

# **Organometallic Reactivity: The Role of Metal-Ligand Bond Energies from a Computational Perspective**

Natalie Fey,\* Benjamin M. Ridgway, Jesús Jover, Claire L. McMullin and Jeremy N. Harvey\*

## **Supporting Information**

## Computational Details

### a) Complex Bond-Dissociation Enthalpies

To estimate the bond energies for the substitution reaction  $[\text{RuCl}_2(\text{p-cymene})]_{2(\text{soln})} + 2 \text{PR}_{3(\text{soln})} \rightarrow 2 [\text{RuCl}_2(\text{p-cymene})(\text{PR}_3)]_{(\text{soln})}$  we optimised the geometry of all complexes with the standard DFT approach used for all LKB-P calculations (described and justified in detail in reference 1), which can be summarised as follows: Optimisations used the standard Becke-Perdew (BP86) functional<sup>2</sup> as implemented in Jaguar.<sup>3</sup> The Jaguar triple- $\zeta$  form of the standard Los Alamos ECP basis set (LACV3P) was used on the transition metal atoms, employing the 6-31G\* basis for all other atoms. “Loose” convergence (5 times larger than default criteria) was used for all geometry optimizations. This functional/basis set combination has been denoted as BE1 throughout the manuscript.

Single point calculations with BP86 were performed with the larger LACV3P\*\*\* basis set in Jaguar, which corresponds to 6-311+G\*\* on all atoms apart from ruthenium, where the Los Alamos ECP basis set as described above was used (denoted as BE2).

Solvation free energies were obtained from single point (SP) calculations in Gaussian<sup>4</sup> on the Jaguar optimized geometries. These calculations used the BP86/LANL2DZ<sup>5</sup> functional/basis set combination with the default Integral Equation Formalism Polarizable Continuum Model (IEF-PCM) continuum dielectric solvation model,<sup>6</sup> using dichloromethane ( $\epsilon = 8.93$ ) as the solvent. A solvation correction was estimated as the difference between the SP potential energy in the gas phase and the SP free energy in solution with all non-electrostatic terms, and this corrections was then applied to the BE2 results; these solvation-corrected binding energies are denoted as BE2 (solv) in the text.

Dispersion-energy contributions were calculated using an in-house programme which uses Grimme’s DFT-D2 approach<sup>7</sup> to determine the dispersion energy for the final geometry in Jaguar output files. These corrections were calculated for the Jaguar optimized geometries and added to BE2 and BE2 (solv) results, these datasets have been labeled as BE2 (disp) and BE2 (solv+disp) in this study.

Table S1 lists all calculated dispersion energies and the optimized geometries can be found below.

### b) Oxidative Addition to Pd(0)

Our results for the oxidative addition of PhBr to  $[\text{PdL}_2]$  have previously been reported in reference 8, where they are summarised in Table 1. Detailed computational details are given in the supporting information of this work, which can be accessed via the following link: <http://www.rsc.org/suppdata/dt/c0/c0dt00778a/c0dt00778a.pdf>.

The geometries for the  $[\text{Pd}(\text{PPh}_3)_n]$  and  $[\text{Pd}(\text{binap})_n]$  complexes as well as the dissociated ligands  $\text{PPh}_3$  and binap were optimised in Jaguar,<sup>3b</sup> using the BP86,<sup>2</sup> B3LYP,<sup>2a,2e,9</sup> M06<sup>10</sup> and M06-L<sup>11</sup> functionals as implemented in the programme. The standard 6-31G\* basis set was used on all atoms except for palladium where the LACV3P basis set was used. As indicated in the text, starting geometries for  $[\text{Pd}(\text{PPh}_3)_4]$  and  $[\text{Pd}(\text{binap})_2]$  were derived from suitable crystal structure data (Refcodes TTPPDB<sup>12</sup> and QIPBEW<sup>13</sup>) as recorded in the Cambridge Structural Database.<sup>14</sup> All other structures were built in Maestro<sup>15</sup> or by modification of these crystal structure geometries. Optimisations used “loose” convergence (5 times larger than default criteria). Test calculations on other complexes using the more stringent default convergence criteria did not lead to significant changes in energies, bond lengths, or angles, but were much more time-consuming.

### c) Ligand Size Effects

P-donor ligand dissociation energies for the complexes  $[\text{PdCl}_3\text{L}]$  and  $[\text{Pt}(\text{PH}_3)_3\text{L}]$  have been reported for 348 ligands in reference 1b, with additional details about LKB-P discussed in our earlier work.<sup>1a</sup> We have also included additional ligand descriptor data as will be reported in a forthcoming publication (N. Fey, M. Garland, J. P. Hopewell, C. L. McMullin, S. Mastroianni, A. G. Orpen, P. G. Pringle, manuscript in preparation for *Angew. Chem. Int. Ed.*) These calculations used BP86 and the 6-31G\*/LACV3P basis set combination as described above for all geometry optimisations in Jaguar.<sup>3</sup>

Dispersion energy contributions have been calculated for the Jaguar output files using our in-house implementation of Grimme’s DFT-D2<sup>7</sup> approach, which have been added to the BP86 energies to give use BP86-D results. Data were analysed in S-Plus<sup>16</sup> and Microsoft Excel 2007.

### Dispersion Effects on Conformer Preferences

Analysis of P-donor ligand conformers as described by Haddow, Orpen and co-workers<sup>17</sup> can be used to generate ideal conformations and hence calculate relative conformer energies for both free ligands and their complexes. In unpublished work, we have used the LKB-P computational methodology described above to explore conformers for a range of different ligands, and then applied our in-house programme to calculate dispersion energy corrections according to Grimme's DFT-D2. These results suggest that dispersion corrections can alter the predicted conformer preferences, which can also contribute to calculated ligand dissociation energies. This is illustrated below for three representative ligands; we also show the resulting ligand dissociation energies for [PdCl<sub>3</sub>L] for the different conformations. As described in,<sup>17</sup> the substituent conformations are labelled according to their M-P-X-C torsion angles as gauche ( $\pm 60^\circ$ ) and anti ( $\pm 180^\circ$ ), with + or - indicating the direction of the torsion angle in the gauche conformation.

a) P(o-tolyl)<sub>3</sub> – Helicity is likely to be maintained in this case,<sup>18</sup> and four different conformations can be adopted: g+g+g+ (exo3), g+g+a (exo2), g+aa (exo1), aaa (exo0)

Calculated relative energies, kcal mol<sup>-1</sup>

Conformer	Rel. E, L	Rel. E <sub>vdw</sub> disp, L	Rel. E, [PdCl <sub>3</sub> L] <sup>-</sup>	Rel. E <sub>vdw</sub> , [PdCl <sub>3</sub> L] <sup>-</sup>	BE(Pd)	BE <sub>vdw</sub> (Pd)
aaa (exo0)	11.92	9.66	9.44	10.48	28.63	45.19
g+aa (exo1)	7.96	6.23	2.89	3.64	31.22	48.59
g+g+a (exo2)	3.03	1.45	0.00	0.00	29.18 (26.15) <sup>a</sup>	47.46 (46.01) <sup>a</sup>
g+g+g+ (exo3)	0.00	0.00	0.75	1.36	25.40	44.64

<sup>a</sup> BE calculated for lowest energy ligand (g+g+g+) and complex (g+g+a) conformations.

b) P(OPh)<sub>3</sub> – seven different conformations can be adopted<sup>17</sup>

Calculated relative energies, kcal mol<sup>-1</sup>

Conformer	Rel. E, L	Rel. E <sub>vdw</sub> disp, L	Rel. E, [PdCl <sub>3</sub> L] <sup>-</sup>	Rel. E <sub>vdw</sub> , [PdCl <sub>3</sub> L] <sup>-</sup>	BE(Pd)	BE <sub>vdw</sub> (Pd)
aaa (A)	6.40	0.59	4.00	2.88	33.74	40.07
g+g+g+ (B)	1.81	3.22	1.82	1.79	31.33	43.78
g+g+a (C)	1.04	1.13	1.29	0.31	31.09	43.18
g+aa (D)	2.84	-0.10	1.29	0.10	32.89	42.16
g+g-a (E)	2.56	2.95	1.30	0.31	32.60	45.00
g-g+a (F)	0.00	0.00	0.00	0.00	31.34	42.35
g+g+g- (G)	2.37	2.75	0.75	-1.54	32.96	46.64

c) PCy<sub>3</sub> – seven different conformations can be adopted<sup>17</sup>

Calculated relative energies, kcal mol<sup>-1</sup>

Conformer	Rel. E, L	Rel. E <sub>vdw</sub> disp, L	Rel. E, [PdCl <sub>3</sub> L] <sup>-</sup>	Rel. E <sub>vdw</sub> , [PdCl <sub>3</sub> L] <sup>-</sup>	BE(Pd)	BE <sub>vdw</sub> (Pd)
aaa (A)	2.41	1.51	9.82	10.82	31.04	45.73
g+g+g+ (B)	2.36	3.13	6.00	7.01	34.82	51.15
g+g+a (C)	0.00	0.00	3.11	3.52	35.34	51.51
g+aa (D)	0.98	0.68	0.27	0.00	39.15	55.71 (55.04) <sup>a</sup>
g+g-a (E)	1.56	1.73	0.77	0.86	39.24	55.90
g-g+a (F)	1.23	1.10	0.00	0.58	39.68 (38.45) <sup>a</sup>	55.55
g+g+g- (G)	3.47	3.71	4.00	3.99	37.91	54.75

<sup>a</sup> BE calculated for lowest energy ligand and complex conformations.

**Tables S1** a) Bond energies (kcal mol<sup>-1</sup>) for [RuCl<sub>2</sub>(p-cymene)]<sub>2(soln)</sub> + 2 PR<sub>3(soln)</sub> → 2 [RuCl<sub>2</sub>(p-cymene)(PR<sub>3</sub>)]<sub>(soln)</sub>

L	Expt. <sup>19</sup>	BE1	BE2	BE2 (solv)	BE2 (disp)	BE2 (solv + disp)
PMe <sub>3</sub>	55.3	39.5	36.8	47.7	48.9	59.9
PEt <sub>3</sub>	51.3	34.9	29.8	39.9	54.4	64.6
PiPr <sub>3</sub>	35.6	19.7	14.9	23.6	48.0	56.7
PCy <sub>3</sub>	34.4	17.2	13.0	17.2	52.1	56.2
PPh <sub>3</sub>	36.3	24.9	17.1	20.6	50.0	53.5
P(p-F-C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub>	36.5	23.5	17.8	20.0	50.4	52.6
P(p-MeO-C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub>	39.0	24.7	20.0	21.6	53.4	54.9
P(p-tolyl) <sub>3</sub>	37.6	25.7	21.4	21.8	54.0	54.5
P(p-Cl-C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub>	34.8	23.1	17.4	18.4	49.6	50.6
P(p-F <sub>3</sub> C-C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub>	33.4	21.0	15.5	16.6	48.3	49.4
P(OMe) <sub>3</sub> <sup>a</sup>	45.9	31.4	22.6	25.0	36.8	39.2
P(OPh) <sub>3</sub> <sup>a</sup>	35.5	19.3	14.4	10.8	41.0	37.5
P(pyr) <sub>3</sub> (pyr = NC <sub>4</sub> H <sub>4</sub> )	30.3	18.6	11.8	13.0	41.9	43.1
P(pyrd) <sub>3</sub> (pyrd = NC <sub>4</sub> H <sub>8</sub> )	44.0	26.0	18.4	24.8	58.2	64.6
PPh <sub>2</sub> Me	45.6	28.7	24.5	29.3	49.0	53.8
PPhMe <sub>2</sub>	52.5	39.6	36.7	43.0	55.4	61.7
PPh <sub>2</sub> Et	45.2	25.0	21.3	25.5	52.0	56.2
P(CH <sub>2</sub> Ph) <sub>3</sub>	40.7	25.7	23.2	20.1	61.6	58.5
PPh <sub>2</sub> pyr	34.4	15.5	10.5	10.6	43.2	43.2
PPh(pyr) <sub>2</sub>	31.1	20.8	15.0	11.0	45.0	41.1
PPh <sub>2</sub> Cy	38.8	22.5	18.7	21.7	53.5	56.5
PPhCy <sub>2</sub>	34.6	17.8	15.6	14.7	53.5	52.6
PiBu <sub>3</sub>	39.6	19.8	14.4	20.9	47.5	54.1

<sup>a</sup> Not included in analysis

b) Calculated energies and corrections for ligands (Hartree)

L	BP86/BS1	BP86/BS2	Solv	Disp
PMe <sub>3</sub>	-461.1001	-461.1584	0.004022	-0.01048345
PEt <sub>3</sub>	-579.0241	-579.1095	0.00642	-0.024131781
PiPr <sub>3</sub>	-696.945638	-697.0567	0.009779	-0.047741048
PCy <sub>3</sub>	-1047.138731	-1047.3261	0.005465	-0.092786664
PPh <sub>3</sub>	-1036.2800	-1036.4697	-0.00417	-0.041847396
P(p-F-C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub>	-1333.9872	-1334.2891	-0.00395	-0.043233438
P(p-MeO-C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub>	-1379.8503	-1380.1393	8.59E-05	-0.059740734
P(p-tolyl) <sub>3</sub>	-1154.2240	-1154.4365	0.004358	-0.055251755
P(p-Cl-C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub>	-2415.1569	-2415.4424	-0.00369	-0.04547713
P(p-F <sub>3</sub> C-C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub>	-2047.3886	-2047.9318	-0.00049	-0.059390824
P(OMe) <sub>3</sub> <sup>a</sup>	-686.7832	-686.9181	0.003502	-0.012831969
P(OPh) <sub>3</sub> <sup>a</sup>	-1261.9953	-1262.2553	-0.00466	-0.040435596
P(pyr) <sub>3</sub> (pyr = NC <sub>4</sub> H <sub>4</sub> )	-970.0766	-970.2622	-0.00569	-0.032836473
P(pyrd) <sub>3</sub> (pyrd = NC <sub>4</sub> H <sub>8</sub> )	-977.3149	-977.5009	0.005673	-0.059413672
PPh <sub>2</sub> Me	-844.5529	-844.6985	-0.00255	-0.030900897
PPhMe <sub>2</sub>	-652.8260	-652.9277	-2.5E-05	-0.020544574
PPh <sub>2</sub> Et	-883.8616	-884.0160	-0.00153	-0.036211907
P(CH <sub>2</sub> Ph) <sub>3</sub>	-1154.2182	-1154.4362	-0.00502	-0.054276844
PPh <sub>2</sub> pyr	-1014.2125	-1014.4008	-0.00503	-0.039012914
PPh(pyr) <sub>2</sub>	-992.1461	-992.3329	-0.00577	-0.035760812
PPh <sub>2</sub> Cy	-1039.9017	-1040.0901	-0.00168	-0.058330824
PPhCy <sub>2</sub>	-1043.5226	-1043.7104	0.001612	-0.0753553
PiBu <sub>3</sub>	-814.885415	-815.0243	0.015626	-0.057077369

<sup>a</sup> Not included in analysis

c) Calculated energies and corrections for complexes (Hartree)

L	BP86/BS1	BP86/BS2	Solv	Disp
PMe <sub>3</sub>	-1865.1485	-1865.3573	-0.0040827	-0.078015551
PEt <sub>3</sub>	-1983.06883	-1983.3029	-0.0010436	-0.101636106
PiPr <sub>3</sub>	-2100.9782	-2101.2382	0.0034833	-0.131987783
PCy <sub>3</sub>	-2451.1693	-2451.5061	0.0027276	-0.18173903
PPh <sub>3</sub>	-2440.31668	-2440.6530	-0.0063541	-0.125907644
P(p-F-C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub>	-2738.0228	-2738.4729	-0.0051452	-0.1270666
P(p-MeO-C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub>	-2783.8868	-2784.3249	-0.00055414	-0.144193743
P(p-tolyl) <sub>3</sub>	-2558.26135	-2558.6232	0.00456086	-0.139154737
P(p-Cl-C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub>	-3819.1922	-3819.6259	-0.0038929	-0.129037323
P(p-F <sub>3</sub> C-C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub>	-3451.4222	-3452.1137	-0.0007475	-0.143441859
P(OMe) <sub>3</sub> <sup>a</sup>	-2090.8251	-2091.1058	0.002225172	-0.082028033
P(OPh) <sub>3</sub> <sup>a</sup>	-2666.0276	-2666.4364	-0.0012238	-0.11951272
P(pyr) <sub>3</sub> (pyr = NC <sub>4</sub> H <sub>4</sub> )	-2374.1084	-2374.4412	-0.00605309	-0.114727828
P(pyrd) <sub>3</sub> (pyrd = NC <sub>4</sub> H <sub>8</sub> )	-2381.3526	-2381.6851	0.00112921	-0.1489846
PPh <sub>2</sub> Me	-2248.5927	-2248.8877	-0.00573613	-0.108261921
PPhMe <sub>2</sub>	-2056.8744	-2057.1266	-0.004397605	-0.093302894
PPh <sub>2</sub> Et	-2287.8984	-2288.2026	-0.00429009	-0.118471157
P(CH <sub>2</sub> Ph) <sub>3</sub>	-2558.2556	-2558.6244	-0.00192513	-0.142707113
PPh <sub>2</sub> pyr	-2418.2417	-2418.5788	-0.00445617	-0.122916782
PPh(pyr) <sub>2</sub>	-2396.1795	-2396.5145	-0.00204447	-0.117579647
PPh <sub>2</sub> Cy	-2443.9365	-2444.2746	-0.00349225	-0.143892279
PPhCy <sub>2</sub>	-2447.5537	-2447.8925	0.002964	-0.163411369
PiBu <sub>3</sub>	-2218.9181	-2219.2054	0.011025247	-0.141339714
[RuCl <sub>2</sub> (p-cymene)] <sub>2</sub>	-2808.033761	-2808.33925	0.0011894	-0.115734863

<sup>a</sup> Not included in analysis

**Table S2** Pd-P bond lengths (Å) in [PdL<sub>n</sub>] complexes, where L = PPh<sub>3</sub> and of [Pd(binap)<sub>n</sub>] complexes

Complex	B3LYP	BP86	M06	M06-L
PdL <sub>4</sub>	2.551, 2.534, 2.536, 2.546	2.475, 2.481, 2.479, 2.477	2.481, 2.484, 2.484, 2.487	2.458, 2.460, 2.461, 2.466
PdL <sub>3</sub>	2.386, 2.385, 2.381	2.347, 2.350, 2.361	2.362, 2.367, 2.373	2.331, 2.333, 2.338
PdL <sub>2</sub>	2.315, 2.314	2.292, 2.294	2.312, 2.313	2.291, 2.292
Pd(binap) <sub>2</sub>	2.481, 2.476, 2.469, 2.474	2.420, 2.424, 2.428, 2.426	2.452, 2.455, 2.447, 2.453	2.413, 2.413, 2.408, 2.418
Pd(binap)	2.292, 2.292	2.263, 2.267	2.310, 2.312	2.274, 2.280

**Table S3** LKB-P Ligand dissociation energies for [PdCl<sub>3</sub>L]<sup>-</sup> and [Pt(PH<sub>3</sub>)<sub>3</sub>L] calculated with BP86 and BP86-D, He<sub>8</sub>\_steric and Δ<sub>vdw</sub>. See supporting information of reference 1 at [http://pubs.acs.org/doi/suppl/10.1021/om100648v/suppl\\_file/om100648v\\_si\\_001.pdf](http://pubs.acs.org/doi/suppl/10.1021/om100648v/suppl_file/om100648v_si_001.pdf) for ligand numbers used here.

No.	BE(Pd), kcal mol <sup>-1</sup>	BE(Pt), kcal mol <sup>-1</sup>	He <sub>8</sub> _steric, kcal mol <sup>-1</sup>	BE <sub>vdw</sub> (Pd), kcal mol <sup>-1</sup>	BE <sub>vdw</sub> (Pt), kcal mol <sup>-1</sup>	Δ <sub>vdw</sub> (Pd), kcal mol <sup>-1</sup>	Δ <sub>vdw</sub> (Pt), kcal mol <sup>-1</sup>
1	29.1	8.8	2.3	32.1	16.3	3.0	7.5
2	38.5	12.9	3.0	46.2	24.2	7.7	11.3
3	32.3	22.8	3.0	41.7	38.0	9.4	15.2
4	16.4	16.6	20.7	28.4	36.8	12.0	20.2
5	37.0	17.1	6.0	48.4	33.1	11.4	16.0
6	27.7	20.4	9.9	39.7	39.1	12.0	18.7
7	40.1	16.6	7.5	52.4	33.7	12.3	17.2
8	30.9	14.0	11.6	40.6	28.9	9.7	15.0
9	37.3	16.6	6.1	49.4	33.3	12.1	16.7
10	37.2	14.4	12.2	52.1	33.4	14.9	19.0
11	42.4	15.4	9.1	55.7	33.8	13.3	18.4
12	43.5	17.0	6.1	56.0	34.1	12.5	17.0
13	37.2	16.7	6.1	49.4	33.7	12.2	17.0
14	35.6	9.1	19.1	52.6	30.2	17.0	21.1
15	30.0	11.7	37.8	46.6	33.2	16.5	21.5
16	23.9	9.8	23.4	49.0	43.1	25.1	33.3
17	29.3	14.5	7.7	40.2	30.2	10.9	15.7
18	40.9	16.2	4.5	54.6	33.0	13.7	16.8
19	28.3	4.3	31.3	47.7	29.6	19.5	25.3
20	35.3	15.1	9.2	50.5	35.6	15.3	20.5
21	36.8	13.3	16.7	53.0	33.2	16.2	19.9
22	38.8	13.3	12.7	53.9	33.4	15.2	20.1
23	29.9	10.5	2.1	34.2	19.4	4.3	8.9
24	36.5	12.0	2.6	42.6	22.0	6.0	10.0
25	36.3	18.1	2.1	44.5	30.9	8.1	12.8
26	38.7	16.8	3.6	47.6	29.9	8.9	13.1
27	38.3	16.7	3.0	46.4	29.5	8.2	12.8
28	39.3	16.3	3.9	49.5	30.4	10.2	14.1
29	38.9	16.9	3.9	48.6	30.9	9.7	14.0
30	37.7	15.7	4.7	48.6	31.2	10.9	15.5
31	39.6	15.6	4.6	49.9	30.1	10.3	14.6
32	34.5	20.0	2.7	43.0	33.7	8.4	13.7
33	36.3	17.0	4.3	46.4	31.5	10.1	14.5
34	36.2	15.6	3.1	45.1	29.6	8.9	14.0
35	39.9	13.0	5.4	51.9	28.6	12.0	15.7
36	34.8	12.0	19.7	49.8	32.4	15.1	20.4
37	35.7	12.4	18.5	51.6	33.9	15.9	21.5
38	30.2	12.5	25.9	45.7	33.8	15.5	21.3
39	31.2	11.9	16.7	46.7	33.6	15.5	21.7
40	36.0	13.4	15.0	51.0	33.9	15.0	20.5

41	21.8	9.5	21.0	36.7	32.6	14.9	23.2
42	29.1	7.9	30.2	47.4	32.3	18.3	24.4
43	34.0	8.2	22.9	51.2	31.4	17.3	23.2
44	35.8	11.3	22.6	53.9	35.6	18.1	24.3
45	23.5	9.5	30.4	40.5	35.0	17.0	25.5
46	28.7	7.5	28.5	45.8	31.3	17.1	23.8
47	28.3	7.3	27.5	45.7	32.4	17.4	25.1
48	39.3	15.4	7.8	52.2	33.5	13.0	18.1
49	34.9	11.3	20.8	50.9	33.3	16.1	22.0
50	38.2	14.1	18.5	53.5	34.9	15.2	20.8
51	36.7	7.5	15.4	53.7	29.5	17.0	22.1
52	36.2	11.1	26.4	56.4	37.0	20.2	26.0
53	36.6	13.6	11.3	50.5	33.1	13.8	19.5
54	36.5	13.6	19.3	54.9	37.1	18.4	23.5
55	23.9	8.6	32.2	41.5	35.2	17.6	26.6
56	34.3	13.1	3.8	43.5	26.3	9.2	13.2
57	36.6	16.4	3.7	45.4	29.3	8.8	12.9
58	31.6	19.8	4.1	41.2	34.6	9.6	14.9
59	31.3	13.1	5.6	42.6	29.3	11.2	16.2
60	29.8	8.2	24.2	50.5	35.4	20.7	27.2
61	17.1	3.0	44.9	39.8	31.9	22.7	28.9
62	28.4	3.3	12.3	42.8	23.4	14.5	20.1
63	31.9	16.9	8.0	45.0	35.5	13.1	18.6
64	28.1	13.3	11.1	42.6	33.4	14.6	20.1
65	33.3	17.4	7.4	46.4	35.9	13.1	18.5
66	35.3	16.8	8.3	48.6	35.3	13.3	18.5
67	21.3	5.7	23.6	38.2	28.8	16.9	23.1
68	33.6	14.2	8.2	47.1	32.8	13.5	18.7
69	37.1	17.0	8.2	50.4	35.7	13.3	18.7
70	32.7	11.9	11.6	48.5	33.1	15.8	21.2
71	47.6	17.5	6.3	62.4	36.6	14.8	19.0
72	31.4	12.6	5.4	42.1	30.4	10.7	17.8
73	25.9	6.3	30.1	44.2	31.5	18.4	25.2
74	31.3	16.1	8.1	44.9	35.3	13.6	19.2
75	32.1	18.3	6.6	45.1	36.5	13.0	18.2
76	22.5	8.2	16.5	40.3	31.3	17.8	23.1
77	30.2	15.9	7.7	43.4	34.9	13.2	18.9
78	30.7	16.2	8.3	44.0	34.8	13.3	18.6
79	18.4	3.3	30.7	39.4	30.5	21.0	27.2
80	38.4	17.1	7.7	51.7	35.7	13.3	18.6
81	28.0	13.1	8.6	41.3	31.3	13.3	18.2
82	25.5	18.8	7.2	55.9	38.4	30.4	19.6
83	32.5	17.1	8.4	46.3		13.8	
84	32.6	14.8	8.2	45.9	34.2	13.3	19.4
85	36.4	13.0	9.7	55.0	38.0	18.7	25.0
86	25.8	8.2	23.5	46.4	34.9	20.5	26.7

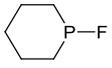
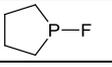
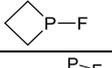
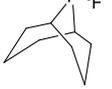
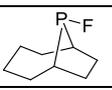
87	35.3	17.0	8.4	48.8	35.9	13.5	18.9
88	41.2	17.3	7.7	55.8	36.4	14.6	19.0
89	31.6	14.4	12.3	55.4	44.2	23.8	29.8
90	29.0	13.6	9.1	42.6	33.4	13.6	19.9
91	28.0	13.1	12.6	43.0	33.9	15.1	20.9
92	33.2	13.0	8.0	46.2	30.8	13.0	17.8
93	33.7	14.2	8.5	48.6	34.6	15.0	20.4
94	29.7	12.0	9.2	44.1	31.9	14.4	19.9
95	30.0	10.9	20.5	46.8	34.1	16.8	23.2
96	24.7	10.9	14.4	40.7	32.6	16.0	21.7
97	35.3	16.0	4.8	46.1	32.2	10.8	16.1
98	31.8	18.9	3.8	44.3	36.7	12.5	17.9
99	33.9	16.1	5.4	46.3	33.8	12.4	17.7
100	35.4	16.4	4.0	47.3	33.9	11.9	17.5
101	33.8	15.6	9.4	47.8	34.9	14.0	19.2
102	31.8	14.4	9.2	46.6	35.0	14.9	20.6
103	33.9	14.9	10.9	47.1	34.8	13.2	20.0
104	34.7	15.7	6.8	48.5	35.0	13.7	19.3
105	32.2	12.4	10.9	49.2	35.2	17.0	22.8
106	29.8	11.7	12.7	47.3	35.1	17.5	23.4
107	37.3	16.5	3.2	46.4	30.5	9.1	14.0
108	31.7	19.3	6.2	42.6	35.1	10.9	15.8
109	37.4	15.8	7.3	49.5	32.6	12.1	16.8
110	35.5	12.2	7.0	46.3	28.0	10.8	15.8
111	36.2	14.8	10.5	50.4	33.9	14.2	19.1
112	31.4	11.2	22.9	48.4	34.5	17.0	23.3
113	35.1	11.3	15.9	51.5	31.9	16.5	20.6
114	35.7	13.7	12.5	44.3	30.1	8.6	16.4
115	37.6	11.9	9.3	53.3	32.9	15.7	21.0
116	31.2	4.8	30.2	49.3	28.8	18.1	24.0
117	37.2	12.7	4.3	47.1	26.7	9.9	14.0
118	36.5	12.4	4.6	46.3	26.1	9.7	13.7
119	31.2	11.8	24.4	49.2	36.2	18.0	24.4
120	29.1	2.5	34.4	50.9	30.3	21.8	27.8
121	29.2	3.1	34.6	51.2	31.0	21.9	28.0
122	40.6	8.7	16.8	61.4	33.7	20.8	25.0
123	29.5	5.6	29.2	50.0		20.5	
124	38.1	15.8	4.9	49.3	32.1	11.2	16.2
125	37.3	15.9	2.9	46.7	29.7	9.5	13.8
126	36.5	11.3	5.8	47.8	27.7	11.3	16.4
127	35.3	12.1	6.2	46.3	28.6	11.0	16.5
128	37.1	16.1	7.1	51.0	35.8	13.9	19.7
129	38.5	15.3	7.7	52.7	35.4	14.2	20.1
130	36.2	13.2	14.0	51.8	33.8	15.6	20.5
131	30.6	6.6	25.7	47.9	29.9	17.4	23.4
132	37.7	15.4	12.2	52.2	35.8	14.5	20.3

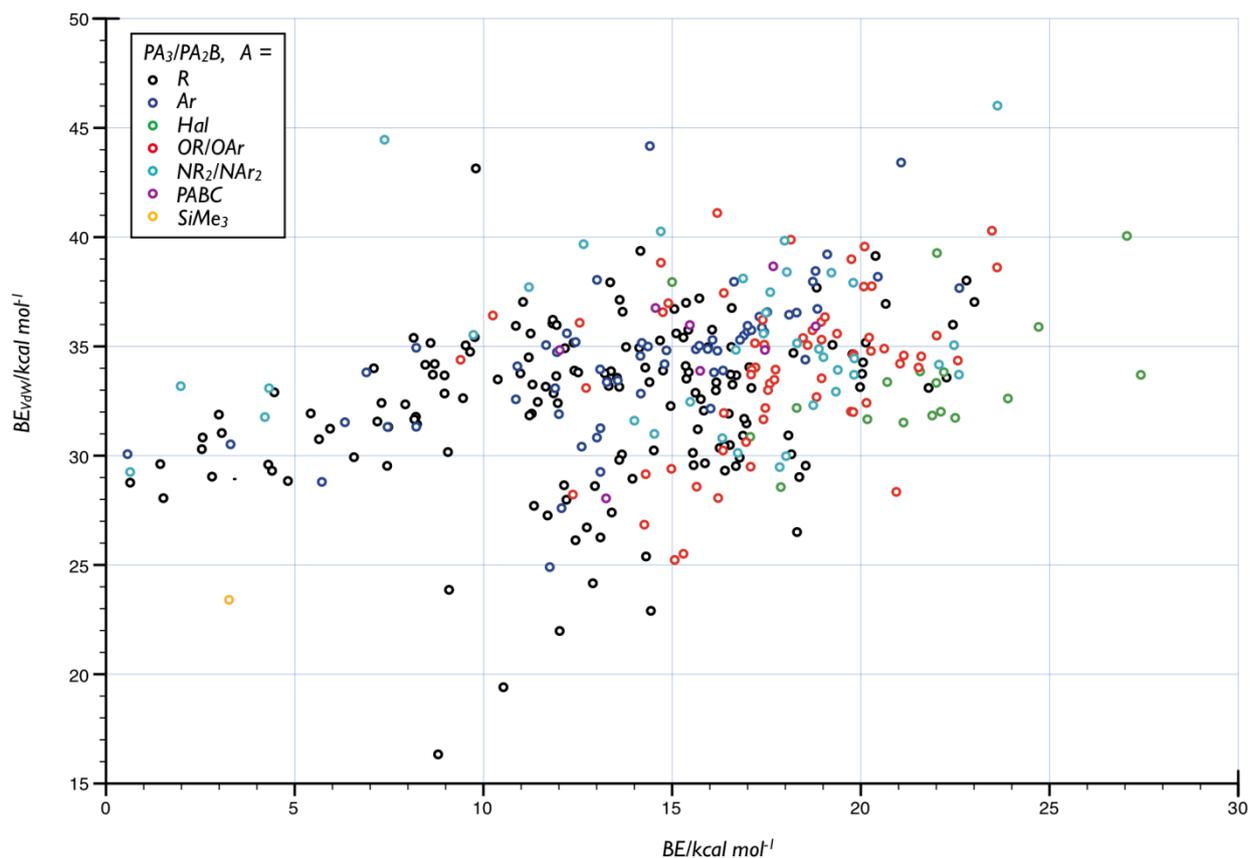
133	37.2	15.4	12.1	52.4	37.0	15.2	21.6
134	29.9	11.9	18.0	45.9	36.0	16.0	24.0
135	35.1	11.8	3.1	44.5	24.9	9.4	13.1
136	33.3	12.1	4.5	44.9	27.6	11.6	15.5
137	39.4	15.4	8.4	52.6	34.1	13.2	18.7
138	37.0	16.4	3.0	46.5	30.4	9.5	14.1
139	42.9	13.6	7.2	54.4	29.8	11.5	16.2
140	30.2	12.4	11.9	46.3	35.2	16.1	22.8
141	35.5	14.2	16.6	53.2	39.4	17.7	25.2
142	31.8	10.9	27.7	49.2	35.9	17.4	25.1
143	33.6	11.0	18.1	50.2	33.8	16.6	22.8
144	39.3	13.5	12.0	54.4	33.6	15.1	20.0
145	36.8	16.9	3.4	47.3	31.7	10.5	14.8
146	40.3	11.7	4.8	51.4	27.3	11.1	15.6
147	41.0	16.5	3.7	51.1	31.9	10.1	15.4
148	38.5	12.2	5.9				
149	39.9	13.4	3.4	49.2	27.4	9.3	14.0
150	38.5	20.7	4.6	49.2	36.9	10.7	16.3
151	32.7	15.0	6.0	44.0	32.3	11.3	17.3
152	37.1	15.6	5.9	48.8	32.9	11.7	17.3
153	33.4	16.6	7.7	46.1	35.0	12.8	18.4
154	31.6	11.4	10.8	45.2	32.5	13.6	21.0
155	33.3	9.0	16.7	50.1	32.8	16.8	23.9
156	33.9	12.2	17.6	49.5	34.9	15.6	22.8
157	31.7	13.8	10.9	45.9	35.0	14.2	21.2
158	32.3	11.2	10.5	45.8	31.8	13.5	20.6
159	35.7	9.1	8.3	48.7	23.9	13.0	14.8
160	32.8	7.2	22.4	51.4	31.6	18.7	24.4
161	29.8	9.0	19.2	48.9	33.7	19.1	24.7
162	22.5	-0.4	45.9	45.0	27.5	22.5	27.9
163	34.2	8.2	20.8	54.1	31.7	19.9	23.5
164	34.8	10.4	21.4	53.3	33.5	18.5	23.1
165	28.0	12.2	13.6	45.5	35.6	17.5	23.4
166	22.4	-0.4	43.0	45.1	28.8	22.8	29.1
167	28.2	5.6	23.5	47.4	30.8	19.2	25.1
168	25.4	1.5	43.7	48.9	28.1	23.5	26.5
169	27.1	9.8	26.1	45.9	35.4	18.8	25.7
170	26.9	7.5	16.2	44.9	31.3	18.0	23.9
171	24.3	1.4	31.7	43.5	29.6	19.2	28.2
172	19.0	-0.7	47.9	42.2	24.7	23.2	25.4
173	29.3	4.4	24.1	51.7	29.3	22.4	24.9
174	20.7	-0.8	48.7	40.9	24.3	20.3	25.1
175	34.3	11.8	18.0	54.5	36.1	20.1	24.2
176	16.6	0.6	28.0	39.7	30.1	23.1	29.5
177	30.0	0.6	29.1	50.0	28.8	20.0	28.1
178	30.3	2.8	33.2	50.6	29.0	20.4	26.2

179	24.8	-0.4	34.6	46.8	27.1	22.0	27.5
180	31.3	8.7	22.2	52.8	34.2	21.5	25.5
181	24.4	2.6	37.5	46.2	30.8	21.8	28.3
182	31.1	8.2	19.9	50.8	31.8	19.8	23.6
183	28.6	9.6	16.8	47.8	34.8	19.2	25.1
184	37.5	7.1	24.9	57.9	34.0	20.4	26.9
185	30.7	5.4	25.3	50.7	31.9	19.9	26.5
186	27.3	6.9	20.4	49.7	33.8	22.4	26.9
187	30.0	5.9	29.0	50.6	31.2	20.6	25.3
188	31.7	13.7	16.0	49.0	36.6	17.3	22.9
189	37.0	22.5	1.5	41.5	31.7	4.5	9.2
190	29.9	22.0	2.2	35.8	33.3	5.9	11.3
191	30.3	27.1	3.1	37.1	40.1	6.8	13.0
192	30.7	27.4	4.1	31.8	33.7	1.1	6.3
193	43.2	23.9	1.6	47.2	32.6	4.0	8.7
194	41.2	22.1	1.2	46.8	32.0	5.6	9.9
195	36.2	21.1	1.7	42.0	31.5	5.9	10.4
196	41.6	24.7	2.2	48.1	35.9	6.5	11.2
197	35.9	21.6	2.5	43.7	33.9	7.7	12.3
198	39.0	20.7	2.5	46.9	33.4	8.0	12.7
199	39.6	22.2	2.4	46.7	33.8	7.1	11.6
200	35.4	21.9	1.9	40.2	31.8	4.8	9.9
201	33.6	20.2	2.4	40.1	31.7	6.5	11.5
202	28.8	17.9	2.1	35.3	28.6	6.5	10.7
203	28.6	17.1	4.3	36.9	30.9	8.4	13.8
204	31.6	18.3	3.7	40.9	32.2	9.3	13.9
205	40.3	18.3	1.9	43.8	26.5	3.5	8.2
206	41.1	18.4	2.5	47.8	29.0	6.7	10.7
207	33.2	22.6	2.5	40.2	34.4	7.0	11.8
208	41.7	22.4	3.3	50.8	36.0	9.0	13.6
209	37.8	19.0	4.3	48.7	34.5	11.0	15.5
210	38.8	18.8	11.0	52.1	37.7	13.3	18.9
211	38.5	22.6	3.0	48.3	37.7	9.8	15.1
212	35.7	14.4	1.8	39.5	22.9	3.8	8.5
213	36.4	14.3	2.5	43.5	25.4	7.1	11.1
214	29.7	19.8	5.4	37.1	32.0	7.5	12.2
215	29.8	14.5	9.4	41.2	31.0	11.4	16.5
216	31.4	14.3	12.8	45.4	34.0	14.0	19.7
217	35.6	16.2	7.2	47.6	33.4	12.0	17.2
218	38.0	20.9	4.2	44.7	28.3	6.7	7.4
219	32.5	23.5	5.1	42.7	40.3	10.2	16.8
220	34.4	21.6	3.0	41.9	34.5	7.5	12.9
221	40.9	23.6	3.1	50.1	38.6	9.1	15.0
222	36.0	18.6	4.4	48.1	35.1	12.2	16.5
223	35.0	17.7	7.1	46.2	33.5	11.1	15.8
224	36.1	20.6	4.4	49.2	34.9	13.1	14.3

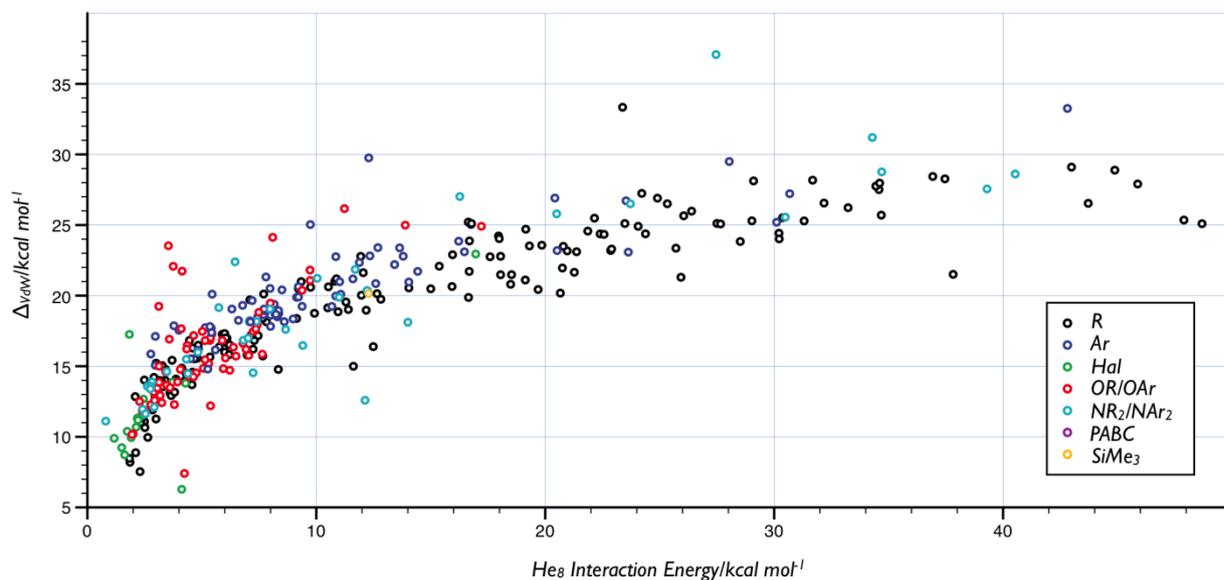
225	32.8	12.7	9.4	47.7	33.1	14.9	20.4
226	19.4	15.0	17.0	35.0	37.9	15.6	22.9
227	36.3	19.4	4.3	47.8	35.6	11.5	16.2
228	35.6	19.0	4.6	48.8	36.1	13.2	17.2
229	31.8	19.8	5.9	43.0	34.6	11.2	14.8
230	37.1	20.3	5.0	49.0	37.8	12.0	17.5
231	41.4	22.0	1.8	55.1	39.3	13.7	17.3
232	33.9	16.4	9.7	48.4	37.4	14.5	21.1
233	31.2	17.2	5.4	43.4	34.0	12.1	16.8
234	31.9	17.1	5.9	43.5	33.9	11.6	16.8
235	43.8	19.1	5.4	55.5	36.3	11.7	17.3
236	35.8	14.9	3.8	48.0	37.0	12.1	22.1
237	29.8	10.3	11.2	51.3	36.4	21.5	26.2
238	26.7	12.6	3.5	45.1	36.1	18.3	23.5
239	31.9	14.7	8.1	47.9	38.8	16.0	24.1
240	29.9	15.7	3.2	38.0	28.6	8.1	12.9
241	35.9	17.1	3.3	43.8	29.5	7.9	12.4
242	34.0	22.0	3.6	42.4	35.5	8.4	13.5
243	35.2	19.0	6.4	46.9	35.3	11.7	16.3
244	40.2	17.5	7.2	52.6	34.9	12.4	17.5
245	35.1	16.4	3.9	44.3	30.2	9.2	13.9
246	35.0	18.7	5.4	46.8	35.7	11.7	17.0
247	30.8	17.4	7.5	43.1	36.2	12.4	18.8
248	33.8	19.8	3.1	48.7	39.0	14.9	19.2
249	34.0	20.1	4.1	45.4	37.7	11.4	17.7
250	33.7	16.0	11.4	47.2	35.0	13.6	19.0
251	36.2	18.2	4.8	48.1	34.7	11.9	16.5
252	41.7	20.0	3.8	50.8	33.1	9.1	13.2
253	37.1	23.0	2.5	44.7	37.0	7.6	14.0
254	36.3	15.7	18.1	52.2	37.2	15.9	21.5
255	32.4	14.7	9.8	47.3	35.3	14.9	20.6
256	37.3	20.5	5.2	49.5	38.2	12.2	17.7
257	37.0	18.1	9.0	50.6	36.5	13.6	18.4
258	38.1	18.1	9.4	53.2		15.1	
259	33.4	13.4	21.9	52.3	37.9	18.9	24.6
260	35.0	19.1	5.5	49.0	39.2	14.1	20.1
261	35.6	16.6	7.8	50.5	38.0	14.9	21.3
262	39.6	21.1	11.9	56.1	43.4	16.6	22.3
263	31.9	19.7	3.8	39.4	32.0	7.5	12.3
264	32.1	17.0	3.5	40.8	30.6	8.8	13.7
265	33.9	21.5	2.3	41.5	34.0	7.7	12.5
266	32.5	16.4	6.0	43.0	32.0	10.5	15.6
267	30.7	20.2	2.8	38.1	32.4	7.4	12.3
268	35.2	15.0	4.7	44.8	29.4	9.6	14.4
269	30.1	16.2	2.4	37.8	28.1	7.7	11.8
270	32.3	14.3	5.1	42.2	29.2	9.9	14.9

271	37.1	11.2	23.7	54.6	37.7	17.5	26.5
272	36.3	21.0	2.9	44.1	34.2	7.8	13.2
273	36.0	20.3	4.8	45.6	34.8	9.7	14.5
274	32.9	17.6	6.5	43.4	33.3	10.5	15.7
275	35.9	20.2	5.3	45.8	35.4	9.9	15.2
276	12.6	9.4	13.9	29.0	34.4	16.4	25.0
277	32.0	17.1	6.8	43.0	33.7	11.0	16.6
278	36.8	21.1	3.1	44.8	34.6	8.0	13.4
279	33.4	17.7	6.9	44.1	33.9	10.8	16.2
280	36.3	17.5	5.1	46.4	33.0	10.2	15.5
281	37.6	18.8	3.1	47.7	32.7	10.1	13.9
282	34.8	17.4	7.4	46.4	35.1	11.7	17.6
283	35.4	14.8	9.7	51.7	36.6	16.3	21.8
284	33.0	17.2	7.4	45.2	35.1	12.1	18.0
285	35.1	20.1	8.0	48.6	39.6	13.5	19.5
286	34.5	19.0	3.4	44.7	33.5	10.2	14.6
287	34.2	14.3	2.9	42.7	26.8	8.5	12.6
288	24.6	15.3	2.0	30.1	25.5	5.5	10.2
289	24.5	15.1	1.9	30.0	25.2	5.5	10.2
290	32.0	17.4	4.6	41.6	31.7	9.6	14.2
291	48.3	22.6	0.8	55.7	33.7	7.4	11.1
292	34.4	22.5	12.1	46.7	35.1	12.4	12.6
293	16.1	0.6	40.5	35.1	29.3	19.1	28.6
294	33.3	19.4	7.2	45.9	33.9	12.6	14.5
295	39.9	17.6	11.0	54.0	37.5	14.1	19.9
296	43.7	23.6	6.5	61.3	46.0	17.7	22.4
297	34.7	19.8	14.0	52.3	37.9	17.6	18.1
298	21.0	-0.5	42.8	47.8	32.8	26.8	33.3
299	27.8	7.4	27.5	56.1	44.5	28.3	37.1
300	35.6	15.5	7.0	48.0	32.5	12.4	17.0
301	38.6	16.7	7.1	51.2	34.8	12.7	18.2
302	47.3	22.1	2.9	55.2	34.2	7.9	12.1
303	27.2	4.3	34.7	49.0	33.1	21.8	28.8
304	30.4	4.2	39.3	51.6	31.8	21.2	27.6
305	35.7	19.8	3.5	45.1	34.4	9.4	14.6
306	33.0	17.4	7.4	45.9	35.6	12.9	18.2
307	29.5	19.2	5.7	44.1	38.4	14.6	19.2
308	36.6	18.0	12.2	52.1	38.4	15.5	20.4
309	33.1	16.9	10.0	50.0	38.1	16.9	21.2
310	24.6	2.0	34.3	45.4	33.2	20.8	31.2
311	30.8	12.7	16.3	51.0	39.7	20.2	27.0
312	26.2	9.7	20.5	45.0	35.5	18.8	25.8
313	42.4	18.5	2.8	52.4	34.4	10.0	15.9
314	42.6	18.2	2.9	50.1	30.1	7.5	11.9
315	33.7	17.5	6.2	43.4	32.2	9.7	14.7
316	39.9	16.7	2.8	48.6	30.1	8.7	13.4

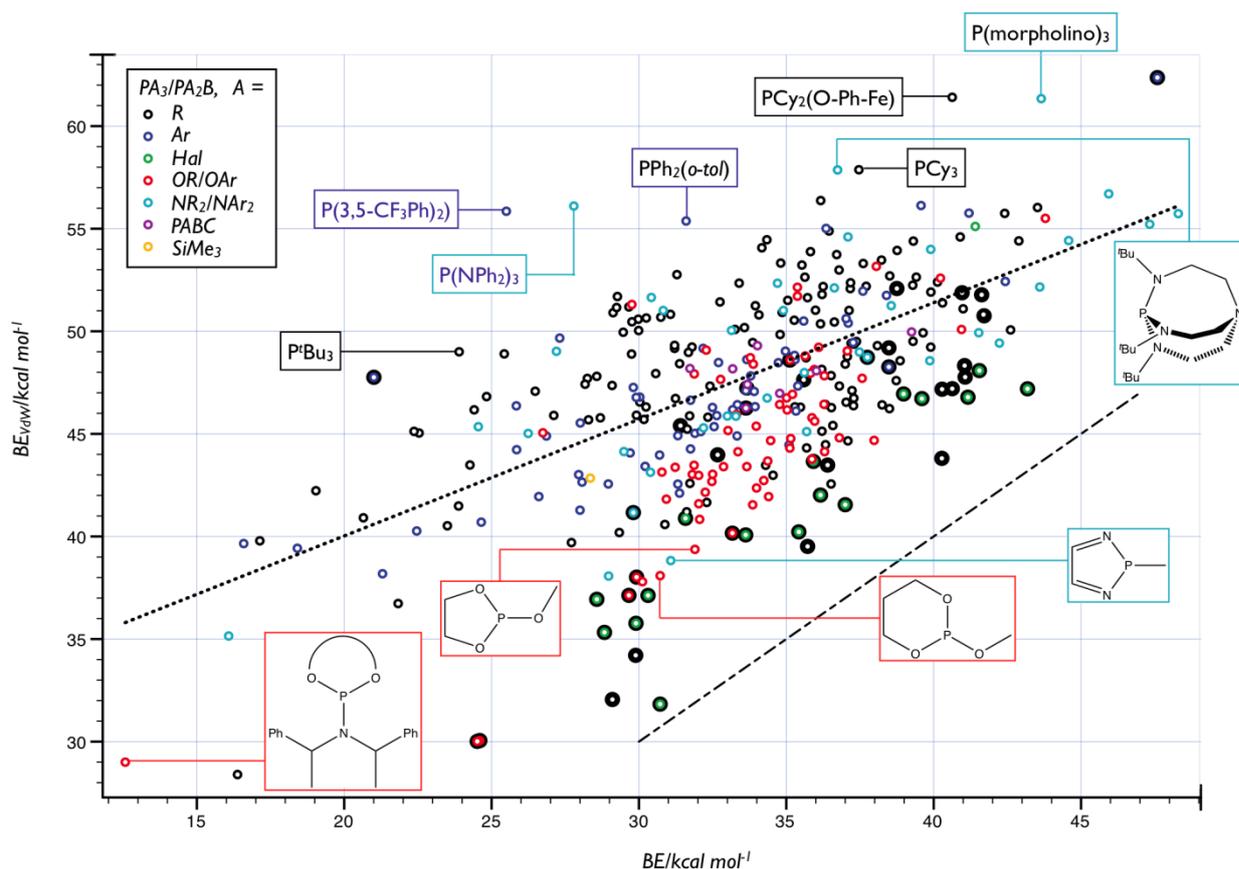
317	26.5	8.5	34.7	47.1	34.2	20.6	25.7
318	34.1	15.1	21.3	50.8	36.7	16.7	21.7
319	34.4	19.8	4.1	43.7	34.6	9.3	14.8
320	32.6	17.4	7.1	45.4	35.7	12.8	18.2
321	33.3	18.5	3.6	45.9	35.4	12.6	16.9
322	37.6	18.7	10.7	52.0	38.0	14.4	19.2
323	30.9	12.4	7.6	41.8	28.2	10.9	15.9
324	29.7	4.5	36.9	51.2	32.9	21.5	28.4
325	29.9	11.9	13.8	46.8	34.7	16.9	22.8
326	26.6	14.2	14.0	41.9	35.2	15.3	21.0
327	42.2	17.9	2.5	49.4	29.5	7.2	11.6
328	44.6	16.3	4.4	54.4	30.8	9.8	14.5
329	43.6	19.8	2.8	52.2	33.7	8.6	13.9
330	37.5	18.3	6.8	49.0	35.1	11.5	16.8
331	30.4	17.5	8.0	43.1	36.5	12.7	19.1
332	31.1	18.0	2.4	38.8	30.0	7.7	12.0
333	29.0	18.7	2.6	38.1	32.3	9.1	13.6
334	45.9	18.9	4.8	56.7	34.9	10.8	16.0
335	41.5	19.3	2.8	49.9	32.9	8.4	13.6
336	32.2	14.0	8.7	45.3	31.6	13.1	17.6
337	34.9	18.0	11.7	51.0	39.8	16.1	21.9
338	36.7	14.7	30.5	57.9	40.3	21.1	25.6
339	36.0	18.8	3.0	48.1	35.9	12.1	17.1
340	33.6	15.7	7.1	46.3	33.9	12.6	18.1
341	34.8	17.5	5.4	47.0	34.8	12.2	17.4
342	39.3	13.3	5.3	50.0	28.0	10.7	14.8
343	31.7	12.0	12.3	48.2	34.8	16.5	22.8
344	33.2	17.7	11.0	48.2	38.7	15.0	21.0
345	34.0	14.6	13.4	49.3	36.8	15.3	22.2
346	33.7	15.5	8.0	47.4	36.0	13.7	20.5
347	32.3	16.2	17.2	49.1	41.1	16.8	24.9
348	35.4	18.1	4.1	52.1	39.9	16.8	21.7
	41.0	18.5	2.3	48.3	29.5	7.3	11.0
	40.3	21.8	2.4	47.2	33.1	6.9	11.3
	40.6	22.3	2.2	47.2	33.6	6.6	11.3
	41.6	20.1	2.9	51.8	34.3	10.2	14.2
	41.0	20.1	3.3	51.9	35.2	10.9	15.0



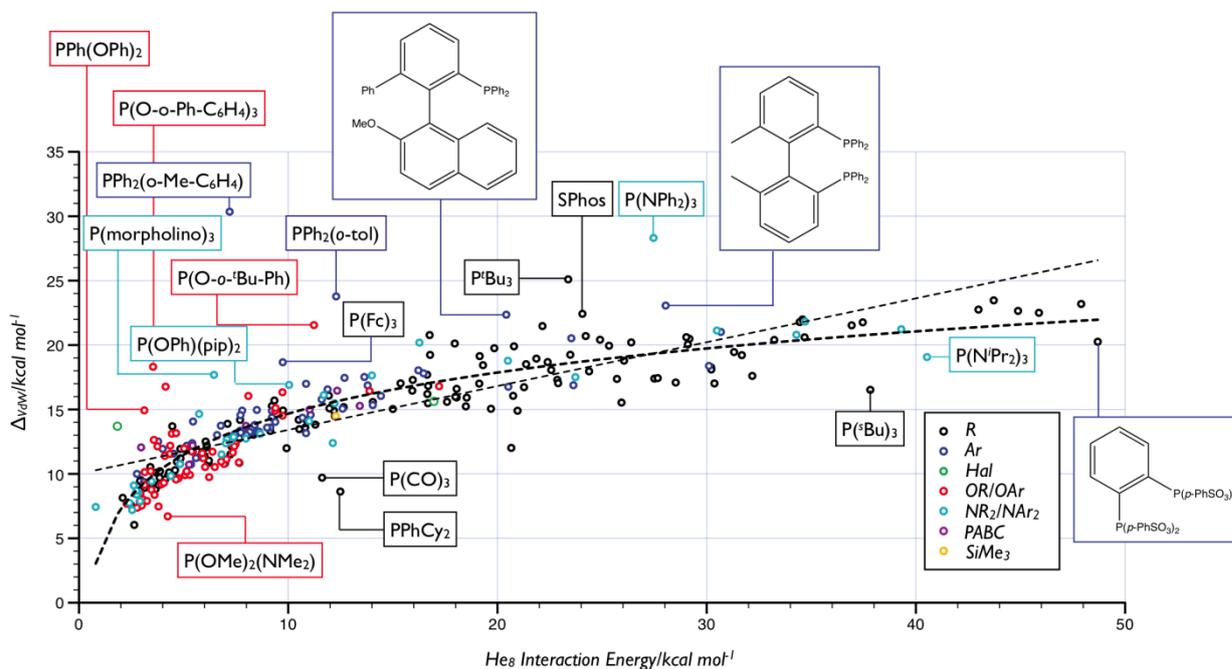
**Fig. S1** Ligand bond energy (kcal mol<sup>-1</sup>) in [Pt(PH<sub>3</sub>)<sub>3</sub>L] calculated at BP86 (BE) and BP86-D (BE<sub>vdW</sub>) level for ligands in LKB-P.



**Fig. S2** Relationship between difference in bond energy for [Pt(PH<sub>3</sub>)<sub>3</sub>L] (kcal mol<sup>-1</sup>) between BP86 and BP86-D, and the LKB-P He<sub>8</sub> steric descriptor (kcal mol<sup>-1</sup>).<sup>1</sup>



**Fig. S3** Ligand bond energy ( $\text{kcal mol}^{-1}$ ) in  $[\text{PdCl}_3\text{L}]^-$  calculated at BP86 (BE) and BP86-D ( $\text{BE}_{\text{vdW}}$ ) level for ligands in LKB-P. – Outliers identified.



**Fig. S4** Relationship between difference in bond energy for  $[\text{PdCl}_3\text{L}]^-$  ( $\text{kcal mol}^{-1}$ ) between BP86 and BP86-D, and the LKB-P  $\text{He}_8$  steric descriptor ( $\text{kcal mol}^{-1}$ ).<sup>1</sup> – Outliers identified.

## References:

1. a) N. Fey, A. C. Tsipis, S. E. Harris, J. N. Harvey, A. G. Orpen and R. A. Mansson, *Chem. Eur. J.*, 2006, **12**, 291-302; b) J. Jover, N. Fey, J. N. Harvey, G. C. Lloyd-Jones, A. G. Orpen, G. J. J. Owen-Smith, P. Murray, D. R. J. Hose, R. Osborne and M. Purdie, *Organometallics*, 2010, **29**, 6245-6258.
2. a) A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098-3100; b) J. P. Perdew, *Physical Review B*, 1986, **33**, 8822-8824; c) J. P. Perdew, *Physical Review B*, 1986, **34**, 7406; d) J. P. Perdew and A. Zunger, *Physical Review B*, 1981, **23**, 5048-5079; e) J. C. Slater, *Quantum Theory of Molecules and Solids, Vol. 4: The Self-Consistent Field for Molecules and Solids*, McGraw-Hill, New York, 1974.
3. a) Jaguar 6.0, Schrödinger-LLC, New York, NY, 2005; b) Jaguar 7.6, Schrödinger-LLC, New York, NY, 2009.
4. Gaussian 03, Revision B.04, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. Montgomery, J. A., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Pittsburgh PA 2003.
5. a) T. H. Dunning and P. J. Hay, ed. H. F. Schaefer III, Plenum, New York, 1976, vol. 3, pp. 1-28; b) P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 270-283; c) W. R. Wadt and P. J. Hay, *J. Chem. Phys.*, 1985, **82**, 284-298; d) P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299-310.
6. a) B. Marten, K. Kim, C. Cortis, R. A. Friesner, R. B. Murphy, M. N. Ringnalda, D. Sitkoff and B. Honig, *J. Phys. Chem.*, 1996, **100**, 11775; b) D. J. Tannor, B. Marten, R. B. Murphy, R. A. Friesner, D. Sitkoff, A. Nicholls, M. N. Ringnalda, W. A. Goddard and B. Honig, *J. Am. Chem. Soc.*, 1994, **116**, 11875.
7. S. Grimme, *J. Comput. Chem.*, 2006, **27**, 1787-1799.
8. C. L. McMullin, J. Jover, J. N. Harvey and N. Fey, *Dalton Trans.*, 2010, **39**, 10833-10836.
9. a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652; b) S. H. Vosko, L. Wilk and M. Nusair, *Can. J. Phys.*, 1980, **58**, 1200-1211.
10. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.
11. Y. Zhao and D. G. Truhlar, *J. Chem. Phys.*, 2006, **125**, 194101.
12. V. G. Andrianov, I. S. Akhrem, N. M. Chistovalova and Y. T. Struchkov, *Zh. Strukt. Khim. (Russ. J. Struct. Chem.)*, 1976, **17**, 135.
13. L. M. Alcazar-Roman, J. F. Hartwig, A. L. Rheingold, L. M. Liable-Sands and I. A. Guzei, *J. Am. Chem. Soc.*, 2000, **122**, 4618-4630.
14. F. Allen, *Acta Cryst. B*, 2002, **58**, 380-388.
15. Maestro 9.0, Schrödinger-LLC, New York, NY, 2009.
16. S-PLUS 7.0, Insightful-Corporation, Seattle, WA, 2005.
17. D. D. Ellis, M. F. Haddow, A. G. Orpen and P. J. Watson, *Dalton Trans.*, 2009, 10436-10445.
18. N. Fey, J. A. S. Howell, J. D. Lovatt, P. C. Yates, D. Cunningham, P. McArdle, H. E. Gottlieb and S. J. Coles, *Dalton Trans.*, 2006, 5464-5475.
19. a) S. Serron, S. P. Nolan, Y. A. Abramov, L. Brammer and J. L. Petersen, *Organometallics*, 1998, **17**, 104-110; b) S. A. Serron and S. P. Nolan, *Organometallics*, 1995, **14**, 4611-4616.

## Cartesian coordinates of optimised geometries

### [RuCl<sub>2</sub>(p-cymene)(PR<sub>3</sub>)] and related complexes

PMe <sub>3</sub>				H14	2.2053851031	0.8277620925	1.9613894159
Ligand				C15	0.8200950851	1.5199748226	-2.2495340710
P1	0.1138764586	-0.1959730931	-0.0811022335	H16	1.2091355754	2.5034696693	-2.5712484536
C2	-0.0345916500	0.0582863268	1.7708965418	H17	1.4944704993	0.7410063014	-2.6477411860
C3	-1.6820436109	0.0600488884	-0.5567288890	H18	-0.1658916125	1.3835924328	-2.7294679473
C4	0.7875309797	1.4888019454	-0.5557434390	C19	-2.5130015200	-1.3138430548	-0.0260515976
H5	0.9732350681	0.0903689447	2.2211997240	H20	-3.5814061189	-1.1958870572	-0.2843733960
H6	-0.5704223287	0.9898290406	2.0336002202	H21	-2.1391431637	-2.2213834037	-0.5327653024
H7	-0.5711215421	-0.7969960409	2.2184180185	H22	-2.4559644451	-1.4932304442	1.0628344302
H8	-2.2831452385	-0.7939622988	-0.1976649195				
H9	-2.1060659441	0.9927695626	-0.1393411230	Complex			
H10	-1.7726877240	0.0910913990	-1.6568161692	Ru1	-0.1324078426	0.2503644455	-0.6191047635
H11	0.8038855495	1.5836503537	-1.6558271582	Cl2	0.3889653850	-1.6208503267	-2.0949051734
H12	0.1917649768	2.3214300252	-0.1365514918	Cl3	-2.4836668015	-0.2673148536	-0.9901190300
H13	1.8282386747	1.5832022120	-0.1985453612	P4	-0.2329070813	-1.3934342071	1.0810005971
				C5	1.6323684963	1.3093841171	-1.5849954708
Complex				C6	0.4187113574	1.8976584892	-2.0985409916
Ru1	3.5950632547	.0856682323	2.3663839138	C7	-0.5790209686	2.3733272905	-1.2078787881
Cl2	5.5715850132	1.4958286158	2.6302246486	C8	-0.4136679518	2.3418076689	0.2235896847
Cl3	2.1568620979	2.0116584585	2.7920089766	C9	0.7910663313	1.7297509373	0.7116720123
P4	3.6555386110	.0046575603	4.7112739771	C10	1.8259873785	1.2601561657	-0.1708546782
C5	4.7797359068	-1.1792296789	.9091668294	C11	-1.0578117096	-0.8481286840	2.6720953799
C6	3.9344589227	-2.785329109	.1468973564	C12	1.4520910036	-1.8748513860	1.7440721469
C7	2.5467893765	-2.015126564	.3945556679	C13	-1.0641008470	-2.9979137552	0.6434613858
C8	1.9077084909	-1.0296769776	1.3961330892	C14	-1.4094410278	2.9697432787	1.1920746832
C9	2.7432894502	-1.9332492305	2.1243959032	C15	2.6749425385	0.7681460146	-2.5293576638
C10	4.1596570130	-2.0277862224	1.8721107570	C16	-0.8833317022	4.3581479390	1.6365875665
C11	6.2722465080	-1.2038766227	.6180694303	C17	-2.8407913733	3.0781842103	0.6354188889
H12	7.5883513225	-1.9467225862	-.9660555533	C18	-1.0744881616	-4.074759005	1.7413731286
H13	6.2392771987	-3.0528195710	-.5739094305	C19	-2.5824174328	-0.6683680519	2.5960776906
H14	.1526927431	-1.4345701942	2.5964355268	C20	2.3707312900	-2.6013144097	0.7488956977
H15	-.1596675955	-1.3366260955	.8389375392	H21	0.2198371011	1.8659062527	-3.1733756494
C16	6.5189423679	-1.9896869474	-.6931143753	H22	-1.5373068529	2.6979577434	-1.6229365413
H17	5.9345296366	-1.5780374064	-1.5350107935	H23	0.9324830952	1.6350242375	1.7956399553
C18	.4314107435	-9.059147400	1.6691924626	H24	2.7282581553	0.7918216617	0.2347018057
H19	.1555538857	.1571767831	1.7831492429	H25	-0.5721046229	0.1035685568	2.9611976011
C20	7.1317100660	-1.7535086448	1.7673023522	H26	-0.7905718500	-1.5839236311	3.4563942895
H21	8.2010733160	-1.6587316261	1.5097529037	H27	1.9221375493	-0.9333461631	2.0886746428
H22	6.9514605182	-1.1802404480	2.6920779180	H28	1.2959211351	-2.4926319614	2.6500194008
H23	6.9364171175	-2.8261308729	1.9564274882	H29	-0.5570353905	-3.3496049330	-0.2714459386
H24	4.4023580357	.4339755473	-.5387624791	H30	-2.0844547170	-2.7190986915	0.3267302470
H25	1.9554499782	.5784168581	-.0955373421	H31	-1.4398885910	2.3182403016	2.0890986696
H26	2.2947731575	-2.5528151570	2.9093811157	H32	2.2051501173	0.3152213026	-3.4166930889
H27	4.7710722552	-2.7025102341	2.4768873693	H33	3.2942869675	-0.0036206485	-2.0449953669
H28	6.5686537166	-.1490477620	.4609476299	H34	3.3382350367	1.5909543483	-2.8608064903
C30	4.0583054481	1.5649175845	5.6057118822	H35	-0.8201642136	5.0463917968	0.7732358090
H31	4.0264374164	1.3946446886	6.6967434491	H36	0.1219208622	4.2926693197	2.0906848693
H32	5.0582282832	1.9013399469	5.2923851048	H37	-1.5669318219	4.8087556225	2.3790964185
H33	3.3254493420	2.3313366227	5.3099852744	H38	-2.9025045906	3.8291996458	-0.1746012553
C34	2.0484925806	-5.0710326250	5.4785148921	H39	-3.5289952065	3.4072687241	1.4342956142
H35	2.1079516371	-4.814876110	6.5811840744	H40	-3.1917784165	2.1102518399	0.2376243682
H36	1.2725487278	.1955648221	5.1324856918	H41	-0.0545503666	-4.3868857028	2.0294745591
H37	1.7764952001	-1.5264710792	5.1571060930	H42	-1.6002240354	-4.9749957583	1.3747275826
C38	4.8743710010	-1.2050515356	5.4126244106	H43	-1.5966954450	-3.7400053529	2.6558209569
H39	4.8579076981	-1.1919468641	6.5171001733	H44	-2.8663831104	0.0139096421	1.7784793160
H40	4.6466109533	-2.2259009282	5.0624562184	H45	-2.9662405241	-0.2654355040	3.5513444869
H41	5.8810894973	-.9264789613	5.0601536261	H46	-3.0925182922	-1.6293630571	2.4089680951
				H47	2.4850484473	-2.5298016247	-0.1869149966
				H48	1.9634727342	-3.5889334835	0.4716686119
				H49	3.3681662837	-2.7620150942	1.1978539756
PEt <sub>3</sub>				PiPr <sub>3</sub>			
Ligand				Ligand			
P1	0.1439132676	-0.2486777656	-0.1018947265	P1	2.9468185395	-1.8715046102	1.6769799020
C2	0.1417245054	0.0914993686	1.7538485412	C2	1.0399930941	-1.8814302496	1.8641015299
C3	-1.7034980309	-0.0729679003	-0.4407895821	C3	.2109344578	-2.4647310316	.7045224932
C4	0.7220423197	1.4387614819	-0.7162935530	C4	.5561300710	-4.597317322	2.2207918595
H5	-0.3437481067	1.0672219601	1.9592605385	C5	3.4231669124	-3.6165066919	2.2811232750
H6	-0.4948801154	-0.6855460184	2.2186681332	C6	2.7247867414	-4.8184115467	1.6220616456
H7	-2.0954898305	0.8352775714	0.0606059506	C7	3.2882324401	-3.6706534411	3.8172566521
H8	-1.8128349461	0.0915568910	-1.5298332993	C8	3.2271996197	-1.9890574477	-1.982052216
H9	0.0547057831	2.2331177562	-0.3244371292	C9	4.6849289462	-2.3979183897	-.4926672763
H10	1.7209455895	1.6139468153	-0.2729128027	C10	2.9266062272	-.6174910761	-.8361932884
C11	1.5476819059	0.0428897565	2.3767068891				
H12	1.5031899297	0.1958940882	3.4706508886				
H13	2.0331472931	-0.9314590516	2.1893450519				

H11	.8738490356	-2.5187185819	2.7570370520	H58	-1.0036858143	-4.4158204299	-0.3945311028
H12	-.8638235084	-2.4685161313	.9717497136				
H13	.4972177429	-3.5001800587	.4565698229				
H14	.3124028111	-1.8580938676	-.2135478988				
H15	.7158012759	.2422731850	1.3814124781				
H16	1.0954237817	-.0565602131	3.0954002035				
H17	-.5270381563	-4.611276695	2.4507973126				
H18	4.5054289239	-3.6718316527	2.0478884611				
H19	3.1704358597	-5.7682171502	1.9771842500				
H20	2.8097288760	-4.8025287411	.5206959644				
H21	1.6507248091	-4.8478458118	1.8806824330				
H22	2.2298948394	-3.6052984760	4.1336271524				
H23	3.8362985738	-2.8441645251	4.3029878369				
H24	3.6854333059	-4.6262557432	4.2093481209				
H25	2.5493546045	-2.7442891006	-.6417767470				
H26	4.8858407512	-2.3412404030	-1.5795805382				
H27	4.9073348537	-3.4295942062	-.1688539971				
H28	5.3986208119	-1.7206609142	.0133531194				
H29	3.5839887783	1.637965903	-4.120864340				
H30	1.8820672586	-.2970560749	-.6759419948				
H31	3.1019334202	-.6521766759	-1.9286597353				
Complex							
Ru1	0.4672308174	1.1866346408	-0.1818950494				
Cl2	-1.2005150561	2.6177533181	0.8795072164				
Cl3	-0.8414158160	1.4078865822	-2.2250052200				
P4	-0.9679422092	-0.6473995911	0.4861690063				
C5	2.3911739191	0.4126972933	-1.1355914463				
C6	2.3223542784	0.0884390839	0.2612177312				
C7	2.1908023076	1.0957925948	1.2773873043				
C8	2.0091657148	2.4639288552	0.9072670177				
C9	2.0210284650	2.8076756668	-0.4897544293				
C10	2.1866261177	1.7937310915	-1.4753405273				
C11	2.7141869772	-0.6649505115	-2.1624675297				
C12	4.2294460736	-0.9831550160	-2.1113264388				
C13	1.8097971968	3.5224529744	1.9593679816				
C14	2.2784982097	-0.3115424436	-3.5959825520				
C15	-2.8376823887	-0.3002379436	0.3476767925				
C16	-0.5780999529	-2.2815117141	-0.4012307655				
C17	-0.7617109805	-1.1531947768	2.3132409634				
C18	-3.7217372035	-0.9933081301	1.4057675148				
C19	0.5378520752	-1.9171096222	2.6345354657				
C20	-0.6316293895	-2.1890824989	-1.9396949307				
C21	-3.4121975292	-0.5684036127	-1.0585355549				
C22	-0.9174269693	0.0455052619	3.2680013891				
C23	-1.3851166376	-3.4991631252	0.0943700292				
H24	2.4095321456	-0.9626671158	0.5581945072				
H25	2.1637644105	0.8165452685	2.3343725856				
H26	1.7907671963	3.8312597799	-0.7962890851				
H27	2.0704663424	2.0681753709	-2.5269872769				
H28	2.1707478630	-1.5797025730	-1.8532369680				
H29	4.8241958208	-0.0951889136	-2.3935986265				
H30	4.4742994216	-1.7956866916	-2.8189938852				
H31	4.5492037083	-1.2985986508	-1.1021276919				
H32	1.3045538035	3.1119569772	2.8479116790				
H33	2.7937911637	3.9244645869	2.2696520187				
H34	1.1941190084	4.3500886335	1.5752124162				
H35	2.9019540333	0.5008111527	-4.0139582632				
H36	2.4050444430	-1.1898738537	-4.2529407142				
H37	1.2233420301	0.0102097290	-3.6326842137				
H38	-2.8591014266	0.7910226495	0.5230365909				
H39	0.4840656007	-2.4343357257	-0.1201854778				
H40	-1.6018772151	-1.8505780316	2.4938911011				
H41	-3.6901410821	-2.0951502985	1.3250014155				
H42	-4.7705467778	-0.6857432672	1.2355194529				
H43	-3.4671978692	-0.7146418761	2.4411978003				
H44	1.4270802939	-1.2740416815	2.5314054039				
H45	0.6861855313	-2.8133389271	2.0089897265				
H46	0.5065368470	-2.2547331198	3.6876560478				
H47	-1.6669308709	-2.2554546315	-2.3102256721				
H48	-0.0670349270	-3.0343054029	-2.3773406673				
H49	-0.2121035035	-1.2420661640	-2.3130426939				
H50	-3.5187366496	-1.6512183704	-1.2553664679				
H51	-2.8026810420	-0.1078139759	-1.8496123417				
H52	-4.4256613052	-0.1280612224	-1.1098412525				
H53	-0.0933434954	0.7649880195	3.1319726712				
H54	-0.9032972456	-0.3129779007	4.3151369475				
H55	-1.8485205695	0.6091556239	3.1014578637				
H56	-2.4514303979	-3.4056911651	-0.1742818008				
H57	-1.3202035795	-3.6528091941	1.1849306191				
				PCy <sub>3</sub>			
				Ligand			
				P1	-1.0826915114	.5407459785	1.2275626072
				C2	-1.2188217523	.5686252832	-.6789563018
				C3	-2.7071374170	.6920547393	-1.0945634649
				C4	-.5325237091	-.5632219156	-1.4778949147
				C5	.5804672628	1.4115459482	1.5247255516
				C6	.4111506227	2.9378198451	1.3252859714
				C7	1.8180665636	.9022334013	.7549677570
				C8	-.6845537108	-1.2704501817	1.6312288261
				C9	-.1257308273	-1.4049623021	3.0682116621
				C10	-1.9759816528	-2.1151051355	1.4908971538
				C11	-2.8617587062	.8974607611	-2.6152209143
				C12	-2.1577840271	-.2168185346	-3.4124620430
				C13	-.6795276432	-.3459764240	-2.9999276406
				C14	.1007990503	-2.8806356207	3.4602258555
				C15	-1.1801873609	-3.7193238126	3.2974590293
				C16	-1.7450612885	-3.5919261754	1.8708215697
				C17	3.0950898346	1.6647651323	1.1708222261
				C18	2.9270932109	3.1843108991	.9810401532
				C19	1.6862008095	3.7071447980	1.7298491373
				H20	-.7238785739	1.5235373510	-.9612404964
				H21	-3.1842244234	1.5223138852	-.5412881291
				H22	-3.2476164899	-.2291566053	-.7932699543
				H23	.5367618996	-.6418331629	-1.2113747547
				H24	-.9940628509	-1.5355461772	-1.2130399932
				H25	.7622797178	1.2512070835	2.6090231595
				H26	.1884994893	3.1480794996	.2581415573
				H27	-.4591378182	3.3002661229	1.9044086460
				H28	1.6548581200	1.0474582555	-1.3205019699
				H29	1.9570348232	-.1843512429	.9124393484
				H30	.0738638234	-1.6678441165	.9256668923
				H31	-.8397580243	-.9396476190	3.7794205880
				H32	.8256644725	-.8504609596	3.1694020036
				H33	-2.7557615714	-1.6830368229	2.1511145096
				H34	-2.3729303000	-2.0503528443	.4601762995
				H35	-2.4210565481	1.8774811528	-2.8929853136
				H36	-3.9340550720	.9479380956	-2.8852405833
				H37	-2.6724644360	-1.1812646804	-3.2219230520
				H38	-2.2396852444	-.0257611045	-4.4994301285
				H39	-.1371556107	.5783100366	-3.2881430232
				H40	-.1963736125	-1.1776164995	-3.5482747058
				H41	.8986276512	-3.3062448280	2.8171748141
				H42	.4722394645	-2.9394915903	4.5013356552
				H43	-1.9419349437	-3.3652409706	4.0221547234
				H44	-.9801872623	-4.7798561738	3.5422902505
				H45	-1.0327462678	-4.0473687733	-1.5222090003
				H46	-2.6915840384	-4.1580610510	1.7772702585
				H47	3.9637518931	1.2967008300	.5915873104
				H48	3.3138532637	1.4507910698	2.2374158311
				H49	3.8351101678	1.1813148912	1.3201297756
				H50	2.8179241656	3.4039950945	-.1012281630
				H51	1.5511520546	4.7899129240	1.5439678265
				H52	1.8440918644	3.5923803489	2.8220706035
				Complex			
				Ru1	-4.0646333169	-5.2162258115	.2959271527
				Cl2	-4.0281600802	-2.7737095350	.2856700261
				Cl3	-6.4897335673	-5.0756884869	.0271129705
				P4	-3.9460026498	-5.2044026557	-2.1289334806
				C5	-4.2097268394	-6.9023982904	-2.9448882722
				C6	-3.0503006922	-7.9158156019	-2.7962739876
				C7	-3.3212639014	-9.1804335508	-3.6413038221
				C8	-4.6613692128	-9.8383773796	-3.2646608309
				C9	-5.8210925157	-8.8289451153	-3.3549005990
				C10	-5.2710870196	-4.1300001956	-2.9765971933
				C11	-5.7508973324	-4.6034160526	-4.3741050920
				C12	-6.9442850898	-3.7506468679	-4.8610758824
				C13	-6.6126441413	-2.2489597129	-4.8831022010
				C14	-6.1015421445	-1.7855239992	-3.5079487755
				C15	-2.2320254820	-4.7513716057	-2.8081483632
				C16	-2.0852657520	-4.8426528942	-4.3487275982
				C17	-.6070484139	-4.6922591870	-4.7705402745
				C18	.0087164620	-3.3867337188	-4.2352609191
				C19	-.1715726056	-3.2734547494	-2.7094774885
				C20	-4.4892698684	-6.8295489002	1.8576774442
				C21	-3.6166465349	-7.3606224722	.8597135693



H61	6.4565412360	.2334898372	5.5034193995
<b>P(p-F-C<sub>6</sub>H<sub>4</sub>)<sub>3</sub></b>			
<b>Ligand</b>			
P1	1.0183890000	0.9210570000	0.0143280000
C2	-0.1276630000	0.3359100000	-1.3249560000
C3	0.6985070000	2.7507540000	0.0380400000
C4	0.1485580000	0.3480770000	1.5523110000
C5	-0.4029920000	4.7838540000	0.8557770000
C6	-1.1997350000	-0.0706330000	1.6016630000
C7	0.3829290000	5.5393650000	-0.0228560000
C8	1.3299580000	4.9442940000	-0.8675980000
C9	1.4881190000	3.5513430000	-0.8217060000
C10	-0.2404920000	3.3885030000	0.8791540000
F11	0.2285050000	6.8870310000	-0.0538430000
H12	1.9317740000	5.5699340000	-1.5337990000
H13	2.2387180000	3.0764640000	-1.4650950000
H14	-0.8530610000	2.7903520000	1.5620600000
H15	-1.1267990000	5.2872460000	1.5042750000
C16	-0.9975780000	-0.5119250000	3.9668830000
C17	0.3451950000	-0.1105940000	3.9576640000
C18	0.9117700000	0.3067630000	2.7437430000
C19	-1.7793330000	-0.5051470000	2.8049540000
F20	-1.5523440000	-0.9259870000	5.1337720000
H21	0.9271580000	-0.1413200000	4.8838200000
H22	1.9667880000	0.6055850000	2.7207790000
H23	-1.8054080000	-0.0605150000	0.6890680000
H24	-2.8221910000	-0.8336970000	2.8532540000
C25	-1.7553070000	-0.6998230000	-3.3650570000
C26	-1.9964720000	0.5965920000	-2.8930810000
C27	-1.1792420000	1.1063970000	-1.8705110000
C28	0.0968270000	-0.9616280000	-1.8438940000
C29	-0.7174690000	-1.4918280000	-2.8555850000
F30	-2.5440020000	-1.2016680000	-4.3482470000
H31	-2.8135460000	1.1856600000	-3.3211550000
H32	-1.3632230000	2.1182670000	-1.4936030000
H33	0.9218520000	-1.5667230000	-1.4488800000
H34	-0.5540570000	-2.4963150000	-3.2578550000
<b>Complex</b>			
Ru1	3.5117536353	.0901767434	2.4163332354
C12	5.5026657485	1.4780033474	2.6575546018
C13	2.0949324509	2.0810594051	2.6045632002
P4	3.6215076308	-0.398731831	4.7898957796
C5	4.0401234479	1.4315457175	5.8333394947
C6	4.3256870910	1.2287640426	7.2033276875
C7	4.5887999566	2.3114716018	8.0521139844
C8	4.5564636568	3.6041171379	7.5128621038
C9	4.2688247763	3.8361919622	6.1639405606
C10	4.0103831613	2.7445956019	5.3204363770
C11	2.0588014344	-.6328197428	5.5984078127
C12	.8405054670	-1.018124146	5.1149778091
C13	-.3775056543	-.4313556221	5.7278803707
C14	-.3695276814	-1.2966781272	6.8290435281
C15	.8197184688	-1.8291462924	7.3403511096
C16	2.0331016426	-1.4855973764	6.7247484936
C17	4.9067015725	-1.2755416600	5.2842685738
C18	6.2301413226	-.8426383530	5.5288004104
C19	7.2505029126	-1.7643441851	5.8060311562
C20	6.9425382653	-3.1295995559	5.8325847617
C21	5.6467946053	-3.5972526458	5.5799526013
C22	4.6365203623	-2.6638662257	5.3018888428
C23	4.7124781005	-1.2124303845	.9966591346
C24	3.8799218942	-.3128604480	.2206254541
C25	2.4871339506	-.2395281313	.4472671962
C26	1.8314307077	-1.0581412837	1.4438699790
C27	2.6604518013	-1.9373895057	2.2068930744
C28	4.0787449735	-2.0374717332	1.9696004103
C29	6.2056813701	-1.2564720786	.7179850032
H30	2.9629242822	-1.8933241401	7.1337314467
H31	7.5159444255	-2.0175776339	-.8609776179
H32	6.1408792134	-3.0965849619	-.4864308136
H33	.0506682360	-1.4124328224	2.6232362957
H34	-.2019752312	-1.4752020346	.8532010992
C35	6.4435772633	-2.0389064872	-.5977927598
H36	5.8753913402	-1.6102253898	-1.4423177293
C37	.3451365968	-.9567648371	1.6635595422
H38	.0324572919	.1020887940	1.6705044781
C39	7.0465629686	-1.8336383487	1.8663085042

H40	8.1191874427	-1.7527187762	1.6172406270
H41	6.8689182013	-1.2767114082	2.8005997532
H42	6.8321656356	-2.9050746409	2.0393259455
H43	8.2748181391	-1.4352878684	6.0036394939
H44	4.8190202342	2.1655831355	9.1115061474
H45	-1.3247821361	-0.0179160014	5.3692159084
F46	4.8107498217	4.6579151484	8.3274026810
H47	.8584739033	.5943059755	4.2666236672
F48	-1.5435450872	-1.6260604375	7.4201237719
H49	.7885132803	-2.4954049127	8.2077198450
F50	7.9213063226	-4.0228302913	6.1092243390
H51	5.4405715842	-4.6713803509	5.6101869879
H52	4.3556443308	.3965396777	-.4627173325
H53	1.9033376360	.5373171808	-.0564769116
H54	2.2047026487	-2.5265425676	3.0107330635
H55	4.6835232648	-2.6824094855	2.6118740523
H56	6.5198930271	-2.056506262	.5688372478
H57	4.3496626222	.2162293277	7.6205981445
H58	4.2521703696	4.8605520599	5.7808598833
H59	3.7825268265	2.9103339843	4.2654003668
H60	3.6212261897	-3.0293208169	5.1131452617
H61	6.4658576121	.2250700117	5.4951287744

<b>P(p-MeO-C<sub>6</sub>H<sub>4</sub>)<sub>3</sub></b>			
<b>Ligand</b>			
P1	0.7860700105	0.8374302977	-0.1046581007
C2	-0.5036388830	0.4502417589	-1.3812139940
C3	0.7144734523	2.6898858176	-0.0140616847
C4	-0.0643521985	0.3372803280	1.4663012226
C5	-0.0831215397	4.8232744959	0.9071820841
C6	-1.4602492399	0.1402769349	1.6003325983
C7	0.7524804812	5.5291162314	0.0179877865
C8	1.5768099048	4.8163999474	-0.8820317992
C9	1.5611194997	3.4197379141	-0.8862886558
C10	-0.0961783406	3.4169182365	0.8807110489
H11	2.2254613190	5.3823825024	-1.5587723687
H12	2.2174498699	2.8787712373	-1.5793220782
H13	-0.7510287257	2.8802013159	1.5761133951
H14	-0.7253113635	5.3520555808	1.6176256377
C15	-1.1998269136	-0.4144860463	3.9587101895
C16	0.1945826375	-0.2352475173	3.8445900155
C17	0.7442727721	0.1274445247	2.6033034812
C18	-2.0231630927	-0.2323379935	2.8252380048
H19	0.8551524852	-0.3827710703	4.7037865735
H20	1.8313518384	0.2519731118	2.5212325896
H21	-2.1121902889	0.2794023912	0.7307397699
H22	-3.1024157932	-0.3850568224	2.9329270715
C23	-2.4151231496	-0.3217743036	-3.3351687469
C24	-2.4110071229	0.9938606793	-2.8213258946
C25	-1.4701409109	1.3689972536	-1.8564385441
C26	-0.5070830586	-0.8521761997	-1.9249874074
C27	-1.4541550117	-1.2503191940	-2.8831752194
H28	-3.1604020718	1.7018926029	-2.9910360309
H29	-1.4833780118	2.3915700544	-1.4633087454
H30	0.2439392020	-1.5786049716	-1.5898743543
H31	-1.4289919180	-2.2719260498	-3.2731035486
O32	0.8435921572	6.8965267717	-0.0526785190
C33	0.0297844021	7.6543451622	0.8425628869
H34	-1.0484355008	7.4637918664	0.6734349027
H35	0.2750107096	7.4360573610	1.9006258675
H36	0.2515578152	8.7104269979	0.6263481879
O37	-3.3864138683	-0.5924687361	-4.2663609070
C38	-3.4404028511	-1.9191619790	-4.7905666669
H39	-2.5103096461	-2.1826651635	-5.3314481309
H40	-3.6188298267	-2.6654943215	-3.9916173066
H41	-4.2865289976	-1.9280366263	-5.4943110858
O42	-1.8508210338	-0.7689751486	5.1138091792
C43	-1.0563329278	-0.9391375677	6.2874926753
H44	-0.3210881818	-1.7588934967	6.1673228424
H45	-0.5198893012	-0.0073661745	6.5545065245
H46	-1.7623406843	-1.1975049159	7.0913506628

<b>Complex</b>			
Ru1	3.4795651543	.0883171935	2.3887403651
C12	5.4606381050	1.5031599236	2.5628001170
C13	2.0453731969	2.0649486191	2.5877109030
P4	3.6234090162	-.0302183416	4.7673364252
C5	4.0588299066	1.4463871317	5.7852970154
C6	4.3685194912	1.2634209986	7.1557194671

C7	4.6525381102	2.3523172811	7.9791344434	C10	-0.2378313437	3.3620069011	0.5286833563
C8	4.6226655666	3.6610109062	7.4477227052	H11	2.7043233276	5.2593858187	-1.1849101522
C9	4.3023679213	3.8569243697	6.0905159156	H12	2.7570680145	2.7727492654	-1.0128948557
C10	4.0221875052	2.7537538250	5.2673526291	H13	-1.0599037232	2.8412417060	1.0322462113
C11	2.0747055827	-.6296367711	5.5895878475	H14	-1.1106143715	5.3146380884	0.8552013910
C12	.8350081677	-.1395692471	5.1107899181	C15	-0.9712931286	-0.5290650570	4.0948973875
C13	-.3621581164	-.4900500247	5.7391741961	C16	-0.1532723761	0.6143804729	4.0048595859
C14	-.3535351660	-1.3400092439	6.8673740747	C17	0.3874515432	1.0295560134	2.7771021995
C15	.8730679083	-1.8206776978	7.3669146771	C18	-1.2228430592	-1.2515882676	2.9089802357
C16	2.0714492724	-1.4565138597	6.7309676188	H19	0.0614545682	1.1949862112	4.9114054102
C17	4.9096022387	-1.2647424465	5.2533892145	H20	1.0162826533	1.9268600624	2.7444663650
C18	6.2421091259	-.8422234941	5.4817549575	H21	-0.9132020351	-1.4222887341	0.7774338740
C19	7.2505178895	-1.7654580792	5.7674366500	H22	-1.8552273742	-2.1483358975	2.9479242369
C20	6.9587669753	-3.1456644191	5.8280696113	C23	-2.1341405526	-0.4390414731	-3.3375905165
C21	5.6429679953	-3.5884884269	5.5831657525	C24	-2.5847945340	0.2248075295	-2.1725658610
C22	4.6389519935	-2.6485389626	5.2956531209	C25	-1.6930685111	0.5870908262	-1.1553297684
C23	4.6737006007	-1.2215814101	.9772499240	C26	0.1363230680	-0.3717774000	-2.4235164840
C24	3.8263386127	-.3414571506	.1940265769	C27	-0.7618141570	-0.7321973198	-3.4442153885
C25	2.4360899561	-.2737484282	.4339764793	H28	-3.6518309149	0.4601579886	-2.0656838703
C26	1.7969254678	-1.0822909801	1.4500525618	H29	-2.0737958225	1.0926722132	-0.2605137534
C27	2.6387805916	-1.9466568418	2.2159683726	H30	1.2012090374	-0.6156196009	-2.5234373204
C28	4.0557254830	-2.0389022331	1.9667984239	H31	-0.3896551868	-1.2522380728	-4.3366254992
C29	6.1655895047	-1.2543290779	.6884005385	C32	0.7518678819	6.9794526238	-0.2823885377
H30	3.0133604409	-1.8332745554	7.1424849255	H33	1.6492850356	7.3752205368	-0.7867614150
H31	7.4760029602	-2.0220829375	-.8878065276	H34	-0.1328969855	7.3224816912	-0.8504766882
H32	6.1164292972	-3.1121150001	-.4886128381	H35	0.6921355214	7.4474904017	0.7182491868
H33	.0268841226	-1.4392086328	2.6449741089	C36	-1.5660641463	-0.9726036974	5.4154885677
H34	-.2396621643	-1.5076545918	.8759412083	H37	-1.2645266232	-0.3028312283	6.2390619629
C35	6.4055199253	-2.0523983543	-.6170868537	H38	-2.6717879324	-0.9814094556	5.3778165716
H36	5.8265180750	-1.6433899879	-1.4641495527	H39	-1.2459005977	-1.9977089458	5.6803147293
C37	.3121217295	-.9862291031	1.6814513877	C40	-3.1091477702	-0.8229859102	-4.4315343449
H38	-.0028942950	-.020990535	1.6886597930	H41	-2.6022243258	-1.3463099763	-5.2608465865
C39	7.0201678190	-1.8042004888	1.8401641537	H42	-3.9043633993	-1.4896253830	-4.0473123442
H40	8.0905841245	-1.7139717402	1.5841906544	H43	-3.6119770207	0.0682814810	-4.8521925566
H41	6.8407724466	-1.2374746632	2.7681567298				
H42	6.8192605255	-2.8754008289	2.0305286241	Complex			
H43	8.2792118634	-1.4392240856	5.9507373190	Ru1	3.5107958207	.0937976652	2.4082538508
H44	4.9002832358	2.2169133617	9.0368373222	Cl2	5.5235785498	1.4569594930	2.6143133571
H45	-1.3228834445	-.1091676647	5.3773518093	Cl3	2.1294667192	2.1035794004	2.6039134500
H46	.8260825616	.5423029982	4.2511945186	P4	3.6324999676	-.0298983041	4.7810931336
H47	.9105763466	-2.4696393801	8.2463691187	C5	4.0455178525	1.4390641317	5.8308117663
H48	5.3871140544	-4.6509931068	5.6218052968	C6	4.2787710428	1.2293490247	7.2097943718
H49	4.2907756537	.3616181889	-.5035719424	C7	4.5433637552	2.3093011808	8.0570636446
H50	1.8411850898	.4913892677	-0.0748310671	C8	4.5772932255	3.6296669154	7.5588330853
H51	2.1954817569	-2.5255444285	3.0339599753	C9	4.3358499330	3.8255562993	6.1868334915
H52	4.6715558642	-2.6676235402	2.6146842859	C10	4.0720404983	2.7499669937	5.3222955267
H53	6.4667508350	-.2020115613	.5233528425	C11	2.0736799795	-.6302716241	5.5897328681
H54	4.3968799868	.2561083152	7.5857170794	C12	.8523691308	-.0832563245	5.1349166045
H55	4.2709431883	4.8598025099	5.6565931574	C13	-.3534293428	-0.4325805246	5.7566372256
H56	3.7729770457	2.9132120408	4.2163297497	C14	-.3868176293	-1.3318006525	6.8440783752
H57	3.6206418390	-3.0133071026	5.1208082107	C15	.8358444309	-1.8603061631	7.2987967812
H58	6.4866296089	.2231127485	5.4310741887	C16	2.0516948648	-1.5125172065	6.6895837460
O60	-1.5801355424	-1.6330925081	7.4021239107	C17	4.9231992010	-1.2584490542	5.2742776764
O61	8.0127721238	-3.9656409811	6.1320083089	C18	6.2357503279	-.8152744296	5.5522665386
O62	4.9195307479	4.6624832534	8.3348030008	C19	7.2506641250	-1.7363848149	5.8414300241
C63	-1.6084542539	-2.4711113772	8.5589283319	C20	7.0007875697	-3.1247474153	5.8633839640
H64	-2.6708249454	-2.5764116599	8.8247843814	C21	5.6948531456	-3.5622509458	5.5690439944
H65	-1.1812870435	-3.4709312876	8.3473166799	C22	4.6718110160	-2.6476602158	5.2741181066
H66	-1.0605921665	-2.0135344257	9.4054642439	C23	4.6835085136	-1.2344348248	.9965750572
C67	7.7523010363	-5.3679627080	6.2165965713	C24	3.8595938459	-.3316767565	.2143112231
H68	8.7143369785	-5.8346127004	6.4755324061	C25	2.4693869390	-.2358890683	.4478382579
H69	7.0086120683	-5.5961276487	7.0050026544	C26	1.8074898294	-1.0363241470	1.4554478275
H70	7.3948689925	-5.7746580250	5.2505059655	C27	2.6271490588	-1.9219127005	2.2215669755
C71	4.9093766818	6.0018079286	7.8365466679	C28	4.0426659801	-2.0441955038	1.9779153729
H72	5.1714838539	6.6398472335	8.6939625022	C29	6.1765038561	-1.2968442988	.7194715938
H73	5.6562554461	6.1403878800	7.0311480550	H30	2.9824101329	-1.9377135710	7.0788796431
H74	3.9088945929	6.2858545423	7.4569866737	H31	7.4827846806	-2.0959921834	-.8446578697
				H32	6.0991359964	-3.1575338485	-.4514580465
				H33	.0285180388	-1.3515888929	2.6476370684
				H34	-.2363516258	-1.4227078323	.8786112068
				C35	6.4100087410	-2.1042602061	-.5816337406
				H36	5.8452489040	-1.6867514860	-1.4341726979
				C37	.3243886465	-.9085908338	1.6826803515
				H38	.0308747664	.1558547099	1.6846783462
				C39	7.0116247480	-1.8588020400	1.8800261401
				H40	8.0852485446	-1.7887775106	1.6309713023
				H41	6.8356051238	-1.2851237886	2.8044251673
				H42	6.7897577727	-2.9254293769	2.0721352435
				H43	8.2608065603	-1.3667331096	6.0594366668
P(p-tolyl) <sub>3</sub>							
Ligand							
P1	0.9668752486	0.7645645958	0.0023438239				
C2	-0.3132613460	0.2960683420	-1.2659014747				
C3	0.8445838181	2.6214865358	-0.0000010527				
C4	0.1156444310	0.3176417444	1.5870594879				
C5	-0.2606014295	4.7595595683	0.4373944483				
C6	-0.6895300057	-0.8417187032	1.6794343235				
C7	0.7916941047	5.4685706571	-0.1852742671				
C8	1.8718590734	4.7301245389	-0.7042173605				
C9	1.9014727285	3.3283044765	-0.6097041225				

H44	4.7269783956	2.1249473549	9.1236513121
H45	-1.2902786697	.0095422392	5.3931991051
H46	.8639384818	.6358532403	4.3060761239
H47	.8408251615	-2.5545114130	8.1487103992
H48	5.4703049266	-4.6363638367	5.5792766864
H49	4.3421330831	.3652136797	-.4772051292
H50	1.8940643093	.5454769484	-.0588330498
H51	2.1679914663	-2.4953056539	3.0347449747
H52	4.6417100489	-2.6899215611	2.6249239885
H53	6.4993301965	-.2513466156	.5524345447
H54	4.2569894854	.2163493314	7.6267360350
H55	4.3553765121	4.8428302011	5.7770170878
H56	3.8855969432	2.9256144289	4.2609031786
H57	3.6653255116	-3.0253765469	5.0611542193
H58	6.4602839643	.2555643640	5.5360926858
C60	4.8630901243	4.7911547275	8.4846675329
H61	4.8511939134	5.7516666803	7.9432666010
H62	4.1148743356	4.8507191219	9.2968605363
H63	5.8526178358	4.6867514045	8.9673856673
C64	8.1017068454	-4.1069472818	6.1967268700
H65	7.7387578382	-5.1480141953	6.1639111185
H66	8.9463694905	-4.025533148	5.4888690547
H67	8.5103787489	-3.9242495710	7.2077342598
C68	-1.6962630312	-1.7062373586	7.5021248540
H69	-1.5421691184	-2.4087274670	8.3384247934
H70	-2.2141397556	-.8145861420	7.9007643781
H71	-2.3872034764	-2.1837298436	6.7829615764

P(p-Cl-C<sub>6</sub>H<sub>4</sub>)<sub>3</sub>

Ligand

P1	1.0260480000	0.9534050000	-0.0267290000
C2	-0.1467190000	0.3760270000	-1.3451100000
C3	0.6880010000	2.7789350000	0.0209380000
C4	0.2028650000	0.3630610000	1.5294130000
C5	-0.3990950000	4.7951780000	0.8957940000
C6	-1.0981950000	-0.1824380000	1.5920820000
C7	0.3318510000	5.5729330000	-0.0163080000
C8	1.2443240000	4.9823920000	-0.9068850000
C9	1.4224920000	3.5917750000	-0.8735720000
C10	-0.2182570000	3.4022090000	0.9064350000
H11	1.8118750000	5.6043120000	-1.6055280000
H12	2.1475470000	3.1311000000	-1.5555780000
H13	-0.7910930000	2.7964760000	1.6167560000
H14	-1.1026420000	5.2729290000	1.5844110000
C15	-0.8634100000	-0.5338700000	3.9770870000
C16	0.4360020000	0.0001900000	3.9456180000
C17	0.9626020000	0.4331270000	2.7203400000
C18	-1.6353800000	-0.6359540000	2.8087900000
H19	1.0267280000	0.0645640000	4.8642950000
H20	1.9830080000	0.8345630000	2.6912910000
H21	-1.7040330000	-0.2558540000	0.6825970000
H22	-2.6439490000	-1.0583500000	2.8511770000
C23	-1.8136850000	-0.6457210000	-3.3721540000
C24	-2.0628960000	0.6350580000	-2.8530580000
C25	-1.2293060000	1.1360460000	-1.8401730000
C26	0.0883720000	-0.9030570000	-1.9003210000
C27	-0.7424350000	-1.4247080000	-2.9032360000
H28	-2.8998010000	1.2282820000	-3.2338930000
H29	-1.4249520000	2.1347430000	-1.4349500000
H30	0.9361600000	-1.5012050000	-1.5446700000
H31	-0.5583000000	-2.4173370000	-3.3248560000
Cl32	0.1079120000	7.3199660000	-0.0400640000
Cl33	-1.5320770000	-1.0912800000	5.5082080000
Cl34	-2.8572900000	-1.2840780000	-4.6393240000

Complex

Ru1	3.5198286759	.0879205557	2.4228658692
Cl2	5.5083465535	1.4777634903	2.6629500265
Cl3	2.1004955518	2.0742357339	2.6252331065
P4	3.6318234101	-.0383340635	4.7938385188
C5	4.0506009732	1.4377756539	5.8367359465
C6	4.3193423350	1.2421001109	7.2101238340
C7	4.5862904392	2.3275359248	8.0546666554
C8	4.5756168421	3.6241369650	7.5144161763
C9	4.3016561432	3.8424651968	6.1566511954
C10	4.0396559550	2.7473414459	5.3168529024
C11	2.0653770770	-.6228218565	5.6076374845
C12	.8503369564	-.0836165512	5.1283462143
C13	-.3708832723	-.4155511931	5.7345370160

C14	-.3793103360	-1.2968200117	6.8279507046
C15	.8152693146	-1.8329527160	7.3328512984
C16	2.0323252588	-1.4860172413	6.7249925218
C17	4.9188730817	-1.2743732866	5.2907751824
C18	6.2405900817	-.8408771345	5.5376658740
C19	7.2627058925	-1.7609176786	5.8163405886
C20	6.9668133355	-3.1329058061	5.8438113788
C21	5.6660253047	-3.5945136248	5.5857602744
C22	4.6537717075	-2.6632526015	5.3058112458
C23	4.7196300900	-1.2080893824	.9958556609
C24	3.8840864372	-2.0378036341	.2264941582
C25	2.4913043862	-.2355471107	.4551308276
C26	1.8382368107	-1.0602669176	1.4481624490
C27	2.6700467667	-1.9415454525	2.2057426192
C28	4.0883394499	-2.0378036341	1.9663535097
C29	6.2121349718	-1.2489615013	.7137617565
H30	2.9580396561	-1.9022949080	7.1346354774
H31	7.5195477803	-2.0036821567	-.8699304942
H32	6.1467454603	-3.0856170736	-.4964211703
H33	.0557434606	-1.4348388190	2.6194114176
H34	-.1932412810	-1.4706681677	.8487109319
C35	6.4477666165	-2.0272625341	-.6048958347
H36	5.8724924218	-1.5966117776	-1.4470038039
C37	.3516666012	-.9637993108	1.6677499696
H38	.0373163785	.0943836795	1.6891114218
C39	7.0563878166	-1.8282663905	1.8586564733
H40	8.1283266930	-1.7443067504	1.6081828840
H41	6.8795190685	-1.2747731785	2.7951901234
H42	6.8450947652	-2.9006579712	2.0287371120
H43	8.2818745081	-1.4153975181	6.0113361322
H44	4.8002166859	2.1712713124	9.1157396442
H45	-1.3083639536	.0103459006	5.3654757006
Cl46	4.9109770003	4.9962512959	8.5685244071
H47	.8707681953	.6200168387	4.2861134177
Cl48	-1.9096481517	-1.7323951256	7.5826236555
H49	.7949862141	-2.5094213290	8.1923673654
Cl50	8.2402069177	-4.2926937225	6.2070754189
H51	5.4474298776	-4.6662232775	5.6098414977
H52	4.3573231512	.4073941879	-.4547948003
H53	1.9057171753	.5423492732	-.0449314495
H54	2.2160658257	-2.5366939049	3.0061527558
H55	4.6952575965	-2.6860850106	2.6033450484
H56	6.5243210358	-.1972778777	.5663635343
H57	4.3276068126	.2331624853	7.6367065030
H58	4.2961232124	4.8588624952	5.7531654970
H59	3.8238975847	2.9113926415	4.2589852222
H60	3.6413715922	-3.0341121926	5.1120215672
H61	6.4774282298	.2267189643	5.5043771835

P(p-F<sub>3</sub>C-C<sub>6</sub>H<sub>4</sub>)<sub>3</sub>

Ligand

P1	1.0449632689	0.9464254716	-0.0626622874
C2	-0.1359246635	0.3950129516	-1.3878493506
C3	0.7531839349	2.7817969408	-0.0098163018
C4	0.1877106184	0.3701904839	1.4831656143
C5	-0.2203619152	4.8266582171	0.9139503408
C6	-1.1265648020	-0.1447042695	1.5203870506
C7	0.4903859436	5.5967772725	-0.0232941387
C8	1.3369602934	4.9643918196	-0.9539091768
C9	1.4733189809	3.5703834922	-0.9383019060
C10	-0.0922633778	3.4287901492	0.9173925186
H11	1.8884734927	5.5640075020	-1.6850341532
H12	2.1478567345	3.0865107219	-1.6550828962
H13	-0.6566931187	2.8384780554	1.6466278218
H14	-0.8828807501	5.3189875677	1.6328905652
C15	-0.9516240612	-0.4904722787	3.9239643719
C16	0.3636869738	0.0099977143	3.8996292524
C17	0.9301687968	0.4243542074	2.6861801961
C18	-1.6910854143	-0.5755059819	2.7304134598
H19	0.9458934861	0.0601636595	4.8250028436
H20	1.9627171529	0.7938611238	2.6715680559
H21	-1.7147191517	-0.2095617322	0.5992267963
H22	-2.7090010749	-0.9781233909	2.7481699450
C23	-1.8501053096	-0.6258024521	-3.3889167360
C24	-2.0515905406	0.6707047984	-2.8834624612
C25	-1.1998075082	1.1764966011	-1.8886722901
C26	0.0702941610	-0.8978465546	-1.9238816811
C27	-0.7835265225	-1.4100359115	-2.9094618914
H28	-2.8741887873	1.2825331233	-3.2667367932



C5	.2716965318	-1.3107189839	.3210450803	C46	5.8072783949	3.9474153148	6.1734556725
C6	.3454000059	2.5214294012	.0024654201	C47	6.1113520744	2.6947383368	5.6223152764
C7	1.4736018788	2.9032366871	-.7402121475	C48	7.3519484171	2.4261255347	5.0294831029
C8	-2.3308438815	2.9142469146	-2.0631121809	C49	8.3028438311	3.4596000922	4.9820311659
C9	-3.4145285847	3.4915785894	-2.7462034149	H50	8.7689690776	5.5222720952	5.4795319097
C10	-4.0805632220	2.7835228883	-3.7591137337	H51	6.5374125883	5.9476416300	6.5411386359
C11	-3.6587748765	1.4834317457	-4.0894723464	H52	4.8260301626	4.1059345386	6.6310206310
C12	-2.5874640686	.8888860861	-3.4080249729	H53	7.5553224732	1.4560932982	4.5643654193
C13	1.1916892359	-2.0137785312	1.1179405147	H54	9.2706353886	3.2661794351	4.5071260402
C14	.9370158622	-3.3535657839	1.4427024089	C55	6.4354026684	-1.5004454961	9.5935922624
C15	-.2323638843	-3.9885849253	.9881169139	C56	7.1880594713	-.5256903191	8.9185803341
C16	-1.1434402384	-3.2750987020	.1937424614	C57	6.9586523010	-.2647321527	7.5583028375
C17	-.8953162685	-1.9366036845	-.1536534208	C58	5.9625631559	-.9894359603	6.8903984283
C18	2.0770426530	2.1083519446	-1.7291231547	C59	5.2017932094	-1.9673598257	7.5452411684
C19	3.2008839487	2.6120595000	-2.4048587879	C60	5.4456097426	-2.2206376793	8.9037411044
C20	3.7188656104	3.8817712318	-2.1035291655	H61	6.6208357890	-1.7001302067	10.6545358019
C21	3.1032430613	4.6610763434	-1.1096281865	H62	7.9619541009	.0393266583	9.4496171482
C22	1.9789775056	4.1763778198	-.4260639280	H63	7.5384945781	.4897009319	7.0180737068
H23	-1.7844022186	3.4812185140	-1.3027709505	H64	4.4353507627	-2.5153317893	6.9896776652
H24	-3.7282950833	4.5092133036	-2.4885510204	H65	4.8553956386	-2.9834434042	9.4237492757
H25	-4.9202219780	3.2421963136	-4.2919019008				
H26	-4.1682133032	.9248256290	-4.8824575876				
H27	-2.2455612608	-.1220672853	-3.6511399486				
H28	2.0911995955	-1.4993536499	1.4693948708				
H29	1.6561467816	-3.9022929412	2.0609944841				
H30	-.4288695405	-5.0337842605	1.2488074535				
H31	-2.0533209151	-3.7628176695	-.1735245013				
H32	-1.5833731797	-1.3943159130	-.8090759430				
H33	1.6842153661	1.1182734456	-1.9648675225				
H34	3.6741545569	1.9952925401	-3.1769959882				
H35	4.5959512920	4.2610292605	-2.6383930232				
H36	3.4969457913	5.6531219865	-.8620210937				
H37	1.4844214490	4.7657021488	.3521531327				

P(pyr)<sub>3</sub> (pyr = NC<sub>4</sub>H<sub>4</sub>)

Ligand

P1	1.9509591153	2.8159207388	7.3142474802
N2	.4694852009	2.0032069769	6.8454193944
C3	-.7421342743	2.7026877446	6.7518386649
C4	-1.7264728022	1.8139130337	6.3651912718
C5	-1.1075958416	.5297839926	6.2036265328
C6	.2369373401	.6650164136	6.4989402584
N7	3.1442655456	1.7511961108	6.5947819379
C8	3.7206828096	2.0502913128	5.3524191133
C9	4.5480868871	1.0031033244	4.9955783127
C10	4.4888885071	.0299867744	6.0478412494
C11	3.6204966433	.5018582800	7.0159047137
N12	2.0644006971	2.3353145294	8.9958965357
C13	1.5522136693	1.2112725342	9.6580143847
C14	1.9549423030	1.2755102793	10.9797981486
C15	2.7396021953	2.4655630989	11.1442311901
C16	2.7867536148	3.1034874227	9.9199511662
H17	-.7792267747	3.7692915216	6.9711965699
H18	-2.7765477025	2.0583982578	6.2042124480
H19	-1.5943627390	-.3932725410	5.8871341112
H20	1.0601376975	-.0470295650	6.4684819143
H21	3.4863292622	2.9877665620	4.8489063581
H22	5.1456934113	.9462399143	4.0856889754
H23	5.0407122223	-.9092279045	6.0990898955
H24	3.3209814907	.0950956688	7.9804919012
H25	.9221061344	.4995647502	9.1270835446
H26	1.6987956946	.5526573017	11.7549828004
H27	3.2038619840	2.8215133078	12.0640765758
H28	3.2623707513	4.0330957761	9.6085502891

Complex

Ru1	4.6061185194	.2866406830	2.6293352556
Cl2	7.0265653148	.2314603301	2.4473060028
Cl3	4.6695421609	2.7149278540	2.6022127644
P4	4.7837377463	.3840895260	4.9020878950
C5	4.5460607014	-1.7587896674	1.6775243165
C6	4.5277675136	-.7655489829	6.164677053
C7	3.5780725870	.2728055160	.5870210095
C8	2.5655889035	.3882522631	1.6204640528
C9	2.5413600968	-.6125208716	2.6339003928
C10	3.5229065197	-1.6669402700	2.6695045962
C11	5.6174464941	-2.8374478256	1.6624403809
H12	6.1099784525	-4.6122883575	.4836919800
H13	4.3632283903	-4.4395597533	.8238927941
H14	.9964591677	1.5682509440	2.5272984391
H15	.8868155823	1.4129053822	.7447128713
C16	5.2849404950	-3.8834465692	.5718092003
H17	5.1389401838	-3.4149397066	-.4181230340
C18	1.5838555500	1.5268865936	1.5963841639
H19	2.1251277854	2.4828887394	1.4836858298
C20	5.8504162121	-3.5039537724	3.0277938736
H21	6.7143397994	-4.1883106770	2.9623801309
H22	6.0691819662	-2.7511649897	3.8034794560
H23	4.9796176267	-4.1072420871	3.3471637310
H24	5.3534521990	-.7560265435	-.1020183691
H25	3.6728511858	1.0739176816	-.1522280838
H26	1.8126869117	-.5263181820	3.4457969108
H27	3.5175577398	-2.3677925273	3.5084674857
H28	6.5546506288	-2.3169365267	1.3821044215
O29	5.1119608257	1.7242497645	5.7925149525
O30	3.4017594982	-.0438158563	5.7303925055
O31	5.7683893045	-.7929293586	5.5049816432
C33	-.1184788184	2.1641302568	6.3282644205
C34	.8726636969	2.6872036845	5.4821705419
C35	2.0713985961	1.9905801927	5.2514269351
C36	2.2649402845	.7520558017	5.8908467841
C37	1.2828125297	.2152094335	6.7406637909
C38	.0934112086	.9255594554	6.9561618125
H39	-1.0471284861	2.7185388378	6.5010860125
H40	.7218157847	3.6539407142	4.9889883478
H41	2.8353087701	2.4095773096	4.5848151907
H42	1.4720266441	-.7458854486	7.2296810152
H43	-.6679584928	.5069490053	7.6238520919
C44	8.0201677721	4.7240662708	5.5226408017
C45	6.7693116844	4.9641174184	6.1169255210

Complex

Ru1	9.9686451757	5.5984808338	7.9479613214
Cl2	10.2517007665	3.3219550292	7.1474635215
Cl3	9.6222733697	6.3497724161	5.6586512676
P4	12.2688010469	5.7842677662	7.6932499728
N5	12.8717670397	7.4267802354	7.6950173789
N6	13.1295134527	4.9865035140	6.4238549158
N7	13.1874120131	5.1673958615	9.0602935234
C8	8.9337430010	7.4348945904	8.7980243500
C9	9.9300866465	6.9533767642	9.7038976494
C10	9.9110507660	5.6063182961	10.2179140654
C11	8.9273642191	4.6786873100	9.7772310562
C12	7.9328777023	5.1471761723	8.8293502456
C13	7.9389151238	6.4810949951	8.3645097079
C14	8.8524600562	3.2407702401	10.2606093291
C15	7.6153701468	3.0883524645	11.1825351068
C16	10.1244322041	2.7394513729	10.9588454046
C17	8.9012106519	8.8565510401	8.3045455478
C18	12.1684606813	8.4586708496	7.0457632536
C19	12.9775914287	9.5773047960	7.0199569131
C20	14.2195513003	9.2344543711	7.6518032182
C21	14.1473005997	7.9110835367	8.0390132404
C22	12.5772452661	6.4656400585	5.1716611918
C23	13.6119397440	4.2682644021	4.3450247852
C24	14.8396432937	4.3835056735	5.0844220996
C25	14.5318968861	4.8345520549	6.3486191826
C26	13.4733249589	3.8042664340	9.2351203144



H15	-1.9356282205	2.3010695028	.4612283756
H16	-4.3525279598	2.4898909588	-.1216744371
C17	1.8663056021	4.0925071436	-.8981459594
C18	1.3019025418	3.2267689250	-1.8521104860
C19	.7366250835	2.0088381930	-1.4506620083
C20	.7037933525	1.6363786383	-.0853424754
C21	1.2767897780	2.5128965666	.8611072570
C22	1.8555283102	3.7291822460	.4568646772
H23	2.3148747663	5.0417435664	-1.2116113848
H24	1.3074635341	3.4995976682	-2.9136448446
H25	.3072762024	1.3376383557	-2.2047641346
H26	1.2756836722	2.2535694822	1.9252250840
H27	2.2948872535	4.3954314627	1.2083726556

H8	-2.3412825279	-.9259757177	-.0909510737
H9	-2.3001142915	.8221486426	.3393778341
C10	1.5089589282	4.1912085012	-.7071546722
C11	1.1726707204	3.3182984024	-1.7564846819
C12	.7243176392	2.0199779904	-1.4740610627
C13	.5771119768	1.5724724799	-1.398257094
C14	.9236365378	2.4581253584	.9028935206
C15	1.3890918284	3.7543041056	.6211589950
H16	1.8694500083	5.2027324817	-.9250910312
H17	1.2707512084	3.6462798229	-2.7977707618
H18	.4903517749	1.3382390851	-2.3019557630
H19	.8331582832	2.1425057528	1.9478074213
H20	1.6549735931	4.4256509910	1.4460423844

Complex

Ru1	3.8190972889	.5124243020	2.6155011961
C12	6.0508435844	1.4659645293	2.8893478203
C13	2.7932949215	2.7027465039	2.9350601470
P4	3.8260831334	.3751312760	4.9683587350
C5	4.2982306929	1.7800436717	6.0739461500
C6	4.8093316509	2.9970891339	5.5838427775
C7	5.2013148391	3.9988408861	6.4891983446
C8	5.0905729711	3.7973858906	7.8736092539
C9	4.5699849099	2.5879654850	8.3648717271
C10	4.1739297250	1.5847801436	7.4694292537
C11	2.1667646070	-.1008409540	5.6270619458
C12	1.7848386611	-1.4497425720	5.7947744194
C13	.4894847710	-1.7791741035	6.2290472596
C14	-.4413991995	-.7620155578	6.4938228887
C15	-.0728144064	.5835007405	6.3180255745
C16	1.2197744278	.9150610041	5.8856869103
C17	4.7186912808	-.8652823192	1.0414050227
C18	3.9409437349	.1585351956	.3775944947
C19	2.5948360225	.3981198458	.7534455050
C20	1.9331689810	-.3752240542	1.7777657804
C21	2.7205355061	-1.3802330140	2.4283718431
C22	4.0829615830	-1.6513334921	2.0471717502
C23	6.1687209742	-1.0692895210	.6322872951
H24	3.7549959780	.6511896780	7.8625939742
H25	7.2463292995	-1.9342633923	-1.0641301472
H26	5.7901608630	-2.8580593370	-.5922392554
H27	.2577589100	-.5634071297	3.1345483307
H28	-.1955337454	-.4499657759	1.4076447445
C29	6.2042852985	-1.8396608044	-.7110034892
H30	5.6214736857	-1.3256557255	-1.4953714010
C31	.5103161096	-.0815778968	2.1759998989
H32	.3660792625	1.0071573396	2.2883969781
C33	7.0351418540	-1.7663730859	1.6928367700
H34	8.0838981504	-1.8012205161	1.3492701427
H35	7.0049122143	-1.2087844857	2.6436340294
H36	6.7152642984	-2.8116155545	1.8659523187
H37	.2100960390	-2.8308326784	6.3624141757
H38	5.5954685060	4.9440537018	6.1013765929
H39	4.8971700985	3.1535148902	4.5070943928
H40	5.4040911080	4.5823482833	8.5706851978
H41	4.4703531561	2.4227533822	9.4437349706
H42	-1.4503073526	-1.0167489502	6.8352261721
H43	-.7967238425	1.3806380450	6.5191552542
H44	4.4328435198	.8270376356	-.3344370205
H45	2.0715610736	1.2639279425	.3349483192
H46	2.2811996456	-1.9332380739	3.2672918035
H47	4.6547635528	-2.4095611625	2.5879792158
H48	6.5869317331	-.0578568604	.4706907482
H49	1.5017397672	1.9629712189	5.7427498975
H50	2.4992402026	-2.2533643051	5.5857338418
C52	4.9718501299	-.9628824329	5.5513651847
H53	4.9418991827	-1.0824345197	6.6474405309
H54	4.7365929987	-1.9231547275	5.0661134730
H55	5.9836218034	-.6534542558	5.2376079232

PPhMe<sub>2</sub>  
Ligand

P1	.0035052603	-.1751721724	.1146474883
C2	-.1009063461	-2.890932474	1.9783279157
H3	.9121877574	-.2823241625	2.4160500900
H4	-.6990235605	.5203130174	2.4357305422
H5	-.5672674624	-1.2563381249	2.2348042442
C6	-1.8242036190	.0333750618	-.2702920804
H7	-1.9465743613	.2880791671	-1.3368569488

Complex

Ru1	3.5168693023	.1316126455	2.4056018256
C12	5.5836294163	1.4145738983	2.6584513983
C13	2.2379725063	2.2032318847	2.6256077436
P4	3.5944507809	.1416069672	4.7561456212
C5	2.1177551646	-.6426271931	5.5420158450
C6	.8537129660	-.0453903649	5.3243162896
C7	-.3034535896	-.6201237934	5.8710742119
C8	-2.199760426	-1.8024608324	6.6285254054
C9	1.0289093498	-2.4065047502	6.8400648487
C10	2.1929063155	-1.8295960064	6.3013351905
C11	4.6101639351	-1.3194839653	1.0638141094
C12	3.8668293473	-.3986721184	.2217854929
C13	2.4865684324	-.1871403203	.4260468694
C14	1.7526049474	-.8896066231	1.4587165309
C15	2.4845641620	-1.8139915819	2.2658159105
C16	3.8913902411	-2.0487234506	2.0570370316
C17	6.1019222414	-1.4938258582	8.270633328
H18	3.1595573734	-2.3106226434	6.4843867813
H19	7.3896387684	-2.4221946140	-.6854830524
H20	5.9300609607	-3.3792747155	-.2973414995
H21	-.0571229669	-1.0391126472	2.6341727340
H22	-.3164010657	-1.0590852189	.8627561371
C23	6.3131894566	-2.3529616524	-.4480518825
H24	5.7966251821	-1.9239813897	-1.3248341821
C25	.2881429092	-.6157194337	1.6767907641
H26	.1068695590	.4735189723	1.6939085534
C27	6.8707996425	-2.0766064260	2.0188311200
H28	7.9514644486	-2.0928226698	1.7941711959
H29	6.7189304167	-1.4563248721	2.9175679393
H30	6.5683624033	-3.1181631360	2.2386728427
H31	-1.2759260037	-.1437374543	5.7027686940
H32	.7878981763	.8606025168	4.7089160218
H33	-1.1263003647	-2.2516599969	7.0498052988
H34	1.1026841682	-3.3291429740	7.4270834999
H35	4.4118854125	.2252796577	-.4927021809
H36	1.9781352701	.6104934703	-.1246860403
H37	1.9724043085	-2.3165584731	3.0935866261
H38	4.4241981645	-2.7358254308	2.197795841
H39	6.5008223341	-.4781776527	.6359401122
C41	3.7214457115	1.7824984572	5.5849172730
H42	3.8005949456	1.6487217511	6.6779461201
H43	4.6120821881	2.2907129189	5.1827008864
H44	2.8354772712	2.3826862147	5.3309141339
C45	5.0450886002	-.7633040714	5.4548845937
H46	5.0568410651	-.7241812515	6.5582425304
H47	5.0563475351	-1.8142198796	5.1226515172
H48	5.9423570704	-.2606476821	5.0573217357

PPh<sub>2</sub>Et

Ligand

P1	.1146005261	-.3377821192	-.0909980287
C2	-.1199536937	-.1780079108	1.7729672619
H3	.8912038459	-.1131316229	2.2178887180
H4	-.6524894140	.7613500838	2.0160492032
C5	-.8681455318	-1.3908827691	2.3509760468
H6	-.9674157843	-1.3023729234	3.4477788450
H7	-1.8840412960	-1.4733715069	1.9260282451
H8	-.3334784059	-2.3327639736	2.1331223921
C9	-4.3263607140	.1377916534	-1.5230325422
C10	-3.6718431479	-1.1024977136	-1.5854763921
C11	-2.3356493931	-1.2137892393	-1.1636776237
C12	-1.6403062636	-.0907974455	-.6645022753
C13	-2.3101755914	1.1519624609	-.6080097919
C14	-3.6419447562	1.2652917161	-1.0351607228





H25	2.5047285269	-1.9160101882	-1.8143940271	H12	-0.7685617861	.3787916674	2.3603964743
H26	-2.8115032842	.4703495639	-1.8843001153	H13	-1.0563774768	-2.1282774788	2.1986478407
H27	-3.5074662955	2.8427576079	-1.6271387645	H14	.6952441948	-2.3194116343	1.9974712605
H28	-1.8677947972	4.5593155088	-.8251200830	H15	-.7317039843	-1.1815007471	4.4916435859
H29	.4806512968	3.8763215943	-.2848119833	H16	.0408880220	-2.7751914339	4.3682351793
H30	1.1860936025	1.5034910118	-.5385100543	H17	2.2765261074	-1.7129897442	4.0507562130
Complex				H18	1.5322494100	-1.0922292011	5.5394172019
Ru1	1.0645324931	-.5183265461	-1.2511317139	C19	-.0915383993	4.3646383013	-.8065353287
Cl2	-.5804530036	-.3377824550	-3.0378510306	C20	1.0516741532	3.5776943276	-1.0199628034
Cl3	.1634558172	-2.7143997207	-.6778133817	C21	1.0088896171	2.1953403254	-.7726035278
P4	-.4986115960	.2765326907	.2667424095	C22	-.1704443940	1.5815662970	-.2949204019
C5	2.9997812853	-1.5600816110	-1.9708046981	C23	-1.3135519471	2.3837866931	-.0867858948
C6	3.0095460259	-1.2664108559	-.5452549984	C24	-1.2746131486	3.7635372509	-.3423722192
C7	2.8684949715	.0604492151	-.0551316127	H25	-.0642499537	5.4414473770	-1.0084740086
C8	2.6055571012	1.1563882622	-.9586287116	H26	1.9757201296	4.0371264871	-1.3894415562
C9	2.4486439613	.8427322309	-2.3421246797	H27	1.8985226038	1.5804153544	-.9561240015
C10	2.6988672089	-.4900058095	-2.8426381278	H28	-2.2455415214	1.9233300816	.2608848870
C11	3.1900432448	-2.9962813079	-2.4246973529	H29	-2.1723741360	4.3720087421	-.1819401923
C12	4.6869064816	-3.3766800000	-2.3175454383	C30	-4.5268863922	-1.5458198619	-.8411982297
C13	2.5243439676	2.5761068661	-.4579896555	C31	-3.5212743947	-1.6229243619	-1.8191602262
C14	2.6311051292	-3.2812233365	-3.8275932727	C32	-2.2093523078	-1.2312374294	-1.5106241690
N15	-1.0300214144	1.9306607140	.0312744210	C33	-1.8786660559	-.7378426261	-.2279756875
C16	-2.0677762810	-.6049675042	.6323514410	C34	-2.9006845129	-.6667089054	.7453452226
N17	.2070927164	.4027549773	1.8889358302	C35	-4.2121317418	-1.0711077645	.4427962049
C18	.7242159669	1.5339568399	2.5332403845	H36	-5.5495473054	-1.8617689328	-1.0760791952
C19	1.4797408036	1.1062874422	3.6133053122	H37	-3.7563944239	-1.9992089637	-2.8213568690
C20	1.4555307546	-.3273495867	3.6220859339	H38	-1.4232399017	-1.3122168454	-2.2714590551
C21	.6783546867	-.7382545434	2.5521913143	H39	-2.6773611530	-.2928887904	1.7537874198
C22	-.8920340209	2.6329112378	-1.1768596705	H40	-4.9899443177	-1.0131302413	1.2130801306
C23	-1.5449821508	3.8433599639	-1.0457910264	Complex			
C24	-2.1150947649	3.8930568160	.2702018156	Ru1	.1507179132	-1.8596117049	.2831353600
C25	-1.8057385464	2.7074020098	.9077049098	Cl2	.1839975487	-2.0737664859	-2.1401866806
C26	-2.7749253882	-1.1968859710	-.4359620510	Cl3	-1.7870144913	-3.3503171674	.3402781875
C27	-4.0193886498	-1.7954857625	-.1919876534	P4	-1.2382561012	.0406095828	-.1164181282
C28	-4.5563260237	-1.8203949514	1.1062368080	C5	2.4271341385	-1.9724666381	-.2164666695
C29	-3.8473323006	-1.2385288625	2.1695007749	C6	1.9079581573	-3.2409314781	.6808888339
C30	-2.6050581586	-.6283130471	1.9371884188	C7	1.0027797149	-3.2965781068	1.7700848366
H31	3.1090267760	-2.0923972070	.1651731913	C8	.5800355017	-2.1125621163	2.4774393853
H32	2.8693859433	.2410054633	1.0255390637	C9	1.0962361154	-.8648650705	1.9985088820
H33	2.1484591524	1.6265786834	-3.0440572517	C10	2.0346413785	-.7895240699	.9086808871
H34	2.5197924551	-.6873667503	-3.9022839829	C11	3.3858353900	-1.9644413834	-.9634289803
H35	2.6172279035	-3.6139690158	-1.7041822834	C12	4.7607253647	-2.5017385415	-.4942157482
H36	5.2971418286	-2.7809270798	-3.0210794305	C13	-.3808803859	-2.2044428400	3.6337257024
H37	4.8241934000	-4.4440278542	-2.5653408812	C14	3.5321138259	-.5989109899	-1.6506769639
H38	5.0821763376	-3.2100816605	-1.2994361270	C15	-2.2877392904	.6078613116	1.3532339507
H39	2.2944687310	2.6043696793	.6193648239	C16	-.1115564683	1.4702498603	-.4582647646
H40	3.5039146037	3.0697408910	-.6080277892	C17	-2.4235772775	.0814385695	-1.5329469095
H41	1.7589600329	3.1597003770	-.9957685345	C18	-3.3413446739	-.4628773867	1.7245516557
H42	3.1947020310	-2.7434954443	-4.6132345275	C19	-2.7880570162	1.3166971841	-2.1170121854
H43	2.7125824768	-4.3598184318	-4.0475214952	C20	.4210593316	1.6245444254	-1.7591208539
H44	1.5668617431	-2.9967797661	-3.8938468757	C21	-2.9710260735	1.9849860866	1.1753614477
H45	.4516316053	2.5329787604	2.1994697988	C22	-3.0257738369	-1.0795666935	-1.9945186433
H46	1.9714706576	1.7579596813	4.3366405011	C23	.3246869125	2.3460758912	.5610247104
H47	1.9361272946	-.9864601953	4.3460624292	C24	-4.1020146785	-.0589608595	3.0043984047
H48	.4269525040	-1.7295208064	2.1745018644	C25	-3.7431308793	1.3623002246	-3.1443191937
H49	-.4181665342	2.1449584178	-2.0272740418	C26	1.3502084217	2.6401147980	-2.0313398814
H50	-1.6217127665	4.6072110368	-1.8200577904	C27	-3.7211349496	2.3922632387	2.4619841566
H51	-2.6939220692	4.7097970103	.7036213969	C28	-3.9840172827	-1.0519016967	-3.0198531677
H52	-2.0633526889	2.3362218861	1.8973262022	C29	1.2605381883	3.3580820486	.2862489266
H53	-2.3445523413	-1.1920961599	-1.4425425184	C30	-4.7564827171	1.3287505807	2.8713647573
H54	-4.5645185599	-2.2566322034	-1.0225822016	C31	-4.3443016364	.1765313980	-3.5969776371
H55	-5.5244214278	-2.2995479167	1.2912192550	C32	1.7732847920	3.5105279209	-1.0118001625
H56	-4.2558425680	-1.2626444983	3.1859202580	H33	2.1255504110	-4.1490838696	.1116657444
H57	-2.0510285960	-.1868912883	2.7715680802	H34	.5219491570	-4.2494931589	2.0129404845
PPh <sub>2</sub> Cy				H35	.7624205302	.0647075177	2.4733424616
Ligand				H36	2.3619083157	.1909334466	.5553731858
P1	-.1043846489	-.2506625316	.0400430130	H37	2.9627806593	-2.6693394748	-1.7047406145
C2	.0416584425	-.2483542466	1.9312044037	H38	5.2125751234	-1.8249721570	-.2544422617
C3	1.5768023607	.3373348914	3.8834829135	H39	5.4515965827	-2.5689230877	-1.3532292775
C4	1.3942464436	.3727934507	2.3521771284	H40	4.6802978557	-3.5051064311	-.0401529464
C5	-.0809350106	-1.6893069031	2.4787280332	H41	-1.2034694803	-2.8999120396	3.3924036697
C6	.1041875878	-1.7299127519	4.0100133504	H42	.1306141049	-2.5755023493	4.5424683851
C7	1.4406434504	-1.0938784409	4.4365779444	H43	-.8177746927	-1.2193221470	3.8701596918
H8	.8114779819	.9873069695	4.3554603221	H44	4.0095176907	.1476698421	-.9884072113
H9	2.5612928087	.7644732394	4.1540415969	H45	4.1714894940	-.6999307165	-2.5452384652
H10	2.2168404999	-.1970627011	1.8720842715	H46	2.5496163957	-2.160309441	-1.9703259466
H11	1.4700484054	1.4120168369	1.9829533606	H47	-1.5622495985	.6771265622	2.1926575106
				H48	-4.0584295879	-.5593988927	.8851957874

H49	-2.8688509606	-1.4532323546	1.8381831286
H50	-2.3148142901	2.2455624197	-1.7822327339
H51	.1088100861	.9369782868	-2.5522567564
H52	-3.6931586255	1.9165299964	.3389980222
H53	-2.2397906644	2.7661699694	.9000558077
H54	-2.7348031377	-2.0668258576	-1.5552262578
H55	-.0699420154	2.2518806027	1.5788096431
H56	-4.8646371778	-.8254604836	3.2378615043
H57	-3.3950940614	-.0480282430	3.8607720684
H58	-4.0110633973	2.3264816588	-3.5913111858
H59	1.7485128909	2.7484543507	-3.0462572575
H60	-4.2102118272	3.3733724135	2.3098639147
H61	-2.9885157950	2.5301289469	3.2846884499
H62	-4.4412904761	-1.9815987123	-3.3756558744
H63	1.5803689821	4.0319390081	1.0892579890
H64	-5.5503976382	1.2826924158	2.0983162829
H65	-5.2516593696	1.6173734453	3.8180120682
H66	-5.0871440420	.2111390156	-4.4020785523
H67	2.4978073147	4.3035105922	-1.2277991454

PPhCy<sub>2</sub>  
Ligand

P1	.1429295241	-.2920130635	.1341045631
C2	.2845123310	-.0139270149	4.4487503924
C3	2.0285463515	-.2112999176	.0019383099
C4	-1.9565315241	-.9866042301	3.7520095788
C5	-1.6618125848	-.6130626708	2.2844440571
C6	-.1415727695	-.5853908630	1.9985040787
C7	.5806411475	.3602698140	2.9794943371
C8	-1.2294789484	-.0445091722	4.7301818675
H9	-1.6253704275	-2.0297372943	3.9352124553
H10	-3.0480207621	-.9664317108	3.9346724174
H11	-2.0877144824	.3885901941	2.0718371239
H12	-2.1633047458	-1.3220738902	1.5981333989
H13	.2433059341	-1.6156127225	2.1577907992
H14	1.6734281778	.3438235711	2.8054788631
H15	.2434565121	1.3991053886	2.7926388162
H16	.7158576588	-1.0134639663	4.6641011481
H17	.7900846865	.6990967561	5.1281446743
H18	-1.6399303285	.9802950651	4.6203256240
H19	-1.4210895660	-.3511429281	5.7761488773
C20	3.9632217248	.1857447213	-1.6214750252
C21	2.4319192966	.1851817136	-1.4386455572
C22	2.6451059385	-1.5819129321	.3737292137
C23	4.1771260776	-1.5844183253	.1887136705
C24	4.5770170802	-1.1750343864	-1.2413290059
H25	4.4059786643	.9783669375	-.9833896683
H26	4.2172921446	.4462373034	-2.6666886651
H27	1.9782298516	-.5369461846	-2.1482221640
H28	2.0162004681	1.1779064644	-1.6927093637
H29	2.4370828814	.5482070517	.7011157082
H30	2.3954129520	-1.8509916277	1.4174165913
H31	2.1968951863	-2.3664646996	-2.703744145
H32	4.6301295446	-.8752040597	.9119141100
H33	4.5836611060	-2.5844117625	.4333478305
H34	4.2190358147	-1.9465725052	-1.9536141419
H35	5.6789544452	-1.1432910418	-1.3382796105
C36	-1.2956488150	4.1476140726	-.3961660523
C37	-2.1244094922	3.0579399933	-.7084653387
C38	-1.6513387044	1.7456458477	-.5461192672
C39	-.3516964509	1.4919530878	-.0492078628
C40	.4697237841	2.6017004537	.2570308449
C41	.0047058507	3.9153750498	.0820285556
H42	-1.6573948907	5.1729286324	-.5322651988
H43	-3.1367476744	3.2287592094	-1.0921999686
H44	-2.2928354114	.8986549446	-.8181283419
H45	1.4852553825	2.4439738468	.6372087163
H46	.6597655853	4.7605951850	.3234475881

Complex

Ru1	1.5412710615	-2.0292892227	-.2506713975
C12	1.3703626463	-3.1123438939	-2.4292769875
C13	-.0620290743	-3.6985408677	.5462719205
P4	-.3841128772	-.6984813354	-7.7622055951
C5	2.3455845427	-1.4106235669	1.7875005808
C6	2.4672879693	-.3495370557	.8312724178
C7	3.1939551489	-.5036697028	-.3999501712
C8	3.7541232579	-1.7700094691	-.7438355352
C9	3.6057918593	-2.8663520831	.1838249226

C10	2.8961979718	-2.6852083626	1.4014193704
C11	1.7050916837	-1.1437663508	3.1411138380
C12	2.7294907412	-.4179017102	4.0488323856
C13	4.4721356620	-1.9787744722	-2.0502050215
C14	1.1499521704	-2.4023567323	3.8295210411
C15	-1.9264316031	-1.5664837499	-1.4382498176
C16	-.9678345604	.0426428236	.8364862475
C17	.0332561710	.8028424620	-1.8269197826
C18	-1.8295960483	-1.8974973241	-2.9483159661
C19	.8009811270	.4493450542	-3.1242659449
C20	-.7289381168	1.3855589293	1.2047132365
C21	-3.2767176466	-.8683461622	-1.1319869038
C22	-1.1392768158	1.7625661328	-2.1477505086
C23	-1.6245675633	-.8022659731	1.7648346767
C24	-3.0075014910	-2.8009028948	-3.3711177724
C25	1.3360399745	1.7336969744	-3.7908311989
C26	-1.1440546207	1.8759255040	2.4559245372
C27	-4.4540793124	-1.7713660207	-1.5588172671
C28	-.6117129683	3.0513331593	-2.8148176054
C29	-2.0478666598	-.3064358475	3.0074457480
C30	-4.3675042361	-2.1565579138	-3.0466246101
C31	.2043151225	2.7384271773	-4.0834251950
C32	-1.8115831119	1.0344791622	3.3584789539
H33	1.9834717193	.6087857560	1.0544869852
H34	3.2666712115	.3296102191	-1.1055774137
H35	3.9399502658	-3.8658669746	-.1081012045
H36	2.6965934584	-3.5596569198	2.0267374853
H37	.8617945192	-.4494463563	2.9653567086
H38	3.6059835218	-1.0621391002	4.2476207790
H39	2.2663840914	-.1640553541	5.0194524655
H40	3.0936287920	.5177895158	3.5878281690
H41	5.5565557536	-2.0995649438	-1.8657097228
H42	4.0919737738	-2.8838699957	-2.5527045899
H43	4.3272616448	-1.1243938759	-2.7309933755
H44	1.9639158359	-3.0717439088	4.1665994473
H45	.5757998249	-2.1111758904	4.7268696767
H46	.4894274223	-2.9688665009	3.1511646076
H47	-1.8868897064	-2.5266331485	-.8842926480
H48	.7528454771	1.3528057201	-1.1803657239
H49	-.8686180407	-2.3884412782	-3.1712256263
H50	-1.8781822788	-.9574999855	-3.5358505964
H51	1.6167429198	-.2618664265	-2.9089594113
H52	.1234507845	-.0721535242	-3.8248903517
H53	-.2207733503	2.0706306421	.5182361399
H54	-3.3702967981	-.6228099445	-.0604409544
H55	-3.3379245603	.0904045116	-1.6829479184
H56	-1.7188052648	2.0108918102	-1.2404822296
H57	-1.8374689574	1.2564872233	-2.8420618036
H58	-1.7697140967	-1.8602874087	1.5211808752
H59	-2.9196623540	-3.7712653261	-2.8426526737
H60	-2.9322455550	-3.0218081910	-4.4528203411
H61	2.0819999217	2.2109471199	-3.1199250290
H62	1.8715172764	1.4760292898	-4.7240791551
H63	-.9484411395	2.9222773361	2.7172179910
H64	-4.4429412717	-2.6913484194	-.9394885625
H65	-5.4101948025	-1.2560224241	-1.3440232718
H66	.0278138989	3.5985090542	-2.0906611642
H67	-1.4585811836	3.7222826286	-3.0544981749
H68	-2.5582447723	-.9766214604	3.7081717477
H69	-5.1962701899	-2.8388779154	-3.3159136895
H70	-4.4952645931	-1.2432963851	-3.6648084788
H71	.6154002391	3.6707155743	-4.5151076287
H72	-.4720631337	2.3062732372	-4.8489877341
H73	-2.1415997304	1.4186383298	4.3301394874

PiBu<sub>3</sub>  
Ligand

P1	0.0309321597	0.0336511008	0.0242492171
C2	-0.0500712502	0.01190983821	1.9106122982
C3	1.9101685299	-0.0284767046	-0.1680401380
C4	-0.2231547073	1.8697987866	-0.3450930244
C5	-1.4780674212	0.1240820974	2.5077257391
C6	-2.2143231964	-1.2046201009	2.2535276596
C7	-1.4238601155	0.4395657388	4.0163216409
C8	2.5426836037	-1.4314932663	-0.0036327456
C9	4.0794575976	-1.3189279025	0.0589346788
C10	2.1104765827	-2.3946389047	-1.1251042968
C11	-0.2956711570	2.2342573702	-1.8475596441
C12	-1.5385413640	1.6307524156	-2.5281766604

C13	-0.2632040439	3.7656745631	-2.0264068354	H50	1.3745005728	-5.1319902557	1.6202645350
H14	0.4993871641	-0.7638993742	2.2966089066	H51		-1.5308266510	-4.6768898042
H15	0.5086373513	1.0143746927	2.2542794114		2.7312407334		
H16	2.3686777209	0.6817145508	0.5511311723	H52	-0.0269032235	-4.9034907201	3.6667247048
H17	2.1422678101	0.3550701153	-1.1827309648	H53	-1.0316552212	-3.4536829472	3.9436071051
H18	-1.1731689913	2.1673725667	0.1443103608	H54	-2.6675500343	-1.5940331162	-0.9193636867
H19	0.5828999460	2.4513063947	0.1488142893	H55	-4.2443766012	0.0518920984	1.1609503436
H20	-2.0561576987	0.9354775399	2.0168950104	H56	-3.4534762936	-1.5110930152	1.4958159376
H21	-1.6907762637	-2.0418277315	2.7552848983	H57	-4.8112670937	-1.4292519146	0.3414033317
H22	-2.2658069289	-1.4386224126	1.1756728255	H58	-3.9063936248	1.2235029457	-1.1450293613
H23	-3.2454490273	-1.1684515721	2.6502007754	H59	-4.5588609376	-0.2581346590	-1.8965275029
H24	-0.8482433673	-0.3353753741	4.5583845464	H60	-2.9768431599	0.3856465082	-2.4208861961
H25	-2.4384401236	0.4702163347	4.4552587996	H61	-1.0557300906	-1.2447354091	-2.4638792277
H26	-0.9398704090	1.4144405526	4.2100068027	H62	1.5874081533	-2.4323500212	-3.5230256474
H27	2.1990653346	-1.8555246109	0.9636178620	H63	0.1086133985	-2.1625647825	-4.4870815613
H28	4.4798157883	-0.8908595670	-0.8803080693	H64	0.9990691314	-0.7699303409	-3.8084903687
H29	4.4051390642	-0.6674740572	0.8906040272	H65	0.1743763444	-4.0425440734	-1.9985893819
H30	4.5475886899	-2.3108102295	0.2002702762	H66	-1.3389468230	-3.4609165757	-1.2661076544
H31	2.4611002059	-2.0280406762	-2.1097065276	H67	-1.2357557681	-3.6797837821	-3.0323960614
H32	2.5399218945	-3.4013285974	-0.9700730685				
H33	1.0116224196	-2.4906802997	-1.1746606157				
H34	0.6046545265	1.8198015054	-2.3486085561	[RuCl <sub>2</sub> (p-cymene)] <sub>2</sub>			
H35	-2.4650484738	2.0421744075	-2.0819805973	Ru1	-1.7618371670	-0.6490459919	-0.0005169187
H36	-1.5694168733	0.5330249036	-2.4133388562	Cl2	-0.7888514036	-2.8390719226	-0.0067056857
H37	-1.5530250907	1.8670404166	-3.6079137649	Cl3	0.0000000000	0.0000000000	1.6215241140
H38	-1.1366701885	4.2362899525	-1.5352075622	Cl4	0.0000000000	0.0000000000	-1.6257469185
H39	-0.2914299223	4.0440986114	-3.0962904909	C5	-3.1050264558	0.8037154015	-0.9750523699
H40	0.6489017826	4.2067389758	-1.5840517950	C6	-3.4653533883	-0.5344135871	-1.3874141240
				H7	-3.4311774920	-0.8079396018	-2.4459317299
				C8	-3.7262511394	-1.5310823304	-0.4001196042
Complex				H9	-3.8732711661	-2.5715575033	-0.7041139505
Ru1	1.4152752978	0.5571392537	1.6692504817	C10	-3.6297463816	-1.2077379367	1.0005029690
Cl2	0.4702449462	-0.3425738982	3.7355483454	C11	-3.2642836622	0.1221537516	1.3867479021
Cl3	2.9280425612	-1.3584299302	1.5353525167	H12	-3.0622692473	0.3361947144	2.4411927909
P4	-0.1009218310	-0.8717195847	0.5116568895	Cl3	-3.0334489736	1.1485832004	0.4036006812
C5	2.8120253149	1.7686365116	0.3915770379	H14	-2.6489078311	2.1268743568	0.7037703110
C6	1.4587364618	2.1183409508	0.0945103785	Ru15	1.7618371670	0.6490459919	-0.0005169187
C7	0.5471870647	2.5571234602	1.1230738425	Cl16	0.7888514036	2.8390719226	-0.0067056857
C8	0.9655381567	2.6274659430	2.4840031157	C17	3.1050264558	-0.8037154015	-0.9750523699
C9	2.3472648248	2.2986601604	2.7865664457	C18	3.4653533883	0.5344135871	-1.3874141240
C10	3.2349430023	1.8756575517	1.7745205379	C19	3.7262511394	1.5310823304	-0.4001196042
C11	-0.7902294227	-2.3430984890	1.4346464226	H20	3.4311774920	0.8079396018	-2.4459317299
C12	0.6594357125	-1.3648279203	-1.1332545544	H21	3.8732711661	2.5715575033	-0.7041139505
C13	-1.6420351020	0.0967982242	0.0317044854	C22	3.6297463816	1.2077379367	1.0005029690
C14	0.0542965405	3.0681059279	3.6219322477	C23	3.2642836622	-0.1221537516	1.3867479021
C15	3.7774085645	1.2999685755	-0.6670469800	H24	3.0622692473	-0.3361947144	2.4411927909
C16	0.3739202606	4.5379715135	3.9898223558	C25	3.0334489736	-1.1485832004	0.4036006812
C17	-1.4451970860	2.8734100356	3.3468405917	H26	2.6489078311	-2.1268743568	0.7037703110
C18	0.1441850797	-3.3932890743	2.0884253841	H29	-2.7728481158	1.5262746259	-1.7262805788
C19	0.7574844480	-4.3859654958	1.0866526856	H30	-3.7309709299	-1.9937696219	1.7530080506
C20	-0.6605326369	-4.1474175820	3.1678727315	H31	2.7728481158	-1.5262746259	-1.7262805788
C21	-2.9353059776	-0.6231636735	-0.4601386026	H32	3.7309709299	1.9937696219	1.7530080506
C22	-3.9111356032	-0.8982414993	0.7015293904				
C23	-3.6310466084	0.2281297164	-1.5432198696	[PdL <sub>n</sub> ] complexes			
C24	-0.1755180637	-1.9040252407	-2.3233577166	L = PPh <sub>3</sub>			
C25	0.6777028833	-1.8085262042	-3.6078747569	B3LYP			
C26	-0.6744518504	-3.3485863675	-2.1396086672	E= -1036.28092 H			
H27	1.0996873495	2.0212625858	-0.9370876896	P1	2.2893556158	0.0002094824	0.0054962915
H28	-0.4919804028	2.7727765748	0.8615024732	C2	4.3601835672	4.1815157805	0.0018481748
H29	2.6626312917	2.2564684353	3.8336090653	C3	4.9008505789	3.1668707007	0.7927601576
H30	4.2287288228	1.5078794151	2.0495426742	C4	4.3122287508	1.9009190076	0.8136215198
H31	-1.5271489029	-2.8420942428	0.7745137343	C5	3.1674411935	1.6329083718	0.0473370651
H32	-1.3555459239	-1.8460339890	2.2450638334	C6	2.6257722854	2.6673050755	-0.7338787373
H33	1.1520405314	-0.4251291802	-1.4503748985	C7	3.2204581251	3.9282557993	-0.7633616505
H34	1.4912822919	-2.0483071697	-0.8832426659	H8	4.8200311022	5.1662936457	-0.0132736305
H35	-1.2814201632	0.7994708147	-0.7456803261	H9	5.7851622721	3.3594750775	1.3954487069
H36	-1.8844952636	0.7191172548	0.9133918941	H10	4.7439311537	1.1198512619	1.4316972857
H37	0.3146176896	2.4241071076	4.4840131725	H11	1.7269433751	2.4831293034	-1.3183954628
H38	4.5488244040	2.0695714655	-0.8594156040	H12	2.7891007811	4.7153992870	-1.3765994896
H39	3.2605484727	1.0905109953	-1.6190627324	Cl3	3.9965500798	-2.1463732420	3.7802076425
H40	4.2816334670	0.3743670126	-0.3364169816	C14	4.6344973395	-2.3390527759	2.5540856214
H41	0.1198940196	5.2199755059	3.1571299219	C15	4.1561460731	-1.7077210261	1.4042052028
H42	1.4434292537	4.6790073005	4.2283740538	C16	3.0265743658	-0.8772059372	1.4630053118
H43	-0.2145928747	4.8449051450	4.8729983731	C17	2.3855000420	-0.7032059355	2.7009282412
H44	-1.8065315401	3.5143812989	2.5200699541	C18	2.8698043943	-1.3250094227	3.8512983465
H45	-2.0268185400	3.1451131701	4.2453886217	H19	4.3707055414	-2.6382603471	4.6742973591
H46	-1.6603318272	1.8171040668	3.1117506948	H20	5.5091403503	-2.9818627982	2.4908522177
H47	0.9623151912	-2.8473095943	2.5884891519	H21	4.6632620328	-1.8643399739	0.4570666973
H48	-0.0249675883	-4.9381436739	0.5298842095	H22	1.4951558556	-0.0810213274	2.7603819368
H49	1.4164352526	-3.8822676487	0.3598105117				

H23	2.3623308206	-1.1759728104	4.8010298270
C24	4.2253518229	-2.2693845274	-3.5808588616
C25	4.8616793015	-1.1293661334	-3.0880549784
C26	4.3141693197	-0.4265501268	-2.0130541781
C27	3.1153053579	-0.8504764547	-1.4194529413
C28	2.4784046874	-1.9923008746	-1.9336380447
C29	3.0315932205	-2.7005596423	-2.9997430814
H30	4.6540567368	-2.8161792558	-4.4167625975
H31	5.7892183733	-0.7857111349	-3.5395572376
H32	4.8208524375	0.4569465433	-1.6369466123
H33	1.5392885112	-2.3247557380	-1.4969832249
H34	2.5266050771	-3.5840732851	-3.3820471649

BP86

E=-1036.280009 H

P1	2.2800271649	0.0003672233	0.0058666352
C2	4.3708751937	4.1906939991	0.0042583064
C3	4.9030184724	3.1721368114	0.8101552706
C4	4.3072208571	1.9007165374	0.8302808655
C5	3.1638613327	1.6335307207	0.0479875728
C6	2.6288197260	2.6707522946	-0.7484339448
C7	3.2321405838	3.9362086564	-0.7776715241
H8	4.8380189756	5.1821958921	-0.009935175
H9	5.7892567636	3.3658582669	1.4261147187
H10	4.7307246605	1.1107683269	1.4600445220
H11	1.7281533260	2.4828887474	-1.3462778767
H12	2.8068982680	4.7283972353	-1.4048542145
C13	4.0013355684	-2.1551146716	3.7906077237
C14	4.6346280217	-2.3558756483	2.5540493911
C15	4.1514387425	-1.7199215467	1.3990848189
C16	3.0211524731	-0.8780225372	1.4652312660
C17	2.3833890032	-0.6951723946	2.7129136829
C18	2.8742928215	-1.3205995826	3.8679546487
H19	4.3807360716	-2.6524754617	4.6907192217
H20	5.5121863030	-3.0098530588	2.4863517898
H21	4.6536264185	-1.8800937321	0.4387830437
H22	1.4907122850	-0.0602522710	2.7750947379
H23	2.3700198745	-1.1643264590	4.8287244100
C24	4.2319770771	-2.2695981090	-3.5951971483
C25	4.8593446087	-1.1121728546	-3.1082125459
C26	4.3060846151	-0.4085855338	-2.0262135092
C27	3.1107449672	-0.8508437259	-1.4209568431
C28	2.4811086898	-2.0094920285	-1.9284103375
C29	3.0413559861	-2.7186104191	-3.0007659940
H30	4.6662834160	-2.8176458028	-4.4393004560
H31	5.7870799555	-0.7547210804	-3.5706491187
H32	4.8036467137	0.4920771790	-1.6503886142
H33	1.5411538712	-2.3538612413	-1.4792473675
H34	2.5425318751	-3.6184721472	-3.3792324773

M06

E=-1035.695557 H

P1	2.2266067184	0.0043723234	0.0001244911
C2	4.4166790230	4.0931988447	0.0159905887
C3	4.8789405200	3.0873833857	0.8566074022
C4	4.2439222328	1.8500774692	0.8854906605
C5	3.1314242847	1.6085124914	0.0763556045
C6	2.6666132524	2.6318185985	-0.7550460277
C7	3.3085369517	3.8627969239	-0.7926939566
H8	4.9180204851	5.0597836299	-0.0064931627
H9	5.7454777452	3.2642710112	1.4928105580
H10	4.6208144248	1.0642942777	1.5407721707
H11	1.7909274399	2.4561844853	-1.3828300876
H12	2.9389058353	4.6478294159	-1.4509924026
C13	4.0424268991	-2.1101882007	3.7084887635
C14	4.6022178152	-2.3581449095	2.4605145819
C15	4.0803552890	-1.7493279579	1.3239178486
C16	2.9848488781	-0.8884620397	1.4238444101
C17	2.4211247437	-0.6574288662	2.6820483752
C18	2.9499739736	-1.2562542496	3.8182107762
H19	4.4552702931	-2.5863392280	4.5967538322
H20	5.4567068823	-3.0279173710	2.3699373749
H21	4.5333015186	-1.9425003377	0.3510232498
H22	1.5568338483	0.0037718745	2.7687323231
H23	2.5038200748	-1.0609384020	4.7924162255
C24	4.2793921570	-2.2238554591	-3.5131278781
C25	4.8251407565	-1.0218675582	-3.0781696311
C26	4.2337797908	-0.3199712236	-2.0327471012
C27	3.0813417666	-0.8112877128	-1.4154165730

C28	2.5333027729	-2.0145450233	-1.8700282609
C29	3.1313123796	-2.7211457157	-2.9051640916
H30	4.7469997871	-2.7726822691	-4.3293593700
H31	5.7234330380	-0.6280698844	-3.5524091537
H32	4.6765134049	0.6163526194	-1.6919558732
H33	1.6269675268	-2.4020231706	-1.4006998196
H34	2.6963979216	-3.6607806084	-3.2431510732

M06-L

E=-1036.177731 H

P1	2.2324760707	0.0039246326	-0.0003672465
C2	4.4172957615	4.0971484503	0.0248078758
C3	4.8646238796	3.0941576966	0.8796261766
C4	4.2292686765	1.8551310974	0.9032997160
C5	3.1292539490	1.6062473375	0.0746520275
C6	2.6790390721	2.6288330281	-0.7715432186
C7	3.3225577392	3.8611658782	-0.8034491350
H8	4.9183577487	5.0637164536	0.0066149210
H9	5.7191510846	3.2743540421	1.5305963391
H10	4.5948603617	1.0738855117	1.5690355357
H11	1.8156070497	2.4518288580	-1.4140471309
H12	2.9644511157	4.6425579842	-1.4720364766
C13	4.0428120027	-2.1162910831	3.7092132858
C14	4.5892124631	-2.3777556191	2.4561580814
C15	4.0673156477	-1.7652288675	1.3195723593
C16	2.9832784036	-0.8858483975	1.4222502931
C17	2.4324246405	-0.6416912258	2.6876483225
C18	2.9626546087	-1.2444135052	3.8232686152
H19	4.4552742913	-2.5948362114	4.5961146446
H20	5.4326972337	-3.0604303415	2.3615133983
H21	4.5100396320	-1.9695585468	0.3451770806
H22	1.5794051268	0.0316778292	2.7800317152
H23	2.5270417387	-1.0385391163	4.7998398065
C24	4.2794512320	-2.2213272530	-3.5207236494
C25	4.8115354436	-1.0072871882	-3.0968815890
C26	4.2198413271	-0.3075978003	-2.0480372925
C27	3.0787457916	-0.8118208479	-1.4137542378
C28	2.5439412323	-2.0286439147	-1.8587992950
C29	3.1435507296	-2.7324454195	-2.8973113209
H30	4.7468631102	-2.7675474734	-4.3385093637
H31	5.6988071758	-2.0625187146	-3.5820153931
H32	4.6522405925	0.6363202736	-1.7176754222
H33	1.6489159654	-2.4280617038	-1.3801254164
H34	2.7193103677	-3.6800412607	-3.2258191623

[PdL<sub>2</sub>]

B3LYP

E=-2199.386214 H

Pd1	-0.0055093235	-0.0205084688	-0.0560172855
P2	2.3076534625	-0.0143680842	0.0177430721
C3	4.2925058228	4.1963275532	0.0978697249
C4	4.8965299477	3.1540658572	0.8019230146
C5	4.3250081045	1.8802376152	0.7982827229
C6	3.1393054894	1.6368687234	0.0900171157
C7	2.5313291798	2.6960317778	-0.6018179054
C8	3.1086098972	3.9650795370	-0.6053506944
H9	4.7386576656	5.1877924477	0.1038005266
H10	5.8140734638	3.3317667396	1.3577910923
H11	4.8012129154	1.0767660195	1.3527440555
H12	1.5954737673	2.5187715337	-1.1277774636
H13	2.6288308624	4.7759464793	-1.1476493167
C14	3.9824449820	-2.1704267117	3.7940503194
C15	4.6433167356	-2.3307993238	2.5759960795
C16	4.1650857856	-1.6977696009	1.4267757120
C17	3.0142648039	-0.8982326383	1.4819550094
C18	2.3477858013	-0.7556848003	2.7098623244
C19	2.8328058642	-1.3796264364	3.8583373027
H20	4.3558291642	-2.6646494586	4.6873129530
H21	5.5341604761	-2.9515116943	2.5172473401
H22	4.6888571187	-1.8318428402	0.4846324253
H23	1.4377113756	-0.1612440373	2.7537247084
H24	2.3069533888	-1.2568686132	4.8020428614
C25	4.2726470874	-2.2408253280	-3.5669789165
C26	4.9134268547	-1.1195733625	-3.0387504135
C27	4.3484020709	-0.4271907083	-1.9659168512
C28	3.1309461367	-0.8480791145	-1.4117139210
C29	2.4866921131	-1.9688668340	-1.9608676070
C30	3.0578131027	-2.6648465629	-3.0249897322
H31	4.7149657541	-2.7778789167	-4.4025669394

H32	5.8559024393	-0.7809636759	-3.4623458232	C39	-4.3289505713	0.4314536058	1.9309332025
H33	4.8563729375	0.4446484820	-1.5637658662	C40	-3.1790496543	0.8382240282	1.2229544272
H34	1.5288997405	-2.2821170591	-1.5514475485	C41	-2.6566246406	2.1310457291	1.4483918211
H35	2.5494778485	-3.5330507202	-3.4374248519	C42	-3.2863283027	3.0071738853	2.3435980602
P36	-2.3103950363	-0.2302629180	-0.0337958742	H43	-4.9218213938	3.2777358099	3.7491566121
C37	-4.3862443389	2.6561051964	2.9725738222	H44	-5.8428862245	0.9785571957	3.3831789278
C38	-4.9188070028	1.3800715633	2.7874315584	H45	-4.7378995518	-0.5741340041	1.7779956536
C39	-4.3220427273	0.4922632513	1.8896898686	H46	-1.7415396744	2.4357123199	0.9236807836
C40	-3.1808829354	0.8719854562	1.1678738829	H47	-2.8715177825	4.0092245379	2.5065892264
C41	-2.6451263571	2.1537034742	1.3724404734	C48	-3.6586143333	-4.5449019770	1.1846111599
C42	-3.2484653222	3.0421923771	2.2616253081	C49	-2.4894406681	-3.9803775291	1.7213160843
H43	-4.8510014833	3.3443940364	3.6742638272	C50	-2.0934000813	-2.6897830116	1.3417543920
H44	-5.8002267878	1.0707528130	3.3443663565	C51	-2.8718054478	-1.9401359726	0.4332540261
H45	-4.7434665831	-0.5003609553	1.7580749775	C52	-4.0402142169	-2.5167752645	-0.1075909644
H46	-1.7428620101	2.4429140522	0.8385877346	C53	-4.4294414823	-3.8129183687	-0.2676348955
H47	-2.8224370789	4.0318255363	2.4080518842	H54	-3.9626623487	-5.5585148187	1.4722687611
C48	-3.6555583145	-4.4752817346	1.3296635454	H55	-1.8759543177	-4.5511695324	2.4287400502
C49	-2.5128376963	-3.8692053368	1.8557230341	H56	-1.1650732526	-2.2521635059	1.7325713597
C50	-2.1273492076	-2.6033522965	1.4169321076	H57	-4.6439302095	-1.9544259248	-0.8296867277
C51	-2.8883018020	-1.9164984172	0.4570685090	H58	-5.3372812668	-4.2530077814	-0.1626967481
C52	-4.0316849784	-2.5352179397	-0.0691969281	C59	-4.3584837477	0.5959786011	-4.0961887429
C53	-4.4103743500	-3.8076704927	0.3647060350	C60	-5.0368347609	0.9296083893	-2.9134705681
H54	-3.9516039706	-5.4662325741	1.6648170995	C61	-4.4381254688	0.6951097488	-1.6648498620
H55	-1.9141035202	-4.3863575955	2.6013601485	C62	-3.1502261344	0.1252723290	-1.5895549853
H56	-1.2232998046	-2.1413085057	1.8067586959	C63	-2.4685440271	-0.1931491068	-2.7840952802
H57	-4.6267378303	-2.0274104315	-0.8228156024	C64	-3.0729289616	0.0327648522	-4.0288899586
H58	-5.2965231475	-4.2773504986	-0.0550399001	H65	-4.8276042065	0.7814152926	-5.0698850405
C59	-4.4246175484	0.4684732282	-4.1281555674	H66	-6.0372602403	1.3769146044	-2.9601855797
C60	-5.0861159274	0.8361470810	-2.9550658052	H67	-4.9727230640	0.9611434228	-0.7452114538
C61	-4.4765373680	0.6438247126	-1.7133428742	H68	-1.4533252927	-0.6072596101	-2.7232642041
C62	-3.1940219101	0.0829886637	-1.6305247177	H69	-2.5331809163	-0.2205453537	-4.9493243597
C63	-2.5298248199	-0.2688491275	-2.8160495167				
C64	-3.1442102155	-0.0848229138	-4.0544946509				
H65	-4.9004037377	0.6196565034	-5.0935386489				
H66	-6.0794004903	1.2755304000	-3.0041496519				
H67	-5.0016261628	0.9363507882	-0.8079304374				
H68	-1.5234295920	-0.6776371951	-2.7585038970				
H69	-2.6175305273	-0.3646088602	-4.9637370528				

BP86

E= -2199.461596 H

Pd1	-0.0013746099	-0.0185254712	-0.0274817084
P2	2.2925959732	-0.0135908253	-0.0024523819
C3	4.2864802223	4.2138712073	-0.0458835030
C4	4.8940429020	3.1854262666	0.6914292765
C5	4.3202019603	1.9039113337	0.7230852048
C6	3.1278243494	1.6410454491	0.0169133456
C7	2.5148296264	2.6851404135	-0.7091208785
C8	3.0958750142	3.9607164240	-0.7475029739
H9	4.7350315374	5.2143046484	-0.0665560990
H10	5.8187775535	3.3800205975	1.2482954798
H11	4.7973802299	1.1068175527	1.3053152197
H12	1.5701006516	2.4874100698	-1.2325992713
H13	2.6110273413	4.7625021431	-1.3174065955
C14	3.9562096065	-2.0556073373	3.8598685091
C15	4.6364424927	-2.2468106725	2.6470274831
C16	4.1638056456	-1.6470614864	1.4676621627
C17	2.9995006191	-0.8517320272	1.4916644049
C18	2.3123583279	-0.6778756086	2.7135243858
C19	2.7933118956	-1.2674304391	3.8909229086
H20	4.3264955499	-2.5263909023	4.7784848870
H21	5.5402183182	-2.8674724724	2.6151976710
H22	4.7000674841	-1.8032997556	0.5243270603
H23	1.3876624406	-0.0854324161	2.7239269262
H24	2.2513143096	-1.1211944337	4.8331390005
C25	4.2546655988	-2.3625946624	-3.5408881575
C26	4.9111903100	-1.2314447273	-3.0300947415
C27	4.3449434777	-0.5005475414	-1.9718956121
C28	3.1099715958	-0.8940759553	-1.4150738910
C29	2.4479934404	-2.0232268368	-1.9457146042
C30	3.0212563166	-2.7571358683	-2.9948066555
H31	4.6987345999	-2.9308556937	-4.3668254673
H32	5.8701002662	-0.9126629585	-3.4566679881
H33	4.8641003516	0.3824949385	-1.5810317431
H34	1.4730016558	-2.3105580108	-1.5295472198
H35	2.4976804067	-3.6343481507	-3.3936853766
P36	-2.2826457336	-0.2361652143	0.0087475854
C37	-4.4357188106	2.5969319662	3.0401726799
C38	-4.9514677776	1.3079166851	2.8354027031

M06

E= -2198.236136 H

Pd1	-0.0035221241	0.0290349017	-0.0398017294
P2	2.3088311388	0.0120253458	-0.0003616568
C3	4.4174499616	4.1142406413	0.3561265734
C4	4.9503541248	3.0261188660	1.0403091407
C5	4.3363755875	1.7795131975	0.9594739275
C6	3.1786940035	1.6153497623	0.1953402263
C7	2.6407424518	2.7168898210	-0.4769851714
C8	3.2620259741	3.9581093723	-0.4047141345
H9	4.9000848302	5.0895970608	0.4218773465
H10	5.8508467225	3.1480620341	1.6422687036
H11	4.7598907109	0.9284051820	1.4959649580
H12	1.7209388913	2.5899795045	-1.0529246594
H13	2.8369316354	4.8098026297	-0.9356401810
C14	3.9256424885	-2.4573434225	3.5651857431
C15	4.5892552320	-2.5302735513	2.3441801738
C16	4.1275806302	-1.8025590276	1.2502283178
C17	2.9920206792	-0.9989834155	1.3702625010
C18	2.3217053334	-0.9426563841	2.5974600983
C19	2.7911938293	-1.6600596261	3.6915443606
H20	4.2890996466	-3.0291534751	4.4196046959
H21	5.4733131093	-3.1591106029	2.2405197120
H22	4.6539678972	-1.8626956305	0.2953529002
H23	1.4172809732	-0.3345849954	2.6797533085
H24	2.2634840890	-1.6064784000	4.6441479117
C25	4.2301059317	-1.9715350764	-3.7132982745
C26	4.8747814730	-0.8881778698	-3.1250392237
C27	4.3196660799	-0.2624552168	-2.0119844105
C28	3.1090479323	-0.7146113996	-1.4826289802
C29	2.4595774878	-1.7948007773	-2.0888560105
C30	3.0216461081	-2.4259412876	-3.1924096073
H31	4.6673681163	-2.4597260058	-4.5846311912
H32	5.8176496528	-0.5264071440	-3.5349272624
H33	4.8322830291	0.5845868956	-1.5524807743
H34	1.4999560266	-2.1292374523	-1.6858715076
H35	2.5095792462	-3.2700200658	-3.6541247914
P36	-2.3022771033	-0.2114615760	0.0112114599
C37	-4.5382365041	2.8033880297	2.7146385433
C38	-4.9818260446	1.4855380766	2.6724228616
C39	-4.3284955757	0.5516398376	1.8731931697
C40	-3.2204069880	0.9307427169	1.1127527099
C41	-2.5420714836	2.2542093286	1.1719389982
C42	-3.4326004922	3.1876902754	1.9612020666
H43	-5.0505223398	3.5319367053	3.3430536072
H44	-5.8429812715	1.1801349524	3.2663671979
H45	-4.6835791888	-0.4799329769	1.8414204732

H46	-1.8887900833	2.5418310948	0.5971075182
H47	-3.0763133933	4.2169694092	1.9979439970
C48	-3.5985264032	-4.3631921145	1.5937387887
C49	-2.4665980525	-3.7220798280	2.0872889881
C50	-2.0921359060	-2.4831538820	1.5796930556
C51	-2.8550192365	-1.8640799804	0.5846361094
C52	-3.9877974706	-2.5146671108	0.0920570668
C53	-4.3550401127	-3.7604059508	0.5945121145
H54	-3.8871112919	-5.3400749351	1.9831725463
H55	-1.8654126512	-4.1951664796	2.8628632798
H56	-1.1894644979	-1.9852533279	1.9425856186
H57	-4.5860796614	-2.0460276185	-0.6907516268
H58	-5.2373947313	-4.2636757372	0.2008979233
C59	-4.3811607277	0.1280145751	-4.1091456896
C60	-5.0405197474	0.6144258255	-2.9850523364
C61	-4.4393803271	0.5364738392	-1.7312013618
C62	-3.1685327917	-0.0256367781	-1.5949592619
C63	-2.5064687672	-0.4991632948	-2.7319996559
C64	-3.1130564561	-0.4309634618	-3.9810040323
H65	-4.8540881281	0.1910720376	-5.0897072028
H66	-6.0307976695	1.0584808249	-3.0834235045
H67	-4.9632112495	0.9155396081	-0.8521219735
H68	-1.5014668628	-0.9149920242	-2.6253097192
H69	-2.5894875141	-0.8052200156	-4.8603503061

M06-L

E= -2199.232371 H

Pd1	-0.0089227895	0.1090941351	-0.0648195954
P2	2.2806293279	0.0410433243	-0.0120383922
C3	4.5369090028	4.0496513909	0.5071311069
C4	5.0107735346	2.9221388988	1.1723829838
C5	4.3505549326	1.7023839398	1.0429553092
C6	3.2020302369	1.6008476520	0.2496791706
C7	2.7239012025	2.7448944278	-0.4024717021
C8	3.3919950653	3.9583502511	-0.2829718518
H9	5.0554593081	5.0018281276	0.6099075030
H10	5.9016626375	2.9905631838	1.7957798967
H11	4.7301862752	0.8225169712	1.5630775331
H12	1.8136987032	2.6713624634	-1.0011648914
H13	3.0120135026	4.8388088804	-0.7990029364
C14	3.7996302094	-2.6115503956	3.4652531285
C15	4.4830775961	-2.6370516231	2.2538316513
C16	4.0490784252	-1.8539430127	1.1870374953
C17	2.9196436386	-1.0397695306	1.3215515707
C18	2.2312606594	-1.0314318036	2.5407254895
C19	2.6729486243	-1.8048955444	3.6079402839
H20	4.1410523641	-3.2256643181	4.2970761587
H21	5.3606344482	-3.2704619983	2.1371020107
H22	4.5902838512	-1.8766730136	0.2417719190
H23	1.3349365889	-0.4145379676	2.6325191644
H24	2.1307867054	-1.7862647025	4.5511547742
C25	4.2001512273	-1.8521177147	-3.7743084000
C26	4.8609787832	-0.8039535466	-3.1406790070
C27	4.3074213669	-0.2078492818	-2.0104336879
C28	3.0795927673	-0.6522195101	-1.5069801031
C29	2.4150893643	-1.6980707744	-2.1607558217
C30	2.9758241733	-2.3002079203	-3.2804155381
H31	4.6354513152	-2.3160642013	-4.6575636745
H32	5.8150412216	-0.4472233161	-3.5266558924
H33	4.8334469371	0.6090734880	-1.5164792028
H34	1.4444333077	-2.0246822924	-1.7800053082
H35	2.4512772936	-3.1152590753	-3.7763026660
P36	-2.2816451635	-0.1819838596	0.0021113948
C37	-4.6102423934	2.8696838044	2.5879425181
C38	-5.0156148365	1.5374271717	2.5939492640
C39	-4.3325336605	0.5931478145	1.8324355298
C40	-3.2298744577	0.9727803401	1.0598342553
C41	-2.8200907671	2.3127241274	1.0736322734
C42	-3.5110508551	3.2564410130	1.8243952406
H43	-5.1459671892	3.6060620703	3.1843901109
H44	-5.8699591838	1.2296422033	3.1947058133
H45	-4.6575896323	-0.4477306583	1.8399412903
H46	-1.9423878573	2.6029851066	0.4934084118
H47	-3.1832610636	4.2951753142	1.8237190445
C48	-3.4382566889	-4.3132352209	1.7445333392
C49	-2.2837939859	-3.6514963976	2.1583037419
C50	-1.9503457210	-2.4203818138	1.6042262065
C51	-2.7755886222	-1.8260222394	0.6413772559
C52	-3.9306545443	-2.5004851920	0.2280376646

C53	-4.2574433800	-3.7382285624	0.7765515947
H54	-3.6950909095	-5.2819283255	2.1707078630
H55	-1.6332367408	-4.1020354664	2.9060943461
H56	-1.0315602276	-1.9072351479	1.8986646382
H57	-4.5761223845	-2.0554046972	-0.5298049353
H58	-5.1566644739	-4.2560343990	0.4449394624
C59	-4.4225045190	-0.0690348372	-4.1012680338
C60	-5.0767437035	0.4516231647	-2.9885603164
C61	-4.4579793428	0.4384447513	-1.7408647542
C62	-3.1719738068	-0.0918490506	-1.5959734594
C63	-2.5155256463	-0.5984094607	-2.7251495647
C64	-3.1399624081	-0.5961970111	-3.9668860308
H65	-4.9084994546	-0.0567871416	-5.0755993676
H66	-6.0766125733	0.8705018126	-3.0906050473
H67	-4.9781389947	0.8446813665	-0.8730324294
H68	-1.4998755866	-0.9847841813	-2.6163083146
H69	-2.6195354597	-0.9962601664	-4.8356449082

[PdL<sub>3</sub>]

B3LYP

E= -3235.677136 H

Pd1	6.9840965099	-1.7454600420	-0.5588489995
C1	6.9070277412	0.8384400827	4.8908570227
C2	8.2632746253	0.9063981833	4.5703654066
C3	8.6918109135	0.6574788791	3.2648511663
C4	7.7682074736	0.3271744451	2.2624928686
C5	6.4082424931	0.2458711062	2.6015513522
C6	5.9788616805	0.5089897960	3.9014318351
H7	6.5756117722	1.0329966615	5.9080165090
H8	8.9926630400	1.1564421465	5.3376488023
H9	9.7502732231	0.7199961518	3.0292641060
H10	5.6879135717	-0.0416282008	1.8386909249
H11	4.9214359554	0.4414035284	4.1452694822
C12	8.2696543320	4.2643536000	-1.4026781025
C13	7.9450219940	4.1279870570	-0.0541601252
C14	7.9347437083	2.8657523631	0.5454442124
C15	8.2421685919	1.7187513491	-0.2002022365
C16	8.5532096752	1.8687903027	-1.5619665674
C17	8.5761919865	3.1280874105	-2.1556907446
H18	8.2782999478	5.2473167463	-1.8676377529
H19	7.7025577159	5.0059601370	0.5405669170
H20	7.6893435746	2.7795000618	1.5992646843
H21	8.7701128495	0.9908769587	-2.1650215131
H22	8.8171762211	3.2201550062	-3.2117401526
C23	12.7579034058	-1.0704752732	0.6995821532
C24	12.3743030293	0.2717758027	0.6888243206
C25	11.0234877475	0.6172153297	0.6264944540
C26	10.0321098086	-0.3761905799	0.5759104800
C27	10.4326040046	-1.7222589465	0.5727945613
C28	11.7831991167	-2.0672568976	0.6403779569
H29	13.8111291571	-1.3370185345	0.7459923004
H30	13.1286350931	1.0543184599	0.7270550275
H31	10.7396620634	1.6656787263	0.6102897684
H32	9.6769452204	-2.5006759104	0.4997353243
H33	12.0713095655	-3.1158059125	0.6369919309
P34	8.2170744118	-0.0029874559	0.4959592440
C35	10.1359100706	-2.6870369534	-5.5146408715
C36	8.8493408752	-2.8950441200	-6.0160051392
C37	7.7302922204	-2.5692597924	-5.2467798059
C38	7.8768652129	-2.0275621440	-3.9592402243
C39	9.1765468361	-1.8365278768	-3.4611965379
C40	10.2948729968	-2.1573740294	-4.2325825088
H41	11.0056087315	-2.9432149763	-6.1146340866
H42	8.7133976590	-3.3145068155	-7.0102717582
H43	6.7366638597	-2.7442159140	-5.6496359832
H44	9.3079190844	-1.4493150715	-2.4538008253
H45	11.2904144962	-2.0007210016	-3.8240390847
C46	5.1536933065	2.7000602259	-4.2750618324
C47	5.9526882174	1.9255804801	-5.1181816411
C48	6.3602004894	0.6475932545	-4.7276592709
C49	5.9818725407	0.1266178395	-3.4812434576
C50	5.1927218239	0.9218464927	-2.6349959517
C51	4.7736667437	2.1922002426	-3.0307751452
H52	4.8369545717	3.6940091840	-4.5811281446
H53	6.2593270463	2.3144518556	-6.08669977416
H54	6.9760836977	0.0560851527	-5.3991525757
H55	4.9198494409	0.5418149109	-1.6528450273
H56	4.1630822997	2.7914556087	-2.3597574050
C57	3.0533005219	-4.2614533646	-4.6351423498





H56	4.7074574876	3.0597749686	-2.3703547896	C29	3.2865116078	4.1521962797	0.5526644344
C57	3.0017284155	-4.0524199786	-4.7415920947	H30	2.7468427607	4.5936146812	1.3848234931
C58	3.2255878509	-2.7644197398	-5.2202293397	C31	5.0677429425	-3.7347036691	0.1453044670
C59	4.2432655190	-1.9805265270	-4.6811007444	H32	5.8510536909	-4.3033758479	0.6411141167
C60	5.0468283249	-2.4752545129	-3.6474075514	C33	-0.8430630213	-4.1916450573	-3.1726925183
C61	4.8029282729	-3.7685572017	-3.1676144753	H34	-1.6702747419	-4.7201414162	-2.7057466841
C62	3.7970970033	-4.5558969147	-3.7142474576	C35	-0.1752615789	-3.1990795739	-2.4549425238
H63	2.2014601922	-4.6599932465	-5.1625926186	H36	-0.5032063406	-2.9661788773	-1.4478663289
H64	2.6028371420	-2.3638568994	-6.0198454121	C37	1.2660346841	-2.7905099073	-4.3402152344
H65	4.4108034400	-0.9735500053	-5.0644126284	H38	2.0895048093	-2.2608993657	-4.8089036883
H66	5.4024459166	-4.1475116361	-2.3359801609	C39	0.5914992451	-3.7783820087	-5.0639094899
H67	3.6214180235	-5.5563122387	-3.3189923401	H40	0.8990790247	-3.9963618957	-6.0844906632
P68	6.3986440027	-1.5311165355	-2.8386116463	C41	-0.4642026619	-4.4846678737	-4.4845640088
C70	2.3385065163	-5.7767443364	0.0807801541	H42	-0.9866180449	-5.2524426198	-5.0500302430
C71	3.4609176547	-6.5470725971	0.3869729872	C43	3.2841113895	-3.6006047818	-1.4890700147
C72	4.6971537234	-5.9363707083	0.5758964491	H44	2.6973543426	-4.0789164180	-2.2666763682
C73	4.8265125752	-4.5472051584	0.4486127449	C45	4.2899522587	-4.3291979555	-0.8486213660
C74	3.6960369674	-3.7853596008	0.1245394901	H46	4.4664647036	-5.3639723709	-1.1343586211
C75	2.4568269479	-4.3938091590	-0.0479099345	C47	4.8280975150	-2.4064607388	-5.0290600800
H76	1.3722330330	-6.2570734630	-0.0672683687	H48	5.4137794821	-1.9314417913	1.2857420449
H77	3.3721072265	-7.6296834047	0.4811981690	C49	3.8183235337	-1.6834877397	-0.1305977940
H78	5.5723589054	-6.5422820091	0.8219012079	H50	3.6311757645	-0.6604052537	0.1766181547
H79	3.8089201067	-2.7064636111	-0.0148843054	C51	4.1202841170	-0.7726356499	-3.5713243062
H80	1.5863061348	-3.7893628148	-0.3053766646	H52	4.5784558622	-1.5944095767	-3.0301016495
C81	6.9278762680	-3.4551243920	5.2885600393	C53	4.8498535091	-0.1278021845	-4.5738585594
C82	5.7464663781	-3.9706283456	4.7670223650	H54	5.8629533884	-0.4582008943	-4.7934304021
C83	5.5706015343	-4.0758194114	3.3877260498	C55	2.2625664919	0.7011579779	-3.9859932361
C84	6.5755267395	-3.6563539434	2.5106684254	H56	1.2664144397	1.0566262335	-3.7491223164
C85	7.7566332039	-3.1244736971	3.0501724667	C57	0.9085499437	5.0670739327	-4.4658461350
C86	7.9374013108	-3.0349341390	4.4232780130	H58	1.4001468149	5.8623618837	-5.0213076385
H87	7.0611643871	-3.3715474386	6.3667067453	C59	0.6199555530	3.7994541643	-2.4283194692
H88	4.9518912302	-4.2984743706	5.4367712183	H60	0.61031773380	3.6100314123	-1.4018577645
H89	4.6429905721	-4.4900115579	2.9932192149	C61	0.5697485546	4.2340575202	4.1405427477
H90	8.5381417465	-2.7623558505	2.3772404892	H62	0.8766987098	4.4296916460	5.1658371214
H91	8.8607004491	-2.6138971857	4.8196754340	C63	1.2529740257	3.2709881551	3.3917873408
C92	9.6383391575	-6.6870933862	-0.7015848078	H64	2.0817290399	2.7372295972	3.8465743553
C93	9.2154923989	-6.7129826454	0.6253539051	C65	-0.1977628035	3.7099849210	1.5206069433
C94	8.2407238094	-5.8238174427	1.0709043523	H66	-0.5291550704	3.4955767575	0.5105578160
C95	7.6722906242	-4.8946792212	0.1908116147	C67	-2.3137914161	1.2819802377	4.1547108880
C96	8.1112406734	-4.8761102688	-1.1412560551	H68	-1.8085114244	2.0339960936	4.7551999723
C97	9.0830178462	-5.7643779059	-1.5862134002	C69	-1.6157680234	0.6476960975	3.1272004640
H98	10.4049704395	-7.3806480641	-1.0434526827	H70	-0.5829627241	0.9247926650	2.9465819946
H99	9.6488662003	-7.4302344267	1.3215436164	C71	-3.6530123280	0.9662030822	4.3944845334
H100	7.9225151996	-5.8459644392	2.1139462654	H72	-4.2018878318	1.4623874377	5.1911008909
H101	7.6956591301	-4.1327847607	-1.8250412370	C73	-4.2804602014	0.0084386795	3.5961557023
H102	9.4125817232	-5.7233288689	-2.6245828661	H74	-5.3230080655	-0.2495392281	3.7703286465
P103	6.4084757976	-3.6564071734	0.6836232653	C75	-3.5770745851	-0.6330992490	2.5721865945

[PdL<sub>4</sub>]

B3LYP

E= -4271.947245 H

Pd1	0.2719247263	0.2637324498	-0.4932662136	C91	-3.6716124107	-0.4835634856	-5.3185703340
P2	1.7395685183	1.7409593461	0.9799314961	H92	-4.2272433782	-0.9982089834	-6.0986609537
P3	-1.1923745564	1.6979450356	-1.9830983178	C93	-4.2755715554	0.5322973648	-4.5755289623
C4	3.0022938091	2.8373817247	0.1481288039	H94	-5.3063298584	0.8164660054	-4.7768518198
C5	-0.3676711357	3.0035722073	-3.0290903016	C95	-3.5644363622	1.1972237906	-3.5721669331
C6	-2.4999221692	2.7468859513	-1.1627642844	H96	-4.0532909638	1.9904815416	-3.0157402778
C7	-3.8697112085	4.7498542253	-0.9652189366	C97	-2.3474255368	-0.8324605793	-5.0463652501
C8	-2.8453591783	4.0384295579	-1.5937581759	H98	-1.8601919536	-1.6282997551	-5.6036831812
H9	-4.1217252430	5.7484582457	-1.3158500778	C99	-1.6424447209	-0.1750952807	-4.0381816428
H10	-2.3192374080	4.4928337778	-2.4271960110	H100	-0.6239689448	-0.4792866834	-3.8270137387
P11	-1.1967765088	-1.1613212383	1.0046967170	C101	4.2854268036	0.9269550063	-5.2941330021
P12	1.7448493748	-1.1986294967	-1.9671219564	H102	4.8549804748	1.4255292200	-6.0746361508
C13	0.8816934967	2.9961954965	2.0652444630	C103	2.9856779109	1.3393709639	-4.9939793780
C14	2.8291101538	0.9062738893	2.2495249447	H104	2.5313461623	2.1683662404	-5.5305852127
C15	-2.2293384983	-0.3250149236	2.3220465487	C105	-2.2317002445	0.8549810003	-3.2884680826
C16	-0.3765404936	-2.4726229637	2.0482784538	C106	-0.1722509118	-3.8493169535	4.0452779598
C17	-2.5140132379	-2.1975949200	0.1817860325	H107	-0.5112082593	-4.0973344624	5.0488091693
C18	3.0361745715	-2.2625354505	-1.1424244603				
C19	2.8099071054	-0.3698463081	-3.2627667231				
C20	0.8938034485	-2.4864544461	-3.0203871027				
C21	-3.2012953056	2.2007671059	-0.0776635885				
H22	-2.9292514616	1.2220021988	0.2998347840				
C23	3.7241716016	2.3085426098	-0.9331914521				
H24	3.5049659611	1.3073528274	-1.2872645585				
C25	4.7100725554	3.0545967968	-1.5789816334				
H26	5.2477104513	2.6149785655	-2.4151780187				
C27	4.2673255795	4.9047326810	-0.1001202770				
H28	4.4708224627	5.9203955220	0.2325402417				

C108	-0.7937033420	-2.8126880923	3.3458002841	C47	4.9598434996	-2.2795929168	0.4691442948
H109	-1.6109140420	-2.2729255818	3.8135302662	H48	5.6163866450	-1.7522320431	1.1704873100
C110	0.6852711567	-3.1937266672	1.4814593185	C49	3.9142189210	-1.5788917697	-0.1492793622
H111	1.0467166401	-2.9289038030	0.4939109240	H50	3.7731632122	-0.5186420202	0.0834561592
C112	4.3457396694	-0.4279708840	4.2258741015	C51	4.0788071197	-0.8242248179	-3.5296664133
H113	4.9310159767	-0.9410222514	4.9850705511	H52	4.5370315762	-1.6452672607	-2.9685203390
C114	4.8902473798	0.6492616773	3.5238639353	C53	4.7960619236	-0.2175257940	-4.5734425849
H115	5.9040619442	0.9820170664	3.7362251916	H54	5.8079339498	-0.5698129094	-4.8090804388
C116	4.1410175506	1.3118787885	2.5471488243	C55	2.2188778126	0.6734349797	-3.9483813658
H117	4.5837699680	2.1512446886	2.0202419935	H56	1.2257379236	1.0529110469	-3.6899345818
C118	4.9862636360	4.3594894332	-1.1657077058	C57	0.9469366289	5.1158232113	-4.4723984509
H119	5.7498303666	4.9466288644	-1.6700277674	H58	1.4274779920	5.9254236119	-5.0342178640
C120	-0.8739793165	4.6778505934	2.2632788529	C59	0.6245249812	3.8860483031	-2.3963535080
H121	-1.7086268495	5.2082591587	1.8119988236	H60	0.8788753338	3.7429617692	-1.3414781987
C122	-0.4937108214	4.9442622835	3.5802133201	C61	0.5993459130	4.0905240501	4.2243963518
H123	-1.0227487495	5.6927376140	4.1650384932	H62	0.9368728012	4.2503697217	5.2561360290
C124	1.2477712685	4.8248595194	-3.1334244136	C63	1.2684924522	3.1536200069	3.4170166861
H125	2.0122908777	5.4206566828	-2.6415154132	H64	2.1199949052	2.6005502575	3.8281563635
C126	-4.2320308243	2.9046089608	0.5438005614	C65	-0.2424111847	3.6603342523	1.5912236834
H127	-4.7548589880	2.4538021375	1.3834852803	H66	-0.6013457296	3.4791007654	0.5729990506
C128	-4.5715418743	4.1834406066	0.1000666287	C67	-2.2800025873	1.2469872273	4.1750224808
H129	-5.3712678382	4.7382948381	0.5851596794	H68	-1.7565185754	1.9678343706	4.8133317406
C130	-0.6974571110	3.2551784015	-4.3705969690	C69	-1.5850725802	0.6331977009	3.1228339770
H131	-1.4575583394	2.6587365775	-4.8649257185	H70	-0.5338130995	0.8893010598	2.9588018061
C132	-0.0618358156	4.2765197725	-5.0820486725	C71	-3.6367265864	0.9544399828	4.3928687184
H133	-0.3331929737	4.4554373724	-6.1203082534	H72	-4.1838409931	1.4364312120	5.2116620741
C134	2.2999866503	-0.1846144563	2.9569613635	C73	-4.2850189166	0.0384479021	3.5488321350
H135	1.3018468568	-0.5401722239	2.7275852685	H74	-5.3436385338	-0.2027013357	3.7072701840
C136	3.0428338587	-0.8404581845	3.9389931236	C75	-3.5853924558	-0.5844539210	2.5001224508
H137	2.6029138498	-1.6849183948	4.4635746813	H76	-4.1055397536	-1.3051605107	1.8603678920
				C77	-4.6124711673	-3.5699766193	-1.1985882224
				H78	-5.4143463727	-4.1220840626	-1.7028490039
BP86				C79	-4.3179342515	-2.2473813301	-1.5682757917
E= -4272.030589 H				H80	-4.8764791645	-1.7558524074	-2.3730213143
Pd1	0.2715646932	0.2761379634	-0.4948199798	C81	-3.2850399019	-1.5482588711	-0.9264971120
P2	1.6964763030	1.7082108059	0.9341903114	H82	-3.0527049276	-0.5294797508	-1.2496277255
P3	-1.1177522092	1.7006081232	-1.9693522053	C83	-2.8387103915	-3.4725320006	0.4748351118
C4	2.9217472848	2.8595562493	0.1055152606	H84	-2.2776102452	-3.9624599234	1.2774666685
C5	-0.2996168755	3.0193770762	-3.0187800641	C85	-3.8665115722	-4.1778458873	-0.1755728272
C6	-2.4389770095	2.7619001541	-1.1723935759	H86	-4.0838528052	-5.2103289074	0.1254979351
C7	-3.8148918725	4.7802475134	-1.0232690795	C87	0.8005013272	-4.5831655302	3.4154327720
C8	-2.7742375949	4.0565865097	-1.6278668880	H88	1.2641728114	-5.4075833647	3.9706747361
H9	-4.0603032118	5.7837950063	-1.3924127602	C89	1.2653368967	-4.2415962638	2.1354218270
H10	-2.2249075508	4.5015537458	-2.4642196775	H90	2.1008473032	-4.7863692231	1.6807940339
P11	-1.1946035237	-1.1187790125	0.9363754162	C91	-3.6187587764	-0.4931021072	-5.3073461413
P12	1.7155076238	-1.1888521705	-1.8822241432	H92	-4.1844668137	-1.0144683869	-6.0885188105
C13	0.8576982547	2.9271574907	2.0844555187	C93	-4.2100915653	0.5545454515	-4.5825945915
C14	2.8442023252	0.8665946932	2.1537587797	H94	-5.2423809310	0.8582838387	-4.7970428064
C15	-2.2214412438	-0.2963057720	2.2726212990	C95	-3.4881160961	1.2263985054	-3.5807971517
C16	-0.4004991240	-2.4531046333	1.9841171075	H96	-3.9645953437	2.0474615566	-3.0347981433
C17	-2.5341945462	-2.1418820241	0.1102683308	C97	-2.2955085269	-0.8656854003	-5.0188933020
C18	3.0412615240	-2.2210777367	-1.0541088050	H98	-1.8168225515	-1.6885174092	-5.5620855590
C19	2.7745074304	-0.3887273608	-3.2048118232	C99	-1.5795419913	-0.2025744540	-4.0111745402
C20	0.8879628728	-2.5126150116	-2.9212219392	H100	-0.5609232124	-0.5277973549	-3.7800649780
C21	-3.1660759054	2.2233379488	-0.0908178504	C101	4.2225942664	0.8261615403	-5.3168428450
H22	-2.8958347726	1.2405682245	0.3066690404	H102	4.7842922289	1.2955069617	-6.1335853520
C23	3.6294238713	2.3823983591	-1.0184016480	C103	2.9296603111	1.2719090359	-4.9990701569
H24	3.4189637771	1.3798970531	-1.4048925520	H104	2.4706820282	2.0973217778	-5.5555028895
C25	4.5824939144	3.1818626964	-1.6675263888	C105	-2.1577707154	0.8576182203	-3.2810908225
H26	5.1118059367	2.7825320594	-2.5403798579	C106	-0.2567596380	-3.8552102951	3.9843265817
C27	4.1307209668	4.9792735526	-0.1052785837	H107	-0.6241620921	-4.1097656420	4.9862897908
H28	4.3181294081	5.9969063719	0.2595549457	C108	-0.8559376244	-2.8016334979	3.2753402403
C29	3.1840910435	4.1740701864	0.5522085148	H109	-1.6867443522	-2.2515623265	3.7295799227
H30	2.6505829878	4.5723172542	1.4219835113	C110	0.6735251071	-3.1817357766	1.4330615756
C31	5.1489007326	-3.6466702860	0.2053659314	H111	1.0670554484	-2.9042288719	0.4507929428
H32	5.9627903320	-4.1979116549	0.6908919796	C112	4.4744968357	-0.4901695595	4.0407213326
C33	-0.8385180623	-4.2462507794	-3.0714869590	H113	5.1060503073	-1.0150424573	4.7672316768
H34	-1.6761467090	-4.7768045455	-2.6044220567	C114	4.9684771716	0.6280016028	3.3489185985
C35	-0.1906626528	-3.2266444612	-2.3577513232	H115	5.9898076901	0.9834743889	3.5347680324
H36	-0.5423865576	-2.9728855031	-1.3534675412	C116	4.1624407882	1.3028235707	2.4154366066
C37	1.2914829940	-2.8405144748	-4.2350210519	H117	4.5631946737	2.1773751741	1.8914607994
H38	2.1273788828	-2.3072640949	-4.6999985810	C118	4.8361079565	4.4876859165	-1.2158672588
C39	0.6351360489	-3.8540265506	-4.9550281007	H119	5.5746475015	5.1175667839	-1.7258143759
H40	0.9659621871	-4.0904639733	-5.9740905542	C120	-0.9033509119	4.6025979646	2.3931303496
C41	-0.4312511269	-4.5629125072	-4.3778509711	H121	-1.7574709621	5.1519991124	1.9808813211
H42	-0.9408142649	-5.3529842799	-4.9420651999	C122	-0.4874327214	4.8210310747	3.7170413299
C43	3.2404099583	-3.5946207747	-1.3141167850	H123	-1.0068513208	5.5513483588	4.3487531162
H44	2.5835405671	-4.1181676713	-2.0168463065	C124	1.2364518798	4.9264476083	-3.1106225145
C45	4.2831964774	-4.2994062068	-0.6866497998	H125	1.9536193025	5.5778559536	-2.5982335018
H46	4.4198279865	-5.3657886711	-0.9056311358				

C126	-4.2144070141	2.9393948514	0.5047639625
H127	-4.7592868563	2.4934616075	1.3448711281
C128	-4.5443090311	4.2221504470	0.0386778186
H129	-5.3596542221	4.7879287211	0.5057003192
C130	-0.5851166746	3.2185761974	-4.3876418010
H131	-1.3025283721	2.5658837835	-4.8963171149
C132	0.0359482451	4.2556132778	-5.1062829249
H133	-0.2024246853	4.3918144326	-6.1685704594
C134	2.3629916531	-0.2618282512	2.8511887331
H135	1.3567335882	-0.6388283738	2.6415872395
C136	3.1631630065	-0.9278848576	3.7912377208
H137	2.7612209654	-1.8049227394	4.3115782697

M06

E= -4269.719487 H

Pd1	0.2544589535	0.2718702993	-0.4959603124
P2	1.6925995495	1.7031194704	0.9430407709
P3	-1.1889560574	1.7085020647	-1.9174958551
C4	2.9620872449	2.7557882675	0.1075620451
C5	-0.3457548193	2.9748174825	-2.9666788059
C6	-2.4539609401	2.7679077136	-1.0773954310
C7	-3.6834765290	4.8274032085	-0.7346789150
C8	-2.7175203041	4.0963871712	-1.4229161453
H9	-3.8741704340	5.8622731936	-1.0161902863
H10	-2.1626240916	4.5692731139	-2.2338786448
P11	-1.1475936460	-1.1833122571	0.9428788537
P12	1.7054522664	-1.1404649385	-1.9353424244
C13	0.8605112259	2.9748302079	1.9958337017
C14	2.7461161644	0.8746751898	2.2160648299
C15	-2.2032747860	-0.3402760217	2.2041724757
C16	-0.3074167095	-2.4494145761	2.0003095224
C17	-2.4156753582	-2.2327385726	0.1051028529
C18	2.9811505448	-2.1895802618	-1.1048768454
C19	2.7520140030	-0.3101569380	-3.2128449781
C20	0.8627749187	-2.4117888010	-2.9794464353
C21	-3.1822319343	2.1963815569	-0.0299831315
H22	-2.9695727100	1.1728026854	0.2772661140
C23	3.6769332247	2.1853748954	-0.9488289765
H24	3.4533555339	1.1662940855	-1.2626652565
C25	4.6505966359	2.9043581368	-1.6285376192
H26	5.1825752526	2.4335228465	-2.4555318824
C27	4.2114766271	4.8042351048	-0.2189216694
H28	4.4171778211	5.8342888092	0.0717705119
C29	3.2382047735	4.0792059191	0.4637405417
H30	2.6929077055	4.549492696	1.2826365350
C31	4.9355018947	-3.6583530576	0.2684956664
H32	5.6906891402	-4.2333834131	0.8033932939
C33	-0.8593569693	-4.1160243272	-3.1002662612
H34	-1.6665920180	-4.6630163787	-2.6132363083
C35	-0.1676373453	-3.1462428791	-2.3870019153
H36	-0.4498369289	-2.9413720682	-1.3540664128
C37	1.1835915429	-2.6673697196	-4.3159703066
H38	1.9826819904	-2.1078118434	-4.8027596630
C39	0.4884993074	-3.6371615872	-5.0347293231
H40	0.7503965652	-3.8259874494	-6.0758768584
C41	-0.5320694663	-4.3634712745	-4.4305942045
H42	-1.0758639788	-5.1176781980	-4.9987510881
C43	3.2492991540	-3.5158621444	-1.4553827754
H44	2.6972086469	-3.9877192055	-2.2691787291
C45	4.2197876307	-4.2436445566	-0.7710890493
H46	4.4169105127	-5.2769940849	-1.0560236916
C47	4.6756770879	-2.3386399228	0.6263458455
H48	5.2130521858	-1.8666670130	1.4494511395
C49	3.7045204545	-1.6171024709	-0.0548397769
H50	3.4900170918	-0.5944484123	0.2539128114
C51	4.0654567439	-0.6861608889	-3.5087639138
H52	4.5313435460	-1.5114800836	-2.9698242532
C53	4.7869326213	-0.0132754802	-4.4917138301
H54	5.8098088717	-0.3184911282	-4.7124115935
C55	2.1862612806	0.7546505663	-3.9177919372
H56	1.1754233568	1.0829994062	-3.6764202606
C57	1.0440507320	4.9251978932	-4.4235524003
H58	1.5853387064	5.6789997784	-4.9938938177
C59	0.7079661307	3.6884613092	-2.3878660317
H60	1.0133093394	3.4668000251	-1.3648341049
C61	0.5316295536	4.2169189572	4.0485243214
H62	0.8195483286	4.4168177849	5.0804773519
C63	1.2131481376	3.2442558925	3.3214827359
H64	2.0282754977	2.6938611387	3.7923621087

C65	-0.1904090745	3.6970924725	1.4246564789
H66	-0.5003494365	3.4802423629	0.4029624834
C67	-2.3576252548	1.4133068080	3.8753709302
H68	-1.8852045796	2.2395248584	4.4077744677
C69	-1.6300717701	0.7140011267	2.9219083792
H70	-0.6026982581	1.0127122404	2.7142617842
C71	-3.6839903871	1.0702730463	4.1229211782
H72	-4.2633855373	1.6199172076	4.8638272070
C73	-4.2693877802	0.0267531382	3.4128116836
H74	-5.3074344256	-0.2467009576	3.6002958860
C75	-3.5360846911	-2.3655934573	2.4597064304
H76	-4.0093267497	-1.4904417425	1.9101727594
C77	-4.3771835656	-3.6818243642	-1.2771820426
H78	-5.1369285251	-4.2488828183	-1.8143147715
C79	-4.1011769270	-2.3653585506	-1.6358077402
H80	-4.6295410790	-1.8879942774	-2.4618614003
C81	-3.1253377774	-1.6539198522	-0.9506085346
H82	-2.8967223401	-0.6331158743	-1.2558581233
C83	-2.6973912524	-3.5559964440	0.4553845333
H84	-2.1556972366	-4.0312621318	1.2740523503
C85	-3.6731122673	-4.2734529164	-0.2329260415
H86	-3.8842274871	-5.3039091341	0.0522536961
C87	1.0846011637	-4.3895021040	3.4804377364
H88	1.6250529434	-5.1372147638	4.0596372485
C89	1.4714496743	-4.0929629691	2.1754171241
H90	2.3246669228	-4.5943667459	1.7177354221
C91	-3.6906623943	-0.5205678005	-5.1506673886
H92	-4.2581766769	-1.0590569821	-5.9079549243
C93	-4.2850761442	0.5141328137	-4.4345990587
H94	-5.3200049330	0.7908515578	-4.6337855849
C95	-3.5663126940	1.2057361747	-3.4615918800
H96	-4.0465371064	2.0150238782	-2.9123477778
C97	-2.3672759883	-0.8632128035	-4.8866711516
H98	-1.8842971504	-1.6801885484	-5.4227948412
C99	-1.6536866006	-0.1741502272	-3.9149305821
H100	-0.6271337166	-0.4705371403	-3.6999286039
C101	4.2078002889	1.0401856844	-5.1918171566
H102	4.7779156425	1.5651274116	-5.9576678508
C103	2.9022045938	1.4253438536	-4.9010482476
H104	2.4362841538	2.2599955476	-5.4249901615
C105	-2.2369564400	-0.8703679983	-3.1916060804
C106	0.0030368561	-3.7165691686	4.0429224012
H107	-0.3089171608	-3.9412527739	5.0633624757
C108	-0.6898514370	-2.7549647307	3.3105790186
H109	-2.1340300764	-2.2361138353	3.7669091256
C110	0.7810165952	-3.1308380692	1.4486708251
H111	1.1161725375	-2.8822143042	0.4412685461
C112	4.2117188488	-0.4845499228	4.1822958018
H113	4.7847895178	-1.0130847713	4.9435018162
C114	4.7941547606	0.5591224028	3.4686572343
H115	5.8230830995	0.8538782614	3.6746023426
C116	4.0682278009	1.2361578744	2.4918295687
H117	4.5361904563	2.0555231896	1.9441736187
C118	4.9209166229	4.2199097723	-1.2632144658
H119	5.6794146491	4.7923481216	-1.7956232232
C120	-0.8688167151	4.6703594313	2.1454949087
H121	-1.6912476906	5.2083749010	1.6733339770
C122	-0.5077225916	4.9330414929	3.4638763410
H123	-1.0394959628	5.6909859764	4.0378038699
C124	1.3974455165	4.6571900761	-3.1035821907
H125	2.2231922783	5.1866432341	-2.6271064578
C126	-4.1506199345	2.9214658754	0.6533296104
H127	-4.6917936558	2.4479135189	1.4723938761
C128	-4.4043216712	4.2447968790	0.3032473600
H129	-5.1561531740	4.8222892855	0.8393096610
C130	-0.6921095672	3.2511593464	-4.2927661099
H131	-1.5090575471	2.7078015756	-4.7690770638
C132	0.0007680064	4.2197579652	-5.0144091817
H133	-0.2803605416	4.4241903716	-6.0477665046
C134	2.1775573617	-0.1810215578	2.9346164504
H135	1.1584205923	-0.4964761662	2.7126060199
C136	2.8979756443	-0.8561233759	3.9113439292
H137	2.4288643738	-1.6829465522	4.4463934412

M06-L

E= -4271.678999 H

Pd1	0.2574620761	0.2725668976	-0.4932658698
P2	1.6746878865	1.6934125194	0.9286759243
P3	-1.1547512940	1.6749067402	-1.9360752660



C68	5.3299046283	4.7587055202	21.4894810601
C69	4.6496739530	3.8499000019	20.7108214589
C70	5.3449183213	2.9312041394	19.8743896690
C71	4.6616983045	1.9798911391	19.0425541685
C72	3.1570129233	1.9809362248	19.0081353116
C73	2.4278537747	1.1717664652	19.9426835675
C74	3.0752128647	0.3757878658	20.9291860957
C75	2.3502263529	-0.3960586264	21.8091629978
C76	0.9363786106	-0.4168635835	21.7524829112
C77	0.2771182309	0.3406773590	20.8116170072
C78	0.9955766077	1.1484968627	19.8909419074
C79	0.3330190994	1.9327535461	18.9136256859
C80	1.0468194559	2.7098338159	18.0361044265
C81	2.4684049679	2.7585185523	18.0770887780
C82	3.2816546287	5.4974525397	17.5625140925
C83	4.2566671257	6.4264222529	17.1658785497
C84	4.2184002639	7.7444588131	17.6231765475
C85	3.2111682637	8.1498648087	18.4993931846
C86	2.2434457073	7.2322017820	18.9133407596
C87	2.2760684470	5.9176370977	18.4471670964
C88	2.2619499150	3.8396870733	15.4291097694
C89	2.0765181441	2.6443407384	14.7102034813
C90	1.2901695930	2.6180375337	13.5605302832
C91	0.6866922823	3.7891145996	13.0950064985
C92	0.8718192191	4.9817321932	13.7928097354
C93	1.6513826804	5.0085265087	14.9522390325
H122	6.3654511713	-1.1704955892	19.3760425747
H123	6.5114389388	-3.3637451759	20.4918085417
H124	3.2503477578	-4.8127004700	18.0893871595
H125	3.0796698873	-2.6023852436	16.9944101358
H126	6.3768244730	-2.3154503818	16.1691344015
H127	7.8461067218	-2.4296324591	14.1888473557
H128	6.7359061529	1.5877325990	13.1257825895
H129	5.2545056419	1.7021679963	15.0938551641
H130	7.3769009939	0.4858322364	17.6230975523
H131	8.5735320048	2.1166807432	19.0216476680
H132	8.5362211176	3.9539867181	20.6582945136
H133	7.2689771575	5.5262555093	22.0911691033
H134	4.7767037175	5.4521807862	22.1171938993
H135	3.5658183389	3.8304433258	20.7264381481
H136	4.1585280170	0.3806762125	20.9802065969
H137	2.8682517752	-0.9972979526	22.5516126372
H138	0.37570111429	-1.0317270399	22.4513905782
H139	-0.8091455832	0.3322737193	20.7563309361
H140	-0.7531574963	1.9079206392	18.8674695736
H141	0.5224655131	3.2919244436	17.2846062188
H142	5.0545181677	6.1104344930	16.4977157643
H143	4.9794015443	8.4508861954	17.3012395109
H144	1.4580424407	7.5414416056	19.5989077401
H145	1.5157098738	5.2155845158	18.7762082910
H146	2.5480515712	1.7272867430	15.0578013665
H147	1.1545204141	1.6829074640	13.0226539652
H148	0.4063375840	5.8983553941	13.4380505416
H149	1.7829229222	5.9453134605	15.4850906851
H154	4.9653087808	-5.2044493455	19.8512675743
H155	8.0408665764	-0.4816478114	12.6561746284
H156	3.1823162168	9.1742470126	18.8621856538
H157	0.0800291474	3.7708115294	12.1931516394

BP86

E= -2378.637521 H

P4	4.4987588837	-0.0403082060	17.1743817896
P5	3.4616294448	3.6992179729	16.8442937808
C50	4.6809591569	-1.6780483164	18.0319687625
C51	5.6314993155	-1.9618152635	19.0358508640
C52	5.6914426662	-3.2358080866	19.6232402831
C53	4.8088719333	-4.2487098086	19.2134400946
C54	3.8559024629	-3.9767137612	18.2180494475
C55	3.7862729955	-2.6994717450	17.6410044142
C56	5.7174279880	-0.1886994288	15.7784528367
C57	6.3821562080	-1.3810838547	15.4255101535
C58	7.2176183848	-1.4228420998	14.2960148289
C59	7.4062486921	-0.2762628592	13.5097296833
C60	6.7476610119	0.9166072795	13.8542422734
C61	5.9046367227	0.9591137559	14.9724215838
C62	5.4038567950	1.1258358953	18.3109916453
C63	6.8302630300	1.1891449897	18.3330236540
C64	7.4957605194	2.0817919523	19.1541201891
C65	6.7742229765	2.9711123761	20.0003373120

C66	7.4382802918	3.9011626294	20.8535829501
C67	6.7178361603	4.7665177970	21.6624777126
C68	5.2970826660	4.7346237399	21.6455469351
C69	4.6202523918	3.8433728285	20.8260455164
C70	5.3300662243	2.9342915509	19.9827787593
C71	4.6558213075	2.00145842826	19.1153485439
C72	3.1512153222	1.9912706663	19.0639981357
C73	2.4106342848	1.2091400078	20.0199825911
C74	3.0534330173	0.4332566817	21.0326672936
C75	2.3142341338	-0.3176731124	21.9345737312
C76	0.8944343917	-0.3327772847	21.8710934161
C77	0.2381021534	0.4063311158	20.8989562456
C78	0.9675344468	1.1880827465	19.9553257276
C79	0.3127633464	1.943670649	18.9421523542
C80	1.0419085295	2.6901210079	18.0333866101
C81	2.4680012206	2.7349773178	18.0878624272
C82	3.3208140983	5.4393177043	17.4733638569
C83	4.3192665760	6.3461797297	17.0547983033
C84	4.2870528249	6.6882319080	17.4633356844
C85	3.2649702468	8.1386610199	18.3137730613
C86	2.2748804277	7.2426041398	18.7492396119
C87	2.3001236441	5.9031657591	18.3307739247
C88	2.3065957097	3.7076306998	15.3907503372
C89	2.1020526056	2.4755809182	14.7249478138
C90	1.3145609215	2.4117746661	13.5675626957
C91	0.7329481017	3.5788246709	13.0426539592
C92	0.9400147909	4.8067751280	13.6887356990
C93	1.7181284614	4.8727473682	14.8569014607
H122	6.3304959991	-1.1824567975	19.3589188776
H123	6.4362479450	-3.4384662551	20.4021612918
H124	3.1573146877	-4.7578657555	17.8962051244
H125	3.0271300223	-2.4868330610	16.8779515554
H126	6.2480300633	-2.2809719262	16.0354812254
H127	7.7282908851	-2.3575657128	14.0349960486
H128	6.8866993161	1.8181379170	13.2457997269
H129	5.3905418329	1.8933364325	15.2331074062
H130	7.3992237852	0.5253737838	17.6731045103
H131	8.5919954194	2.1181096719	19.1595359094
H132	8.5351104823	3.9189003445	20.8543452467
H133	7.2402805888	5.4768046227	22.3131291909
H134	4.7315278378	5.4240140670	22.2826574912
H135	3.5260434111	3.8300343090	20.8144035557
H136	4.1466229959	0.4351894888	21.0846470301
H137	2.8293114916	-0.9080408413	22.7008673218
H138	0.3221627722	-0.89308903804	22.5890991140
H139	-0.8570922937	0.3991853045	20.8363923171
H140	-0.7823101521	1.9206798202	18.8890790080
H141	0.5248163991	3.2492105401	17.2460906111
H142	5.1297620865	5.9920290296	16.4059295904
H143	5.0672694486	8.3801401836	17.1253301262
H144	1.4762584196	7.5884488604	19.4164325207
H145	1.5212307076	5.2126991930	18.6730836256
H146	2.5604118490	1.5612355140	15.1238324080
H147	1.1603551547	1.4476602770	13.0686965505
H148	0.4886428166	5.7220046394	13.2871674128
H149	1.8675010487	5.8363531824	15.3557267619
H154	4.8599068770	-5.2431112475	19.6712734221
H155	8.0587733308	-0.3120756281	12.6295638932
H156	3.2420898805	9.1847603403	18.6406674462
H157	0.1242349442	3.5299567435	12.1322951822

M06

E= -2377.264125 H

P4	4.5999158558	0.0505686710	16.9648490602
P5	3.3605509731	3.6345129354	16.6807563640
C50	4.5868977383	-1.3820141994	18.1231850580
C51	5.6591027655	-1.7079994942	18.9609971476
C52	5.5683899980	-2.7818598230	19.8376248677
C53	4.3999796730	-3.5382636681	19.8943033370
C54	3.3246447072	-3.2171834154	19.0745202973
C55	3.4199040042	-2.1444587384	18.1931807410
C56	5.9351135888	-0.3749368429	15.7750053648
C57	6.6516295134	-1.5724061743	15.7514580445
C58	7.6156749049	-1.7975122202	14.7721053007
C59	7.8793916657	-0.8293001835	13.8109753675
C60	7.1646782000	0.3657301677	13.8207970581
C61	6.1938274457	0.5849531545	14.7880190459
C62	5.4676753623	1.2958247328	18.0285713571
C63	6.8640381239	1.5206265836	17.9806520630

C64	7.4464843656	2.4940138487	18.7498725195	C61	6.4615108993	0.7514873977	14.8794625608
C65	6.6721500307	3.2935068452	19.6200167488	C62	5.4839367016	1.3648929627	18.0020769975
C66	7.2538544446	4.3050404818	20.4206458402	C63	6.8783040339	1.6099542907	17.9946920949
C67	6.4809269038	5.0697081692	21.2555159391	C64	7.4366181281	2.5513977192	18.8242554957
C68	5.0881059463	4.8524636015	21.3269106490	C65	6.6384201241	3.3043315096	19.7132880792
C69	4.4957615673	3.8789890444	20.5648587395	C66	7.1881836903	4.2889676688	20.5674067992
C70	5.2657951445	3.0742485726	19.6876976869	C67	6.3857357027	5.0148236027	21.4148929981
C71	4.6785015368	2.0747825005	18.8613076024	C68	4.9947290080	4.7826552894	21.4427224366
C72	3.1989588192	1.8981488619	18.8415696379	C69	4.4302673074	3.8294599671	20.6295517469
C73	2.5748367085	1.0213334460	19.7730502355	C70	5.2283530115	3.0647010595	19.7422899083
C74	3.3063710650	0.3491277035	20.7845234784	C71	4.6693059381	2.0902696574	18.8670471877
C75	2.6816924041	-0.5138325684	21.6474624847	C72	3.1964834055	1.8682356004	18.8548986608
C76	1.2930833554	-0.7459569847	21.5473809480	C73	2.6013398956	1.0160227118	19.8287594284
C77	0.5567186961	-0.1060831211	20.5840433107	C74	3.3640699568	0.3700427162	20.8340089497
C78	1.1723267259	0.7891178057	19.6774250738	C75	2.7660252019	-0.4665992978	21.7454016692
C79	0.4359063677	1.4591067671	18.6751369974	C76	1.3749660227	-0.6949127895	21.7018424497
C80	1.0527766435	2.3179574803	17.8032096819	C77	0.6061885981	-0.0832066642	20.7406621012
C81	2.4470596793	2.5506548607	17.8754077475	C78	1.1908907210	0.7799374814	19.7841925093
C82	3.3453375847	5.2171285629	17.6230864383	C79	0.4279065118	1.4153215860	18.7794794140
C83	4.5197962959	5.9706689164	17.6365008715	C80	1.0213548403	2.2398309126	17.8546305246
C84	4.5936796070	7.1569058862	18.3600733026	C81	2.4170164528	2.4779521423	17.8763505464
C85	3.4893087378	7.6008331719	19.0775085338	C82	3.3514667867	5.1117234286	17.5637830947
C86	2.3122557871	6.8559063448	19.0754812070	C83	4.5602102454	5.8129902804	17.6050510478
C87	2.2425208763	5.6694993200	18.3560973330	C84	4.6712348545	6.9955466818	18.3321293463
C88	2.0710854685	3.8948920208	15.3993806197	C85	3.5717417768	7.4907087347	19.0256306080
C89	1.8125013421	2.8007010365	14.5632839728	C86	2.3616748075	6.7989367954	18.9965769811
C90	0.8866183535	2.8975059027	13.5337582827	C87	2.2540192546	5.6159304237	18.2744565395
C91	0.2199235937	4.0993121897	13.3079030844	C88	1.9676040608	3.8073692413	15.4020859469
C92	0.4853340509	5.1965779528	14.1180541859	C89	1.5774830053	2.6931537641	14.6417817408
C93	1.4031075595	5.0961966818	15.1603183167	C90	0.6222035970	2.8131281781	13.6414290877
H122	6.5697460296	-1.1068366810	18.9310262193	C91	0.0534546049	4.0551552883	13.3635409459
H123	6.4098380393	-3.0279380277	20.4844231142	C92	0.4471246492	5.1700835626	14.0951846661
H124	2.4045252240	-3.7974193121	19.1266627544	C93	1.3954059851	5.0494154523	15.1091931080
H125	2.5695244763	-1.8747746614	17.5646927771	H122	6.6031780503	-1.1397617562	18.7505123881
H126	6.4582893976	-2.3370710158	16.5034425820	H123	6.3825844656	-3.0575081817	20.3042116182
H127	8.1685880903	-2.7362390114	14.7660706636	H124	2.2993477780	-3.5923646955	19.0656109481
H128	7.3629932945	1.1282358433	13.0687619855	H125	2.5256867205	-1.6761098794	17.5038504024
H129	5.6285945002	1.5206623664	14.7916689315	H126	6.2838065734	-2.3433744074	16.2779289299
H130	7.4802318174	0.9172422944	17.3143101975	H127	8.0387033155	-2.7674086571	14.5919111904
H131	8.5224660040	2.6646422454	18.7026899429	H128	7.7871385955	1.3210255934	13.2877590975
H132	8.3314815314	4.4613744337	20.3591212817	H129	6.0075474884	1.7417519161	14.9552330346
H133	6.9388715925	5.8453551297	21.8676665724	H130	7.5154808992	1.0442196878	17.3167855964
H134	4.4790696126	5.4675597966	21.9877588319	H131	8.5119755816	2.7289716190	18.8079746972
H135	3.4193550224	3.7189734975	20.6195107179	H132	8.2642348095	4.4615396727	20.5375069556
H136	4.3795258965	0.5213550868	20.8618956587	H133	6.8209236263	5.7713579082	22.0659427043
H137	3.2618572080	-1.0294109765	22.4114504085	H134	4.3627203999	5.3687318964	22.1081749463
H138	0.8089752427	-1.4331959175	22.2397819374	H135	3.3542700644	3.6614899968	20.6476769598
H139	-0.5175383449	-0.2745521062	20.4996374448	H136	4.4400969373	0.5354242822	20.8658398154
H140	-0.6383122549	1.2807953792	18.6086748142	H137	3.3714058737	-0.9632250300	22.5021356285
H141	0.4666464573	2.8216316751	17.0346777155	H138	0.9125667751	-1.3574600199	22.4317939137
H142	5.3921099441	5.6057340732	17.0916771610	H139	-0.4698336649	-0.2535459237	20.6988126915
H143	5.5198281474	7.7297451443	18.3711763394	H140	-0.6484816938	1.2424083920	18.7513240747
H144	1.4477604320	7.1997045853	19.6424307665	H141	0.4115570692	2.7159563757	17.0886618750
H145	1.3240346866	5.0799286549	18.3685614512	H142	5.4264395441	5.4114482169	17.0776827560
H146	2.3416326067	1.8595738875	14.7352153769	H143	5.6223991960	7.5246847510	18.3655933040
H147	0.6874877710	2.0339451968	12.9005438484	H144	1.5010644998	7.1814454980	19.5439224915
H148	-0.0298420023	6.1404703702	13.9432675249	H145	1.3099399061	5.0688269239	18.2625452640
H149	1.5987879786	5.9622842078	15.7925129827	H146	2.0286034236	1.7208722202	14.8504772156
H154	4.3270331197	-4.3759794746	20.5867749509	H147	0.3237530885	1.9349413373	13.0706934934
H155	8.6377841270	-1.0066036164	13.0497301443	H148	0.0098224399	6.1444419125	13.8810291855
H156	3.5453161890	8.5276648588	19.6471037691	H149	1.6887162112	5.9298867193	15.6791487854
H157	-0.5025007915	4.1798151692	12.4969065448	H154	4.2296229565	-4.2863543285	20.4661149485
				H155	8.8083989732	-0.9402267074	13.0962496154
				H156	3.6580913931	8.4131194511	19.5981692479
				H157	-0.6911789916	4.1521911024	12.5751948542

M06-L

E= -2378.432621 H

P4	4.6600096119	0.1522083219	16.8762354334
P5	3.2918588868	3.5294437970	16.6327333952
C50	4.5841522294	-1.2956880441	18.0040327396
C51	5.6619532109	-1.6887875656	18.8088545011
C52	5.5374749524	-2.7614563126	19.6839651282
C53	4.3294862741	-3.4517539729	19.7735341574
C54	3.2493582156	-3.0660626144	18.9863250540
C55	3.3777185996	-1.9946623795	18.1059420536
C56	6.0326223755	-0.2672005689	15.7449604334
C57	6.6085687690	-1.5354995455	15.6233091196
C58	7.5990998797	-1.7741070001	14.6727389000
C59	8.0312192470	-0.7514519491	13.8350400719
C60	7.4584313105	0.5150585907	13.9421872013

[Pd(binap)]

B3LYP

E= -2505.424423 H

Pd1	3.8951243007	1.7714380750	14.0934269446
P2	5.1336450760	3.1725409462	12.7688891699
P3	2.7599368228	0.0570987921	13.0808204587
C6	4.4335387283	4.6837786279	11.9724807561
C7	3.4715038305	5.4153483387	12.6844388185
C8	2.9630439352	6.6110236899	12.1733587879
C9	3.4042092013	7.0908832584	10.9391900900
C10	4.3524839537	6.3648573041	10.2159963446
C11	4.8627614430	5.1706764450	10.7276896837
C12	6.7891862952	3.7733369745	13.3672386196

C13	7.3623441601	3.0613410059	14.4348603500	C10	4.1878950846	6.3265644370	10.3046496628
C14	8.5934051376	3.4388125388	14.9714850702	C11	4.7710923387	5.1476316478	10.7933988860
C15	9.2658830592	4.5516803829	14.4634607487	C12	6.8183749983	3.7919704330	13.3688028564
C16	8.6988760778	5.2788645885	13.4157753386	C13	7.4555543691	3.0759349817	14.4071748694
C17	7.4728174491	4.8934842709	12.8695524576	C14	8.6860970198	3.5035023699	14.9271269145
C18	5.5585022146	2.0193033825	11.3484155959	C15	9.2910806684	4.6721840509	14.4341404236
C19	6.9420966019	1.7384579671	11.1517938873	C16	8.6570350183	5.4026330863	13.4158898357
C20	7.3799501567	0.8194640828	10.2340901168	C17	7.4329315705	4.9658966821	12.8833583540
C21	6.4584909168	0.1212792087	9.4225500367	C18	5.5942047537	2.0129676085	11.3629210291
C22	6.8981561525	-0.8096715517	8.4437167366	C19	6.9815901159	1.7279584957	11.1674872867
C23	6.0008275180	-1.4544493030	7.6274853542	C20	7.4185088983	0.8075449419	10.2359775189
C24	4.6184645016	-1.1895190097	7.7663809566	C21	6.4892781527	0.1138227541	9.4177988307
C25	4.1635380449	-0.3037347946	8.7159050640	C22	6.9242559420	-0.8232768009	8.4348221368
C26	5.0606493981	0.3848766239	9.5863832738	C23	6.0155781824	-1.4700659129	7.6150747449
C27	4.6064474761	1.3283361708	10.5803569063	C24	4.6289847319	-1.1975256950	7.7555010786
C28	3.1090216890	1.5709564924	10.6213607910	C25	4.1760574369	-0.2991448911	8.7091010359
C29	2.5711004379	2.3911809024	9.5633356159	C26	5.0812809136	0.3878803255	9.5806561577
C30	3.3976883512	2.9881048047	8.5653493944	C27	4.6289657197	1.3355712509	10.5792675905
C31	2.8669763679	3.7607181175	7.5582174395	C28	3.1358909685	1.5998118594	10.6083389456
C32	1.4737232795	3.9924701850	7.4824912529	C29	2.6101062622	2.4171644268	9.5328893633
C33	0.6414181927	3.4295433559	8.4196709673	C30	3.4517968516	2.9994886786	8.5315504743
C34	1.1594134907	2.6184137727	9.4638874778	C31	2.9300977901	3.7670973326	7.5014378232
C35	0.3081412987	1.9994460832	10.4064342079	C32	1.5331107516	4.0070567687	7.4077423775
C36	0.8245547704	1.1984134723	11.3916656239	C33	0.6838639304	3.4572535236	8.3537837504
C37	2.2241470139	0.9634110697	11.5284256462	C34	1.1891305550	2.6536905122	9.4184506560
C38	3.6575028718	-1.4547253508	12.5224977033	C35	0.3214240579	2.0473858034	10.3649708599
C39	4.6834289000	-1.9430255379	13.3456352130	C36	0.8280248101	1.2453869851	11.3691907975
C40	5.3548223701	-3.1236493688	13.0234791852	C37	2.2302421731	1.0021078183	11.5175162047
C41	5.0168833706	-3.8307217346	11.8683370609	C38	3.6107268827	-1.4622144976	12.4994420039
C42	4.0066761068	-3.3470011241	11.0348946780	C39	4.6379845557	-1.9758691995	13.3189052536
C43	3.3314614952	-2.1693712990	11.3592454873	C40	5.2747035214	-3.1836224131	12.9940691762
C44	1.1795231372	-0.6527852380	13.7612491436	C41	4.9002123906	-3.8900353885	11.8392438909
C45	0.5553567188	0.0753243928	14.7878147325	C42	3.8883808444	-3.3795708063	11.0094294064
C46	-0.6240937258	-0.3804667792	15.3782761504	C43	3.2462285688	-2.1744749825	11.3366689933
C47	-1.1917410362	-1.5875506213	14.9669488560	C44	1.1628613466	-0.5919713509	13.7584132085
C48	-0.5708677730	-2.3309722088	13.9614336178	C45	0.5212389398	0.2009130122	14.7367498896
C49	0.6026261923	-1.8689708222	13.3625721530	C46	-0.6671471553	-0.2281350885	15.3461936573
H94	3.1197654251	5.0380817216	13.6417527645	C47	-1.2226456517	-1.4732372053	15.0061915156
H95	2.2179755415	7.1648323198	12.7391611979	C48	-0.5825635756	-2.2788997146	14.0503947835
H96	4.6925039269	6.7244310043	9.2477731034	C49	0.5981615936	-1.8422289827	13.4273979532
H97	5.5958603706	4.6115234780	10.1522198792	H94	3.0965955947	4.8930827647	13.7671225948
H98	6.8285900795	2.2058636428	14.8448829836	H95	2.0619039217	7.0041578466	12.9034075991
H99	9.0208215931	2.8694009068	15.7932279646	H96	4.4866374633	6.7152029178	9.3240736529
H100	9.2117569495	6.1525204680	13.0203244915	H97	5.5211048952	4.6201573668	10.1924672537
H101	7.0463153501	5.4762321907	12.0592695305	H98	6.9651213501	2.1788961476	14.8089451639
H102	7.6764076832	2.2665003544	11.7477111827	H99	9.1656041990	2.9305936297	15.7295861161
H103	8.4444853518	0.6289150806	10.1137189781	H100	9.1160997746	6.3216814854	13.0321101135
H104	7.9662160155	-0.9941914526	8.3495022713	H101	6.9479476775	5.5519260196	12.0950481222
H105	6.3473781497	-2.1593559725	6.8759148397	H102	7.7196345486	2.2563512416	11.7777107684
H106	3.9062526127	-1.6907533254	7.1152615354	H103	8.4912508756	0.6118584848	10.1122587808
H107	3.0994532269	-0.1189207807	8.7995011659	H104	8.0003190826	-1.0154872691	8.3380199559
H108	4.4680034817	2.8229577721	8.5989393824	H105	6.3615864389	-2.1844304931	6.8590475401
H109	3.5267345877	4.1976358335	6.8124337361	H106	3.9074700181	-1.7017020256	7.1016961823
H110	1.0672579490	4.6079135700	6.6838959904	H107	3.1041842631	-0.1027985126	8.7958144618
H111	-0.4337786947	3.5890561968	8.3744264821	H108	4.5302210148	2.8244189579	8.5789151656
H112	-0.7660946788	2.1565312849	10.3350018202	H109	3.6058017170	4.1919253376	6.7496180795
H113	0.1424741745	0.7315093520	12.0919056096	H110	1.1330098847	4.6168749476	6.5897696783
H114	4.9567898175	-1.3857614415	14.2384912419	H111	-0.3994365063	3.6223159255	8.2969361828
H115	6.1470117754	-3.4869107833	13.6735344961	H112	-0.7604819887	2.2111621603	10.2813249919
H116	3.7478329405	-3.8813922170	10.1241852284	H113	0.1347212181	0.7799786419	12.0755498233
H117	2.5547713225	-1.7987431501	10.6958362228	H114	4.9368339852	-1.4123485819	14.2116166520
H118	1.0085783767	1.0055862892	15.1251192647	H115	6.0711602300	3.5691185057	13.6413888643
H119	-1.0918197061	0.2033678367	16.1672362455	H116	3.6017911347	-3.9164445556	10.0976903109
H120	-0.9996140498	-3.2777679116	13.6412619694	H117	2.4641507763	-1.7788178497	10.6785408879
H121	1.0742346132	-2.4680298864	12.5898132821	H118	0.9746254361	1.1600889110	15.0208969645
H150	3.0060741868	8.0197794346	10.5389484305	H119	-1.1511217181	0.4047928436	16.0993493659
H151	10.2204801232	4.8552383261	14.8860274431	H120	-1.0027780219	-3.2570171944	13.7868778296
H152	5.5424989346	-4.7475278532	11.6139688241	H121	1.0895640157	-2.4870452799	12.6907334518
H153	-2.1048360235	-1.9509092656	15.4314119385	H150	2.7607689637	7.9190280645	10.6789267762
H151	10.2453429376	5.0172409712	14.8485199908	H151	5.4012657238	-4.8300962877	11.5811313511
H152	5.4012657238	-4.8300962877	11.5811313511	H153	-2.1428223454	-1.8184917632	15.4915019882
H153	-2.1428223454	-1.8184917632	15.4915019882				
BP86							
E= -2505.506111 H							
Pd1	3.9581721015	1.7114301487	14.0793911016	M06			
P2	5.1678343393	3.1367954819	12.8047559593	E= -2504.069693 H			
P3	2.7586205548	0.0772935731	13.0655995002	Pd1	3.9754576267	1.7033034400	14.2689991138
C6	4.3895883777	4.6298572156	12.0495229561	P2	5.1567032719	3.1076247190	12.8656635584
C7	3.4064114078	5.3072955492	12.7995757849	P3	2.7768887676	0.1008655572	13.1112781765
C8	2.8265193596	6.4877243342	12.3114435259	C6	4.3121833985	4.4563090815	11.9626911252
C9	3.2179410410	7.0000933051	11.0641534274				

C7	3.1773624549	5.0208131370	12.5479718693	P2	5.0972794639	3.1637780596	12.7513721676
C8	2.4956599863	6.0532423146	11.9125264359	P3	2.7392240448	0.1522729755	13.2054020694
C9	2.9423530058	6.5301233445	10.6849896623	C6	4.6228560541	4.5703427941	11.6774981393
C10	4.0684518302	5.9697415817	10.0904404847	C7	3.3598817597	5.1492147778	11.8248959128
C11	4.7462675250	4.9352103671	10.7226986212	C8	2.9399224050	6.1618690186	10.9649153569
C12	6.7973172215	3.8314792339	13.2993018457	C9	3.7839691919	6.6163628616	9.9560548957
C13	7.4492492477	3.2539599575	14.3937289306	C10	5.0485786622	6.0492249744	9.8026303205
C14	8.7026410618	3.7011831232	14.7951607661	C11	5.4590514326	5.0244812645	10.6476748457
C15	9.3132904841	4.7524823331	14.1197703627	C12	6.7431693836	3.6225030257	13.4167256840
C16	8.6650941423	5.3502038120	13.0440732945	C13	7.3750591777	2.6713060080	14.2368016154
C17	7.4176780270	4.8925423605	12.6340053995	C14	8.5849986862	2.9487921828	14.8577598481
C18	5.5750387952	1.8840508284	11.5260114539	C15	9.1820712062	4.1998565536	14.6999226849
C19	6.9237064328	1.4476223033	11.4584004699	C16	8.5532893507	5.1604111118	13.9150746899
C20	7.3233204062	0.4767599270	10.5842399833	C17	7.3472952619	4.8763482546	13.2746806149
C21	6.4052025663	-0.0973230381	9.6816781921	C18	5.4868771263	1.8928168481	11.4536976128
C22	6.8229153051	-1.0450995530	8.7171186491	C19	6.8340447610	1.5025413907	11.2444325541
C23	5.9413980074	-1.5500059668	7.7980540612	C20	7.1739150554	0.5501171712	10.3198792775
C24	4.5958000487	-1.1297494779	7.8221764202	C21	6.1892188116	-0.0507420881	9.5102323998
C25	4.1583060269	-0.2358261776	8.7657749683	C22	6.5283454697	-1.0066802408	8.5240639199
C26	5.0446181304	0.3182508838	9.7289581627	C23	5.5683915023	-1.5498341294	7.7056349220
C27	4.6200637714	1.2865905366	10.6988699954	C24	4.2238671023	-1.1543895441	7.8531289052
C28	3.1628287345	1.6509162980	10.7160303369	C25	3.8618684152	-0.2420846735	8.8159378712
C29	2.6778387230	2.5039022685	9.6691289862	C26	4.8250743012	0.3412247571	9.6821151225
C30	3.5109061168	2.9582771003	8.6113022231	C27	4.4741059792	1.2934039296	10.6961045518
C31	3.0175926664	3.7395299249	7.5979406036	C28	3.0184446702	1.6456748707	10.7848327706
C32	1.6661295914	4.1409487636	7.5919266744	C29	2.5045715414	2.5065194902	9.7622488921
C33	0.8337757024	3.7289297537	8.5994073904	C30	3.3415748522	3.0982944742	8.7809306025
C34	1.3087660739	2.8962783461	9.6404170273	C31	2.8272946085	3.9128283624	7.8009382274
C35	0.4444628621	2.4100000177	10.6431171468	C32	1.4455706362	4.1833900542	7.7411165235
C36	0.9028121381	1.5479161149	11.6001512637	C33	0.6034038335	3.6282704528	8.6740712733
C37	2.2616538279	1.1398700025	11.6524692882	C34	1.1022501523	2.7853365999	9.6941050694
C38	3.6495427721	-1.3306396083	12.3701716504	C35	0.2484255710	2.1790850979	10.6386870998
C39	4.8125449126	-1.7767238027	13.0023408686	C36	0.7498970342	1.3473472435	11.6057474589
C40	5.5186545311	-2.8654677737	12.5003674633	C37	2.1367128423	1.0635422220	11.7060510367
C41	5.0719851936	-3.5191599366	11.3567209670	C38	3.8115828191	-1.1727378586	12.564379314
C42	3.9187142096	-3.0771134247	10.7147970889	C39	5.0712803672	-1.3641878504	13.1224847599
C43	3.2144854271	-1.9882615600	11.2151517229	C40	5.9271944423	-2.3532976263	12.6452765719
C44	1.1815915896	-0.6113985319	13.7039056455	C41	5.5341230563	-3.1640214158	11.5833199745
C45	0.5551292732	0.0776529076	14.7476981842	C42	4.2833874501	-2.9787997985	10.9978067733
C46	-0.6640961110	-0.3538745087	15.2578129910	C43	3.4297053997	-1.9890820261	11.4734605544
C47	-1.2656730033	-1.4993768103	14.74539937692	C44	1.2560394512	-0.7453693392	13.8160275412
C48	-0.6404219347	-2.2056447396	13.7231745838	C45	0.3674840101	-0.0063452826	14.6130502779
C49	0.5718631758	-1.7646463758	13.2029258260	C46	-0.7628879348	-0.5953561598	15.1646948911
H94	2.8254536411	4.6290738779	13.5040624033	C47	-1.0107725222	-1.9512575970	14.9601259535
H95	1.6071415171	6.4813617186	12.3743566981	C48	-0.1218978841	-2.7044196275	14.2006678099
H96	4.4069682157	6.3235753793	9.1170830049	C49	1.0004983273	-2.1089260242	13.6298878058
H97	5.6040761949	4.4713655501	10.2319757402	H94	2.6948660551	4.7744554570	12.6054027483
H98	6.9551757189	2.4406760494	14.9311597312	H95	1.9443819083	6.5883485873	11.0774896978
H99	9.1987764729	3.2340920668	15.6447581189	H96	5.7095296696	6.3932741750	9.0077312240
H100	9.1340925229	6.1808784786	12.5178107508	H97	6.4370967547	4.5606864358	10.5045824675
H101	6.9226596625	5.3783283512	11.7947827714	H98	6.8942564799	1.7013427005	14.3860332737
H102	7.6621313005	1.8987171579	12.1186508952	H99	9.0589344237	2.1902742517	15.4792975957
H103	8.3647790710	0.1552560402	10.5532962361	H100	9.0035937394	6.1447962990	13.7942156373
H104	7.8702733736	-1.3496269083	8.7128018223	H101	6.8722738663	5.6446397552	12.6670125823
H105	6.2759770205	-2.2661622736	7.0489207577	H102	7.6204077850	1.9731344187	11.8295031673
H106	3.8941658116	-1.5236465479	7.0876457255	H103	8.2166215031	0.2620444383	10.1841819082
H107	3.1134991999	0.0688511015	8.7707493689	H104	7.5753471998	-1.2938829514	8.4217938987
H108	4.5593732469	2.6662253397	8.6005633066	H105	5.8426116418	-2.2771710556	6.9430669020
H109	3.6793147370	4.0588630628	6.7933887620	H106	3.4620012307	-1.5784803940	7.2005397209
H110	1.2877338731	4.7684007255	6.7862158366	H107	2.8160078331	0.0386795952	8.9197230750
H111	-0.2173469355	4.0196964883	8.6097263272	H108	4.4126656359	2.9118522001	8.8173955602
H112	-0.6041125987	2.7098075848	10.6262319115	H109	3.4981328337	4.3600727329	7.0682981882
H113	0.2044677234	1.1637574691	12.3415069790	H110	1.0505399630	4.8269662867	6.9566189243
H114	5.1682015524	-1.2470983668	13.8881986387	H111	-0.4691523084	3.8213933464	8.6410696494
H115	6.4274617988	-3.1979643451	13.0001737852	H112	-0.8237610540	2.3689080111	10.5792065509
H116	3.5775629160	-3.5681871692	9.8039723882	H113	0.0633626560	0.8827907497	12.3097406703
H117	2.3336006580	-1.6240348914	10.6830714104	H114	5.3783998576	-0.7091399415	13.9403780251
H118	1.0422437052	0.9657846392	15.1582145695	H115	6.9087242455	-2.4841759377	13.0987408287
H119	-1.1395737904	0.2008813509	16.0654728952	H116	3.9799257604	-3.5924736849	10.1507246546
H120	-1.0997908063	-3.1094442794	13.3245727979	H117	2.4641940027	-1.8271813773	10.9910805729
H121	1.0499232913	-2.3352480276	12.4080571895	H118	0.5806936757	1.0481303073	14.8017985436
H150	2.4049516581	7.3328903929	10.1818868735	H119	-1.4434312216	0.0012582438	15.7702419233
H151	10.2914495452	5.1121035159	14.4363368026	H120	-0.3007312331	-3.7680227644	14.0483089299
H152	5.6281097146	-4.3657917111	10.9568008905	H121	1.6872720858	-2.7192335158	13.0471946009
H153	-2.2159362685	-1.8462220658	15.1488953877	H150	3.4538382265	7.4041845832	9.2805753279
				H151	10.1243957204	4.4253489161	15.1959288852
				H152	6.2058226407	-3.9317944643	11.2025115647
				H153	-1.8876169948	-2.4208404516	15.4028852221
M06-L							
E=-2505.276964 H							
Pd1	3.7419706248	1.9750664336	14.1377929918				

[Pd(binap) <sub>2</sub> ]				C77	0.7352728539	-0.0028672602	21.0538750172
B3LYP				C78	1.2516314662	0.7340215863	19.9563923978
E= -4884.073251 H				C79	0.4065726708	1.2010137957	18.9221200846
Pd1	3.9849297488	1.7111964493	14.6640854662	C80	0.9141775569	1.9442054778	17.8894872910
P2	5.0861372240	2.9883689726	12.8437605511	C81	2.2974058846	2.2837566501	17.8058310750
P3	2.8384328813	0.2256124833	13.0486780997	C82	3.6788206074	4.7167823699	16.9656602554
P4	5.1195048806	0.4795548574	16.4781607330	C83	4.7469331159	5.2753912248	16.2527625469
P5	2.8448732463	3.1999713308	16.2774148975	C84	5.3384631128	6.4736627840	16.6605021385
C6	4.3000543971	4.4650035496	12.0279384129	C85	4.8762956398	7.1345032685	17.7978869992
C7	3.4548721092	5.2797746153	12.7930519050	C86	3.8280273604	6.5760328835	18.5334227366
C8	2.9295279940	6.4635079581	12.2711485129	C87	3.2419015079	5.3785773341	18.1259801955
C9	3.2332178968	6.8537965080	10.9667431029	C88	1.2537497979	3.9668774177	15.6643538560
C10	4.0639151904	6.0451623246	10.1887875139	C89	0.8382515965	3.6266952929	14.3704115760
C11	4.5922740021	4.8657072824	10.7144377090	C90	-0.3248961723	4.1684110508	13.8181167498
C12	6.7313940372	3.7629382457	13.2890665789	C91	-1.0994268951	5.0587779002	14.5575022190
C13	7.2910037702	3.4379110758	14.5310063960	C92	-0.6979501366	5.4120248319	15.8484584392
C14	8.5103279354	3.9827247188	14.9395857405	C93	0.4648465381	4.8733351405	16.3944993705
C15	9.1915508961	4.8697375001	14.1091053879	H94	3.2054811011	4.9922398372	13.8077230691
C16	8.6414874484	5.2135263552	12.8715061514	H95	2.2767082385	7.0752708383	12.8892227924
C17	7.4232183902	4.6702265339	12.4680260540	H96	4.2970828344	6.3262565774	9.1642847511
C18	5.5566213996	1.8920389877	11.4055340908	H97	5.2324787289	4.2480250615	10.0918941839
C19	6.9357132564	1.5385156970	11.3087804759	H98	6.7516930749	2.7621790297	15.1872127717
C20	7.4004151413	0.6654864253	10.3625615367	H99	8.9162579730	3.7181434381	15.9129727549
C21	6.5143532355	0.0732215416	9.4332059711	H100	9.1611717679	5.9116340604	12.2187233588
C22	6.9892548664	-0.8133951764	8.4315787321	H101	7.0094528599	4.9627575904	11.5086025098
C23	6.1292590156	-1.3770759869	7.5199904756	H102	7.6433039618	1.9850640501	11.9969750581
C24	4.7499453359	-1.0751762149	7.5868115384	H103	8.4616288846	0.4292446903	10.3072404260
C25	4.2611208611	-0.2256960157	8.5534535386	H104	8.0543128290	-1.0340609031	8.4000460403
C26	5.1209003598	0.3889061086	9.5113834021	H105	6.5033277407	-2.0513805102	6.7534600130
C27	4.6398811547	1.3046844554	10.5211513094	H106	4.0653502167	-1.5214374508	6.8691968648
C28	3.1624719478	1.6188853008	10.5303052187	H107	3.1986373271	-0.0166504330	8.5842885601
C29	2.6244180034	2.3871223565	9.4292748084	H108	4.5021925376	2.6796303792	8.3788542051
C30	3.4366703105	2.8759415982	8.3638803460	H109	3.5466535600	3.9262077547	6.5091216093
C31	2.8975093739	3.5764779859	7.3085770661	H110	1.0972909888	4.4032911239	6.4160129923
C32	1.5113063337	3.8479917487	7.2540742713	H111	-0.3747836293	3.6032682754	8.2447907267
C33	0.6946523218	3.4038669367	8.2662730441	H112	-0.6854634442	2.3995645511	10.3498229358
C34	1.2214338324	2.6706570868	9.3614329014	H113	0.2269613534	1.0907216524	12.1939434065
C35	0.3823222046	2.1911177977	10.3938826122	H114	4.9651481647	-1.4886794211	14.0595210167
C36	0.8992550844	1.4548180297	11.4264709220	H115	5.9313638215	-3.6417820343	13.3662743284
C37	2.2871564906	1.1347557044	11.5139404815	H116	3.4450488634	-3.6172334124	9.8547713438
C38	3.6295560019	-1.3223474947	12.3784883209	H117	2.4870268575	-1.4611451075	10.5484468079
C39	4.6181214286	-1.9539520870	13.1442822543	H118	1.3606939879	0.6045520835	15.4871729864
C40	5.1659367461	-3.1766000634	12.7495759267	H119	-0.7333161305	-0.3018156242	16.4429637313
C41	4.7404351141	-3.7905638889	11.5722102460	H120	-1.2684591782	-2.7211569467	12.9242693851
C42	3.7706399654	-3.1626522564	10.7876655023	H121	0.8176489761	-1.8283509763	11.9903305088
C43	3.2244121411	-1.9420731912	11.1846287557	H122	5.4396200041	-0.8498118735	19.1837822984
C44	1.2343845504	-0.5162534776	13.6617863381	H123	4.5435392621	-2.9376545440	20.1236398355
C45	0.7723372285	-0.1097834982	14.9195067121	H124	2.1811700893	-3.5198789116	16.5747720594
C46	-0.4082170330	-0.6272488448	15.4581672984	H125	3.0842302858	-1.4326637178	15.6362713428
C47	-1.1518030700	-1.5616266017	14.7415657361	H126	7.2175976818	-1.2302710463	17.9186246837
C48	-0.7002019423	-1.9853383835	13.4891266054	H127	9.3401299727	-2.2138475636	17.1763193262
C49	0.4806391569	-1.4714480977	12.9575631881	H128	8.7489969415	-0.5390349123	13.2555343796
C50	4.3551246346	-0.9964027675	17.3193953695	H129	6.6188116146	0.4622630159	14.0161168783
C51	4.7435731049	-1.4395364524	18.5944666625	H130	7.6566601044	1.5709294325	17.2978181983
C52	4.2320950108	-2.6208912825	19.1307655069	H131	8.4364180371	3.1488924997	18.9861805395
C53	3.3149648657	-3.3854200710	18.4063418472	H132	7.9983975889	4.5874452877	20.9078048801
C54	2.9065462903	-2.9466090592	17.1472110669	H133	6.4240760373	5.5537299154	22.5633266603
C55	3.4197861112	-1.7627704542	16.6125192443	H134	4.0010054091	4.9599816596	22.4494662603
C56	6.7647707626	-0.2882377585	16.0226319586	H135	3.1723732159	3.4358068064	20.7308130131
C57	7.5472152800	-1.0604007955	16.8990652581	H136	4.5339245166	0.7688928813	20.9348600012
C58	8.7500142834	-1.6233112530	16.4788003747	H137	3.5953462701	-0.4838737067	22.91110804428
C59	9.1946851894	-1.4359988667	15.1672299872	H138	1.1522384877	-0.9907109606	22.9074216140
C60	8.4254123809	-0.6832590617	14.2834310047	H139	-0.3315860213	-0.2155303231	21.0771959388
C61	7.2229169201	-0.1140232374	14.7109616776	H140	-0.6583057188	0.9781755010	18.9657249276
C62	5.5735942796	1.5935150174	17.9070215637	H141	0.2378652455	2.3016545679	17.1221546129
C63	6.9401822333	1.9932577285	17.9921695354	H142	5.1229691972	4.7693122204	15.3713231487
C64	7.3839330974	2.8776450107	18.9383994735	H143	6.1656781980	6.8824890797	16.0849846258
C65	6.4873663534	3.4384778554	19.8766076638	H144	3.4746423902	7.0648246450	19.4384521212
C66	6.9400649541	4.3359053513	20.8792040009	H145	2.4521896451	4.9456595391	18.7326159590
C67	6.0669900811	4.8715625764	21.7956357481	H146	1.4474820201	2.9428126468	13.7863630930
C68	4.6962453324	4.5328233618	21.7304547646	H147	-0.6130705204	3.8935450708	12.8065846298
C69	4.2291628723	3.6726115986	20.7627793934	H148	-1.2932173992	6.1098905095	16.4333942404
C70	5.1043306162	3.0820167617	19.8044965206	H149	0.7580834338	5.1721444857	17.3946936652
C71	4.6460088506	2.1543597998	18.7971702185	H150	2.8217569772	7.7728558838	10.5566599163
C72	3.1768801330	1.8113591456	18.7895367925	H151	10.1406835166	5.2979750844	14.4234246929
C73	2.6505782946	1.0354139911	19.8886674903	H152	5.1665185415	-4.7414327262	11.2616427572
C74	3.4705987651	0.5604441129	20.9537521315	H153	-2.0711531788	-1.9679050819	15.1572242646
C75	2.9413758415	-0.1444431894	22.0111372834	H154	2.9155492692	-4.3057332062	18.8253987090
C76	1.5585440002	-0.4325200300	22.0675262543	H155	10.1315899314	-1.8806913438	14.8393011023

H156 5.3341912820 8.0676169651 18.1170959029  
 H157 -2.0050710515 5.4844695464 14.1313094633

BP86

E= -4884.171364 H

Pd1 3.9781041972 1.7280981684 14.6621876485  
 P2 5.0669250269 2.9618984754 12.8789111746  
 P3 2.8894791818 0.2304326384 13.1031584683  
 P4 5.0753561845 0.5083561539 16.4466862905  
 P5 2.8740572452 3.2183438235 16.2293043711  
 C6 4.2720081282 4.4220792475 12.0318803285  
 C7 3.3763648747 5.2257270040 12.7642713036  
 C8 2.8570016868 6.4107687290 12.2184721144  
 C9 3.2179654687 6.8115611516 10.9228489526  
 C10 4.0964324133 6.0101315329 10.1757083897  
 C11 4.6172046763 4.8281983838 10.7241289169  
 C12 6.7053077725 3.7553722819 13.3293221828  
 C13 7.2488659270 3.4621451412 14.5946515148  
 C14 8.4772370987 4.0095529355 14.9984483382  
 C15 9.1816491936 4.8636708105 14.1386995007  
 C16 8.6437463077 5.1772446574 12.8786343640  
 C17 7.4153543319 4.6329641596 12.4795402529  
 C18 5.5600742594 1.8750537590 11.4423538265  
 C19 6.9469433249 1.5329381162 11.3389761408  
 C20 7.4217734099 0.6837717163 10.3609823835  
 C21 6.5355521234 0.1081259060 9.4112168411  
 C22 7.0166363522 -0.7495207320 8.3798324247  
 C23 6.1520230005 -1.3008211448 7.4492932753  
 C24 4.7646942069 -1.0137091629 7.5309260752  
 C25 4.2684577178 -0.1887592661 8.5292548809  
 C26 5.1291681378 0.4124620923 9.5023097983  
 C27 4.6370641092 1.2995152647 10.5391394973  
 C28 3.1605661489 1.6040658458 10.5647467387  
 C29 2.5947344540 2.3607331258 9.4648666173  
 C30 3.3907820976 2.8610823736 8.3861377380  
 C31 2.8255554242 3.5547192654 7.3265393802  
 C32 1.4291870234 3.8036510397 7.2853387158  
 C33 0.6248342026 3.3462531591 8.3158810335  
 C34 1.1766448042 2.6232568781 9.4124584320  
 C35 0.3536610015 2.1331194495 10.4615863694  
 C36 0.8988834202 1.4099716819 11.5022118874  
 C37 2.2985206142 1.1162316192 11.5728902102  
 C38 3.7187633037 -1.2931473143 12.4169408906  
 C39 4.6789488998 -1.9571036215 13.2057387038  
 C40 5.2328493952 -3.1797954142 12.7934779206  
 C41 4.8414307508 -3.7599958139 11.5771579647  
 C42 3.8978127469 -3.0996356867 10.7732396502  
 C43 3.3420503992 -1.8800385447 11.1889039143  
 C44 1.3020514105 -0.5567487111 13.7151570245  
 C45 0.7658024754 -0.0876765903 14.9298167363  
 C46 -0.4261296629 -0.6192827673 15.4470055005  
 C47 -1.1012983583 -1.6338161779 14.7542088164  
 C48 -0.5692766861 -2.1225961501 13.5488059733  
 C49 0.6231643646 -1.5930372469 13.0359837810  
 C50 4.2986772568 -0.9562115269 17.3079836719  
 C51 4.6878612623 -1.3737616702 18.6002023879  
 C52 4.1832688248 -2.5584989168 19.1568144932  
 C53 3.2731235410 -3.3492934489 18.4363777193  
 C54 2.8631850789 -2.9335039113 17.1605370466  
 C55 3.3698052335 -1.7475643320 16.6047048923  
 C56 6.7111432887 -0.2826267441 15.9820186264  
 C57 7.4675861708 -1.0997132886 16.8521543374  
 C58 8.6788260176 -1.6654671154 16.4318529565  
 C59 9.1533764761 -1.4351264060 15.1291981690  
 C60 8.4054655938 -0.6385776083 14.2514856121  
 C61 7.1954915170 -0.0668180227 14.6777727020  
 C62 5.5658276859 1.5983338745 17.8777876277  
 C63 6.9474231861 1.9608343806 17.9731925907  
 C64 7.4149822909 2.8136825979 18.9514976269  
 C65 6.5243620055 3.3757244474 19.9050135551  
 C66 6.9995525335 4.2347046458 20.9377679116  
 C67 6.1317966872 4.7758491520 21.8711845527  
 C68 4.7465441131 4.4791372664 21.7889023701  
 C69 4.2556865724 3.6522162111 20.7893038412  
 C70 5.1209271616 3.0566880826 19.8165224291  
 C71 4.6376504702 2.1609491040 18.7825572713  
 C72 3.1658362349 1.8361714999 18.7591938953  
 C73 2.6145156090 1.0653632694 19.8568901219  
 C74 3.4238486966 0.5596390692 20.9233201485

C75 2.8720533197 -0.1446082573 21.9827199410  
 C76 1.4770366838 -0.3984790097 22.0363455276  
 C77 0.6605893977 0.0618314165 21.0168338511  
 C78 1.1984482892 0.7942475822 19.9194642342  
 C79 0.3641780588 1.2864358096 18.8803169103  
 C80 0.8967325160 2.0174431800 17.8380509566  
 C81 2.2936270167 2.3214294831 17.7582181476  
 C82 3.7244207417 4.7254085451 16.9267160735  
 C83 4.7349886590 5.3463558287 16.1662119611  
 C84 5.3215925855 6.5502808478 16.5888941191  
 C85 4.9120818310 7.1539938459 17.7874526341  
 C86 3.9224088206 6.5326542557 18.5672612758  
 C87 3.3363903411 5.3302298653 18.1431709775  
 C88 1.2845279192 4.0162840808 15.6259650719  
 C89 0.7612909876 3.5771260430 14.3942785990  
 C90 -0.4284695434 4.1165715420 13.8777097621  
 C91 -1.1184411218 5.1109957474 14.5862938197  
 C92 -0.5975901528 5.5714309023 15.8083980724  
 C93 0.5926010140 5.0342357875 16.3206205485  
 H94 3.0778476285 4.9224399336 13.7717114595  
 H95 2.1615587594 7.0161182626 12.8118047472  
 H96 4.3736416315 6.2991631885 9.1547729076  
 H97 5.2948256965 4.2090722176 10.1255222008  
 H98 6.6822342652 2.8099150326 15.2708562383  
 H99 8.8727494746 3.7732654688 15.9933328075  
 H100 9.1821717021 5.8538141778 12.2033187445  
 H101 7.0043750480 4.9006888855 11.5005506398  
 H102 7.6554225560 1.9754821659 12.0451696768  
 H103 8.4941025628 0.4567558346 10.2964036950  
 H104 8.0928120833 -0.9614569647 8.3392513424  
 H105 6.5330017235 -1.9559842147 6.6569383052  
 H106 4.0747817064 -1.4501299873 6.7984630171  
 H107 3.1951505666 0.0165383478 8.5694438455  
 H108 4.4690237871 2.6782233248 8.3927920480  
 H109 3.4666949657 3.9151576401 6.5129399893  
 H110 0.9928495925 4.3538872025 6.4433781779  
 H111 -0.4573100980 3.5291223549 8.3055025800  
 H112 -0.7270122742 2.3204028180 10.4235735056  
 H113 0.2384402480 1.0302527057 12.2871702304  
 H114 5.0005323515 -1.5144809025 14.1527463372  
 H115 5.9785191660 -3.673049832 13.4282450456  
 H116 3.5967504781 -3.5294769569 9.8103525780  
 H117 2.6147960402 -1.3719709212 10.5457748356  
 H118 1.3118738141 0.6882861202 15.4806453151  
 H119 -0.8123806768 -0.2447171401 16.4021553840  
 H120 -1.0832408047 -2.9254814900 13.0057857464  
 H121 1.0316797857 -1.9986191133 12.1044288188  
 H122 5.3826084220 -0.7582884841 19.1831753983  
 H123 4.4960784597 -2.8576147065 16.1238398711  
 H124 2.1397403986 -3.5278611369 16.5900658559  
 H125 3.0325804818 -1.4319913967 15.6134261311  
 H126 7.1059586066 -1.3045755442 17.8651889379  
 H127 9.2522732843 -2.2946976922 17.1238398748  
 H128 8.7511093277 -0.4648981940 13.2257281924  
 H129 6.5975016134 0.5442136300 13.9895077079  
 H130 7.6583080182 1.5252425252 17.2647978118  
 H131 8.4842730717 3.0552319920 19.0130613547  
 H132 8.0740869740 4.4549660587 20.9773320984  
 H133 6.5087055304 5.4310478979 22.6654409582  
 H134 4.0536795519 4.9099494177 22.5218672238  
 H135 3.1835974890 3.4408854154 20.7481499567  
 H136 4.5013755028 0.7455248722 20.9060279666  
 H137 3.5226709991 -0.5095398782 22.7867176472  
 H138 1.0512939173 -0.9560765252 22.8789002757  
 H139 -0.4206095160 -0.1256526941 21.0371730059  
 H140 -0.7151983898 1.0939270265 18.9270418681  
 H141 0.2278514432 2.3985598421 17.0609028896  
 H142 5.0730495338 4.8799414746 15.2359384241  
 H143 6.1067500697 7.0094640253 15.9765917995  
 H144 3.6119279167 6.9778428322 19.5201382795  
 H145 2.5818954638 4.8464972021 18.7742219110  
 H146 1.3143208949 2.8162083140 13.8294878973  
 H147 -0.8020672708 3.7618313603 12.9099859792  
 H148 -1.1190572876 6.3584942608 16.3672897172  
 H149 0.9884761204 5.4201614831 17.2658399764  
 H150 2.8113370003 7.7348536480 10.4938233480  
 H151 10.1412767116 5.2939232401 14.4503123904  
 H152 5.2745252342 -4.7132818116 11.2521015489  
 H153 -2.0313723561 -2.0538241219 15.1563161861

H154	2.8779730584	-4.2741470860	18.8727051769
H155	10.0983328644	-1.8845289844	14.8002069081
H156	5.3697358356	8.0929147293	18.1204835891
H157	-2.0462951112	5.5363090885	14.1857954722

M06

E= -4881.408692 H

Pd1	3.9727691117	1.7225721459	14.6712412066
P2	5.1048736987	2.9257697635	12.8596040726
P3	2.8290044117	0.2785432798	13.0481373201
P4	5.1291096838	0.5628149549	16.4893151240
P5	2.8178692569	3.1572795470	16.2918404671
C6	4.2775699567	4.3254252173	12.0018951388
C7	3.2556231875	4.9839946622	12.6853267573
C8	2.5971043636	6.0677838473	12.1149243482
C9	2.9606103552	6.5107502152	10.8485804327
C10	3.9815747662	5.8655375050	10.1572198302
C11	4.6328247387	4.7794155913	10.7278879516
C12	6.7364261703	3.6957919033	13.2890042588
C13	7.2704569989	3.3873468235	14.5411813202
C14	8.4929484020	3.9087005043	14.9511583362
C15	9.1982863059	4.7601757478	14.1098452062
C16	8.6715085869	5.0892832181	12.8632512806
C17	7.4509383599	4.5644226941	12.4574981226
C18	5.5568573708	1.7923121732	11.4661238435
C19	6.8985216663	1.3253742519	11.4303514797
C20	7.3081057369	0.3862761972	10.5272393526
C21	6.4091018577	-0.1330331932	9.5718897194
C22	6.8354960552	-1.0698747634	8.6024570781
C23	5.9688771347	-1.5464894115	7.6540707378
C24	4.6305338745	-1.1040372612	7.6515496182
C25	4.1871950162	-0.2104602004	8.5933672283
C26	5.0589622129	0.3142632586	9.5843833936
C27	4.6268912456	1.2646943626	10.5684119662
C28	3.1829173236	1.6679098818	10.5703863932
C29	2.6973456049	2.4932435910	9.5022907073
C30	3.5241214160	2.9086682359	8.4250176035
C31	3.0319409811	3.6770676415	7.4012179756
C32	1.6880010041	4.1015839932	7.4035622788
C33	0.8627903956	3.7287649501	8.4323545340
C34	1.3380870452	2.9170216950	9.4881307358
C35	0.4817834680	2.4868037271	10.5239401635
C36	0.9421798895	1.6595041890	11.5087309618
C37	2.2953895286	1.2263827755	11.5506515087
C38	3.6678885780	-1.2029321206	12.3404705012
C39	4.7260690191	-1.7519513202	13.0663326432
C40	5.3933132986	-2.8872630864	12.6158378896
C41	5.0050773915	-3.4960388533	11.4274758815
C42	3.9483312046	-2.9605747060	10.6946319619
C43	3.2885621398	-1.8234407824	11.1449509308
C44	1.2301365522	-0.4677136055	13.6154921780
C45	0.7352450817	-0.0432939335	14.8491000835
C46	-0.4586770563	-0.5459827529	15.3563623487
C47	-1.1792085142	-1.4849793281	14.6290084952
C48	-0.6941924070	-1.9240840888	13.3996124997
C49	0.4992294926	-1.4211030147	12.8982363560
C50	4.3050282847	-0.8312197235	17.3605856971
C51	4.6896752608	-1.2977511991	18.6227617539
C52	4.0490352102	-2.3866135938	19.1990119996
C53	3.0081507810	-3.0218973080	18.5267614307
C54	2.6126697824	-2.5640184141	17.2741893680
C55	3.2621203663	-1.4779633574	16.6969867844
C56	6.7564347794	-0.2147415382	16.0614126442
C57	7.5460565405	-0.9542585506	16.9488317989
C58	8.7461959915	-1.5144204496	16.5326971091
C59	9.1775076851	-1.3516232925	15.2183777598
C60	8.4013156221	-0.6263446425	14.3241623133
C61	7.2019311361	-0.0621582784	14.7477856143
C62	5.5753330018	1.6988175023	17.8800765486
C63	6.9098394365	2.1856529186	17.9139324183
C64	7.3075141670	3.1333424763	18.8136265595
C65	6.3992304903	3.6448134490	19.7649514118
C66	6.8091522786	4.5954013094	20.7285920630
C67	5.9319868943	5.0673461224	21.6701952807
C68	4.5989701973	4.6082199045	21.6702531704
C69	4.1716325551	3.7004766730	20.7345756632
C70	5.0553369601	3.1778254798	19.7530501875
C71	4.6384256094	2.2141702681	18.7765455255
C72	3.2003832152	1.7891771401	18.7765052341

C73	2.7287910792	0.9550643765	19.8446031627
C74	3.5629118661	0.5518208876	20.9207190355
C75	3.0841426686	-0.2279965580	21.9434150981
C76	1.7467997903	-0.6736054677	21.9428115955
C77	0.9148030065	-0.3124922815	20.9152026023
C78	1.3763157773	0.5096567630	19.8606206461
C79	0.5122072934	0.9268246368	18.8261554287
C80	0.9584610526	1.7614341137	17.8408777654
C81	2.3047237340	2.2157254515	17.7973377708
C82	3.6944218382	4.6319430730	16.9675655363
C83	4.7896522462	5.1096920813	16.2471188545
C84	5.4883309095	6.2383265023	16.6653817778
C85	5.0943944243	6.9110664192	17.8170092624
C86	4.0063948776	6.4411269933	18.5495353043
C87	3.3161485827	5.3095622738	18.1318004208
C88	1.2208101297	3.9154185099	15.7408817258
C89	0.7578053694	3.5536819253	14.4754020264
C90	-0.4243165352	4.0800856697	13.9649492657
C91	-1.1660775578	4.9765599958	14.7228080924
C92	-0.7160802061	5.3492012872	15.9872193025
C93	0.4651111153	4.8220850292	16.4921728108
H94	2.9666210055	4.6339992365	13.6763946772
H95	1.7936109223	6.5575957073	12.6645379299
H96	4.2583047496	6.1950551909	9.1558293556
H97	5.4058261820	4.2582173370	10.1611684333
H98	6.6982633774	2.7361083049	15.2053566251
H99	8.8847326258	3.6550927700	15.9366185061
H100	9.2154111195	5.7631878414	12.2019532269
H101	7.0512840023	4.8411084846	11.4825516515
H102	7.6211188040	1.7310238279	12.1383751986
H103	8.3432841998	0.0431293031	10.5154540223
H104	7.8755788830	-1.3970647168	8.6241492098
H105	6.3091619082	-2.2604489764	6.9056188466
H106	3.9389897025	-1.4792565298	6.8980419562
H107	3.1472220241	0.1089468675	8.5799805324
H108	4.5665547035	2.5973076384	8.4076665858
H109	3.6891436906	3.9682017707	6.5828341689
H110	1.3092591198	4.7175058092	6.5893411705
H111	-0.1813071117	4.0424391040	8.4526232226
H112	-0.5629448529	2.8019628438	10.5073541279
H113	0.2511521024	1.3163490889	12.2779424429
H114	5.0336572719	-1.2767972866	13.9978143232
H115	6.2229210518	-3.2880803147	13.1984975870
H116	3.6485498337	-3.4177638926	9.7517483229
H117	2.4909320652	-1.3925986762	10.5374779189
H118	1.3177891618	0.6804426533	15.4235892155
H119	-0.8158558622	-0.2056352383	16.3278370768
H120	-1.2508102529	-2.6651199906	12.8267707317
H121	0.8674476331	-1.7852716180	11.9406685446
H122	5.4732085699	-0.7822806511	19.1805564455
H123	4.3509950106	-2.7267086242	20.1899799380
H124	1.7921241044	-3.0437238008	16.7399026046
H125	2.9489054244	-1.1143071160	15.7177123657
H126	7.2241604661	-1.0968928373	17.9788663713
H127	9.3497017734	-2.0842873634	17.2384122804
H128	8.7171397379	-0.5026379903	13.2887367188
H129	6.5808648336	0.4989483729	14.0451683069
H130	7.6387685335	1.7820839018	17.2112544014
H131	8.3381270523	3.4922895174	18.8238177340
H132	7.8453633993	4.9356906093	20.7095744733
H133	6.2594157780	5.7920943943	22.4141197815
H134	3.8985898929	4.9826056182	22.4160802211
H135	3.1356229147	3.3670065335	20.7457272019
H136	4.6010570169	0.8784259934	20.9362546089
H137	3.7464583223	-0.5100571162	22.7612956414
H138	1.3794546698	-1.2985511008	22.7560294177
H139	-0.1245464202	-0.6425859798	20.8953086052
H140	-0.5264275279	0.5935706598	18.8430824074
H141	0.2613954871	2.0955716439	17.0725310885
H142	5.1022479194	4.5796828616	15.3472759942
H143	6.3448980903	6.5829103291	16.0855327888
H144	3.7058547407	6.9455849582	19.4679247266
H145	2.4956344831	4.9297994789	18.7422104584
H146	1.3570441839	2.8636981651	13.8765710981
H147	-0.7539872494	3.7917372689	12.9666258584
H148	-1.2923292729	6.0540107912	16.5857930285
H149	0.8037307176	5.1303810891	17.4803382344
H150	2.4435445236	7.3548581617	10.3932672415
H151	10.1555568928	5.1744494439	14.4246036010

H152 5.5280877300 -4.3808649517 11.0665229179  
H153 -2.1140596248 -1.8846191310 15.0207619528  
H154 2.5003287834 -3.8684823321 18.9870447152  
H155 10.1177361665 -1.7959385272 14.8950049237  
H156 5.6391633848 7.7927424321 18.1529968133  
H157 -2.0913432436 5.3953196238 14.3280106169

M06-L

E= -4883.793883 H

Pd1 3.9786829395 1.7146732614 14.6675489177  
P2 5.1105250585 2.8787573036 12.8821118012  
P3 2.8335774452 0.3150601881 13.0694268411  
P4 5.1172548244 0.5744829037 16.4567237543  
P5 2.8273499966 3.1215605913 16.2623308827  
C6 4.2750987254 4.2866075753 12.0582730269  
C7 3.2864346651 4.9635035175 12.7784330868  
C8 2.6304119587 6.0628678941 12.2338470166  
C9 2.9605819514 6.5038856379 10.9554319618  
C10 3.9461287363 5.8398817032 10.2270569088  
C11 4.5969124428 4.7391095282 10.7729960170  
C12 6.7315343559 3.6547327562 13.3063693551  
C13 7.2731346331 3.3869799049 14.5662540930  
C14 8.4957860783 3.9278645915 14.9535739295  
C15 9.1937315110 4.7572960758 14.0827260412  
C16 8.6604725184 5.0447944168 12.8275994983  
C17 7.4403522017 4.5003705716 12.4436500294  
C18 5.5729150376 1.7703001892 11.4854435519  
C19 6.9147432993 1.3027850956 11.4372960090  
C20 7.3266889267 0.3832734502 10.5108372719  
C21 6.4290691186 -0.1175629586 9.5432574248  
C22 6.8500114362 -1.0381322127 8.5566735886  
C23 5.9772995920 -1.5032721679 7.6029995494  
C24 4.6391134455 -1.0633946728 7.6138894079  
C25 4.1986357948 -0.1798289400 8.5709737779  
C26 5.0731655506 0.3320599875 9.5661962970  
C27 4.6421232064 1.2642159800 10.5686257705  
C28 3.2040765783 1.6735525872 10.5758860359  
C29 2.7236475948 2.4901096126 9.4978793303  
C30 3.5588966390 2.9070603310 8.4276170376  
C31 3.0746563368 3.6780421446 7.3972221426  
C32 1.7301085008 4.0976529742 7.3852234475  
C33 0.8940660347 3.7232852562 8.4093799564  
C34 1.3591206238 2.9164931254 9.4730533099  
C35 0.5012341272 2.5007702355 10.5134124438  
C36 0.9600439030 1.6889532082 11.5152792823  
C37 2.3117252257 1.2491586803 11.5692574197  
C38 3.6759416384 -1.1776863667 12.4087023711  
C39 4.6922723120 -1.7465888048 13.1816149543  
C40 5.3516407991 -2.8995197830 12.7642207655  
C41 5.0019973189 -3.5044643105 11.5597290232  
C42 3.9912518553 -2.9470094208 10.7785288913  
C43 3.3348789931 -1.7944586632 11.1984691147  
C44 1.2336586942 -0.4027272323 13.6398937144  
C45 0.7217710579 0.0495716137 14.8592341306  
C46 -0.4907709571 -0.4256910275 15.3499133535  
C47 -1.2112736418 -1.3663672139 14.6218266858  
C48 -0.7069247384 -1.8362798348 13.4100811090  
C49 0.5039121473 -1.3585061274 12.9224433132  
C50 4.2985530351 -0.8349824379 17.3039890208  
C51 4.6712950894 -1.3022589599 18.5710871212  
C52 4.0401739071 -2.4063111751 19.1345243176  
C53 3.0219349257 -3.0616364920 18.4438215840  
C54 2.6375773498 -2.6017305464 17.1863759907  
C55 3.2737438005 -1.4982387242 16.6243498592  
C56 6.7435275984 -0.1793672102 16.0114071337  
C57 7.5290445658 -0.9298198343 16.8963985977  
C58 8.7415163927 -1.4711645924 16.4850739398  
C59 9.1904616583 -1.2767771155 15.1790474858  
C60 8.4175705941 -0.5411469211 14.2874138151  
C61 7.2052262170 0.0012469132 14.7043880466  
C62 5.5735653566 1.6962696913 17.8440700594  
C63 6.9097231809 2.1793854837 17.8832577837  
C64 7.3159984034 3.1089643593 18.8015108057  
C65 6.4165678542 3.6097582940 19.7667337940  
C66 6.8315843930 4.5447433353 20.7422364959  
C67 5.9570678677 5.0115343719 21.6934531944  
C68 4.6222043138 4.5615513612 21.6882301786  
C69 4.1868294449 3.6652966551 20.7402458025  
C70 5.0646981186 3.1480805301 19.7506307453

C71 4.6401897805 2.2034742949 18.7572248035  
C72 3.2051751552 1.7844981161 18.7583632594  
C73 2.7327014220 0.9775810448 19.8453451299  
C74 3.5772569386 0.5676339205 20.9102020536  
C75 3.1003393964 -0.1925087646 21.9520350975  
C76 1.7535641107 -0.6042923237 21.9823496702  
C77 0.9083827257 -0.2356653727 20.9634035586  
C78 1.3658578860 0.5601468556 19.8881748950  
C79 0.4982551250 0.9761443795 18.8555627831  
C80 0.9513782514 1.7777055821 17.8425987670  
C81 2.3055869600 2.2053100332 17.7709079347  
C82 3.6902749910 4.6013541400 16.9162534112  
C83 4.7530919448 5.1140966325 16.1672166446  
C84 5.4332504630 6.2562036831 16.5780147618  
C85 5.0553266954 6.9035229220 17.5505852908  
C86 4.0030155775 6.3980073324 18.5126633058  
C87 3.3293247494 5.2535247139 18.1019208343  
C88 1.2363116034 3.8588686506 15.6884037720  
C89 0.7412346195 3.4321849490 14.4530624444  
C90 -0.4608376224 3.9228598786 13.9517678374  
C91 -1.1890303253 4.8529058687 14.6857005551  
C92 -0.7031765414 5.2969795372 15.9145264322  
C93 0.4964092959 4.8021379414 16.4132021437  
H94 3.0266371564 4.6099562114 13.7771703083  
H95 1.8544843439 6.5658588310 12.8117568989  
H96 4.1947668218 6.1663524314 9.2173270214  
H97 5.3421956056 4.2029164541 10.1819583590  
H98 6.7023539475 2.7580177499 15.2523490235  
H99 8.8939580837 3.7088055220 15.9440589422  
H100 9.1986999362 5.6993642132 12.1434336173  
H101 7.0341447998 4.7398884366 11.4617612542  
H102 7.6352798128 1.6925424557 12.1551818897  
H103 8.3630353681 0.0427561975 10.4938832007  
H104 7.8900595177 -1.3658006560 8.5669997474  
H105 6.3151955336 -2.2065812355 6.8433547237  
H106 3.9427031626 -1.4314574494 6.8614021576  
H107 3.1572250351 0.1341570300 8.5683375997  
H108 4.6037311986 2.6037877946 8.4233024988  
H109 3.7409772238 3.9741890239 6.5878601126  
H110 1.3574972467 4.7129601413 6.5676678666  
H111 -0.1499593465 4.0376287767 8.4187040572  
H112 -0.5423838008 2.8180633597 10.4938946198  
H113 0.2680568848 1.3646010630 12.2909878522  
H114 4.9701237460 -1.2671367554 14.1212202133  
H115 6.1462606504 -3.3158329222 13.3826489751  
H116 3.7257126099 -3.3992529644 9.8232145441  
H117 2.5704952401 -1.3463777769 10.5616659424  
H118 1.3091542669 0.7706675305 15.4331124715  
H119 -0.8631587164 -0.0641779707 16.3082926938  
H120 -1.2627651631 -2.5792788881 12.8395808677  
H121 0.8883282573 -1.7395018424 11.9769601586  
H122 5.4347618866 -0.7699123248 19.1406272539  
H123 4.3307974793 -2.7426199534 20.1300975887  
H124 1.8341965006 -3.0934070088 16.6378417632  
H125 2.9683940248 -1.1296136060 15.6439068010  
H126 7.1924830694 -1.0913452998 17.9194427936  
H127 9.3407969387 -2.0491263167 17.1875267100  
H128 8.7481814291 -0.3939685928 13.2595051150  
H129 6.5817815739 0.5648678254 14.0056832135  
H130 7.6319270192 1.7912452494 17.1669206848  
H131 8.3477897769 3.4614506734 18.8108676629  
H132 7.8686053819 4.8813950693 20.7257925986  
H133 6.2904199846 5.7254497247 22.4451994066  
H134 3.9238398658 4.9329979908 22.4371383887  
H135 3.1473974149 3.3452426931 20.7464318510  
H136 4.6238347475 0.8650393407 20.8987901800  
H137 3.7734418156 -0.4842685806 22.7573381682  
H138 1.3868665946 -1.2107438511 22.8091847648  
H139 -0.1375494102 -0.5436779825 20.9688455657  
H140 -0.5478019568 0.6678204753 18.8987222515  
H141 0.2528596723 2.1039097248 17.0735622617  
H142 5.0497694161 4.5974462199 15.2537289487  
H143 6.2638414123 6.6313091752 15.9797417086  
H144 3.7208281148 6.8834801136 19.4463248245  
H145 2.5387820753 4.8382580958 18.7288185646  
H146 1.3359958396 2.7216835297 13.8734096810  
H147 -0.8179341980 3.5831421190 12.9798755156  
H148 -1.2652114009 6.0311830779 16.4905268935  
H149 0.8647434256 5.1639141221 17.3718042792

H150	2.4447170957	7.3585986459	10.5198533945
H151	10.1495180194	5.1864850518	14.3808847431
H152	5.5207698572	-4.4009790500	11.2233015483
H153	-2.1602044971	-1.7437916696	15.0006924391
H154	2.5230690746	-3.9196063090	18.8925179227
H155	10.1398374086	-1.7047436074	14.8591748160
H156	5.5873885272	7.7947691020	18.0810648684
H157	-2.1291923742	5.2433161745	14.2980252297