6-31G(d,p)(E)

Pt	0	-0.05128	-0.36498	0.02145
Cl	0	1.45534	0.72564	-1.46809
Cl	0	1.17489	0.36846	1.92831
N	0	-1.53782	-1.47579	1.07315
C	0	-1.57138	-2.8079	0.41657
C	0	-1.43894	-2.64863	-1.11057
N	0	-1.32529	-1.21082	-1.46561

C	0	-2.6333	-0.51059	-1.51314
C	0	-3.51176	-0.87415	-0.32051
C	0	-2.84624	-0.77547	1.04827
O	0	-1.19741	1.32935	0.09823
O	0	1.05915	-2.08302	-0.06087
H	0	-1.21781	-1.57122	2.03584
H	0	-2.49607	-3.31882	0.70192
H	0	-0.72052	-3.37236	0.7913
H	0	-0.52399	-3.1346	-1.4423
H	0	-2.28932	-3.07952	-1.64787
H	0	-0.85072	-1.11065	-2.36182
H	0	-3.13842	-0.80588	-2.4392
H	0	-2.42017	0.55907	-1.53531
H	0	-3.92359	-1.87936	-0.45863
H	0	-4.37244	-0.19923	-0.32229
H	0	-2.65655	0.26324	1.32256
H	0	-3.49156	-1.24287	1.79992
H	0	-0.54899	2.03825	0.19162
H	0	1.95602	-1.77771	0.1202

$Pt(mhpip)_2Cl_2(OH)_2$ (water)
(PCM) 6-31G(d,p)(E)

Pt	0	0.00852	-0.35915	-0.02811
Cl	0	1.46165	0.62937	-1.63987
Cl	0	1.36656	0.50359	1.73795
N	0	-1.47126	-1.45105	1.11884
C	0	-1.53146	-2.77841	0.44239
C	0	-1.43399	-2.64352	-1.08707
N	0	-1.29384	-1.21754	-1.46728
C	0	-2.58773	-0.49675	-1.5217
C	0	-3.45454	-0.83941	-0.3175
C	0	-2.77512	-0.73069	1.04184
C	0	-1.07138	-1.61322	2.52707
O	0	-1.11718	1.35034	0.04906
O	0	1.09753	-2.09076	-0.08899
H	0	-2.45131	-3.28233	0.75839
H	0	-0.67696	-3.35109	0.79839
H	0	-0.53865	-3.15688	-1.43012
H	0	-2.3065	-3.06234	-1.59789
H	0	-0.81509	-1.13972	-2.36363
H	0	-3.10265	-0.79523	-2.44146
H	0	-2.36074	0.56972	-1.56013
H	0	-3.88027	-1.84062	-0.44053
H	0	-4.30761	-0.15459	-0.31204
H	0	-2.56877	0.31084	1.29336
H	0	-3.43225	-1.16876	1.80268
H	0	-1.77786	-2.28346	3.02968
H	0	-1.07949	-0.638	3.01369
H	0	-0.06542	-2.02995	2.56692

H	0	-0.4882	2.0163	0.35424
H	0	2.00669	-1.78096	-0.1781

$Pt(dmhpip)_2Cl_2(OH)_2$ (water)
(PCM) 6-31G(d,p)(E)

Pt	0	-0.46261	0.00013	-0.00727
Cl	0	-2.18552	1.64688	-0.17413
Cl	0	-2.18109	-1.65122	-0.17692
N	0	1.23556	-1.32303	0.20686
C	0	1.9917	-0.76036	1.35749
C	0	1.99332	0.7746	1.3497
N	0	1.23457	1.32642	0.19556
C	0	2.03585	1.28572	-1.05936
C	0	2.82553	-0.00389	-1.22008
C	0	2.03831	-1.29335	-1.0473
C	0	0.82696	-2.70733	0.50324
C	0	0.82544	2.71295	0.48016
O	0	-0.28707	-0.00738	-2.04836
O	0	-0.59233	0.00695	2.03493
H	0	3.00432	-1.17808	1.3399
H	0	1.48802	-1.10195	2.26001
H	0	1.49281	1.1259	2.25009
H	0	3.00664	1.19018	1.3242
H	0	2.73441	2.13051	-1.02715
H	0	1.33494	1.42678	-1.88385
H	0	3.68623	0.00012	-0.54342
H	0	3.2453	-0.0082	-2.23061
H	0	1.33806	-1.44275	-1.87084
H	0	2.73822	-2.13661	-1.00584
H	0	1.7175	-3.29938	0.74248
H	0	0.32807	-3.12793	-0.36941
H	0	0.13939	-2.70477	1.34824
H	0	1.71592	3.30796	0.71217
H	0	0.13973	2.71741	1.32669
H	0	0.32431	3.12538	-0.39512
H	0	-1.20365	-0.04566	-2.34883
H	0	-1.54039	0.07286	2.20028

$Pt(1,4\text{-}DACH)_2(OH)_2Cl_2$ (water)
(PCM) 6-31G(d,p)(E)

Pt	0	0.46517	0.34396	-0.21232
O	0	0.60241	0.5973	1.81003
N	0	-1.16606	1.67806	-0.0949
N	0	-0.60635	-1.45602	0.04544
Cl	0	1.75727	2.31664	-0.57164
Cl	0	2.38002	-1.07592	-0.29813
O	0	0.13765	0.05782	-2.20826
C	0	-2.59174	1.24833	-0.09643
C	0	-2.03968	-1.51909	0.44396

C	0	-3.00472	0.70369	1.26444
C	0	-2.85883	0.24484	-1.22811
C	0	-2.95337	-1.20313	-0.73268
C	0	-2.31197	-0.60857	1.65054
H	0	1.48841	0.95536	1.94633
H	0	-0.99147	2.30808	-0.87686
H	0	-0.94533	2.18898	0.76183
H	0	-0.03401	-1.95732	0.72365
H	0	-0.46514	-1.9045	-0.86157
H	0	1.02252	0.00502	-2.59037
H	0	-3.16006	2.16666	-0.28471
H	0	-2.20326	-2.56358	0.73388
H	0	-4.08867	0.55146	1.21185
H	0	-2.84274	1.45898	2.04129
H	0	-2.07291	0.33658	-1.98369
H	0	-3.80049	0.51067	-1.71642
H	0	-3.97217	-1.41336	-0.38809
H	0	-2.76398	-1.89785	-1.55832
H	0	-2.94901	-1.14653	2.35809
H	0	-1.36927	-0.40235	2.16606

$Pt(1,4\text{-}DACH)_2(OH)_2Cl_2$ (DMF)
(PCM) 6-31G(d,p)(E)

Pt	0	0.46495	0.34392	-0.21229
O	0	0.60049	0.59884	1.80992
N	0	-1.16654	1.67839	-0.0961
N	0	-0.60636	-1.45643	0.04671
Cl	0	1.7558	2.31566	-0.57551
Cl	0	2.37938	-1.07531	-0.29397
O	0	0.13643	0.05574	-2.20772
C	0	-2.59198	1.24833	-0.09745
C	0	-2.03963	-1.51913	0.44501
C	0	-3.00497	0.70432	1.26372
C	0	-2.85833	0.24382	-1.22849
C	0	-2.9532	-1.20378	-0.73195
C	0	-2.31176	-0.60743	1.65082
H	0	1.49377	0.93698	1.94929
H	0	-0.99137	2.30715	-0.87891
H	0	-0.94536	2.19003	0.76008
H	0	-0.03369	-1.95631	0.72566
H	0	-0.46436	-1.90542	-0.85992
H	0	1.02054	0.02399	-2.5938
H	0	-3.16107	2.16609	-0.28644
H	0	-2.2039	-2.5633	0.73584
H	0	-4.0889	0.55172	1.21113
H	0	-2.84329	1.46006	2.04021
H	0	-2.07171	0.3349	-1.98345
H	0	-3.79964	0.50912	-1.71784

```
 H                    0    -3.9721   -1.41364  -0.38736
 H                    0    -2.76383  -1.89901  -1.55719
 H                    0    -2.94838  -1.14472   2.3593
 H                    0    -1.3688   -0.40038   2.1656
```

Output file for NMR calculation of $[PtCl_4]^{2-}$

```
Entering Link 1 = C:\G03W\l1.exe PID=      6248.

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 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,
 V. Bakken, 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.

 ****************************************
 Gaussian 03:  IA32W-G03RevE.01 11-Sep-2007
               17-Jan-2014
 ****************************************
 %chk=PtCl4_2-PBE0_SARCZORANMR
 %nproc=2
 Will use up to    2 processors via shared memory.
 %mem=800mb
 ----------------------------------------------------------------
------
 #p PBE1PBE/gen nmr=giao integral(ultrafine) SCRF(solvent=water)
SCF(No
 VarAcc,maxcycles=1000)
 ----------------------------------------------------------------
------
 1/38=1/1;
```

```
 2/17=6,18=5,40=1/2;
 3/5=7,11=2,16=1,25=1,30=1,70=2201,72=1,74=-13,75=5/1,2,8,3;
 4//1;
 5/5=2,7=1000,38=1,53=1/2;
 8/6=1,10=90,11=11/1;
 10/13=100,45=16/2;
 6/7=2,8=2,9=2,10=2,28=1/1;
 99/9=1/99;
 Leave Link    1 at Fri Jan 17 09:22:40 2014, MaxMem=  104857600
cpu:       0.0
 (Enter C:\G03W\l101.exe)
 ------------------------
 PtCl4_2-PBE0_SARCZORANMR
 ------------------------
 Symbolic Z-matrix:
 Charge = -2 Multiplicity = 1
 Pt                    0.         0.         0.
 Cl                    0.         2.4384     0.
 Cl                    2.4384     0.         0.
 Cl                   -2.4384     0.         0.
 Cl                    0.        -2.4384     0.

                     Isotopes and Nuclear Properties:
 (Nuclear quadrupole moments (NQMom) in fm**2, nuclear magnetic
moments (NMagM)
  in nuclear magnetons)

  Atom         1           2           3           4           5
 IAtWgt=         195          35          35          35
35
 AtmWgt= 194.9648000  34.9688527  34.9688527  34.9688527
34.9688527
 NucSpn=           1           3           3           3
3
 AtZEff=   0.0000000   0.0000000   0.0000000   0.0000000
0.0000000
 NQMom=    0.0000000  -8.1650000  -8.1650000  -8.1650000  -
8.1650000
 NMagM=    0.6095000   0.8218740   0.8218740   0.8218740
0.8218740
 Leave Link  101 at Fri Jan 17 09:22:40 2014, MaxMem=  104857600
cpu:       0.0
 (Enter C:\G03W\l202.exe)
                          Input orientation:
 ---------------------------------------------------------------
-----
 Center     Atomic     Atomic              Coordinates
(Angstroms)
 Number     Number      Type              X           Y
Z
```

```
 ---------------------------------------------------------------------
-----
    1         78             0        0.000000    0.000000
0.000000
    2         17             0        0.000000    2.438400
0.000000
    3         17             0        2.438400    0.000000
0.000000
    4         17             0       -2.438400    0.000000
0.000000
    5         17             0        0.000000   -2.438400
0.000000
 ---------------------------------------------------------------------
-----
                    Distance matrix (angstroms):
                    1          2          3          4          5
     1  Pt   0.000000
     2  Cl   2.438400   0.000000
     3  Cl   2.438400   3.448418   0.000000
     4  Cl   2.438400   3.448418   4.876800   0.000000
     5  Cl   2.438400   4.876800   3.448418   3.448418   0.000000
 Stoichiometry    Cl4Pt(2-)
 Framework group  D4H[O(Pt),2C2'(Cl.Cl)]
 Deg. of freedom     1
 Full point group                 D4H
 Largest Abelian subgroup         D2H     NOp   8
 Largest concise Abelian subgroup D2      NOp   4
                         Standard orientation:
 ---------------------------------------------------------------------
-----
 Center     Atomic     Atomic              Coordinates
(Angstroms)
 Number     Number      Type              X           Y
Z
 ---------------------------------------------------------------------
-----
    1         78             0        0.000000    0.000000
0.000000
    2         17             0        0.000000    2.438400
0.000000
    3         17             0        2.438400    0.000000
0.000000
    4         17             0       -2.438400    0.000000
0.000000
    5         17             0        0.000000   -2.438400
0.000000
 ---------------------------------------------------------------------
-----
 Rotational constants (GHZ):      1.2153348      1.2153348
0.6076674
```

```
 Leave Link  202 at Fri Jan 17 09:22:41 2014, MaxMem=  104857600
cpu:       0.0
 (Enter C:\G03W\l301.exe)
 General basis read from cards:  (5D, 7F)
 Centers:   1
 S  6 1.00
      Exponent=  1.6896015676D+06 Coefficients=  5.7974482200D-02
      Exponent=  7.5093403004D+05 Coefficients= -1.3148538600D-02
      Exponent=  3.3374845779D+05 Coefficients=  1.2503763310D-01
      Exponent=  1.4833264791D+05 Coefficients=  9.1535752600D-02
      Exponent=  6.5925621293D+04 Coefficients=  3.2913880880D-01
      Exponent=  2.9300276130D+04 Coefficients=  5.3748713720D-01
 S  1 1.00
      Exponent=  1.3022344947D+04 Coefficients=  1.0000000000D+00
 S  1 1.00
      Exponent=  5.7877088650D+03 Coefficients=  1.0000000000D+00
 S  1 1.00
      Exponent=  2.5723150510D+03 Coefficients=  1.0000000000D+00
 S  1 1.00
      Exponent=  1.1432511340D+03 Coefficients=  1.0000000000D+00
 S  1 1.00
      Exponent=  5.0811161500D+02 Coefficients=  1.0000000000D+00
 S  1 1.00
      Exponent=  2.2582738400D+02 Coefficients=  1.0000000000D+00
 S  1 1.00
      Exponent=  1.0036772600D+02 Coefficients=  1.0000000000D+00
 S  1 1.00
      Exponent=  4.4607878000D+01 Coefficients=  1.0000000000D+00
 S  1 1.00
      Exponent=  1.9825724000D+01 Coefficients=  1.0000000000D+00
 S  1 1.00
      Exponent=  8.8114330000D+00 Coefficients=  1.0000000000D+00
 S  1 1.00
      Exponent=  3.9161920000D+00 Coefficients=  1.0000000000D+00
 S  1 1.00
      Exponent=  1.7405300000D+00 Coefficients=  1.0000000000D+00
 S  1 1.00
      Exponent=  7.7356900000D-01 Coefficients=  1.0000000000D+00
 S  1 1.00
      Exponent=  3.4380800000D-01 Coefficients=  1.0000000000D+00
 S  1 1.00
      Exponent=  1.5280400000D-01 Coefficients=  1.0000000000D+00
 S  1 1.00
      Exponent=  6.7913000000D-02 Coefficients=  1.0000000000D+00
 P  5 1.00
      Exponent=  2.3642643991D+04 Coefficients=  1.1403826400D-02
      Exponent=  9.4570575960D+03 Coefficients=  1.7083256700D-02
      Exponent=  3.7828230390D+03 Coefficients=  8.0886502700D-02
      Exponent=  1.5131292150D+03 Coefficients=  2.5252184340D-01
      Exponent=  6.0525168600D+02 Coefficients=  7.4017959180D-01
```

```
P 1 1.00
    Exponent=  2.4210067400D+02 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  9.6840270000D+01 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  3.8736108000D+01 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  1.5494443000D+01 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  6.1977770000D+00 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  2.4791110000D+00 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  9.9164400000D-01 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  3.9665800000D-01 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  1.5866300000D-01 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  6.3465000000D-02 Coefficients=  1.0000000000D+00
D 4 1.00
    Exponent=  1.8110792460D+03 Coefficients=  7.6859038000D-03
    Exponent=  6.5857427100D+02 Coefficients=  4.3883054800D-02
    Exponent=  2.3948155300D+02 Coefficients=  2.4558000620D-01
    Exponent=  8.7084201000D+01 Coefficients=  8.0580963240D-01
D 1 1.00
    Exponent=  3.1666982000D+01 Coefficients=  1.0000000000D+00
D 1 1.00
    Exponent=  1.1515266000D+01 Coefficients=  1.0000000000D+00
D 1 1.00
    Exponent=  4.1873700000D+00 Coefficients=  1.0000000000D+00
D 1 1.00
    Exponent=  1.5226800000D+00 Coefficients=  1.0000000000D+00
D 1 1.00
    Exponent=  5.5370200000D-01 Coefficients=  1.0000000000D+00
D 1 1.00
    Exponent=  2.0134600000D-01 Coefficients=  1.0000000000D+00
D 1 1.00
    Exponent=  7.3217000000D-02 Coefficients=  1.0000000000D+00
F 4 1.00
    Exponent=  8.5141859000D+01 Coefficients=  6.3002593000D-02
    Exponent=  2.8380620000D+01 Coefficients=  2.9424498280D-01
    Exponent=  9.4602070000D+00 Coefficients=  5.6544272570D-01
    Exponent=  3.1534020000D+00 Coefficients=  3.7760481600D-01
F 1 1.00
    Exponent=  1.0511340000D+00 Coefficients=  1.0000000000D+00
F 1 1.00
    Exponent=  3.5037800000D-01 Coefficients=  1.0000000000D+00
****
Centers:   2  3  4  5
```

```
 6-31+G(d)
 ****
 There are    55 symmetry adapted basis functions of AG
symmetry.
 There are    18 symmetry adapted basis functions of B1G
symmetry.
 There are    14 symmetry adapted basis functions of B2G
symmetry.
 There are    14 symmetry adapted basis functions of B3G
symmetry.
 There are     5 symmetry adapted basis functions of AU
symmetry.
 There are    27 symmetry adapted basis functions of B1U
symmetry.
 There are    33 symmetry adapted basis functions of B2U
symmetry.
 There are    33 symmetry adapted basis functions of B3U
symmetry.
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   199 basis functions,   417 primitive gaussians,   220
cartesian basis functions
    74 alpha electrons       74 beta electrons
       nuclear repulsion energy      1391.1768971787 Hartrees.
 IExCor=1009 DFT=T Ex=PBE+HF Corr=PBE ExCW=0 ScaHFX=  0.250000
 ScaDFX=  0.750000  0.750000  1.000000  1.000000
 IRadAn=       5 IRanWt=     -1 IRanGd=            0 ICorTp=0
 NAtoms=    5 NActive=    5 NUniq=    2 SFac= 3.00D+00 NAtFMM=
80 NAOKFM=F Big=F
 ---------------------------------------------------------------
--------------
 United Atom Topological Model (UA0  parameters set).
  Nord Group  Hybr  Charge Alpha Radius          Bonded to
    1  Pt     *     0.00   1.00  1.377  Cl2   [s] Cl3   [s] Cl4
[s] Cl5   [s]
    2  Cl     *     0.00   1.00  1.973  Pt1   [s]
    3  Cl     *     0.00   1.00  1.973  Pt1   [s]
    4  Cl     *     0.00   1.00  1.973  Pt1   [s]
    5  Cl     *     0.00   1.00  1.973  Pt1   [s]
 ---------------------------------------------------------------
--------------
 Polarizable Continuum Model (PCM)
 =================================
 Model                : PCM.
 Atomic radii         : UA0 (Simple United Atom Topological
Model).
 Polarization charges : Total charges.
 Charge compensation  : None.
 Solution method      : Matrix inversion.
```

```
 Cavity                 : GePol (RMin=0.200 OFac=0.890).
                          Default sphere list used, NSphG=    5.
                          Tesserae with average area of 0.200
Ang**2.
 Solvent                : Water, Eps     =  78.390000
                                 Eps(inf)=   1.776000
                                 RSolv   =   1.385000 Ang.
 ----------------------------------------------------------------
--------------
 Using symmetry in molecular cavity generation.
 GePol: Number of tesserae being generated         =    1720
 GePol: Average area of tesserae                   =       0.09
Ang**2
 GePol: Minimum area of tessera                    =   0.15D-02
Ang**2
 GePol: Maximum area of tessera                    =    0.19991
Ang**2
 GePol: Number of small tesserae                   =       0
 GePol: Fraction of small tesserae (<1% of avg)    =       0.00%
 GePol: Total count of vertices                    =    6464
 GePol: Maximum number of vertices in a tessera    =       8
 GePol: Cavity surface area                        =    154.292
Ang**2
 GePol: Cavity volume                              =    135.840
Ang**3
 DisRep: Neglecting contributions from atom    1
 Leave Link  301 at Fri Jan 17 09:22:42 2014, MaxMem=  104857600
cpu:       1.0
 (Enter C:\G03W\l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1
NCelD=      1
         NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=
0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
 NBasis=   199 RedAO= T  NBF=    55    18    14    14     5    27
33    33
 NBsUse=   199 1.00D-06 NBFU=    55    18    14    14     5    27
33    33
 Precomputing XC quadrature grid using
 IXCGrd= 2 IRadAn=           5 IRanWt=          -1 IRanGd=
0.
 Defaulting to unpruned grid for atomic number  78.
 NRdTot=     407 NPtTot=      132060 NUsed=      133903 NTot=
133919
 NSgBfM=   207   207   207   207.
 Leave Link  302 at Fri Jan 17 09:22:43 2014, MaxMem=  104857600
cpu:       0.0
 (Enter C:\G03W\l308.exe)
```

```
 Leave Link  308 at Fri Jan 17 09:22:44 2014, MaxMem=  104857600
cpu:       0.0
 (Enter C:\G03W\l303.exe)
 DipDrv:  MaxL=1.
 Leave Link  303 at Fri Jan 17 09:22:44 2014, MaxMem=  104857600
cpu:       0.0
 (Enter C:\G03W\l401.exe)
 Harris functional with IExCor= 1009 diagonalized for initial
guess.
 ExpMin= 4.83D-02 ExpMax= 1.69D+06 ExpMxC= 1.69D+06 IAcc=4
IRadAn=    199590 AccDes= 0.00D+00
 HarFok:  IExCor=1009 AccDes= 0.00D+00 IRadAn=    199590 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Harris En= -19167.4255278408
 Initial guess orbital symmetries:
       Occupied  (A1G) (A1G) (EU) (EU) (A2U) (A1G) (B1G) (EU)
(EU)
                 (A1G) (EU) (EU) (A2U) (B1G) (B2G) (EG) (EG)
(A1G)
                 (A1G) (EU) (EU) (A2U) (B1G) (B2G) (EG) (EG)
(A1G)
                 (A1G) (B1G) (EU) (EU) (B1G) (EU) (EU) (A1G)
(A2G)
                 (EU) (EU) (B2G) (B2U) (EG) (EG) (A2U) (A1G) (EU)
                 (EU) (B2U) (B1U) (EU) (EU) (A2U) (EU) (EU) (A2U)
                 (A1G) (B1G) (EU) (EU) (A1G) (B1G) (B2G) (EU)
(EU)
                 (EG) (EG) (A2U) (B2U) (EU) (EU) (A2G) (A1G)
(B2G)
                 (EG) (EG)
       Virtual   (B1G) (A1G) (A2U) (EU) (EU) (B1G) (A1G) (B2G)
                 (EG) (EG) (A2U) (A1G) (EU) (EU) (EU) (EU) (B2U)
                 (A2G) (B1G) (A1G) (EG) (EG) (EU) (EU) (B2G)
(A2U)
                 (EU) (EU) (A1G) (B1G) (B1G) (A1G) (B2G) (A2U)
                 (EU) (EU) (B2U) (EU) (EU) (EG) (EG) (B2U) (B1G)
                 (EU) (EU) (EG) (EG) (A2G) (EU) (EU) (A2U) (B2G)
                 (A1G) (B1U) (A1U) (EU) (EU) (EG) (EG) (A2G)
(A1G)
                 (B1G) (A1G) (B1U) (EU) (EU) (EG) (EG) (B1G)
(A2U)
                 (B2G) (EU) (EU) (B2U) (A1G) (EU) (EU) (B1G)
(A2U)
                 (A1G) (EU) (EU) (B1U) (EU) (EU) (A2U) (B2U) (EU)
                 (EU) (EG) (EG) (A1G) (B2G) (B1G) (A1G) (A2U)
(EU)
                 (EU) (EG) (EG) (B2G) (A1G) (B1G) (A1G) (A2U)
(EU)
                 (EU) (EG) (EG) (B2G) (A1G) (B1G) (A1G) (A2U)
(EU)
```

```
                (EU) (A1G) (A2U) (EU) (EU) (A1G) (A1G) (A1G)
(A1G)
                (A1G)
 The electronic state of the initial guess is 1-A1G.
 Leave Link  401 at Fri Jan 17 09:22:46 2014, MaxMem=  104857600
cpu:       1.0
 (Enter C:\G03W\l502.exe)
 Closed shell SCF:
 Requested convergence on RMS density matrix=1.00D-08 within1000
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Using DIIS extrapolation, IDIIS=  1040.
 Integral symmetry usage will be decided dynamically.
       133902 words used for storage of precomputed grid.
 IEnd=   1299438 IEndB=   1299438 NGot= 104857600 MDV= 104608783
 LenX= 104608783
 Fock matrices will be formed incrementally for  20 cycles.

 Cycle   1  Pass 1  IDiag  1:
 Petite list used in FoFDir.
 MinBra= 0 MaxBra= 3 Meth= 1.
 IRaf=       0 NMat=   1 IRICut=       1 DoRegI=T DoRafI=F
ISym2E= 1 JSym2E=1.
 Defaulting to unpruned grid for atomic number  78.
 Defaulting to unpruned grid for atomic number  78.
 E= -19152.4955574018
 DIIS: error= 1.81D+00 at cycle   1 NSaved=   1.
 NSaved= 1 IEnMin= 1 EnMin= -19152.4955574018     IErMin= 1
ErrMin= 1.81D+00
 ErrMax= 1.81D+00 EMaxC= 1.00D-01 BMatC= 3.09D+02 BMatP= 3.09D+02
 IDIUse=3 WtCom= 0.00D+00 WtEn= 1.00D+00
 Coeff-Com:  0.100D+01
 Coeff-En:   0.100D+01
 Coeff:      0.100D+01
 Gap=    -0.454 Goal=   None    Shift=    0.000
 GapD=   -0.454 DampG=0.250 DampE=0.125 DampFc=0.1250 IDamp=-1.
 Damping current iteration by 1.25D-01
 RMSDP=1.34D-02 MaxDP=4.47D-01              OVMax= 9.06D-01

 Cycle   2  Pass 1  IDiag  1:
 RMSU=  1.65D-03    CP:  1.01D+00
 E= -19153.1337740957     Delta-E=       -0.638216693878 Rises=F
Damp=T
 DIIS: error= 1.57D+00 at cycle   2 NSaved=   2.
 NSaved= 2 IEnMin= 2 EnMin= -19153.1337740957     IErMin= 2
ErrMin= 1.57D+00
 ErrMax= 1.57D+00 EMaxC= 1.00D-01 BMatC= 2.25D+02 BMatP= 3.09D+02
 IDIUse=3 WtCom= 0.00D+00 WtEn= 1.00D+00
```

```
 Coeff-Com: -0.553D+01 0.653D+01
 Coeff-En:   0.000D+00 0.100D+01
 Coeff:      0.000D+00 0.100D+01
 Gap=     0.017 Goal=   None    Shift=    0.000
 RMSDP=8.61D-03 MaxDP=3.05D-01 DE=-6.38D-01 OVMax= 1.44D-01

 Cycle   3  Pass 1  IDiag  1:
 RMSU=  6.10D-03    CP:  1.03D+00  3.00D+00
 E= -19153.3421198504     Delta-E=       -0.208345754658 Rises=F
Damp=F
 DIIS: error= 3.64D-01 at cycle   3 NSaved=   3.
 NSaved= 3 IEnMin= 3 EnMin= -19153.3421198504     IErMin= 3
ErrMin= 3.64D-01
 ErrMax= 3.64D-01 EMaxC= 1.00D-01 BMatC= 1.46D+01 BMatP= 2.25D+02
 IDIUse=3 WtCom= 0.00D+00 WtEn= 1.00D+00
 EnCoef did   100 forward-backward iterations
 Coeff-Com:  0.657D+01-0.740D+01 0.183D+01
 Coeff-En:   0.398D+00 0.220D-01 0.580D+00
 Coeff:      0.398D+00 0.220D-01 0.580D+00
 Gap=    -0.253 Goal=   None    Shift=    0.000
 RMSDP=8.50D-03 MaxDP=2.59D-01 DE=-2.08D-01 OVMax= 9.62D-01

 Cycle   4  Pass 1  IDiag  1:
 RMSU=  3.80D-03    CP:  1.00D+00  1.32D+00  1.39D-01
 E= -19154.7896737787     Delta-E=       -1.447553928396 Rises=F
Damp=F
 DIIS: error= 9.78D-02 at cycle   4 NSaved=   4.
 NSaved= 4 IEnMin= 4 EnMin= -19154.7896737787     IErMin= 4
ErrMin= 9.78D-02
 ErrMax= 9.78D-02 EMaxC= 1.00D-01 BMatC= 1.16D+00 BMatP= 1.46D+01
 IDIUse=3 WtCom= 2.21D-02 WtEn= 9.78D-01
 Coeff-Com: -0.151D+01 0.177D+01-0.854D-01 0.826D+00
 Coeff-En:   0.000D+00 0.000D+00 0.282D+00 0.718D+00
 Coeff:     -0.334D-01 0.392D-01 0.274D+00 0.720D+00
 Gap=     0.109 Goal=   None    Shift=    0.000
 RMSDP=5.59D-03 MaxDP=1.33D-01 DE=-1.45D+00 OVMax= 5.03D-01

 Cycle   5  Pass 1  IDiag  1:
 RMSU=  2.43D-03    CP:  1.01D+00  2.89D+00  4.42D-01 -1.78D-02
 E= -19155.2408762008     Delta-E=       -0.451202422009 Rises=F
Damp=F
 DIIS: error= 5.35D-02 at cycle   5 NSaved=   5.
 NSaved= 5 IEnMin= 5 EnMin= -19155.2408762008     IErMin= 5
ErrMin= 5.35D-02
 ErrMax= 5.35D-02 EMaxC= 1.00D-01 BMatC= 3.28D-01 BMatP= 1.16D+00
 IDIUse=3 WtCom= 4.65D-01 WtEn= 5.35D-01
 Coeff-Com: -0.611D+00 0.705D+00-0.776D-01 0.395D+00 0.588D+00
 Coeff-En:   0.000D+00 0.000D+00 0.000D+00 0.306D+00 0.694D+00
 Coeff:     -0.284D+00 0.328D+00-0.361D-01 0.347D+00 0.645D+00
 Gap=     0.154 Goal=   None    Shift=    0.000
```

```
 RMSDP=2.60D-03 MaxDP=8.32D-02 DE=-4.51D-01 OVMax= 2.96D-01

 Cycle   6  Pass 1  IDiag  1:
 RMSU=  1.08D-03    CP:  1.01D+00  2.19D+00  3.17D-01  4.18D-01
6.13D-01
 E= -19155.4646562030     Delta-E=       -0.223780002274 Rises=F
Damp=F
 DIIS: error= 1.02D-02 at cycle   6 NSaved=   6.
 NSaved= 6 IEnMin= 6 EnMin= -19155.4646562030     IErMin= 6
ErrMin= 1.02D-02
 ErrMax= 1.02D-02 EMaxC= 1.00D-01 BMatC= 1.20D-02 BMatP= 3.28D-01
 IDIUse=3 WtCom= 8.98D-01 WtEn= 1.02D-01
 Coeff-Com: -0.909D-01 0.104D+00-0.117D-01 0.225D-01 0.171D+00
0.805D+00
 Coeff-En:   0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00
0.100D+01
 Coeff:     -0.816D-01 0.931D-01-0.105D-01 0.202D-01 0.154D+00
0.825D+00
 Gap=     0.148 Goal=   None    Shift=    0.000
 RMSDP=6.16D-04 MaxDP=1.73D-02 DE=-2.24D-01 OVMax= 5.58D-02

 Cycle   7  Pass 1  IDiag  1:
 RMSU=  1.99D-04    CP:  1.01D+00  2.36D+00  3.49D-01  3.21D-01
7.27D-01
                    CP:  8.89D-01
 E= -19155.4737885748     Delta-E=       -0.009132371782 Rises=F
Damp=F
 DIIS: error= 3.63D-03 at cycle   7 NSaved=   7.
 NSaved= 7 IEnMin= 7 EnMin= -19155.4737885748     IErMin= 7
ErrMin= 3.63D-03
 ErrMax= 3.63D-03 EMaxC= 1.00D-01 BMatC= 1.30D-03 BMatP= 1.20D-02
 IDIUse=3 WtCom= 9.64D-01 WtEn= 3.63D-02
 Coeff-Com:  0.107D-01-0.124D-01-0.134D-02-0.334D-02-0.925D-02
0.193D+00
 Coeff-Com:  0.822D+00
 Coeff-En:   0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00
0.977D-01
 Coeff-En:   0.902D+00
 Coeff:      0.103D-01-0.119D-01-0.129D-02-0.321D-02-0.892D-02
0.190D+00
 Coeff:      0.825D+00
 Gap=     0.147 Goal=   None    Shift=    0.000
 RMSDP=1.75D-04 MaxDP=5.59D-03 DE=-9.13D-03 OVMax= 1.81D-02

 Cycle   8  Pass 1  IDiag  1:
 RMSU=  6.74D-05    CP:  1.01D+00  2.31D+00  3.39D-01  3.42D-01
7.00D-01
                    CP:  9.47D-01  8.31D-01
 E= -19155.4748215935     Delta-E=       -0.001033018674 Rises=F
Damp=F
```

```
 DIIS: error= 2.72D-04 at cycle   8 NSaved=   8.
 NSaved= 8 IEnMin= 8 EnMin= -19155.4748215935     IErMin= 8
ErrMin= 2.72D-04
 ErrMax= 2.72D-04 EMaxC= 1.00D-01 BMatC= 1.46D-05 BMatP= 1.30D-03
 IDIUse=3 WtCom= 9.97D-01 WtEn= 2.72D-03
 Coeff-Com:  0.498D-02-0.572D-02-0.616D-04-0.145D-02-0.994D-02
0.104D-01
 Coeff-Com:  0.252D+00 0.750D+00
 Coeff-En:   0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00
0.000D+00
 Coeff-En:   0.000D+00 0.100D+01
 Coeff:      0.497D-02-0.570D-02-0.614D-04-0.145D-02-0.991D-02
0.104D-01
 Coeff:      0.252D+00 0.750D+00
 Gap=     0.148 Goal=   None    Shift=    0.000
 RMSDP=2.83D-05 MaxDP=9.59D-04 DE=-1.03D-03 OVMax= 9.43D-04

 Cycle   9  Pass 1  IDiag  1:
 RMSU=  1.49D-05    CP:  1.01D+00  2.31D+00  3.40D-01  3.42D-01
7.02D-01
                    CP:  9.45D-01  9.29D-01  9.39D-01
 E= -19155.4748375750     Delta-E=       -0.000015981561 Rises=F
Damp=F
 DIIS: error= 4.49D-05 at cycle   9 NSaved=   9.
 NSaved= 9 IEnMin= 9 EnMin= -19155.4748375750     IErMin= 9
ErrMin= 4.49D-05
 ErrMax= 4.49D-05 EMaxC= 1.00D-01 BMatC= 3.49D-07 BMatP= 1.46D-05
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com:  0.736D-03-0.840D-03 0.934D-05-0.264D-03-0.234D-02-
0.624D-02
 Coeff-Com:  0.315D-01 0.197D+00 0.780D+00
 Coeff:      0.736D-03-0.840D-03 0.934D-05-0.264D-03-0.234D-02-
0.624D-02
 Coeff:      0.315D-01 0.197D+00 0.780D+00
 Gap=     0.147 Goal=   None    Shift=    0.000
 RMSDP=5.94D-06 MaxDP=1.47D-04 DE=-1.60D-05 OVMax= 4.66D-04

 Cycle  10  Pass 1  IDiag  1:
 RMSU=  3.18D-06    CP:  1.01D+00  2.31D+00  3.40D-01  3.42D-01
7.02D-01
                    CP:  9.45D-01  9.35D-01  9.98D-01  8.56D-01
 E= -19155.4748381483     Delta-E=       -0.000000573284 Rises=F
Damp=F
 DIIS: error= 1.43D-05 at cycle  10 NSaved=  10.
 NSaved=10 IEnMin=10 EnMin= -19155.4748381483     IErMin=10
ErrMin= 1.43D-05
 ErrMax= 1.43D-05 EMaxC= 1.00D-01 BMatC= 2.57D-08 BMatP= 3.49D-07
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com: -0.263D-03 0.301D-03 0.177D-04 0.700D-05 0.465D-03-
0.198D-02
```

```
 Coeff-Com: -0.192D-01-0.432D-01 0.155D+00 0.909D+00
 Coeff:     -0.263D-03 0.301D-03 0.177D-04 0.700D-05 0.465D-03-
0.198D-02
 Coeff:     -0.192D-01-0.432D-01 0.155D+00 0.909D+00
 Gap=     0.147 Goal=   None    Shift=    0.000
 RMSDP=2.14D-06 MaxDP=6.40D-05 DE=-5.73D-07 OVMax= 1.49D-04

 Cycle  11  Pass 1  IDiag  1:
 RMSU=  4.80D-07    CP:  1.01D+00  2.31D+00  3.40D-01  3.42D-01
7.02D-01
                    CP:  9.46D-01  9.38D-01  1.01D+00  9.52D-01
1.06D+00
 E= -19155.4748381955     Delta-E=       -0.000000047119 Rises=F
Damp=F
 DIIS: error= 1.51D-06 at cycle  11 NSaved=  11.
 NSaved=11 IEnMin=11 EnMin= -19155.4748381955     IErMin=11
ErrMin= 1.51D-06
 ErrMax= 1.51D-06 EMaxC= 1.00D-01 BMatC= 2.89D-10 BMatP= 2.57D-08
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com: -0.141D-04 0.162D-04-0.675D-06 0.816D-05 0.210D-04-
0.816D-04
 Coeff-Com: -0.712D-03-0.629D-02-0.143D-01-0.208D-02 0.102D+01
 Coeff:     -0.141D-04 0.162D-04-0.675D-06 0.816D-05 0.210D-04-
0.816D-04
 Coeff:     -0.712D-03-0.629D-02-0.143D-01-0.208D-02 0.102D+01
 Gap=     0.147 Goal=   None    Shift=    0.000
 RMSDP=2.50D-07 MaxDP=9.40D-06 DE=-4.71D-08 OVMax= 2.06D-05

 Cycle  12  Pass 1  IDiag  1:
 RMSU=  9.01D-08    CP:  1.01D+00  2.31D+00  3.40D-01  3.42D-01
7.02D-01
                    CP:  9.46D-01  9.39D-01  1.01D+00  9.58D-01
1.09D+00
                    CP:  1.13D+00
 E= -19155.4748381961     Delta-E=       -0.000000000680 Rises=F
Damp=F
 DIIS: error= 1.38D-07 at cycle  12 NSaved=  12.
 NSaved=12 IEnMin=12 EnMin= -19155.4748381961     IErMin=12
ErrMin= 1.38D-07
 ErrMax= 1.38D-07 EMaxC= 1.00D-01 BMatC= 2.96D-12 BMatP= 2.89D-10
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com:  0.208D-05-0.239D-05-0.401D-06 0.106D-05-0.347D-05
0.143D-04
 Coeff-Com:  0.220D-03 0.858D-03-0.594D-03-0.788D-02 0.756D-02
0.100D+01
 Coeff:      0.208D-05-0.239D-05-0.401D-06 0.106D-05-0.347D-05
0.143D-04
 Coeff:      0.220D-03 0.858D-03-0.594D-03-0.788D-02 0.756D-02
0.100D+01
 Gap=     0.147 Goal=   None    Shift=    0.000
```

```
 RMSDP=2.40D-08 MaxDP=8.45D-07 DE=-6.80D-10 OVMax= 1.48D-06

 Cycle  13  Pass 1  IDiag  1:
 RMSU=  7.57D-09    CP:  1.01D+00  2.31D+00  3.40D-01  3.42D-01
7.02D-01
                    CP:  9.46D-01  9.39D-01  1.01D+00  9.58D-01
1.09D+00
                    CP:  1.14D+00  1.15D+00
 E= -19155.4748381964     Delta-E=       -0.000000000317 Rises=F
Damp=F
 DIIS: error= 7.46D-08 at cycle  13 NSaved=  13.
 NSaved=13 IEnMin=13 EnMin= -19155.4748381964     IErMin=13
ErrMin= 7.46D-08
 ErrMax= 7.46D-08 EMaxC= 1.00D-01 BMatC= 5.99D-13 BMatP= 2.96D-12
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com:  0.318D-06-0.365D-06-0.120D-07 0.105D-07-0.390D-06
0.313D-05
 Coeff-Com: -0.100D-05 0.215D-04-0.593D-04 0.777D-04-0.126D-01-
0.406D-01
 Coeff-Com:  0.105D+01
 Coeff:      0.318D-06-0.365D-06-0.120D-07 0.105D-07-0.390D-06
0.313D-05
 Coeff:     -0.100D-05 0.215D-04-0.593D-04 0.777D-04-0.126D-01-
0.406D-01
 Coeff:      0.105D+01
 Gap=     0.147 Goal=   None    Shift=    0.000
 RMSDP=4.85D-09 MaxDP=1.94D-07 DE=-3.17D-10 OVMax= 2.67D-07

 Error on total polarization charges =  0.07401
 SCF Done:  E(RPBE+HF-PBE) =  -19155.4748382     A.U. after   13
cycles
             Convg  =    0.4847D-08             -V/T =  2.0014
             S**2   =   0.0000
 KE= 1.912955091943D+04 PE=-4.842245318434D+04 EE=
8.746250529529D+03
 ---------------------------------------------------------------
----
 Variational PCM results
 =======================
 <psi(f)|   H    |psi(f)>                    (a.u.) =  -
19155.178895
 <psi(f)|H+V(f)/2|psi(f)>                    (a.u.) =  -
19155.474838
 Total free energy in solution:
  with all non electrostatic terms           (a.u.) =  -
19155.462012
 ---------------------------------------------------------------
----
 (Polarized solute)-Solvent               (kcal/mol) =    -185.71
```

```
 ------------------------------------------------------------------
----
 Cavitation energy                        (kcal/mol) =      19.64
 Dispersion energy                        (kcal/mol) =     -13.23
 Repulsion energy                         (kcal/mol) =       1.64
 Total non electrostatic                  (kcal/mol) =       8.05
 ------------------------------------------------------------------
----
 Partition over spheres:
 Sphere  on Atom  Surface  Charge   GEl     GCav    GDR
    1     Pt1       0.96  -0.043    2.83    0.83   -0.11
    2     Cl2      29.05   0.398  -37.37    4.70   -2.87
    3     Cl3      29.05   0.398  -37.37    4.70   -2.87
    4     Cl4      29.05   0.398  -37.38    4.70   -2.87
    5     Cl5      29.05   0.398  -37.38    4.70   -2.87
 Added spheres:    37.15   0.353  -39.04    0.00    0.00
 ------------------------------------------------------------------
----
 After PCM corrections, the SCF energy is  -19155.4748382
a.u.
 ------------------------------------------------------------------
----
 Leave Link  502 at Fri Jan 17 09:25:37 2014, MaxMem=  104857600
cpu:     171.0
 (Enter C:\G03W\l801.exe)
 Range of M.O.s used for correlation:     1   199
 NBasis=   199 NAE=    74 NBE=    74 NFC=     0 NFV=     0
 NROrb=    199 NOA=    74 NOB=    74 NVA=   125 NVB=   125

 **** Warning!!: The largest alpha MO coefficient is
0.12899776D+02

 Leave Link  801 at Fri Jan 17 09:25:38 2014, MaxMem=  104857600
cpu:       0.0
 (Enter C:\G03W\l1002.exe)
 Minotr:  Closed-shell wavefunction.
          Direct CPHF calculation.
          Solving linear equations simultaneously.
          Differentiating once with respect to magnetic field
using GIAOs.
          Electric field/nuclear overlap derivatives assumed to
be zero.
          Using symmetry in CPHF.
          Requested convergence is 1.0D-08 RMS, and 1.0D-07
maximum.
          Secondary convergence is 1.0D-12 RMS, and 1.0D-12
maximum.
          NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F.
          MDV=     104857568 using IRadAn=       1.
 Defaulting to unpruned grid for atomic number  78.
```

```
 Generate precomputed XC quadrature information.
 Symmetry not used in FoFDir.
 MinBra= 0 MaxBra= 3 Meth= 1.
 IRaf=       0 NMat=   1 IRICut=       1 DoRegI=T DoRafI=F
ISym2E= 0 JSym2E=0.
 Defaulting to unpruned grid for atomic number  78.
 Defaulting to unpruned grid for atomic number  78.
          There are   3 degrees of freedom in the 1st order CPHF.
     3 vectors were produced by pass  0.
 AX will form   3 AO Fock derivatives at one time.
     3 vectors were produced by pass  1.
     3 vectors were produced by pass  2.
     3 vectors were produced by pass  3.
     3 vectors were produced by pass  4.
     3 vectors were produced by pass  5.
     3 vectors were produced by pass  6.
 Inv2:  IOpt= 1 Iter= 1 AM= 3.84D-16 Conv= 1.00D-12.
 Inverted reduced A of dimension   21 with in-core refinement.
 Calculating GIAO nuclear magnetic shielding tensors.
 SCF GIAO Magnetic shielding tensor (ppm):
  1  Pt   Isotropic = -3294.4355   Anisotropy =  7190.6898
   XX=  1499.3577   YX=     0.0001   ZX=     0.0000
   XY=     0.0001   YY=  1499.3577   ZY=     0.0000
   XZ=    -0.0002   YZ=    -0.0002   ZZ=-12882.0218
   Eigenvalues:-12882.0218  1499.3576  1499.3578
  2  Cl   Isotropic =  1247.9666   Anisotropy =   279.5088
   XX=  1182.5464   YX=     0.0000   ZX=    -0.0003
   XY=    -0.0001   YY=  1127.0477   ZY=     0.0001
   XZ=    -0.0003   YZ=    -0.0003   ZZ=  1434.3058
   Eigenvalues:  1127.0477  1182.5464  1434.3058
  3  Cl   Isotropic =  1247.9666   Anisotropy =   279.5088
   XX=  1127.0477   YX=    -0.0001   ZX=     0.0001
   XY=     0.0000   YY=  1182.5464   ZY=    -0.0003
   XZ=    -0.0003   YZ=    -0.0003   ZZ=  1434.3058
   Eigenvalues:  1127.0477  1182.5464  1434.3058
  4  Cl   Isotropic =  1247.9664   Anisotropy =   279.5092
   XX=  1127.0479   YX=     0.0000   ZX=     0.0000
   XY=     0.0000   YY=  1182.5454   ZY=     0.0000
   XZ=    -0.0002   YZ=     0.0000   ZZ=  1434.3058
   Eigenvalues:  1127.0479  1182.5454  1434.3058
  5  Cl   Isotropic =  1247.9664   Anisotropy =   279.5092
   XX=  1182.5454   YX=     0.0000   ZX=     0.0000
   XY=     0.0000   YY=  1127.0479   ZY=     0.0000
   XZ=     0.0000   YZ=    -0.0002   ZZ=  1434.3058
   Eigenvalues:  1127.0479  1182.5454  1434.3058
 End of Minotr Frequency-dependent properties file   721 does not
exist.
 Leave Link 1002 at Fri Jan 17 09:29:33 2014, MaxMem=  104857600
cpu:     235.0
 (Enter C:\G03W\l601.exe)
```

```
 Copying SCF densities to generalized density rwf, ISCF=0
IROHF=0.

**********************************************************************
*****

            Population analysis using the SCF density.

**********************************************************************
*****

 Orbital symmetries:
       Occupied  (A1G) (A1G) (EU) (EU) (A2U) (A1G) (A1G) (B1G)
                 (EU) (EU) (EU) (EU) (A2U) (B1G) (B2G) (EG) (EG)
                 (A1G) (A1G) (EU) (EU) (A2U) (B1G) (B2G) (EG)
(EG)
                 (A1G) (A1G) (B1G) (EU) (EU) (B1G) (EU) (EU)
(A1G)
                 (B2U) (EG) (EG) (A2U) (A2G) (EU) (EU) (B2G) (EU)
                 (EU) (B2U) (B1U) (EU) (EU) (A2U) (A1G) (EU) (EU)
                 (A2U) (A1G) (B1G) (EU) (EU) (B1G) (A1G) (B2G)
                 (EG) (EG) (EU) (EU) (A2U) (B2U) (EU) (EU) (A2G)
                 (B2G) (EG) (EG) (A1G)
       Virtual   (B1G) (A1G) (EU) (EU) (A2U) (B1G) (B2G) (EG)
(EG)
                 (A1G) (A2U) (EU) (EU) (A1G) (B2U) (EU) (EU)
(A2G)
                 (B1G) (EG) (EG) (A1G) (EU) (EU) (B2G) (A2U) (EU)
                 (EU) (A1G) (B1G) (B1G) (A1G) (B2G) (A2U) (EU)
                 (EU) (EU) (EU) (EG) (EG) (B2U) (EU) (EU) (B1G)
                 (EG) (EG) (B2U) (B2G) (A2G) (EU) (EU) (A2U)
(A1G)
                 (B1U) (A1G) (A1U) (EU) (EU) (EG) (EG) (A2G)
(B1G)
                 (A1G) (B1U) (EU) (EU) (EG) (EG) (B1G) (A2U) (EU)
                 (EU) (B2G) (B2U) (A1G) (EU) (EU) (B1G) (A2U)
(A1G)
                 (EU) (EU) (B1U) (EU) (EU) (A2U) (B2U) (EU) (EU)
                 (EG) (EG) (B2G) (A1G) (B1G) (A1G) (A2U) (EU)
(EU)
                 (EG) (EG) (B2G) (A1G) (B1G) (A1G) (A2U) (EU)
(EU)
                 (EG) (EG) (B2G) (A1G) (B1G) (A1G) (A2U) (EU)
(EU)
                 (A1G) (A2U) (EU) (EU) (A1G) (A1G) (A1G) (A1G)
                 (A1G)
 The electronic state is 1-A1G.
```

```
 Alpha  occ. eigenvalues -- **********-437.47350-419.60446-
419.60446-419.60024
 Alpha  occ. eigenvalues -- -102.75330-101.64787-101.64786-
101.64784-101.64784
 Alpha  occ. eigenvalues --  -94.36327 -94.36327 -94.35457 -
79.56625 -79.56566
 Alpha  occ. eigenvalues --  -79.56086 -79.56086 -79.55930 -
21.82478 -18.24232
 Alpha  occ. eigenvalues --  -18.24232 -18.22299 -11.88985 -
11.88499 -11.87410
 Alpha  occ. eigenvalues --  -11.87410 -11.87067  -9.47362  -
9.47361  -9.47356
 Alpha  occ. eigenvalues --   -9.47356  -7.20592  -7.20592  -
7.20592  -7.20588
 Alpha  occ. eigenvalues --   -7.20154  -7.20153  -7.20153  -
7.20152  -7.20118
 Alpha  occ. eigenvalues --   -7.20116  -7.20116  -7.20116  -
3.32218  -3.32218
 Alpha  occ. eigenvalues --   -3.31199  -3.30623  -3.30267  -
3.30267  -3.30110
 Alpha  occ. eigenvalues --   -3.10517  -1.98927  -1.98927  -
1.95102  -0.77846
 Alpha  occ. eigenvalues --   -0.76723  -0.76675  -0.76675  -
0.38217  -0.37283
 Alpha  occ. eigenvalues --   -0.36632  -0.32915  -0.32915  -
0.32013  -0.32013
 Alpha  occ. eigenvalues --   -0.30688  -0.28842  -0.28360  -
0.28360  -0.26772
 Alpha  occ. eigenvalues --   -0.25543  -0.24529  -0.24529  -
0.24086
 Alpha virt. eigenvalues --   -0.09346   0.01887   0.05260
0.05260   0.06074
 Alpha virt. eigenvalues --    0.08187   0.09074   0.09640
0.09640   0.10127
 Alpha virt. eigenvalues --    0.10543   0.11488   0.11488
0.13253   0.13378
 Alpha virt. eigenvalues --    0.13392   0.13392   0.16168
0.18241   0.23766
 Alpha virt. eigenvalues --    0.23766   0.24492   0.27021
0.27021   0.28017
 Alpha virt. eigenvalues --    0.40824   0.42348   0.42348
0.43081   0.43181
 Alpha virt. eigenvalues --    0.55482   0.58887   0.63608
0.64063   0.64178
 Alpha virt. eigenvalues --    0.64178   0.66532   0.66532
0.67510   0.67510
 Alpha virt. eigenvalues --    0.68199   0.74534   0.74534
0.74553   0.75025
 Alpha virt. eigenvalues --    0.75025   0.75545   0.76654
0.77501   0.79877
```

```
 Alpha virt. eigenvalues --    0.79877   0.81616   0.82606
0.86827   0.90285
 Alpha virt. eigenvalues --    0.93331   0.94145   0.94145
0.94527   0.94527
 Alpha virt. eigenvalues --    0.94613   0.96521   1.00345
1.00658   1.00939
 Alpha virt. eigenvalues --    1.00939   1.08144   1.08144
1.11700   1.16527
 Alpha virt. eigenvalues --    1.18395   1.18395   1.18885
1.19583   1.39277
 Alpha virt. eigenvalues --    1.45935   1.45935   1.57471
1.69118   1.73289
 Alpha virt. eigenvalues --    1.90756   1.90756   2.75708
2.81343   2.81343
 Alpha virt. eigenvalues --    2.83094   2.83306   3.07825
3.07825   3.12927
 Alpha virt. eigenvalues --    3.12927   3.13920   3.15781
3.39397   5.59232
 Alpha virt. eigenvalues --    7.11194   7.25810   7.25810
14.67361  14.67361
 Alpha virt. eigenvalues --   14.67567  14.69632  14.83089
22.53352  39.90847
 Alpha virt. eigenvalues --   40.03051  40.03051  90.07503
90.07503  90.07723
 Alpha virt. eigenvalues --   90.08767  90.16020 104.70853
234.47383 234.56329
 Alpha virt. eigenvalues --  234.56329
455.885401328.617951328.687801328.68780
 Alpha virt. eigenvalues --
1661.825775146.30464******************************
          Condensed to atoms (all electrons):
               1          2          3          4          5
     1  Pt  77.201606   0.081350   0.081350   0.081350   0.081350
     2  Cl   0.081350  17.587219  -0.021347  -0.021347  -0.007626
     3  Cl   0.081350  -0.021347  17.587219  -0.007626  -0.021347
     4  Cl   0.081350  -0.021347  -0.007626  17.587219  -0.021347
     5  Cl   0.081350  -0.007626  -0.021347  -0.021347  17.587219
 Mulliken atomic charges:
               1
     1  Pt   0.472995
     2  Cl  -0.618249
     3  Cl  -0.618249
     4  Cl  -0.618249
     5  Cl  -0.618249
 Sum of Mulliken charges=  -2.00000
 Atomic charges with hydrogens summed into heavy atoms:
               1
     1  Pt   0.472995
     2  Cl  -0.618249
     3  Cl  -0.618249
```

```
     4  Cl  -0.618249
     5  Cl  -0.618249
 Sum of Mulliken charges=  -2.00000
 Electronic spatial extent (au):  <R**2>=  1686.5699
 Charge=    -2.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=     0.0000    Y=     0.0000    Z=     0.0000  Tot=
0.0000
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=  -119.9608   YY=  -119.9608   ZZ=   -86.5697
   XY=     0.0000   XZ=     0.0000   YZ=     0.0000
 Traceless Quadrupole moment (field-independent basis, Debye-
Ang):
   XX=   -11.1304   YY=   -11.1304   ZZ=    22.2608
   XY=     0.0000   XZ=     0.0000   YZ=     0.0000
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=     0.0000  YYY=     0.0000  ZZZ=     0.0000  XYY=
0.0000
  XXY=     0.0000  XXZ=     0.0000  XZZ=     0.0000  YZZ=
0.0000
  YYZ=     0.0000  XYZ=     0.0000
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX= -1341.0040 YYYY= -1341.0040 ZZZZ=  -110.7755 XXXY=
0.0000
 XXXZ=     0.0000 YYYX=     0.0000 YYYZ=     0.0000 ZZZX=
0.0000
 ZZZY=     0.0000 XXYY=  -395.5491 XXZZ=  -216.1846 YYZZ=  -
216.1846
 XXYZ=     0.0000 YYXZ=     0.0000 ZZXY=     0.0000
 N-N= 1.391176897179D+03 E-N=-4.842245314061D+04  KE=
1.912955091943D+04
 Symmetry AG   KE= 9.805135748241D+03
 Symmetry B1G  KE= 6.698604994282D+02
 Symmetry B2G  KE= 6.241812730076D+02
 Symmetry B3G  KE= 6.241812730076D+02
 Symmetry AU   KE= 9.566891969803D+01
 Symmetry B1U  KE= 2.220637150669D+03
 Symmetry B2U  KE= 2.544943027691D+03
 Symmetry B3U  KE= 2.544943027691D+03
 Calculating spin-rotation constants.
 Leave Link  601 at Fri Jan 17 09:29:35 2014, MaxMem=  104857600
cpu:       2.0
 (Enter C:\G03W\l9999.exe)
 1|1|UNPC-UNK|SP|RPBE1PBE|Gen|Cl4Pt1(2-)|PCUSER|17-Jan-2014|0||#p
PBE1P
 BE/gen nmr=giao integral(ultrafine) SCRF(solvent=water)
SCF(NoVarAcc,m
 axcycles=1000)||PtCl4_2-PBE0_SARCZORANMR||-
2,1|Pt,0,0.,0.,0.|Cl,0,0.,2
```

```
 .4384,0.|Cl,0,2.4384,0.,0.|Cl,0,-2.4384,0.,0.|Cl,0,0.,-
2.4384,0.||Vers
 ion=IA32W-G03RevE.01|State=1-A1G|HF=-19155.4748382|RMSD=4.847e-
009|The
 rmal=0.|Dipole=0.,0.,0.|PG=D04H [O(Pt1),2C2'(Cl1.Cl1)]||@


 JUST WHEN YOU THINK YOU'VE GOT THE WORLD ON A STRING,
 YOU FIND OUT IT'S YOUR LEASH.
 Job cpu time:  0 days  0 hours  6 minutes 56.0 seconds.
 File lengths (MBytes):  RWF=    108 Int=      0 D2E=      0 Chk=
9 Scr=      1
 Normal termination of Gaussian 03 at Fri Jan 17 09:29:36 2014.
```

Output file for NMR calculation of $[PtCl_6]^{2-}$

```
Entering Link 1 = C:\G09W\l1.exe PID=       344.

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 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
 M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B.
Mennucci,
 G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P.
Hratchian,
 A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
 M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T.
Nakajima,
 Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
 J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
 K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J.
Normand,
 K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J.
Tomasi,
 M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B.
Cross,
 V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
 O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
 R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
 P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
 O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
 and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

 ******************************************
 Gaussian 09:  IA32W-G09RevB.01 12-Aug-2010
               30-Nov-2013
 ******************************************
```

```
 %chk=PtCl62-SARCZORANMR
 %nproc=2
 Will use up to    2 processors via shared memory.
 %mem=800mb
 ----------------------------------------------------------------------
 #p pbe1pbe/gen nmr=giao integral(ultrafine) SCRF(solvent=water)
SCF(No
 VarAcc,maxcycles=1000)
 ----------------------------------------------------------------------
 1/38=1/1;
 2/12=2,17=6,18=5,40=1/2;
 3/5=7,11=2,16=1,25=1,30=1,70=2201,72=1,74=-13,75=-5/1,2,8,3;
 4//1;
 5/5=2,7=1000,38=1,53=1/2;
 8/6=1,10=90,11=11/1;
 10/13=100,45=16/2;
 6/7=2,8=2,9=2,10=2,28=1/1;
 99/9=1/99;
 Leave Link    1 at Sat Nov 30 20:45:07 2013, MaxMem=  104857600
cpu:       0.0
 (Enter C:\G09W\l101.exe)
 ---------------
 PtCl62-SARCZORA
 ---------------
 Symbolic Z-matrix:
 Charge = -2 Multiplicity = 1
 Pt                    0.         0.         0.
 Cl                    0.         0.         2.3961
 Cl                    0.         2.3961     0.
 Cl                   -2.3961     0.         0.
 Cl                    2.3961     0.         0.
 Cl                    0.        -2.3961     0.
 Cl                    0.         0.        -2.3961

 NAtoms=       7 NQM=       7 NQMF=       0 NMic=       0 NMicF=
0 NTot=       7.
                    Isotopes and Nuclear Properties:
 (Nuclear quadrupole moments (NQMom) in fm**2, nuclear magnetic
moments (NMagM)
  in nuclear magnetons)

  Atom         1           2           3           4           5
6           7
 IAtWgt=         195          35          35          35
35          35          35
 AtmWgt= 194.9648000  34.9688527  34.9688527  34.9688527
34.9688527  34.9688527  34.9688527
```

```
 NucSpn=           1           3           3           3
3           3           3
 AtZEff=    0.0000000   0.0000000   0.0000000   0.0000000
0.0000000   0.0000000   0.0000000
 NQMom=     0.0000000  -8.1650000  -8.1650000  -8.1650000  -
8.1650000  -8.1650000  -8.1650000
 NMagM=     0.6095000   0.8218740   0.8218740   0.8218740
0.8218740   0.8218740   0.8218740
 Leave Link  101 at Sat Nov 30 20:45:07 2013, MaxMem=  104857600
cpu:       0.0
 (Enter C:\G09W\l202.exe)
                         Input orientation:
 ---------------------------------------------------------------------
-----
 Center     Atomic      Atomic             Coordinates
(Angstroms)
 Number     Number       Type              X           Y
Z
 ---------------------------------------------------------------------
-----
      1         78           0        0.000000    0.000000
0.000000
      2         17           0        0.000000    0.000000
2.396100
      3         17           0        0.000000    2.396100
0.000000
      4         17           0       -2.396100    0.000000
0.000000
      5         17           0        2.396100    0.000000
0.000000
      6         17           0        0.000000   -2.396100
0.000000
      7         17           0        0.000000    0.000000   -
2.396100
 ---------------------------------------------------------------------
-----
                  Distance matrix (angstroms):
                  1          2          3          4          5
     1  Pt   0.000000
     2  Cl   2.396100   0.000000
     3  Cl   2.396100   3.388597   0.000000
     4  Cl   2.396100   3.388597   3.388597   0.000000
     5  Cl   2.396100   3.388597   3.388597   4.792200   0.000000
     6  Cl   2.396100   3.388597   4.792200   3.388597   3.388597
     7  Cl   2.396100   4.792200   3.388597   3.388597   3.388597
                  6          7
     6  Cl   0.000000
     7  Cl   3.388597   0.000000
 Stoichiometry    Cl6Pt(2-)
 Framework group  OH[O(Pt),3C4(Cl.Cl)]
```

```
 Deg. of freedom     1
 Full point group                 OH      NOp  48
 Largest Abelian subgroup         D2H     NOp   8
 Largest concise Abelian subgroup D2H     NOp   8
                         Standard orientation:
 ---------------------------------------------------------------------
-----
 Center     Atomic      Atomic             Coordinates
(Angstroms)
 Number     Number       Type              X           Y
Z
 ---------------------------------------------------------------------
-----
      1         78           0        0.000000    0.000000
0.000000
      2         17           0        0.000000    0.000000
2.396100
      3         17           0        0.000000    2.396100
0.000000
      4         17           0       -2.396100    0.000000
0.000000
      5         17           0        2.396100    0.000000
0.000000
      6         17           0        0.000000   -2.396100
0.000000
      7         17           0        0.000000    0.000000   -
2.396100
 ---------------------------------------------------------------------
-----
 Rotational constants (GHZ):      0.6293119      0.6293119
0.6293119
 Leave Link  202 at Sat Nov 30 20:45:07 2013, MaxMem=  104857600
cpu:       0.0
 (Enter C:\G09W\l301.exe)
 General basis read from cards:  (5D, 7F)
 Centers:   1
 S 6 1.00
     Exponent=  1.6896015676D+06 Coefficients=  5.7974482200D-02
     Exponent=  7.5093403004D+05 Coefficients= -1.3148538600D-02
     Exponent=  3.3374845779D+05 Coefficients=  1.2503763310D-01
     Exponent=  1.4833264791D+05 Coefficients=  9.1535752600D-02
     Exponent=  6.5925621293D+04 Coefficients=  3.2913880880D-01
     Exponent=  2.9300276130D+04 Coefficients=  5.3748713720D-01
 S 1 1.00
     Exponent=  1.3022344947D+04 Coefficients=  1.0000000000D+00
 S 1 1.00
     Exponent=  5.7877088650D+03 Coefficients=  1.0000000000D+00
 S 1 1.00
     Exponent=  2.5723150510D+03 Coefficients=  1.0000000000D+00
 S 1 1.00
```

```
    Exponent=  1.1432511340D+03 Coefficients=  1.0000000000D+00
S 1 1.00
    Exponent=  5.0811161500D+02 Coefficients=  1.0000000000D+00
S 1 1.00
    Exponent=  2.2582738400D+02 Coefficients=  1.0000000000D+00
S 1 1.00
    Exponent=  1.0036772600D+02 Coefficients=  1.0000000000D+00
S 1 1.00
    Exponent=  4.4607878000D+01 Coefficients=  1.0000000000D+00
S 1 1.00
    Exponent=  1.9825724000D+01 Coefficients=  1.0000000000D+00
S 1 1.00
    Exponent=  8.8114330000D+00 Coefficients=  1.0000000000D+00
S 1 1.00
    Exponent=  3.9161920000D+00 Coefficients=  1.0000000000D+00
S 1 1.00
    Exponent=  1.7405300000D+00 Coefficients=  1.0000000000D+00
S 1 1.00
    Exponent=  7.7356900000D-01 Coefficients=  1.0000000000D+00
S 1 1.00
    Exponent=  3.4380800000D-01 Coefficients=  1.0000000000D+00
S 1 1.00
    Exponent=  1.5280400000D-01 Coefficients=  1.0000000000D+00
S 1 1.00
    Exponent=  6.7913000000D-02 Coefficients=  1.0000000000D+00
P 5 1.00
    Exponent=  2.3642643991D+04 Coefficients=  1.1403826400D-02
    Exponent=  9.4570575960D+03 Coefficients=  1.7083256700D-02
    Exponent=  3.7828230390D+03 Coefficients=  8.0886502700D-02
    Exponent=  1.5131292150D+03 Coefficients=  2.5252184340D-01
    Exponent=  6.0525168600D+02 Coefficients=  7.4017959180D-01
P 1 1.00
    Exponent=  2.4210067400D+02 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  9.6840270000D+01 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  3.8736108000D+01 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  1.5494443000D+01 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  6.1977770000D+00 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  2.4791110000D+00 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  9.9164400000D-01 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  3.9665800000D-01 Coefficients=  1.0000000000D+00
P 1 1.00
    Exponent=  1.5866300000D-01 Coefficients=  1.0000000000D+00
P 1 1.00
```

```
     Exponent=  6.3465000000D-02 Coefficients=  1.0000000000D+00
 D 4 1.00
     Exponent=  1.8110792460D+03 Coefficients=  7.6859038000D-03
     Exponent=  6.5857427100D+02 Coefficients=  4.3883054800D-02
     Exponent=  2.3948155300D+02 Coefficients=  2.4558000620D-01
     Exponent=  8.7084201000D+01 Coefficients=  8.0580963240D-01
 D 1 1.00
     Exponent=  3.1666982000D+01 Coefficients=  1.0000000000D+00
 D 1 1.00
     Exponent=  1.1515266000D+01 Coefficients=  1.0000000000D+00
 D 1 1.00
     Exponent=  4.1873700000D+00 Coefficients=  1.0000000000D+00
 D 1 1.00
     Exponent=  1.5226800000D+00 Coefficients=  1.0000000000D+00
 D 1 1.00
     Exponent=  5.5370200000D-01 Coefficients=  1.0000000000D+00
 D 1 1.00
     Exponent=  2.0134600000D-01 Coefficients=  1.0000000000D+00
 D 1 1.00
     Exponent=  7.3217000000D-02 Coefficients=  1.0000000000D+00
 F 4 1.00
     Exponent=  8.5141859000D+01 Coefficients=  6.3002593000D-02
     Exponent=  2.8380620000D+01 Coefficients=  2.9424498280D-01
     Exponent=  9.4602070000D+00 Coefficients=  5.6544272570D-01
     Exponent=  3.1534020000D+00 Coefficients=  3.7760481600D-01
 F 1 1.00
     Exponent=  1.0511340000D+00 Coefficients=  1.0000000000D+00
 F 1 1.00
     Exponent=  3.5037800000D-01 Coefficients=  1.0000000000D+00
 ****
 Centers:   2  3  4  5  6  7
 6-31G(d,p)
 ****
 Ernie: Thresh=  0.10000D-02 Tol=  0.10000D-05 Strict=F.
 There are    60 symmetry adapted basis functions of AG
symmetry.
 There are    17 symmetry adapted basis functions of B1G
symmetry.
 There are    17 symmetry adapted basis functions of B2G
symmetry.
 There are    17 symmetry adapted basis functions of B3G
symmetry.
 There are     6 symmetry adapted basis functions of AU
symmetry.
 There are    34 symmetry adapted basis functions of B1U
symmetry.
 There are    34 symmetry adapted basis functions of B2U
symmetry.
 There are    34 symmetry adapted basis functions of B3U
symmetry.
```

```
 Integral buffers will be    262144 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
   219 basis functions,   505 primitive gaussians,   242
cartesian basis functions
    91 alpha electrons       91 beta electrons
       nuclear repulsion energy      2394.3929937619 Hartrees.
 IExCor= 1009 DFT=T Ex+Corr=PBE1PBE ExCW=0 ScaHFX=  0.250000
 ScaDFX=  0.750000  0.750000  1.000000  1.000000 ScalE2=
1.000000  1.000000
 IRadAn=      5 IRanWt=     -1 IRanGd=            0 ICorTp=0
 NAtoms=    7 NActive=    7 NUniq=    2 SFac= 4.00D+00 NAtFMM=
50 NAOKFM=F Big=F
 ---------------------------------------------------------------
--------------
 Polarizable Continuum Model (PCM)
 =================================
 Model                : PCM.
 Atomic radii         : UFF (Universal Force Field).
 Polarization charges : Total charges.
 Charge compensation  : None.
 Solution method      : Matrix inversion.
 Cavity type          : Scaled VdW (van der Waals Surface)
(Alpha=1.100).
 Cavity algorithm     : GePol (No added spheres)
                        Default sphere list used, NSphG=    7.
                        Lebedev-Laikov grids with approx.  5.0
points / Ang**2.
                        Smoothing algorithm: Karplus/York
(Gamma=1.0000).
                        Polarization charges: spherical
gaussians, with
                                              point-specific
exponents (IZeta= 3).
                        Self-potential: point-specific (ISelfS=
7).
                        Self-field    : sphere-specific E.n sum
rule (ISelfD= 2).
 Solvent              : Water, Eps=  78.355300 Eps(inf)=
1.777849
 ---------------------------------------------------------------
--------------
 Spheres list:
 ISph  on   Nord    Re0     Alpha      Xe            Ye
Ze
    1  Pt      1    1.377   1.100      0.000000      0.000000
0.000000
    2  Cl      2    1.974   1.100      0.000000      0.000000
2.396100
```

```
    3  Cl      3    1.974   1.100      0.000000      2.396100
0.000000
    4  Cl      4    1.974   1.100     -2.396100      0.000000
0.000000
    5  Cl      5    1.974   1.100      2.396100      0.000000
0.000000
    6  Cl      6    1.974   1.100      0.000000     -2.396100
0.000000
    7  Cl      7    1.974   1.100      0.000000      0.000000
-2.396100
 ---------------------------------------------------------------
--------------
 GePol: Number of generator spheres                  =       7
 GePol: Total number of spheres                      =       7
 GePol: Number of exposed spheres                    =       6 (
85.71%)
 GePol: Number of points                             =    1182
 GePol: Average weight of points                     =       0.19
 GePol: Minimum weight of points                     =   0.96D-05
 GePol: Maximum weight of points                     =    0.21616
 GePol: Number of points with low weight             =      24
 GePol: Fraction of low-weight points (<1% of avg)   =
2.03%
 GePol: Cavity surface area                          =    222.591
Ang**2
 GePol: Cavity volume                                =    226.465
Ang**3
 Leave Link  301 at Sat Nov 30 20:45:07 2013, MaxMem=  104857600
cpu:       0.0
 (Enter C:\G09W\l302.exe)
 NPDir=0 NMtPBC=     1 NCelOv=     1 NCel=       1 NClECP=     1
NCelD=      1
         NCelK=      1 NCelE2=     1 NClLst=     1 CellRange=
0.0.
 One-electron integrals computed using PRISM.
 One-electron integral symmetry used in STVInt
 NBasis=   219 RedAO= T  NBF=    60    17    17    17     6    34
34    34
 NBsUse=   219 1.00D-06 NBFU=    60    17    17    17     6    34
34    34
 Precomputing XC quadrature grid using
 IXCGrd= 2 IRadAn=           5 IRanWt=          -1 IRanGd=
0 AccXCQ= 0.00D+00.
 Defaulting to unpruned grid for atomic number  78.
 NRdTot=     559 NPtTot=      173268 NUsed=      175867 NTot=
175883
 NSgBfM=   227   227   227   227   231 NAtAll=     7     7.
 Leave Link  302 at Sat Nov 30 20:45:08 2013, MaxMem=  104857600
cpu:       1.0
 (Enter C:\G09W\l308.exe)
```

```
 Leave Link  308 at Sat Nov 30 20:45:08 2013, MaxMem=  104857600
cpu:       0.0
 (Enter C:\G09W\l303.exe)
 DipDrv:  MaxL=1.
 Leave Link  303 at Sat Nov 30 20:45:08 2013, MaxMem=  104857600
cpu:       0.0
 (Enter C:\G09W\l401.exe)
 Harris functional with IExCor= 1009 diagonalized for initial
guess.
 ExpMin= 6.35D-02 ExpMax= 1.69D+06 ExpMxC= 1.69D+06 IAcc=4
IRadAn=          5 AccDes= 0.00D+00
 HarFok:  IExCor= 1009 AccDes= 0.00D+00 IRadAn=          5 IDoV= 1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Defaulting to unpruned grid for atomic number  78.
 Defaulting to unpruned grid for atomic number  78.
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=     500 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1
NMtDS0=    0 NMtDT0=    0
         I1Cent=           4 NGrid=           0.
 Petite list used in FoFCou.
 Harris En= -20085.9406129799
 Initial guess orbital symmetries:
       Occupied  (A1G) (A1G) (T1U) (T1U) (T1U) (A1G) (EG) (EG)
                 (T1U) (T1U) (T1U) (A1G) (T1U) (T1U) (T1U) (EG)
                 (EG) (T2G) (T2G) (T2G) (A1G) (T1U) (T1U) (T1U)
                 (EG) (EG) (T2G) (T2G) (T2G) (A1G) (EG) (EG)
(T1U)
                 (T1U) (T1U) (T1U) (T1U) (T1U) (EG) (EG) (A1G)
                 (T2G) (T2G) (T2G) (T1U) (T1U) (T1U) (T1G) (T1G)
                 (T1G) (T2U) (T2U) (T2U) (A1G) (T1U) (T1U) (T1U)
                 (T2U) (T2U) (T2U) (A2U) (T1U) (T1U) (T1U) (A1G)
                 (EG) (EG) (T1U) (T1U) (T1U) (A1G) (EG) (EG)
(T2G)
                 (T2G) (T2G) (T1U) (T1U) (T1U) (T2U) (T2U) (T2U)
                 (T1U) (T1U) (T1U) (T1G) (T1G) (T1G) (T2G) (T2G)
                 (T2G)
       Virtual   (EG) (EG) (A1G) (T1U) (T1U) (T1U) (EG) (EG)
(A1G)
                 (T2G) (T2G) (T2G) (T1U) (T1U) (T1U) (T1U) (T1U)
                 (T1U) (EG) (EG) (A1G) (T2G) (T2G) (T2G) (T2U)
                 (T2U) (T2U) (T1U) (T1U) (T1U) (T1G) (T1G) (T1G)
                 (EG) (EG) (T2U) (T2U) (T2U) (T2G) (T2G) (T2G)
                 (T1U) (T1U) (T1U) (A2U) (EU) (EU) (A2G) (T2U)
                 (T2U) (T2U) (T1G) (T1G) (T1G) (T1U) (T1U) (T1U)
                 (T2G) (T2G) (T2G) (A1G) (EG) (EG) (A2U) (EG)
(EG)
```

```
                 (T1U) (T1U) (T1U) (T2G) (T2G) (T2G) (T2U) (T2U)
                 (T2U) (A1G) (T1U) (T1U) (T1U) (EG) (EG) (A1G)
                 (T1U) (T1U) (T1U) (A2U) (T2U) (T2U) (T2U) (T1U)
                 (T1U) (T1U) (T2G) (T2G) (T2G) (EG) (EG) (A1G)
                 (T1U) (T1U) (T1U) (T2G) (T2G) (T2G) (EG) (EG)
                 (A1G) (T1U) (T1U) (T1U) (T2G) (T2G) (T2G) (EG)
                 (EG) (A1G) (T1U) (T1U) (T1U) (A1G) (T1U) (T1U)
                 (T1U) (A1G) (A1G) (A1G) (A1G) (A1G)
 The electronic state of the initial guess is 1-A1G.
 Leave Link  401 at Sat Nov 30 20:45:09 2013, MaxMem=  104857600
cpu:       1.0
 (Enter C:\G09W\l502.exe)
 Closed shell SCF:
 Requested convergence on RMS density matrix=1.00D-08 within1000
cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on             energy=1.00D-06.
 No special actions if energy rises.
 Using DIIS extrapolation, IDIIS=  1040.
 Integral symmetry usage will be decided dynamically.
       175798 words used for storage of precomputed grid.
 IEnd=     1362924 IEndB=     1362924 NGot=   104857600 MDV=
104555483
 LenX=   104555483 LenY=   104496478
 Fock matrices will be formed incrementally for  20 cycles.

 Cycle   1  Pass 1  IDiag  1:
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=
0
         NFxFlg=           0 DoJE=F BraDBF=F KetDBF=F FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=       0 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1
NMtDS0=    0 NMtDT0=    0
         I1Cent=           0 NGrid=           0.
 Petite list used in FoFCou.
 Defaulting to unpruned grid for atomic number  78.
 Defaulting to unpruned grid for atomic number  78.
 E= -20071.6528367638
 DIIS: error= 1.68D+00 at cycle   1 NSaved=   1.
 NSaved= 1 IEnMin= 1 EnMin= -20071.6528367638     IErMin= 1
ErrMin= 1.68D+00
 ErrMax= 1.68D+00 EMaxC= 1.00D-01 BMatC= 3.15D+02 BMatP= 3.15D+02
 IDIUse=3 WtCom= 0.00D+00 WtEn= 1.00D+00
 Coeff-Com:  0.100D+01
 Coeff-En:   0.100D+01
 Coeff:      0.100D+01
 Gap=     0.046 Goal=   None    Shift=    0.000
 GapD=    0.046 DampG=0.250 DampE=0.125 DampFc=0.1250 IDamp=-1.
 Damping current iteration by 1.25D-01
```

```
 RMSDP=1.80D-02 MaxDP=7.71D-01              OVMax= 9.19D-01

 Cycle   2  Pass 1  IDiag  1:
 Density matrix breaks symmetry, PCut= 1.00D-04
 Density has only Abelian symmetry.
 RMSU=  1.58D-03    CP:  1.01D+00
 E= -20072.5968600722     Delta-E=       -0.944023308348 Rises=F
Damp=T
 DIIS: error= 1.47D+00 at cycle   2 NSaved=   2.
 NSaved= 2 IEnMin= 2 EnMin= -20072.5968600722     IErMin= 2
ErrMin= 1.47D+00
 ErrMax= 1.47D+00 EMaxC= 1.00D-01 BMatC= 2.28D+02 BMatP= 3.15D+02
 IDIUse=3 WtCom= 0.00D+00 WtEn= 1.00D+00
 Coeff-Com: -0.533D+01 0.633D+01
 Coeff-En:   0.000D+00 0.100D+01
 Coeff:      0.000D+00 0.100D+01
 Gap=     0.000 Goal=   None    Shift=    0.000
 RMSDP=1.18D-02 MaxDP=4.10D-01 DE=-9.44D-01 OVMax= 1.93D-01

 Cycle   3  Pass 1  IDiag  1:
 Density matrix breaks symmetry, PCut= 1.00D-04
 Density has only Abelian symmetry.
 RMSU=  5.75D-03    CP:  1.03D+00  3.00D+00
 E= -20070.6464423890     Delta-E=        1.950417683140 Rises=F
Damp=F
 DIIS: error= 3.87D-01 at cycle   3 NSaved=   3.
 NSaved= 3 IEnMin= 2 EnMin= -20072.5968600722     IErMin= 3
ErrMin= 3.87D-01
 ErrMax= 3.87D-01 EMaxC= 1.00D-01 BMatC= 2.02D+01 BMatP= 2.28D+02
 IDIUse=3 WtCom= 0.00D+00 WtEn= 1.00D+00
 EnCoef did   100 forward-backward iterations
 Coeff-Com:  0.146D+01-0.150D+01 0.104D+01
 Coeff-En:   0.519D+00 0.369D-01 0.444D+00
 Coeff:      0.519D+00 0.369D-01 0.444D+00
 Gap=     0.063 Goal=   None    Shift=    0.000
 RMSDP=1.15D-02 MaxDP=5.09D-01 DE= 1.95D+00 OVMax= 6.24D-01

 Cycle   4  Pass 1  IDiag  1:
 Density matrix breaks symmetry, PCut= 1.00D-04
 Density has only Abelian symmetry.
 RMSU=  2.64D-03    CP:  1.01D+00  1.26D+00  6.65D-02
 E= -20075.0629684166     Delta-E=       -4.416526027617 Rises=F
Damp=F
 DIIS: error= 9.23D-02 at cycle   4 NSaved=   4.
 NSaved= 4 IEnMin= 4 EnMin= -20075.0629684166     IErMin= 4
ErrMin= 9.23D-02
 ErrMax= 9.23D-02 EMaxC= 1.00D-01 BMatC= 1.41D+00 BMatP= 2.02D+01
 IDIUse=3 WtCom= 7.67D-02 WtEn= 9.23D-01
 Coeff-Com: -0.587D+00 0.727D+00-0.663D-01 0.926D+00
 Coeff-En:   0.000D+00 0.000D+00 0.963D-01 0.904D+00
```

```
 Coeff:     -0.450D-01 0.557D-01 0.838D-01 0.905D+00
 Gap=     0.024 Goal=   None    Shift=    0.000
 RMSDP=6.72D-03 MaxDP=4.08D-01 DE=-4.42D+00 OVMax= 7.70D-01

 Cycle   5  Pass 1  IDiag  1:
 Density matrix breaks symmetry, PCut= 1.00D-04
 Density has only Abelian symmetry.
 RMSU=  3.69D-03    CP:  1.02D+00  2.89D+00  9.75D-02  4.26D-01
 E= -20074.5962490756     Delta-E=        0.466719341046 Rises=F
Damp=F
 DIIS: error= 7.21D-02 at cycle   5 NSaved=   5.
 NSaved= 5 IEnMin= 4 EnMin= -20075.0629684166     IErMin= 5
ErrMin= 7.21D-02
 ErrMax= 7.21D-02 EMaxC= 1.00D-01 BMatC= 1.12D+00 BMatP= 1.41D+00
 IDIUse=3 WtCom= 2.79D-01 WtEn= 7.21D-01
 Coeff-Com:  0.995D-01-0.103D+00-0.625D-01 0.534D+00 0.532D+00
 Coeff-En:   0.000D+00 0.000D+00 0.000D+00 0.627D+00 0.373D+00
 Coeff:      0.277D-01-0.287D-01-0.174D-01 0.601D+00 0.417D+00
 Gap=     0.103 Goal=   None    Shift=    0.000
 RMSDP=3.81D-03 MaxDP=2.72D-01 DE= 4.67D-01 OVMax= 2.89D-01

 Cycle   6  Pass 1  IDiag  1:
 Density matrix breaks symmetry, PCut= 1.00D-04
 Density has only Abelian symmetry.
 RMSU=  6.37D-04    CP:  1.01D+00  1.77D+00  7.42D-02  7.45D-01
5.29D-01
 E= -20075.4996116995     Delta-E=       -0.903362623871 Rises=F
Damp=F
 DIIS: error= 1.25D-02 at cycle   6 NSaved=   6.
 NSaved= 6 IEnMin= 6 EnMin= -20075.4996116995     IErMin= 6
ErrMin= 1.25D-02
 ErrMax= 1.25D-02 EMaxC= 1.00D-01 BMatC= 2.27D-02 BMatP= 1.12D+00
 IDIUse=3 WtCom= 8.75D-01 WtEn= 1.25D-01
 Coeff-Com: -0.449D-01 0.531D-01 0.145D-02 0.901D-01-0.474D-01
0.948D+00
 Coeff-En:   0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00
0.100D+01
 Coeff:     -0.393D-01 0.465D-01 0.127D-02 0.788D-01-0.414D-01
0.954D+00
 Gap=     0.149 Goal=   None    Shift=    0.000
 RMSDP=6.48D-04 MaxDP=3.07D-02 DE=-9.03D-01 OVMax= 5.71D-02

 Cycle   7  Pass 1  IDiag  1:
 Density matrix breaks symmetry, PCut= 1.00D-04
 Density has only Abelian symmetry.
 RMSU=  2.22D-04    CP:  1.01D+00  1.68D+00  7.12D-02  8.10D-01
4.45D-01
                    CP:  8.28D-01
 E= -20075.5083283120     Delta-E=       -0.008716612516 Rises=F
Damp=F
```

```
 DIIS: error= 3.50D-03 at cycle   7 NSaved=   7.
 NSaved= 7 IEnMin= 7 EnMin= -20075.5083283120     IErMin= 7
ErrMin= 3.50D-03
 ErrMax= 3.50D-03 EMaxC= 1.00D-01 BMatC= 1.67D-03 BMatP= 2.27D-02
 IDIUse=3 WtCom= 9.65D-01 WtEn= 3.50D-02
 Coeff-Com: -0.290D-01 0.335D-01 0.198D-02 0.235D-01-0.200D-01
0.413D+00
 Coeff-Com:  0.577D+00
 Coeff-En:   0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00
0.141D+00
 Coeff-En:   0.859D+00
 Coeff:     -0.280D-01 0.324D-01 0.191D-02 0.226D-01-0.193D-01
0.403D+00
 Coeff:      0.587D+00
 Gap=     0.148 Goal=   None    Shift=    0.000
 RMSDP=2.03D-04 MaxDP=1.08D-02 DE=-8.72D-03 OVMax= 1.42D-02

 Cycle   8  Pass 1  IDiag  1:
 Density matrix breaks symmetry, PCut= 1.00D-04
 Density has only Abelian symmetry.
 RMSU=  2.97D-05    CP:  1.01D+00  1.70D+00  7.24D-02  7.98D-01
4.62D-01
                    CP:  9.22D-01  5.55D-01
 E= -20075.5098738114     Delta-E=       -0.001545499465 Rises=F
Damp=F
 DIIS: error= 3.00D-04 at cycle   8 NSaved=   8.
 NSaved= 8 IEnMin= 8 EnMin= -20075.5098738114     IErMin= 8
ErrMin= 3.00D-04
 ErrMax= 3.00D-04 EMaxC= 1.00D-01 BMatC= 1.14D-05 BMatP= 1.67D-03
 IDIUse=3 WtCom= 9.97D-01 WtEn= 3.00D-03
 Coeff-Com: -0.672D-02 0.771D-02-0.249D-04 0.296D-02-0.844D-03
0.648D-01
 Coeff-Com:  0.151D+00 0.781D+00
 Coeff-En:   0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00
0.000D+00
 Coeff-En:   0.000D+00 0.100D+01
 Coeff:     -0.670D-02 0.769D-02-0.249D-04 0.295D-02-0.841D-03
0.646D-01
 Coeff:      0.151D+00 0.782D+00
 Gap=     0.148 Goal=   None    Shift=    0.000
 RMSDP=2.33D-05 MaxDP=8.82D-04 DE=-1.55D-03 OVMax= 1.96D-03

 Cycle   9  Pass 1  IDiag  1:
 Density matrix breaks symmetry, PCut= 1.00D-04
 Density has only Abelian symmetry.
 RMSU=  7.98D-06    CP:  1.01D+00  1.70D+00  7.24D-02  7.98D-01
4.64D-01
                    CP:  9.17D-01  6.08D-01  8.49D-01
 E= -20075.5098860747     Delta-E=       -0.000012263266 Rises=F
Damp=F
```

```
 DIIS: error= 1.34D-04 at cycle   9 NSaved=   9.
 NSaved= 9 IEnMin= 9 EnMin= -20075.5098860747     IErMin= 9
ErrMin= 1.34D-04
 ErrMax= 1.34D-04 EMaxC= 1.00D-01 BMatC= 2.38D-06 BMatP= 1.14D-05
 IDIUse=3 WtCom= 9.99D-01 WtEn= 1.34D-03
 EnCoef did     1 forward-backward iterations
 Coeff-Com: -0.190D-03 0.210D-03-0.554D-04 0.244D-03-0.128D-03
0.566D-02
 Coeff-Com:  0.243D-01 0.229D+00 0.741D+00
 Coeff-En:   0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00
0.000D+00
 Coeff-En:   0.000D+00 0.104D-01 0.990D+00
 Coeff:     -0.190D-03 0.210D-03-0.553D-04 0.244D-03-0.128D-03
0.565D-02
 Coeff:      0.243D-01 0.229D+00 0.741D+00
 Gap=     0.148 Goal=   None    Shift=    0.000
 RMSDP=4.68D-06 MaxDP=1.77D-04 DE=-1.23D-05 OVMax= 1.67D-04

 Cycle  10  Pass 1  IDiag  1:
 Restarting incremental Fock formation.
 E= -20075.5098871556     Delta-E=       -0.000001080847 Rises=F
Damp=F
 DIIS: error= 4.83D-05 at cycle  10 NSaved=  10.
 NSaved=10 IEnMin=10 EnMin= -20075.5098871556     IErMin=10
ErrMin= 4.83D-05
 ErrMax= 4.83D-05 EMaxC= 1.00D-01 BMatC= 4.19D-07 BMatP= 2.38D-06
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com:  0.357D-03-0.409D-03 0.136D-04-0.219D-04-0.349D-03-
0.579D-04
 Coeff-Com:  0.299D-02 0.638D-01 0.189D+00 0.744D+00
 Coeff:      0.357D-03-0.409D-03 0.136D-04-0.219D-04-0.349D-03-
0.579D-04
 Coeff:      0.299D-02 0.638D-01 0.189D+00 0.744D+00
 Gap=     0.148 Goal=   None    Shift=    0.000
 RMSDP=2.95D-06 MaxDP=2.01D-04 DE=-1.08D-06 OVMax= 1.86D-04

 Cycle  11  Pass 1  IDiag  1:
 RMSU=  2.05D-06    CP:  1.00D+00
 E= -20075.5098875284     Delta-E=       -0.000000372831 Rises=F
Damp=F
 DIIS: error= 6.85D-06 at cycle  11 NSaved=  11.
 NSaved=11 IEnMin=11 EnMin= -20075.5098875284     IErMin=11
ErrMin= 6.85D-06
 ErrMax= 6.85D-06 EMaxC= 1.00D-01 BMatC= 5.40D-09 BMatP= 4.19D-07
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com:  0.357D-04-0.407D-04 0.696D-06 0.234D-04-0.179D-04
0.146D-03
 Coeff-Com:  0.418D-03 0.114D-02-0.212D-01 0.256D-01 0.994D+00
 Coeff:      0.357D-04-0.407D-04 0.696D-06 0.234D-04-0.179D-04
0.146D-03
```

```
 Coeff:      0.418D-03 0.114D-02-0.212D-01 0.256D-01 0.994D+00
 Gap=     0.148 Goal=   None    Shift=    0.000
 RMSDP=2.32D-07 MaxDP=9.22D-06 DE=-3.73D-07 OVMax= 1.25D-05

 Cycle  12  Pass 1  IDiag  1:
 RMSU=  1.10D-07    CP:  1.00D+00  1.05D+00
 E= -20075.5098875305     Delta-E=       -0.000000002110 Rises=F
Damp=F
 DIIS: error= 5.57D-07 at cycle  12 NSaved=  12.
 NSaved=12 IEnMin=12 EnMin= -20075.5098875305     IErMin=12
ErrMin= 5.57D-07
 ErrMax= 5.57D-07 EMaxC= 1.00D-01 BMatC= 5.37D-11 BMatP= 5.40D-09
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com:  0.808D-05-0.917D-05-0.584D-07 0.904D-05-0.405D-05
0.654D-04
 Coeff-Com:  0.154D-03 0.427D-03-0.665D-02 0.105D-02 0.279D+00
0.726D+00
 Coeff:      0.808D-05-0.917D-05-0.584D-07 0.904D-05-0.405D-05
0.654D-04
 Coeff:      0.154D-03 0.427D-03-0.665D-02 0.105D-02 0.279D+00
0.726D+00
 Gap=     0.148 Goal=   None    Shift=    0.000
 RMSDP=4.39D-08 MaxDP=1.68D-06 DE=-2.11D-09 OVMax= 1.03D-06

 Cycle  13  Pass 1  IDiag  1:
 RMSU=  2.49D-08    CP:  1.00D+00  1.05D+00  8.99D-01
 E= -20075.5098875308     Delta-E=       -0.000000000302 Rises=F
Damp=F
 DIIS: error= 3.28D-07 at cycle  13 NSaved=  13.
 NSaved=13 IEnMin=13 EnMin= -20075.5098875308     IErMin=13
ErrMin= 3.28D-07
 ErrMax= 3.28D-07 EMaxC= 1.00D-01 BMatC= 1.55D-11 BMatP= 5.37D-11
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com:  0.236D-06-0.259D-06 0.136D-07 0.774D-06-0.691D-06
0.919D-05
 Coeff-Com:  0.267D-04 0.142D-03-0.374D-03-0.226D-02-0.824D-02
0.164D+00
 Coeff-Com:  0.846D+00
 Coeff:      0.236D-06-0.259D-06 0.136D-07 0.774D-06-0.691D-06
0.919D-05
 Coeff:      0.267D-04 0.142D-03-0.374D-03-0.226D-02-0.824D-02
0.164D+00
 Coeff:      0.846D+00
 Gap=     0.148 Goal=   None    Shift=    0.000
 RMSDP=1.35D-08 MaxDP=5.45D-07 DE=-3.02D-10 OVMax= 9.67D-07

 Cycle  14  Pass 1  IDiag  1:
 RMSU=  2.33D-09    CP:  1.00D+00  1.06D+00  9.46D-01  8.95D-01
 E= -20075.5098875309     Delta-E=       -0.000000000146 Rises=F
Damp=F
```

```
 DIIS: error= 4.02D-08 at cycle  14 NSaved=  14.
 NSaved=14 IEnMin=14 EnMin= -20075.5098875309     IErMin=14
ErrMin= 4.02D-08
 ErrMax= 4.02D-08 EMaxC= 1.00D-01 BMatC= 2.07D-13 BMatP= 1.55D-11
 IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00
 Coeff-Com: -0.361D-07 0.405D-07-0.367D-08-0.531D-07 0.104D-06-
0.431D-06
 Coeff-Com:  0.110D-05 0.784D-05-0.437D-04-0.545D-03-0.346D-02
0.102D-03
 Coeff-Com:  0.368D-01 0.967D+00
 Coeff:     -0.361D-07 0.405D-07-0.367D-08-0.531D-07 0.104D-06-
0.431D-06
 Coeff:      0.110D-05 0.784D-05-0.437D-04-0.545D-03-0.346D-02
0.102D-03
 Coeff:      0.368D-01 0.967D+00
 Gap=     0.148 Goal=   None    Shift=    0.000
 RMSDP=1.93D-09 MaxDP=8.24D-08 DE=-1.46D-10 OVMax= 1.44D-07

 Error on total polarization charges =  0.01774
 SCF Done:  E(RPBE1PBE) =  -20075.5098875     A.U. after   14
cycles
             Convg  =    0.1932D-08             -V/T =  2.0014
 KE= 2.004828796335D+04 PE=-5.262142360706D+04 EE=
1.010323276242D+04
 Leave Link  502 at Sat Nov 30 20:47:18 2013, MaxMem=  104857600
cpu:     129.0
 (Enter C:\G09W\l801.exe)
 Range of M.O.s used for correlation:     1   219
 NBasis=   219 NAE=    91 NBE=    91 NFC=     0 NFV=     0
 NROrb=    219 NOA=    91 NOB=    91 NVA=   128 NVB=   128

 **** Warning!!: The largest alpha MO coefficient is
0.12744021D+02

 Leave Link  801 at Sat Nov 30 20:47:18 2013, MaxMem=  104857600
cpu:       0.0
 (Enter C:\G09W\l1002.exe)
 Minotr:  Closed shell wavefunction.
 NEqPCM:  Using equilibrium solvation (IEInf=0, Eps=  78.3553,
EpsInf=   1.7778)
          Direct CPHF calculation.
          Differentiating once with respect to magnetic field
using GIAOs.
          Electric field/nuclear overlap derivatives assumed to
be zero.
          Using symmetry in CPHF.
          Requested convergence is 1.0D-08 RMS, and 1.0D-07
maximum.
          Secondary convergence is 1.0D-12 RMS, and 1.0D-12
maximum.
```

```
          NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F
KeepMc=T.
          MDV=     104857554 using IRadAn=       1.
 Defaulting to unpruned grid for atomic number  78.
 Generate precomputed XC quadrature information.
          Solving linear equations simultaneously, MaxMat=
0.
 FoFCou: FMM=F IPFlag=           0 FMFlag=    10101102 FMFlg1=
0
         NFxFlg=    40000000 DoJE=F BraDBF=F KetDBF=T FulRan=T
         Omega=  0.000000  0.000000  1.000000  0.000000  0.000000
ICntrl=    6100 IOpCl=  0
         NMat0=    1 NMatS0=    1 NMatT0=    0 NMatD0=    1
NMtDS0=    0 NMtDT0=    0
         I1Cent=           7 NGrid=        1189.
 Symmetry not used in FoFCou.
 Defaulting to unpruned grid for atomic number  78.
 Defaulting to unpruned grid for atomic number  78.
 Integrals replicated using symmetry in FoFDir.
 MinBra= 0 MaxBra= 3 Meth= 1.
 IRaf=       0 NMat=   3 IRICut=       1 DoRegI=T DoRafI=F
ISym2E= 2 JSym2E=2.
          There are     3 degrees of freedom in the 1st order
CPHF.  IDoFFX=0.
      3 vectors produced by pass  0 Test12= 3.88D-13 3.33D-08
XBig12= 5.13D+00 1.57D+00.
 AX will form     3 AO Fock derivatives at one time.
      3 vectors produced by pass  1 Test12= 3.88D-13 3.33D-08
XBig12= 6.45D-02 1.72D-01.
      3 vectors produced by pass  2 Test12= 3.88D-13 3.33D-08
XBig12= 1.52D-03 2.72D-02.
      3 vectors produced by pass  3 Test12= 3.88D-13 3.33D-08
XBig12= 1.26D-05 1.85D-03.
      3 vectors produced by pass  4 Test12= 3.88D-13 3.33D-08
XBig12= 8.51D-08 1.35D-04.
      3 vectors produced by pass  5 Test12= 3.88D-13 3.33D-08
XBig12= 2.74D-10 6.75D-06.
      3 vectors produced by pass  6 Test12= 3.88D-13 3.33D-08
XBig12= 6.47D-13 2.70D-07.
 Inverted reduced A of dimension    21 with in-core refinement.
 Calculating GIAO nuclear magnetic shielding tensors.
 SCF GIAO Magnetic shielding tensor (ppm):
  1  Pt   Isotropic = -1600.4199   Anisotropy =     0.0001
   XX= -1600.4199   YX=     0.0000   ZX=     0.0000
   XY=     0.0000   YY= -1600.4199   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ= -1600.4199
   Eigenvalues: -1600.4199 -1600.4199 -1600.4199
  2  Cl   Isotropic =   846.4486   Anisotropy =   374.8435
   XX=   721.5008   YX=     0.0000   ZX=     0.0000
   XY=     0.0000   YY=   721.5008   ZY=     0.0000
```

```
   XZ=     0.0000   YZ=     0.0000   ZZ=  1096.3443
   Eigenvalues:   721.5008   721.5008  1096.3443
  3  Cl   Isotropic =   846.4486   Anisotropy =   374.8435
   XX=   721.5008   YX=     0.0000   ZX=     0.0000
   XY=     0.0000   YY=  1096.3443   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   721.5008
   Eigenvalues:   721.5008   721.5008  1096.3443
  4  Cl   Isotropic =   846.4487   Anisotropy =   374.8435
   XX=  1096.3443   YX=     0.0000   ZX=     0.0000
   XY=     0.0000   YY=   721.5008   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   721.5008
   Eigenvalues:   721.5008   721.5008  1096.3443
  5  Cl   Isotropic =   846.4487   Anisotropy =   374.8435
   XX=  1096.3443   YX=     0.0000   ZX=     0.0000
   XY=     0.0000   YY=   721.5008   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   721.5008
   Eigenvalues:   721.5008   721.5008  1096.3443
  6  Cl   Isotropic =   846.4486   Anisotropy =   374.8435
   XX=   721.5008   YX=     0.0000   ZX=     0.0000
   XY=     0.0000   YY=  1096.3443   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=   721.5008
   Eigenvalues:   721.5008   721.5008  1096.3443
  7  Cl   Isotropic =   846.4486   Anisotropy =   374.8435
   XX=   721.5008   YX=     0.0000   ZX=     0.0000
   XY=     0.0000   YY=   721.5008   ZY=     0.0000
   XZ=     0.0000   YZ=     0.0000   ZZ=  1096.3443
   Eigenvalues:   721.5008   721.5008  1096.3443
 End of Minotr Frequency-dependent properties file   721 does not
exist.
 End of Minotr Frequency-dependent properties file   722 does not
exist.
 Leave Link 1002 at Sat Nov 30 20:53:50 2013, MaxMem=  104857600
cpu:     392.0
 (Enter C:\G09W\l601.exe)
 Copying SCF densities to generalized density rwf, IOpCl= 0
IROHF=0.


*****************************************************************
*****

            Population analysis using the SCF density.


*****************************************************************
*****

 Orbital symmetries:
       Occupied  (A1G) (A1G) (T1U) (T1U) (T1U) (A1G) (A1G) (EG)
                 (EG) (T1U) (T1U) (T1U) (T1U) (T1U) (T1U) (EG)
```

```
                    (EG)  (T2G)  (T2G)  (T2G)  (A1G)  (T1U)  (T1U)  (T1U)
                    (EG)  (EG)  (T2G)  (T2G)  (T2G)  (A1G)  (EG)  (EG)
(T1U)
                    (T1U)  (T1U)  (T1U)  (T1U)  (T1U)  (EG)  (EG)  (A1G)
                    (T2G)  (T2G)  (T2G)  (T1U)  (T1U)  (T1U)  (T1G)  (T1G)
                    (T1G)  (T2U)  (T2U)  (T2U)  (T1U)  (T1U)  (T1U)  (T2U)
                    (T2U)  (T2U)  (A2U)  (A1G)  (T1U)  (T1U)  (T1U)  (A1G)
                    (EG)  (EG)  (T1U)  (T1U)  (T1U)  (EG)  (EG)  (T2G)
(T2G)
                    (T2G)  (A1G)  (T1U)  (T1U)  (T1U)  (T2U)  (T2U)  (T2U)
                    (T1U)  (T1U)  (T1U)  (T2G)  (T2G)  (T2G)  (T1G)  (T1G)
                    (T1G)
       Virtual      (EG)  (EG)  (A1G)  (T1U)  (T1U)  (T1U)  (EG)  (EG)
(A1G)
                    (T2G)  (T2G)  (T2G)  (T1U)  (T1U)  (T1U)  (EG)  (EG)
                    (T1U)  (T1U)  (T1U)  (A1G)  (T2G)  (T2G)  (T2G)  (T2U)
                    (T2U)  (T2U)  (T1U)  (T1U)  (T1U)  (T1G)  (T1G)  (T1G)
                    (EG)  (EG)  (T2U)  (T2U)  (T2U)  (T2G)  (T2G)  (T2G)
                    (T1U)  (T1U)  (T1U)  (A2U)  (T1U)  (T1U)  (T1U)  (EU)
                    (EU)  (A2G)  (T1G)  (T1G)  (T1G)  (T2U)  (T2U)  (T2U)
                    (A1G)  (EG)  (EG)  (T2G)  (T2G)  (T2G)  (A2U)  (EG)
(EG)
                    (T1U)  (T1U)  (T1U)  (T2U)  (T2U)  (T2U)  (T2G)  (T2G)
                    (T2G)  (A1G)  (T1U)  (T1U)  (T1U)  (A1G)  (EG)  (EG)
                    (T1U)  (T1U)  (T1U)  (A2U)  (T2U)  (T2U)  (T2U)  (T2G)
                    (T2G)  (T2G)  (T1U)  (T1U)  (T1U)  (EG)  (EG)  (A1G)
                    (T1U)  (T1U)  (T1U)  (T2G)  (T2G)  (T2G)  (EG)  (EG)
                    (A1G)  (T1U)  (T1U)  (T1U)  (T2G)  (T2G)  (T2G)  (EG)
                    (EG)  (A1G)  (T1U)  (T1U)  (T1U)  (A1G)  (T1U)  (T1U)
                    (T1U)  (A1G)  (A1G)  (A1G)  (A1G)  (A1G)
 The electronic state is 1-A1G.
 Alpha  occ. eigenvalues -- **********-437.58229-419.71174-
419.71174-419.71174
 Alpha  occ. eigenvalues -- -102.86118-101.65848-101.65846-
101.65846-101.65845
 Alpha  occ. eigenvalues -- -101.65845-101.65845 -94.46828 -
94.46828 -94.46828
 Alpha  occ. eigenvalues --  -79.67096 -79.67096 -79.67046 -
79.67046 -79.67046
 Alpha  occ. eigenvalues --  -21.93240 -18.34345 -18.34345 -
18.34345 -11.98855
 Alpha  occ. eigenvalues --  -11.98855 -11.98455 -11.98455 -
11.98455  -9.48463
 Alpha  occ. eigenvalues --   -9.48460  -9.48460  -9.48457  -
9.48457  -9.48457
 Alpha  occ. eigenvalues --   -7.21858  -7.21858  -7.21858  -
7.21858  -7.21858
 Alpha  occ. eigenvalues --   -7.21854  -7.21136  -7.21136  -
7.21136  -7.21135
```

```
 Alpha  occ. eigenvalues --   -7.21135  -7.21135  -7.21135  -
7.21135  -7.21135
 Alpha  occ. eigenvalues --   -7.21133  -7.21133  -7.21133  -
3.42006  -3.42006
 Alpha  occ. eigenvalues --   -3.42006  -3.41627  -3.41627  -
3.41627  -3.41154
 Alpha  occ. eigenvalues --   -3.20767  -2.07611  -2.07611  -
2.07611  -0.79746
 Alpha  occ. eigenvalues --   -0.77930  -0.77930  -0.77672  -
0.77672  -0.77672
 Alpha  occ. eigenvalues --   -0.43028  -0.43028  -0.41422  -
0.41422  -0.41422
 Alpha  occ. eigenvalues --   -0.38636  -0.33931  -0.33931  -
0.33931  -0.29286
 Alpha  occ. eigenvalues --   -0.29286  -0.29286  -0.28702  -
0.28702  -0.28702
 Alpha  occ. eigenvalues --   -0.28275  -0.28275  -0.28275  -
0.27140  -0.27140
 Alpha  occ. eigenvalues --   -0.27140
 Alpha virt. eigenvalues --   -0.12350  -0.12350   0.12910
0.15794   0.15794
 Alpha virt. eigenvalues --    0.15794   0.19625   0.19625
0.20678   0.23974
 Alpha virt. eigenvalues --    0.23974   0.23974   0.30480
0.30480   0.30480
 Alpha virt. eigenvalues --    0.43183   0.43183   0.43670
0.43670   0.43670
 Alpha virt. eigenvalues --    0.44974   0.47937   0.47937
0.47937   0.53055
 Alpha virt. eigenvalues --    0.53055   0.53055   0.58233
0.58233   0.58233
 Alpha virt. eigenvalues --    0.61943   0.61943   0.61943
0.69252   0.69252
 Alpha virt. eigenvalues --    0.69255   0.69255   0.69255
0.71745   0.71745
 Alpha virt. eigenvalues --    0.71745   0.78049   0.78049
0.78049   0.80795
 Alpha virt. eigenvalues --    0.89358   0.89358   0.89358
0.92727   0.92727
 Alpha virt. eigenvalues --    0.92790   0.93961   0.93961
0.93961   0.94023
 Alpha virt. eigenvalues --    0.94023   0.94023   0.95769
0.96705   0.96705
 Alpha virt. eigenvalues --    0.96830   0.96830   0.96830
1.00239   1.08958
 Alpha virt. eigenvalues --    1.08958   1.17408   1.17408
1.17408   1.17603
 Alpha virt. eigenvalues --    1.17603   1.17603   1.19745
1.19745   1.19745
```

```
 Alpha virt. eigenvalues --    1.23434   1.44128   1.44128
1.44128   1.54749
 Alpha virt. eigenvalues --    1.54999   1.54999   1.75760
1.75760   1.75760
 Alpha virt. eigenvalues --    2.67569   2.75715   2.75715
2.75715   3.02636
 Alpha virt. eigenvalues --    3.02636   3.02636   3.03835
3.03835   3.03835
 Alpha virt. eigenvalues --    3.27427   3.27427   5.33624
7.06218   7.06218
 Alpha virt. eigenvalues --    7.06218  14.55243  14.55243
14.55243  14.71416
 Alpha virt. eigenvalues --   14.71416  22.27823  39.84732
39.84732  39.84732
 Alpha virt. eigenvalues --   89.95852  89.95852  89.95852
90.04589  90.04589
 Alpha virt. eigenvalues --  104.46728 234.40143 234.40143
234.40143 455.66079
 Alpha virt. eigenvalues --
1328.538651328.538651328.538651661.614915146.10521
 Alpha virt. eigenvalues -- ******************************
          Condensed to atoms (all electrons):
               1          2          3          4          5
6
     1  Pt  76.871706   0.196741   0.196741   0.196741   0.196741
0.196741
     2  Cl   0.196741  17.194420  -0.015756  -0.015756  -0.015756
-0.015756
     3  Cl   0.196741  -0.015756  17.194420  -0.015756  -0.015756
-0.003495
     4  Cl   0.196741  -0.015756  -0.015756  17.194420  -0.003495
-0.015756
     5  Cl   0.196741  -0.015756  -0.015756  -0.003495  17.194420
-0.015756
     6  Cl   0.196741  -0.015756  -0.003495  -0.015756  -0.015756
17.194420
     7  Cl   0.196741  -0.003495  -0.015756  -0.015756  -0.015756
-0.015756
               7
     1  Pt   0.196741
     2  Cl  -0.003495
     3  Cl  -0.015756
     4  Cl  -0.015756
     5  Cl  -0.015756
     6  Cl  -0.015756
     7  Cl  17.194420
 Mulliken atomic charges:
               1
     1  Pt  -0.052152
     2  Cl  -0.324641
```

```
     3  Cl  -0.324641
     4  Cl  -0.324641
     5  Cl  -0.324641
     6  Cl  -0.324641
     7  Cl  -0.324641
 Sum of Mulliken atomic charges =  -2.00000
 Mulliken charges with hydrogens summed into heavy atoms:
               1
     1  Pt  -0.052152
     2  Cl  -0.324641
     3  Cl  -0.324641
     4  Cl  -0.324641
     5  Cl  -0.324641
     6  Cl  -0.324641
     7  Cl  -0.324641
 Sum of Mulliken charges with hydrogens summed into heavy atoms =
-2.00000
 Electronic spatial extent (au):  <R**2>=           2382.8298
 Charge=             -2.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=              0.0000    Y=              0.0000    Z=
0.0000  Tot=              0.0000
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=           -130.7243   YY=           -130.7243   ZZ=
-130.7243
   XY=              0.0000   XZ=              0.0000   YZ=
0.0000
 Traceless Quadrupole moment (field-independent basis, Debye-
Ang):
   XX=              0.0000   YY=              0.0000   ZZ=
0.0000
   XY=              0.0000   XZ=              0.0000   YZ=
0.0000
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=              0.0000  YYY=              0.0000  ZZZ=
0.0000  XYY=              0.0000
  XXY=              0.0000  XXZ=              0.0000  XZZ=
0.0000  YZZ=              0.0000
  YYZ=              0.0000  XYZ=              0.0000
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=          -1132.2790 YYYY=          -1132.2790 ZZZZ=
-1132.2790 XXXY=              0.0000
 XXXZ=              0.0000 YYYX=              0.0000 YYYZ=
0.0000 ZZZX=              0.0000
 ZZZY=              0.0000 XXYY=           -360.5399 XXZZ=
-360.5399 YYZZ=           -360.5399
 XXYZ=              0.0000 YYXZ=              0.0000 ZZXY=
0.0000
 N-N= 2.394392993762D+03 E-N=-5.262142356470D+04  KE=
2.004828796335D+04
```

```
 Symmetry AG   KE= 1.016728155800D+04
 Symmetry B1G  KE= 6.706929152014D+02
 Symmetry B2G  KE= 6.706929152014D+02
 Symmetry B3G  KE= 6.706929152014D+02
 Symmetry AU   KE= 9.568189544165D+01
 Symmetry B1U  KE= 2.591081921435D+03
 Symmetry B2U  KE= 2.591081921435D+03
 Symmetry B3U  KE= 2.591081921435D+03
 Calculating spin-rotation constants.
 Leave Link  601 at Sat Nov 30 20:53:53 2013, MaxMem=  104857600
cpu:       3.0
 (Enter C:\G09W\l9999.exe)
 1|1|UNPC-DHRT3V4J|SP|RPBE1PBE|Gen|Cl6Pt1(2-)|PC2|30-Nov-
2013|0||#p pbe
 1pbe/gen nmr=giao integral(ultrafine) SCRF(solvent=water)
SCF(NoVarAcc
 ,maxcycles=1000)||PtCl62-SARCZORA||-
2,1|Pt,0,0.,0.,0.|Cl,0,0.,0.,2.396
 1|Cl,0,0.,2.3961,0.|Cl,0,-
2.3961,0.,0.|Cl,0,2.3961,0.,0.|Cl,0,0.,-2.39
 61,0.|Cl,0,0.,0.,-2.3961||Version=IA32W-G09RevB.01|State=1-
A1G|HF=-200
 75.5098875|RMSD=1.932e-
009|Dipole=0.,0.,0.|Quadrupole=0.,0.,0.,0.,0.,0
 .|PG=OH [O(Pt1),3C4(Cl1.Cl1)]||@


 BE NOT THE FIRST BY WHOM THE NEW ARE TRIED,
 NOR YET THE THE LAST TO LAY THE OLD ASIDE.

                          -- ALEXANDER POPE
 Job cpu time:  0 days  0 hours  8 minutes 46.0 seconds.
 File lengths (MBytes):  RWF=     57 Int=      0 D2E=      0 Chk=
4 Scr=      1
 Normal termination of Gaussian 09 at Sat Nov 30 20:53:53 2013.
```