

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

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### **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 TPPDB<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 calculated 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  $[PdCl_3L]^-$  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)  $P(o\text{-tolyl})_3$  – 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, $[PdCl_3L]^-$	Rel. E <sub>vdW</sub> , $[PdCl_3L]^-$	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)  $P(OPh)_3$  – 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, $[PdCl_3L]^-$	Rel. E <sub>vdW</sub> , $[PdCl_3L]^-$	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)  $PCy_3$  – 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, $[PdCl_3L]^-$	Rel. E <sub>vdW</sub> , $[PdCl_3L]^-$	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 (55.04) <sup>a</sup>	55.71
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	<b>BP86/BS1</b>	<b>BP86/BS2</b>	<b>Solv</b>	<b>Disp</b>
PM <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	<b>B3LYP</b>	<b>BP86</b>	<b>M06</b>	<b>M06-L</b>
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  $[PdCl_3L]$  and  $[Pt(PH_3)_3L]$  calculated with BP86 and BP86-D,  $He_8$ \_steric and  $\Delta_{vdW}$ . 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>	$\Delta_{vdW}(Pd)$ , kcal mol <sup>-1</sup>	$\Delta_{vdW}(Pt)$ , 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
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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
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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
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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
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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
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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
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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
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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
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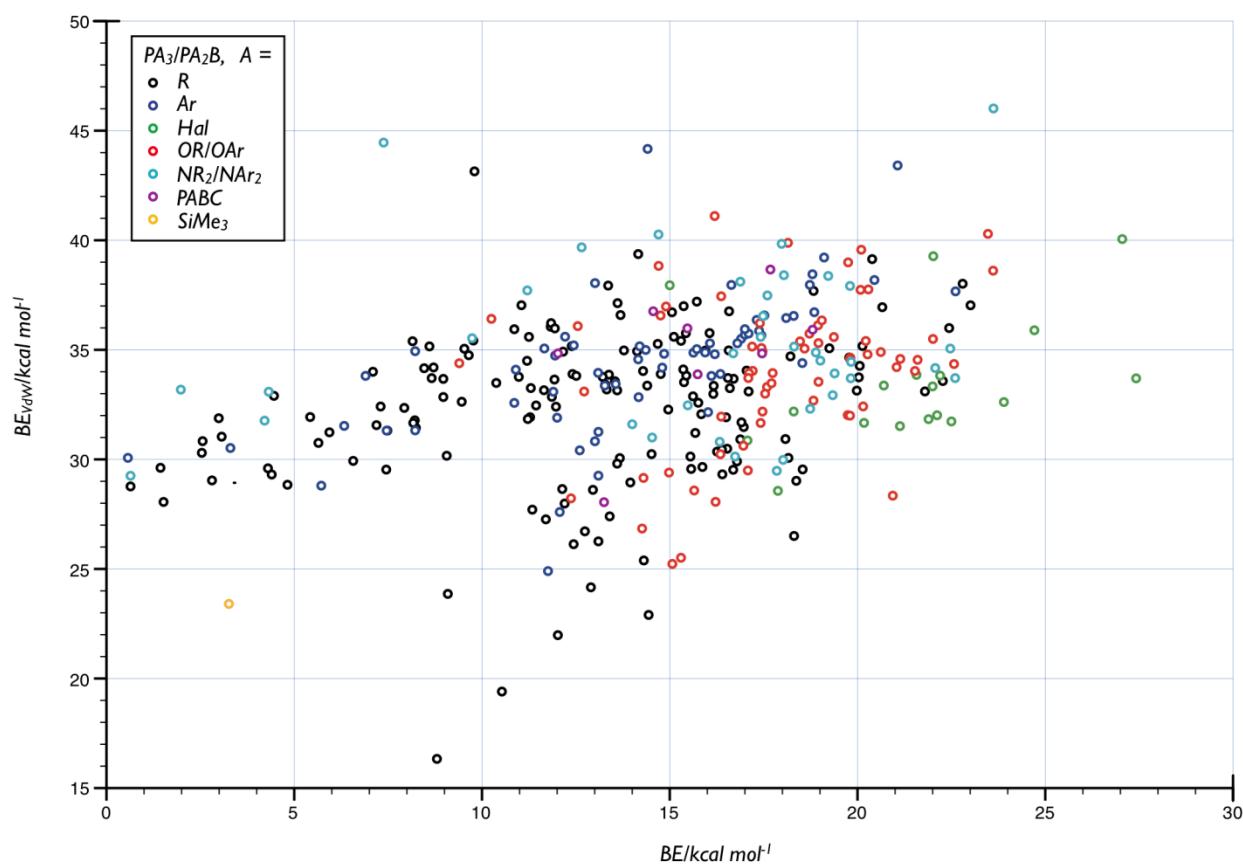
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138	37.0	16.4	3.0	46.5	30.4	9.5	14.1
139	42.9	13.6	7.2	54.4	29.8	11.5	16.2
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141	35.5	14.2	16.6	53.2	39.4	17.7	25.2
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144	39.3	13.5	12.0	54.4	33.6	15.1	20.0
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148	38.5	12.2	5.9				
149	39.9	13.4	3.4	49.2	27.4	9.3	14.0
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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
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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
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185	30.7	5.4	25.3	50.7	31.9	19.9	26.5
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187	30.0	5.9	29.0	50.6	31.2	20.6	25.3
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189	37.0	22.5	1.5	41.5	31.7	4.5	9.2
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193	43.2	23.9	1.6	47.2	32.6	4.0	8.7
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195	36.2	21.1	1.7	42.0	31.5	5.9	10.4
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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
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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
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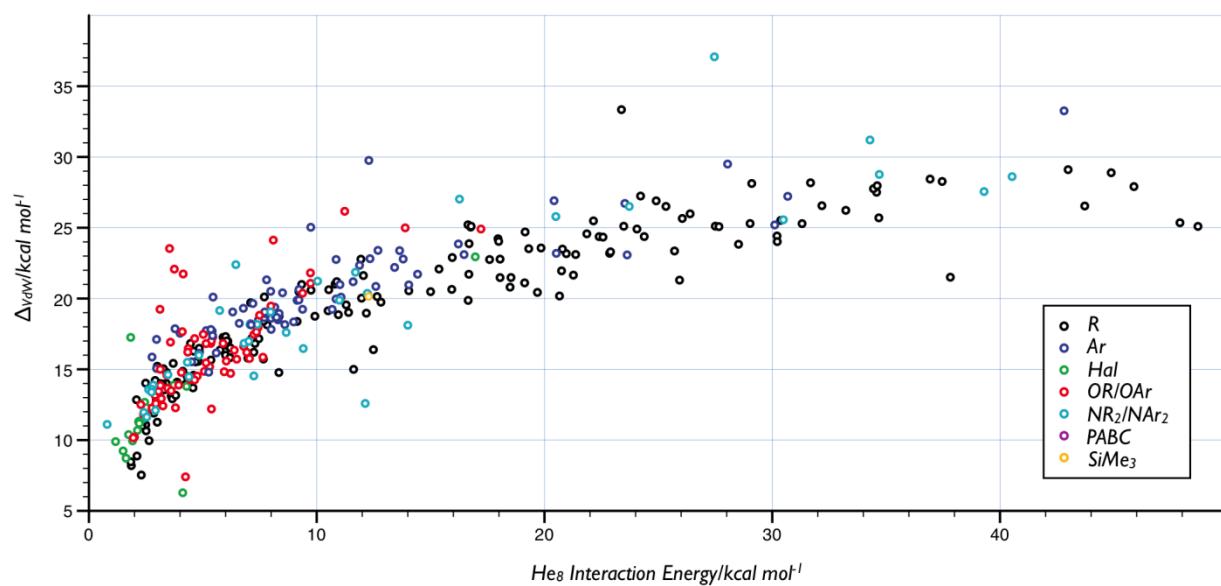
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229	31.8	19.8	5.9	43.0	34.6	11.2	14.8
230	37.1	20.3	5.0	49.0	37.8	12.0	17.5
231	41.4	22.0	1.8	55.1	39.3	13.7	17.3
232	33.9	16.4	9.7	48.4	37.4	14.5	21.1
233	31.2	17.2	5.4	43.4	34.0	12.1	16.8
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236	35.8	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
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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
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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
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260	35.0	19.1	5.5	49.0	39.2	14.1	20.1
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263	31.9	19.7	3.8	39.4	32.0	7.5	12.3
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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
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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
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276	12.6	9.4	13.9	29.0	34.4	16.4	25.0
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278	36.8	21.1	3.1	44.8	34.6	8.0	13.4
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281	37.6	18.8	3.1	47.7	32.7	10.1	13.9
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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
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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

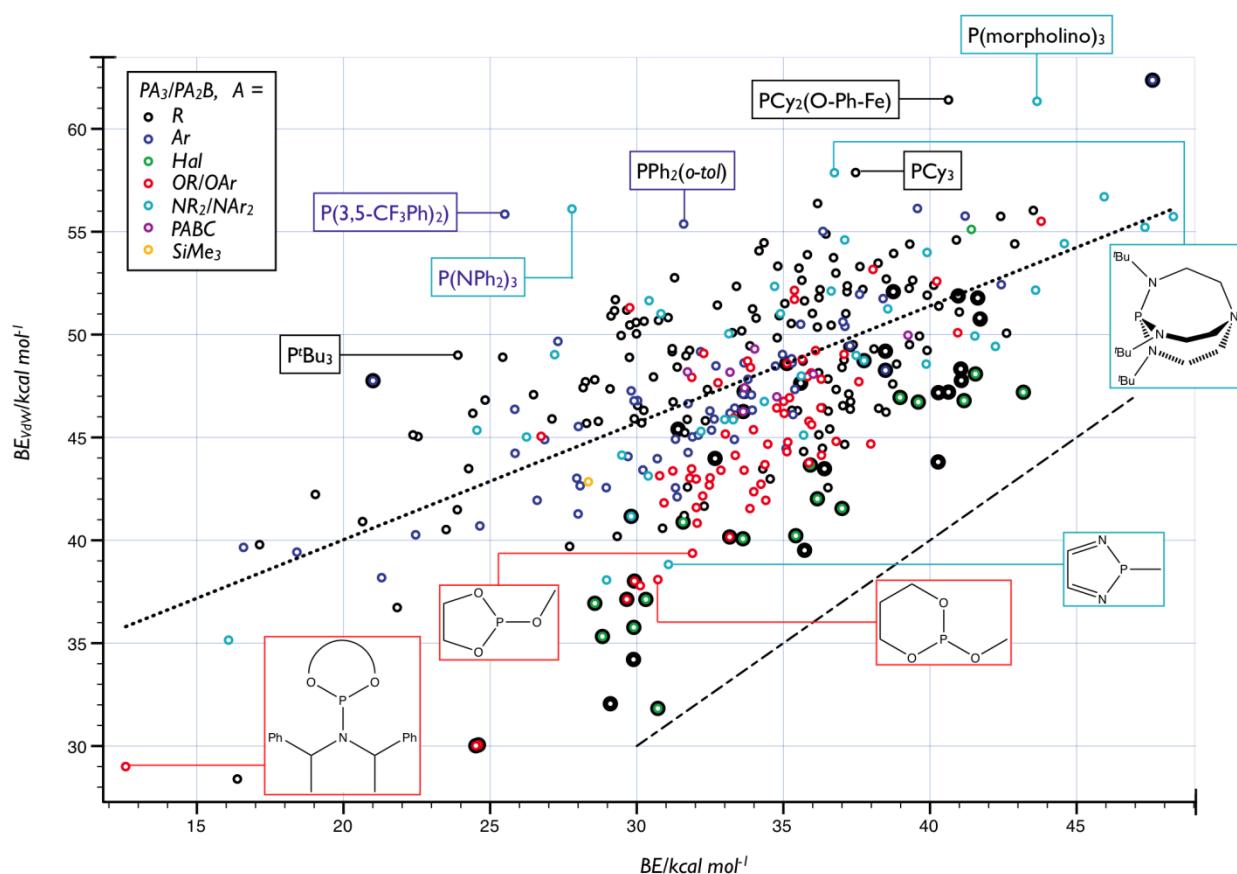
317	26.5	8.5	34.7	47.1	34.2	20.6	25.7
318	34.1	15.1	21.3	50.8	36.7	16.7	21.7
319	34.4	19.8	4.1	43.7	34.6	9.3	14.8
320	32.6	17.4	7.1	45.4	35.7	12.8	18.2
321	33.3	18.5	3.6	45.9	35.4	12.6	16.9
322	37.6	18.7	10.7	52.0	38.0	14.4	19.2
323	30.9	12.4	7.6	41.8	28.2	10.9	15.9
324	29.7	4.5	36.9	51.2	32.9	21.5	28.4
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



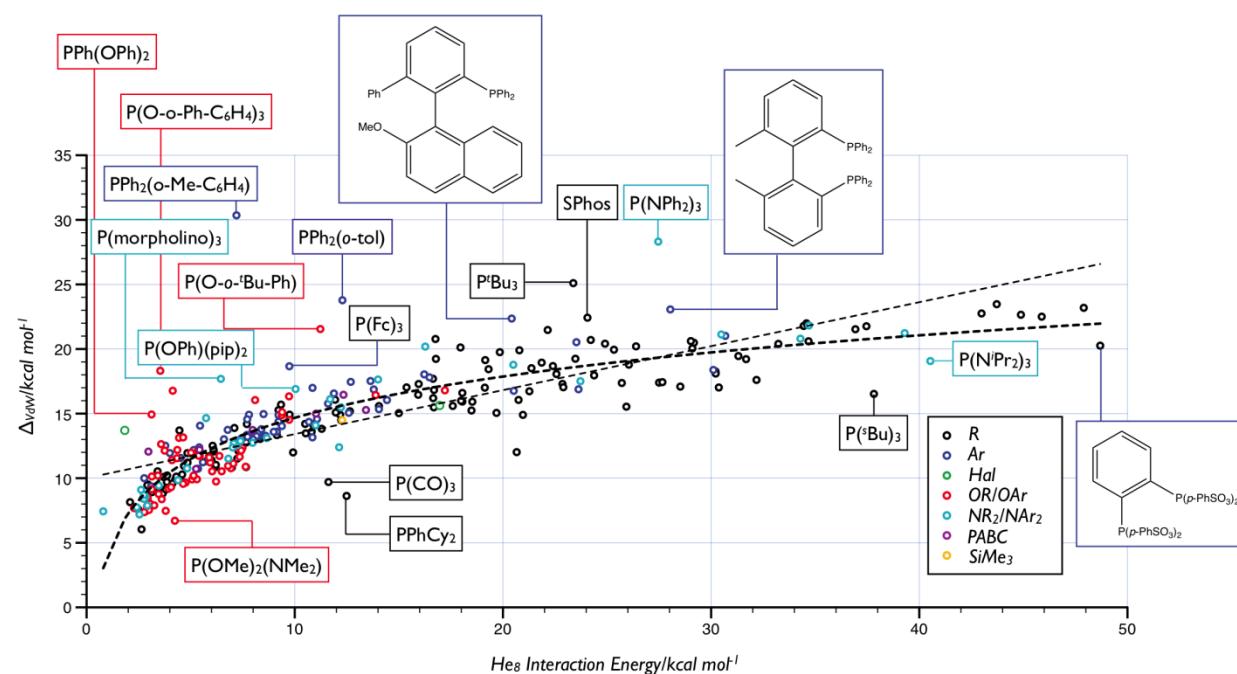
**Fig. S1** Ligand bond energy (kcal mol<sup>-1</sup>) in [Pt(PH<sub>3</sub>)<sub>3</sub>L] calculated at BP86 (BE) and BP86-D (BE<sub>vdW</sub>) level for ligands in LKB-P.



**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 ( $\text{kcal mol}^{-1}$ ). – Outliers identified.

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## Cartesian coordinates of optimised geometries

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

PM <sub>3</sub>								
Ligand								
P1	0.1138764586	-0.1959730931	-0.0811022335	H14	2.2053851031	0.8277620925	1.9613894159	
C2	-0.0345916500	0.0582863268	1.7708965418	C15	0.8200950851	1.5199748226	-2.2495340710	
C3	-1.6820436109	0.0600488884	-0.5567288890	H16	1.2091355754	2.5034696693	-2.5712484536	
C4	0.7875309797	1.4888019454	-0.5557434390	H17	1.4944704993	0.7410063014	-2.6477411860	
H5	0.9732350681	0.0903689447	2.2211997240	H18	-0.1658916125	1.3835924328	-2.7294679473	
H6	-0.5704223287	0.9898290406	2.0336002202	C19	-2.5130015200	-1.3138430548	-0.0260515976	
H7	-0.5711215421	-0.7969960409	2.2184180185	H20	-3.5814061189	-1.1958870572	-0.2843733960	
H8	-2.2831452385	-0.7939622988	-0.1976649195	H21	-2.1391431637	-2.2213834037	-0.5327653024	
H9	-2.1060659441	0.9927695626	-0.1393411230	H22	-2.4559644451	-1.4932304442	1.0628344302	
H10	-1.7726877240	0.0910913990	-1.6568161692	Complex				
H11	0.8038855495	1.5836503537	-1.6558271582	Ru1	-0.1324078426	0.2503644455	-0.6191047635	
H12	0.1917649768	2.3214300252	-0.1365514918	C12	0.3889653850	-1.6208503267	-2.0949051734	
H13	1.8282386747	1.5832022120	-0.1985453612	C13	-2.4836668015	-0.2673148536	-0.9901190300	
Complex				P4	-0.2329070813	-1.3934342071	1.0810005971	
Ru1	3.5950632547	.0856682323	2.3663839138	C5	1.6323684963	1.3093841171	-1.5849954708	
C12	5.5715850132	1.4958286158	2.6302246486	C6	0.4187113574	1.8976584892	-2.0985409916	
C13	2.1568620979	2.0116584585	2.7920089766	C7	-0.5790209686	2.3733272905	-1.2078787881	
P4	3.6555386110	.0046575603	4.7112739771	C8	-0.4136679518	2.3418076689	0.2235896847	
C5	4.7797359068	-1.1792296789	.9091668294	C9	0.7910663313	1.7297509373	0.7116720123	
C6	3.9344589227	-2.2785329109	1.468973564	C10	1.8259873785	1.2601561657	-0.1708546782	
C7	2.5467893765	-2.015126564	.3945556679	C11	-1.0578117096	-0.8481286840	2.6720953799	
C8	1.9077084909	-1.0296769776	1.3961330892	C12	1.4520910036	-1.8748513860	1.7440721469	
C9	2.7432894502	-1.9332492305	2.1243959032	C13	-1.0641008470	-2.9979137552	0.6434613858	
C10	4.1596570130	-2.0277862224	1.8721107570	C14	-1.4094410278	2.9697432787	1.1920746832	
C11	6.2722465080	-1.2038766227	.6180694303	C15	2.6749425385	0.7681460146	-2.5293576638	
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C16	6.5189423679	-1.9896869474	-.6931143753	C20	2.3707312900	-2.6013144097	0.7488956977	
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H32	5.0582282832	1.9013399469	5.2923851048	H35	-0.8201642136	5.0463917968	0.7732358090	
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C34	2.0484925806	-.5071032650	5.4785148921	H37	-1.5669318219	4.8087556225	2.3790964185	
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C38	4.8743710010	-1.2050515356	5.4126244106	H41	-0.0545503666	-4.3868857028	2.0294745591	
H39	4.8579076981	-1.1919468641	6.5171001733	H42	-1.6002240354	-4.9749957583	1.3747275826	
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H41	5.8810894973	-.9264789613	5.0601536261	H44	-2.8663831104	0.0139096421	1.7784793160	
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Ligand				H46	-3.0925182922	-1.6293630571	2.4089680951	
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C3	-1.7034980309	-.0729679003	-0.4407895821	H49	3.3681662837	-2.7620150942	1.1978539756	
PiPr <sub>3</sub>				PiPr <sub>3</sub>				
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P1	2.9468185395	-1.8715046102	1.6769799020	C2	1.0399930941	-1.8814302496	1.8641015299	
C3	.2109344578	-2.4647310316	.7045224932	C4	.5561300710	-4.597317322	2.2207918595	
C4	3.4231669124	-3.6165066919	2.2811232750	C5	2.7247867414	-4.8184115467	1.6220616456	
C6	2.7247867414	-4.8184115467	1.6220616456	C7	3.2882324401	-3.6706534411	3.8172566521	
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C10	2.9266062272	-.6174910761	-.8361932884	C10				

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H12	-.8638235084	-2.4685161313	.9717497136					
H13	.4972177429	-3.5001800587	.4565698229	PCy <sub>3</sub>				
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H15	.7158012759	.2422731850	1.3814124781	P1	-1.0826915114	.5407459785	1.2275626072	
H16	1.0954237817	-.0565602131	3.0954002035	C2	-1.2188217523	.5686252832	-.6789563018	
H17	-.5270381563	-.4611276695	2.4507973126	C3	-2.7071374170	.6920547393	-1.0945634649	
H18	4.5054289239	-3.6718316527	2.0478884611	C4	-.5325237091	-.5632219156	-1.4778949147	
H19	3.1704358597	-5.7682171502	1.9771842500	C5	.5804672628	1.4115459482	1.5247255516	
H20	2.8097288760	-4.8025287411	.5206959644	C6	.4111506227	2.9378198451	1.3252859714	
H21	1.6507248091	-4.8478458118	1.8806824330	C7	1.8180665636	.9022334013	.7549677570	
H22	2.2298948394	-3.6052984760	4.1336271524	C8	-.6845537108	-1.2704501817	1.6312288261	
H23	3.8362985738	-2.8441645251	4.3029878369	C9	-.1257308273	-1.4049623021	3.0682116621	
H24	3.685433059	-4.6262557432	4.2093481209	C10	-1.9759816528	-2.1151051355	1.4908971538	
H25	2.5493546045	-2.7442891006	-.6417767470	C11	-2.8617587062	.8974607611	-2.6152209143	
H26	4.8858407512	-2.3412404030	-1.5795805382	C12	-2.1577840271	-.2168185346	-3.4124620430	
H27	4.9073348537	-3.4295942062	-1.688539971	C13	-.6795276432	-.3459764240	-2.9999276406	
H28	5.3986208119	-1.7206609142	.0133531194	C14	.1007990503	-2.8806356207	3.4602258555	
H29	3.5839887783	.1637965903	-.4120864340	C15	-1.1801873609	-3.7193238126	3.2974590293	
H30	1.8820672586	-.2970560749	-.6759419948	C16	-1.7450612885	-3.5919261754	1.8708215697	
H31	3.1019334202	-.6521766759	-1.9286597353	C17	3.0950898346	1.6647651323	1.1708222261	
Complex				C18	2.9270932109	3.1843108991	.9810401532	
Ru1	0.4672308174	1.1866346408	-0.1818950494	C19	1.6862008095	3.7071447980	1.7298491373	
C12	-1.2005150561	2.6177533181	0.8795072164	C20	-.7238785739	1.5235373510	-.9612404964	
C13	-.8414158160	1.4078865822	-2.2250052200	C21	-3.1842244234	1.5223138852	-.5412881291	
P4	-.9679422092	-.6473995911	0.4861690063	C22	-3.2476164899	-.2291566053	-.7932699543	
C5	2.3911739191	0.4126972933	-1.1355914463	C23	.5367618996	-.6418331629	-1.2113747547	
C6	2.3223542784	0.0884390839	0.2612177312	C24	-.9940628509	-1.5355461772	-1.2130399932	
C7	2.1908023076	1.0957925948	1.2773873043	C25	.7622797178	1.2512070835	2.6090231595	
C8	2.0091657148	2.4639288552	0.9072670177	C26	.1884994893	3.1480794996	.2581415573	
C9	2.0210284650	2.8076756668	-.4897544293	C27	-.4591378182	3.3002661229	1.9044086460	
C10	2.186621177	1.7937310915	-.14753405273	C28	1.6548581200	1.0474582555	-.3320501969	
C11	2.7141869772	-.6649505115	-2.1624675297	C29	1.9570348232	-.1843512429	9.124393484	
C12	4.2294460736	-.9831550160	-2.1113264388	C30	.0738638234	-1.6678441165	.9256668923	
C13	1.8097971968	3.5224529744	1.9593679816	C31	-.8397580243	-.9396476190	3.7794205880	
C14	2.2784982097	-.3115424436	-3.5959825520	C32	.8256644725	-.8504609596	3.1694020036	
C15	-2.8376823887	-.3002379436	0.3476767925	C33	-2.7557615714	-.16830368229	2.1511145096	
C16	-.05780999529	-2.2815117141	-.4012307655	C34	-2.3729303000	-2.0503528443	.4601762995	
C17	-.07617109805	-1.1531947768	2.3132409634	C35	-.24210565481	1.8774811528	-2.8929853136	
C18	-.37217372035	-.9933081301	1.4057675148	C36	-.3.9340550720	.9479380956	-2.8852405833	
C19	0.5378520752	-.19171096222	2.6345354657	C37	-2.6724644360	-.1.1812646804	-3.2219230520	
C20	-.6316293895	-2.1890824989	-.1.9396949307	C38	-2.2396852444	-.0257611045	-4.4994301285	
C21	-3.4121975292	-.5684036127	-1.0585355549	C39	-.1371556107	.5783100366	-3.2881430232	
C22	-.09174269693	0.0455052619	3.2680013891	C40	-.1963736125	-1.1776164995	-3.5482747058	
C23	-.13851166376	-3.4991631252	0.0943700292	C41	.8986276512	-3.3062448280	2.8171748141	
H24	2.4095321456	-.9626671158	0.5581945072	C42	.4722394645	-.2.9394915903	4.5013356552	
H25	2.1637644105	0.8165452685	2.3343725856	C43	-.1.9419349437	-3.3652409706	4.0221547234	
H26	1.7907671963	3.8312597799	-.7962890851	C44	-.9801872623	-.4.779561738	3.5422902505	
H27	2.0704663424	2.0681753709	-.2.5269872769	C45	-.1.0327462678	-.4.0473687733	1.1522209003	
H28	2.1707478630	-.1.5797025730	-.1.8532369680	C46	-.2.6915840384	-.4.1580610510	1.7772702585	
H29	4.8241958208	-.0951889136	-.2.3935986265	C47	3.9637518931	1.2967008300	.5915873104	
H30	4.4742994216	-.1.7956866916	-.2.8189938852	C48	3.3138532637	1.4507910698	2.2374158311	
H31	4.5492037083	-.1.2985986508	-.1.1021276919	C49	3.8351101678	3.7183148912	1.3201297756	
H32	1.3045538035	3.1119569772	2.8479116790	C50	2.8179241656	3.4039950945	-.1012281630	
H33	2.7937911637	3.9244645869	2.2696520187	C51	1.5511520546	4.7899129240	1.5439678265	
H34	1.1941190084	4.3500886335	1.5752124162	C52	1.8440918644	3.5923803489	2.8220706035	
H35	2.9019540333	0.5008111527	-.4.0139582632	Complex				
H36	2.4050444430	-.1.1898738537	-.4.2529407142	Ru1	-4.0646333169	-.5.2162258115	.2959271527	
H37	1.2233420301	0.0102097290	-.3.6326842137	C12	-4.0281600802	-.2.7737095350	.2856700261	
H38	-.2.8591014266	0.7910226495	0.5230365909	C13	-6.4897335673	-.5.0756884869	.0271129705	
H39	0.4840656007	-.2.4343357257	-.0.1201854778	P4	-3.9460026498	-.5.2044026557	-2.1289334806	
H40	-.1.6018772151	-.1.8505780316	2.4938911011	C5	-.4.2097268394	-.6.9023982904	-.2.9448882722	
H41	-.3.6901410821	-.2.0951502985	1.3250014155	C6	-.3.0503006922	-.7.9158156019	-.2.7962739876	
H42	-.4.7705467778	-.6.857432672	1.2355194529	C7	-.3.3212639014	-.9.1804343508	-.3.6413038221	
H43	-.3.4671978692	-.0.7146418761	2.4411978003	C8	-.4.6613692128	-.9.8383773796	-.3.2646608309	
H44	1.4270802939	-.1.2740416815	2.5314054039	C9	-.5.8210925157	-.8.8289451153	-.3.3549005990	
H45	0.6861855313	-.2.8133389271	2.0089897265	C10	-.5.2710870196	-.4.1300001956	-.2.9765971933	
H46	0.5065368470	-.2.2547331198	3.6876560478	C11	-.5.7508973324	-.4.6034160526	-.4.3741050920	
H47	-.1.6669308709	-.2.2554546315	-.2.3102256721	C12	-.6.9442850898	-.3.7506456879	-.4.8610758824	
H48	-.0.0670349270	-.3.0343054029	-.2.3773406673	C13	-.6.6126441413	-.2.489597129	-.4.8831022010	
H49	-.0.2121035035	-.1.2420661640	-.2.3130426939	C14	-.6.1015421445	-.1.7855239992	-.3.5079487755	
H50	-.3.5187366496	-.1.6512183704	-.1.2553664679	C15	-.2.2320254820	-.4.7513716057	-.2.8081483632	
H51	-.2.8026810420	-.0.1078139759	-.1.8496123417	C16	-.2.0852657520	-.4.8426528942	-.4.3487275982	
H52	-.4.4256613052	-.0.1280612224	-.1.1098412525	C17	-.6.070484139	-.4.6922591870	-.4.7705402745	
H53	-.0.0933434954	0.7649880195	3.1319726712	C18	-.0087164620	-.3.3867337188	-.4.2352609191	
H54	-.0.9032972456	-.0.3129779007	4.3151369475	C19	-.1715726056	-.3.2734547494	-.2.7094774885	
H55	-.1.8485205695	0.6091556239	3.1014578637	C20	-.4.4892698684	-.6.8295489002	1.8576774442	
H56	-.2.4514303979	-.3.4056911651	-.0.1742818008	C21	-.3.6166465349	-.7.3606224722	.8597135693	
H57	-.1.3202035795	-.3.6528091941	1.1849306191					

C22	-2.4117195396	-6.6559624450	.5059222377	C19	-0.4027887222	-1.3665934988	3.2320569664
C23	-1.9937994543	-5.4688024645	1.1907403762	H20	-1.3869024244	-0.6440397261	5.0304383270
C24	-2.9010710221	-4.9454505186	2.1764592337	H21	-1.4371746324	1.7350592760	4.2507947153
C25	-4.1077565825	-5.6083764475	2.5235750162	H22	-0.4968206735	2.3450129373	2.0230848999
C26	-5.7751233598	-7.5127390087	2.2993515708	H23	0.5960061755	-1.7932386900	1.3543432540
C28	-6.4014140015	-8.4592128254	1.2652812463	H24	-0.3723430598	-2.4087190518	3.5687127282
H29	-7.3361604237	-8.8842582351	1.6715810842	C25	-2.6555163422	-0.1526467961	-3.1519851306
H30	-6.6482392467	-7.9077319916	.3493526463	C26	-2.9538363106	-0.0459192603	-1.7820263470
H31	-5.7368435584	-9.3098720497	1.0216650068	C27	-1.9308200632	0.2072820299	-0.8518300130
C32	-5.4978482915	-8.2492150031	3.6344396659	C28	-0.3014509577	0.2243678738	-2.6598029700
H33	-6.4337058189	-8.6866207173	4.0250859812	C29	-1.3257444176	-0.0137405736	-3.5897873260
H34	-4.7726197582	-9.0707772147	3.4869624725	H30	-3.4547911069	-0.3485655070	-3.8758790065
H35	-5.0887149740	-7.5694342317	4.4025005524	H31	-3.9880037010	-0.1565458625	-1.4337555979
C36	-6.683213897	-4.7834358915	.9062895536	H32	-2.1715050437	0.2913577407	0.2140168814
H37	-8.045348982	-3.6868035771	.9120890868	H33	0.7371731151	0.3128132909	-3.0037694719
H38	.0653071388	-5.0463833407	1.6788944365	H34	-1.0841887668	-0.1015668948	-4.6561316826
H39	-2.735732411	-5.0830422279	-.0729852820				
H40	-4.2835854894	-6.6685469142	-4.0264574707				
H41	-2.0845119931	-7.4736821668	-3.1017519619				
H42	-2.9475670505	-8.2136951572	-1.7354491251				
H43	-3.3386034211	-8.8984404073	-4.7142820083				
H44	-2.4871968809	-9.8977585358	-3.5181830123				
H45	-4.8554021164	-10.7137448495	-3.9131729021				
H46	-4.5958713905	-10.2237824501	-2.2258973888				
H47	-5.9721274412	-8.5398817450	-4.4159004821				
H48	-6.7661812051	-9.2963065812	-3.0195643662				
H49	-6.1125293351	-4.2355464537	-2.2632424993				
H50	-4.9232337291	-4.5228356338	-5.1079078458				
H51	-6.0655042487	-5.6610169716	-4.3617728979				
H52	-7.2562577619	-4.0976286349	-5.8653823041				
H53	-7.8042600129	-3.9254544006	-4.1833216694				
H54	-5.8289959134	-2.0602192077	-5.6467426187				
H55	-7.5007690290	-1.6643383989	-5.1904918458				
H56	-5.8130313500	-.7175668065	-3.5416587912				
H57	-6.9134357712	-1.8718684386	-2.7585819991				
H58	-1.5982796059	-5.5520954618	-2.3669311393				
H59	-2.4820163887	-5.7970457324	-4.7398879255				
H60	-2.6819570446	-4.0358196646	-4.8174865670				
H61	-.0318351635	-5.5572514415	-4.3788630831				
H62	-.5277403390	-4.7366284213	-5.8737438280				
H63	1.0798710044	-3.3283172034	-4.5072986728				
H64	-.4898556155	-2.5244877855	-4.7235884681				
H65	.4243848859	-4.0697616694	-2.2146535476				
H66	.2295924289	-2.3089121903	-2.3447528436				
H67	-3.8915423058	-8.2698724833	.3200572457				
H68	-1.7777716291	-7.0504259595	-.2956113520				
H69	-2.6928373431	-3.9616864226	2.6089305703				
H70	-4.8025178103	-5.1394758018	3.2258267720				
H71	-6.5031430067	-6.7007999981	2.4880727945				
C72	-1.6530004714	-3.4093781037	-2.2997282198				
H73	-2.2230317486	-2.5690611940	-2.7336679982				
H74	-1.7793543906	-3.3241703065	-1.2083422298				
C75	-4.8969895033	-2.6277534052	-3.0399573542				
H76	-4.5468088745	-2.2791767953	-2.0554553433				
H77	-4.0711684585	-2.4852108442	-3.7674416028				
C78	-5.5394425417	-7.5641544069	-2.5180345240				
H79	-5.4743197192	-7.8301049019	-1.4474539101				
H80	-6.3822146983	-6.8550828368	-2.5923444471				
PPh <sub>3</sub>							
Ligand							
P1	0.8459087076	0.6547819123	-0.1431096914	C19	8.1115100014	-1.7563083304	1.633222176
C2	-0.5918775311	0.3495599284	-1.2800875123	H41	6.8566036179	-1.2801938449	2.8121995214
C3	0.9723105574	2.5088294652	-0.1539725552	H42	6.8257088622	-2.9100580432	2.0569435039
C4	0.1016716663	0.3167376921	1.5257981783	H43	8.2626180518	-1.4065502482	5.9965203418
C5	0.1811234712	4.7661720299	-0.6655615360	H44	4.7920264526	2.1306522166	9.1137197072
C6	0.1386314514	-1.0203631041	1.9839361923	H45	-1.3140416274	-.0258653792	5.3447614944
C7	1.3554538017	5.3127723693	-0.1218471877	H46	4.7683294479	4.4660844045	8.1972938605
C8	2.3435157202	4.4603691475	0.4020824277	H47	.8562812350	.5840806059	4.2577130326
C9	2.1579360932	3.0693483407	0.3755356357	H48	-1.3437008751	-1.5808266408	7.3113915046
C10	-0.0126183865	3.3738233557	-0.6788159605	H49	.8113925804	-2.4980714012	8.1995069700
H11	1.5036796840	6.3986232944	-0.1112663056	H50	7.7629056582	-3.8621058460	6.0344310452
H12	3.2651752575	4.8787626708	0.8220340323	H51	5.4324997103	-4.6595671514	5.5678976560
H13	2.9392717356	2.4066186936	0.7678925367	H52	4.3516597682	.3787493347	-.4650269329
H14	-0.9316814559	2.9546241545	-1.1017536620	H53	1.8999130228	.5264711604	-.0581962263
H15	-0.5911981344	5.4253175381	-1.0788452040	H54	2.1962381023	-2.5224969215	3.0240411678
C16	-0.9716860992	-0.3764940893	4.0520083719	H55	4.6742546691	-2.6850155796	2.6257131672
C17	-0.9984705918	0.9579246706	3.6146363936	H56	6.5126302642	-.2174215827	.5745084354
C18	-0.4684534811	1.3033395589	2.3591849069	H57	4.3211375653	.2062604724	7.6217455269
				H58	4.2708909717	4.8423000589	5.7712869160
				H59	3.8038838076	2.9060416827	4.2661937526
				H60	3.6263967652	-3.0267437290	5.0871989149

H61	6.4565412360	.2334898372	5.5034193995		H40	8.1191874427	-1.7527187762	1.6172406270
P(p-F-C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub>				Ligand	H41	6.8689182013	-1.2767114082	2.8005997532
C1	1.0183890000	0.9210570000	0.0143280000		H42	6.8321656356	-2.9050746409	2.0393259455
C2	-0.1276630000	0.3359100000	-1.3249560000		H43	8.2748181391	-1.4352878684	6.0036394939
C3	0.6985070000	2.7507540000	0.0380400000		H44	4.8190202342	2.1655831355	9.1115061474
C4	0.1485580000	0.3480770000	1.5523110000		H45	-1.3247821361	-.0179160014	5.3692159084
C5	-0.4029920000	4.7838540000	0.8557770000		F46	4.8107498217	4.6579151484	8.3274026810
C6	-1.1997350000	-0.0706330000	1.6016630000		H47	.8584739033	.5943059755	4.2666236672
C7	0.3829290000	5.5393650000	-0.0228560000		F48	-1.5435450872	-1.6260604375	7.4201237719
C8	1.3299580000	4.9442940000	-0.8675980000		H49	.7885132803	-2.4954049127	8.2077198450
C9	1.4881190000	3.5513430000	-0.8217060000		F50	7.9213063226	-4.0243302913	6.1092243390
C10	-0.2404920000	3.3885030000	0.8791540000		H51	5.4405715842	-4.6713803509	5.6101869879
F11	0.2285050000	6.8870310000	-0.0538430000		H52	4.3556443308	.3965396777	-.4627173325
H12	1.9317740000	5.5699340000	-1.5337990000		H53	1.9033376360	.5373171808	-.0564769116
H13	2.2387180000	3.0764640000	-1.4650950000		H54	2.2047026487	-2.5265425676	3.0107330635
H14	-0.8530610000	2.7903520000	1.5620600000		H55	4.6835232648	-2.6824094855	2.6118740523
H15	-1.1267990000	5.2872460000	1.5042750000		H56	6.5198930271	-.2056506262	5.688372478
C16	-0.9975780000	-0.5119250000	3.9668830000		H57	4.3496626222	.2162293277	7.6205981445
C17	0.3451950000	-0.1105940000	3.9576640000		H58	4.2521703696	4.8605520599	5.7808598833
C18	0.9117700000	0.3067630000	2.7437430000		H59	3.7825268265	2.9103339843	4.2654003668
C19	-1.7793330000	-0.5051470000	2.8049540000		H60	3.6212261897	-3.0293208169	5.1131452617
F20	-1.5523440000	-0.9259870000	5.1337720000		H61	6.4658576121	.2250700117	5.4951287744
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					
Complex								
Ru1	3.5117536353	.0901767434	2.4163332354					
Cl2	5.5026657485	1.4780033474	2.6575546018					
Cl3	2.0949324509	2.0810594051	2.6045632002					
P4	3.6215076308	-0.0398731831	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	-.1018124146	5.1149778091					
C13	-.3775056543	-.4313556221	5.7278803707					
C14	-.3695276814	-1.2966781272	6.8290435281					
C15	.8197184688	-1.8291462924	7.3403511096					
C16	2.0331016426	-.14855973764	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	-3.5972826458	5.5799526013					
C22	4.6365203623	-2.6638662257	5.301888428					
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					
Complex								
Ru1	3.4795651543	.0883171935	2.3887403651					
Cl2	5.4606381050	1.5031599236	2.5628001170					
Cl3	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	2.7444696350
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	9.772499240	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	.0720990535	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	Complex			
H42	6.8192605255	-2.8754008289	2.0305286241	Ru1	3.5107958207	.0937976652	2.4082538508
H43	8.2792118634	-1.4392240856	5.9507373190	Cl2	5.5235785498	1.4569594930	2.6143133571
H44	4.9002832358	2.2169133617	9.0368373222	Cl3	2.1294667192	2.1035794004	2.6039134500
H45	-1.3228834445	-.1091676647	5.3773518093	P4	3.6324999676	-0.298983041	4.7810931336
H46	.8260825616	.5423029982	4.2511945186	C5	4.0455178525	1.4390641317	5.8308117663
H47	.9105763466	-2.4696393801	8.2463691187	C6	4.2787710428	1.2293490247	7.2097943718
H48	5.3871140544	-4.6509931068	5.6218052968	C7	4.5433637552	2.3093011808	8.0570636446
H49	4.2907756537	.3616181889	-.5035719424	C8	4.5772932255	3.6296669154	7.5588330853
H50	1.8411850898	.4913892677	-.0748310671	C9	4.3358499330	3.8255562993	6.1868334915
H51	2.1954817569	-2.5255444285	3.0339599753	C10	4.0720404983	2.7499669937	5.3222955267
H52	4.6715558642	-2.6676235402	2.6146842859	C11	2.0736799795	-.6302716241	5.5897328681
H53	6.4667508350	-.2020115613	.5233528425	C12	.8523691308	-.0832563245	5.1349166045
H54	4.3968799868	.2561083152	7.5857170794	C13	-.3534293428	-.4324805246	5.7566372256
H55	4.2709431883	4.8598025099	5.6565931574	C14	-.3868176293	-.13318006525	6.8440783752
H56	3.7729770457	2.9132120408	4.2163297497	C15	.8358444309	-.18603061631	7.2987967812
H57	3.6206418390	-3.0133071026	5.1208082107	C16	2.0516948648	-1.5125172065	6.6895837460
H58	6.4866296089	.2231127485	5.4310741887	C17	4.9231992010	-1.2584490542	5.2742776764
O60	-1.5801355424	-1.6330925081	7.4021239107	C18	6.2357503279	-.8152744296	5.5522665386
O61	8.0127721238	-.39656409811	6.1320083089	C19	7.2506641250	-1.7363848149	5.8414300241
O62	4.9195307479	4.6624832534	8.3348030008	C20	7.0007875697	-.3.1247474153	5.8633839640
C63	-1.608452539	-2.4711113772	8.5589283319	C21	5.6948531456	-3.5622509458	5.5690439944
H64	-2.6708249454	-2.5764116599	8.8247843814	C22	4.6718110160	-2.6476602158	5.2741181066
H65	-1.1812870435	-3.4709312876	8.3473166799	C23	4.6835085136	-1.2344348248	.9965750572
H66	-1.0605921665	-2.0135344257	9.4054642439	C24	3.8559538459	-.3316767565	.2143112231
C67	7.7523010363	-5.3679627080	6.2165965713	C25	2.4693869390	-.2358890683	.4478382579
H68	8.7143369785	-.58346127004	6.4755324061	C26	1.8074898294	-1.0363241470	1.4554478275
H69	7.0086120683	-.55961276487	7.0050026544	C27	2.6271490588	-.19219127005	2.2215669755
H70	7.3948689925	-.57746580250	5.2505059655	C28	4.0426659801	-.2.0441955038	1.9779153729
C71	4.9093766818	6.0018079286	7.8365466679	C29	6.1765038561	-.1.2968442988	.7194715938
H72	5.1714838539	6.6398472335	8.6939625022	H30	2.9824101329	-1.9377135710	7.0788796431
H73	5.6562554461	6.1403878800	7.0311480550	H31	7.4827846806	-2.0959921834	-.8446578697
H74	3.9088945929	6.2858545423	7.4569866737	H32	6.0991359964	-.3.1575338485	-.4514580465
P(p-tolyl) <sub>3</sub> Ligand				H33	.0285180388	-.1.3515888929	2.6476370684
P1	0.9668752486	0.7645645958	0.0023438239	H34	-.2363516258	-1.4227078323	.8786112068
C2	-0.3132613460	0.2960683420	-1.2659014747	C35	6.4100087410	-2.1042602061	-.5816337406
C3	0.8445838181	2.6214865358	-0.0000010527	H36	5.8452489040	-.1.6867514860	-1.4341726979
C4	0.1156444310	0.3176417444	1.5870594879	C37	.3243886465	-.9085908338	1.6826803515
C5	-0.2606014295	4.7595595683	0.4373944483	H38	.0308747664	.1558547099	1.6846783462
C6	-0.6895300057	-0.8417187032	1.6794343235	C39	7.0116247480	-1.8588020400	1.8800261401
C7	0.7916941047	5.4685706571	-.0.1852742671	H40	8.0852485446	-1.7887775106	1.6309713023
C8	1.8718590734	4.7301245389	-.0.7042173605	H41	6.8356051238	-1.2851237886	2.8044251673
C9	1.9014727285	3.3283044765	-.0.6097041225	H42	6.7897577727	-2.9254293769	2.0721352435
				H43	8.2608065603	-1.3667331096	6.0594366668

H44	4.7269783956	2.1249473549	9.1236513121	C14	-3.793103360	-1.2968200117	6.8279507046
H45	-1.2902786697	.0095422392	5.3931991051	C15	.8152693146	-1.8329527160	7.3328512984
H46	.8639384818	.6358532403	4.3060761239	C16	2.0323252588	-1.4860172413	6.7249925218
H47	.8408251615	-2.5545114130	8.1487103992	C17	4.9188730817	-1.2743732866	5.2907751824
H48	5.4703049266	-4.6363638367	5.5792766864	C18	6.2405900817	-.8408771345	5.5376658740
H49	4.3421330831	.3652136797	-4.772051292	C19	7.2627058925	-1.7609176786	5.8163405886
H50	1.8940643093	.5454769484	-.0588330498	C20	6.9668133355	-3.1329058061	5.8438113788
H51	2.1679914663	-2.4953056539	3.0347449747	C21	5.6660253047	-3.5945136248	5.5857602744
H52	4.6417100489	-2.6899215611	2.6249239885	C22	4.6537717075	-2.6632526015	5.3058112458
H53	6.4993301965	-.2513466156	.5524345447	C23	4.7196300900	-1.2080893824	.9958556609
H54	4.2569894854	.2163493314	7.6267360350	C24	3.8840864372	-.3056333247	.2264941582
H55	4.3553765121	4.8428302011	5.7770170878	C25	2.4913043862	-.2355471107	.4551308276
H56	3.8855969432	2.9256144289	4.2609031786	C26	1.8382368107	-.10602669176	1.4481624490
H57	3.6653255116	-3.0253765469	5.0611542193	C27	2.6700467667	-1.9415454525	2.2057426192
H58	6.4602839643	.2555643640	5.5360926858	C28	4.0883394499	-2.0378036341	1.9663535097
C60	4.8630901243	4.7911547275	8.4846675329	C29	6.2121349718	-1.2489615013	.7137617565
H61	4.8511939134	5.7516666803	7.9432666010	H30	2.9580396561	-.19022949080	7.1346354774
H62	4.1148743356	4.8507191219	9.2968605363	H31	7.5195477803	-2.0036821567	-.8699304942
H63	5.8526178358	4.6867514045	8.9673856673	H32	6.1467454603	-3.0856170736	-.4960211703
C64	8.1017068454	-4.1069472818	6.1967268700	H33	.0557434606	-1.4348388190	2.6194114176
H65	7.7387578382	-5.1480141953	6.1639111185	H34	-.1932412810	-1.4706681677	.8487109319
H66	8.9463694905	-4.0205533148	5.4888690547	C35	6.4477666165	-2.0272625341	-.6048958347
H67	8.5103787489	-3.9242495710	7.2077342598	H36	5.8774924218	-1.5966117776	-1.4470038039
C68	-1.6962363012	-1.7062373586	7.5021248540	C37	.3516666012	-.9637993108	1.6677499696
H69	-1.5421691184	-2.4087274670	8.3384247934	H38	.0373163785	.0943836795	1.6891114218
H70	-2.2141397556	-.8145861420	7.9007643781	C39	7.0563878166	-1.8282663905	1.8586564733
H71	-2.3872034764	-2.1837298436	6.7829615764	H40	8.1283266930	-1.7443067504	1.6081828840
P(p-Cl-C <sub>6</sub> H <sub>4</sub> ) <sub>3</sub>				H41	6.8795190685	-1.2747731785	2.7951901234
Ligand				H42	6.8450947652	-2.9006579712	2.0287371120
P1	1.0260480000	0.9534050000	-0.0267290000	H43	8.2818745081	-1.4153975181	6.0113361322
C2	-0.1467190000	0.3760270000	-1.3451100000	H44	4.8002166859	2.1712713124	9.1157396442
C3	0.6880010000	2.7789350000	0.0209380000	H45	-1.3083639356	.0103459006	5.3654757006
C4	0.2028650000	0.3630610000	1.5294130000	C146	4.9109770003	4.9962512959	8.5685244071
C5	-0.3990950000	4.7951780000	0.8957940000	H47	.8707681953	.6200168387	4.2861134177
C6	-1.0981950000	-0.1824380000	1.5920820000	C148	-1.9096481517	-1.7323951256	7.5826236555
C7	0.3318510000	5.5729330000	-0.0163080000	H49	.7949862141	-2.5094213290	8.1923673654
C8	1.2443240000	4.9823920000	-0.9068850000	C150	8.2402069177	-4.2926937225	6.2070754189
C9	1.4224920000	3.5917750000	-0.8735720000	H51	5.4474298776	-4.6662232775	5.6098414977
C10	-0.2182570000	3.4022090000	0.9064350000	H52	4.3573231512	.4073941879	-.4547948003
H11	1.8118750000	5.6043120000	-1.6055280000	H53	1.9057171753	.5423492732	-.0449314495
H12	2.1475470000	3.1311000000	-1.5555780000	H54	2.2160658257	-2.5366939049	3.0061527558
H13	-0.7910930000	2.7964760000	1.6167560000	H55	4.6952575965	-2.6860850106	2.6033450484
H14	-1.1026420000	5.2729290000	1.5844110000	H56	6.5243210358	-.1972778777	.5663635343
C15	-0.8634100000	-0.5338700000	3.9770870000	H57	4.3276068126	.2331624853	7.6367065030
C16	0.4360020000	0.0001900000	3.9456180000	H58	4.2961232124	4.8588624952	5.7531654970
C17	0.9626020000	0.4331270000	2.7203400000	H59	3.8238975847	2.9113926415	4.2589852222
C18	-1.6353800000	-0.6359540000	2.8087900000	H60	3.6413715922	-3.0341121926	5.1120215672
H19	1.0267280000	0.0645640000	4.8642950000	H61	6.4774282298	.2267189643	5.5043771835
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				
C132	0.1079120000	7.3199660000	-0.0400640000				
C133	-1.5320770000	-1.0912800000	5.5082080000				
C134	-2.8572900000	-1.2840780000	-4.6393240000				
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	5.5967577275	-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				
Complex							
Ru1	3.5198286759	.0879205557	2.4228658692				
C12	5.5083465535	1.4777634903	2.662950265				
C13	2.1004955518	2.0742357339	2.6252331065				
P4	3.6318234101	-.0383340635	4.793835188				
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				

H29	-1.3662605545	2.1859744217	-1.4978751518	C64	8.0765338246	-4.1447918273	6.0690822032				
H30	0.9096203223	-1.5059881077	-1.5656284125	F65	7.5933828207	-5.3892471414	6.3459536188				
H31	-0.6167803560	-2.4122116418	-3.3172345366	F66	8.8857085758	-4.2578253909	4.9744389921				
C32	0.4001751310	7.1061109870	0.0049879689	F67	8.8701369946	-3.7651648347	7.1108098588				
F33	0.5316657744	7.6440737863	-1.2415228058	C68	-1.6413358243	-1.6956828170	7.5229693973				
F34	-0.7892401330	7.5360195121	0.5138493801	F69	-1.4707754945	-2.2562188395	8.7534075710				
F35	1.3855585813	7.6515232134	0.7777560715	F70	-2.4861551119	-6344649513	7.6612738065				
C36	-1.5947382425	-0.8836287439	5.2354323131	F71	-2.2850281849	-2.6174170321	6.7448634216				
F37	-0.6720478249	-1.2624393431	6.1641155508	P(OMe) <sub>3</sub>							
F38	-2.3002070996	0.1548253004	5.7755457640	Ligand							
F39	-2.4709464495	-1.9164896711	5.0796191560	P1	.5576009586	-.0644202679	-.5224599110				
C40	-2.8073798827	-1.2135154262	-4.4017332537	O2	.4325293987	.1139489936	1.1369337545				
F41	-2.1624586933	-2.0096080357	-5.3017965788	C3	1.1094468713	1.2426264769	1.7115151300				
F42	-3.7535918329	-1.9900676523	-3.7944781207	O4	-.4607679184	1.2304401522	-.9016992960				
F43	-3.4696749380	-0.2512157820	-5.1029140875	C5	-.4262735864	1.6863733350	-2.2645386706				
Complex											
Ru1	3.5313075506	.1053877319	2.4179160841	O6	-.4131437697	-1.3912726305	-.6741314909				
C12	5.5210273136	1.4897245107	2.6588845956	C7	-1.7016801982	-1.4513913343	-.0155501168				
C13	2.1127140582	2.0950424467	2.6240983980	H8	1.1309085071	1.0822778622	2.8014510612				
P4	3.6544184688	-.0153687015	4.7856891133	H9	2.1524898402	1.3300017133	1.3447652842				
C5	4.0831048929	1.4574576275	5.8333151436	H10	.5726005623	2.1829021532	1.4895030245				
C6	4.3666937138	1.2495428211	7.2033218777	H11	-.7308984430	2.7460608975	-2.2645920957				
C7	4.5975952620	2.3353033001	8.0527315562	H12	-1.1303942592	1.1109108229	-2.8946320975				
C8	4.5391157095	3.6459460623	7.5417421236	H13	.5877804720	1.6051208833	-2.7044153468				
C9	4.2575598042	3.8578483912	6.1837911317	H14	-2.2736064343	-2.2472200193	-5184484558				
C10	4.0310491813	2.7684547551	5.3250990528	H15	-.15735285850	-1.7000946393	1.0510786089				
C11	2.0963550376	-.5946410759	5.6277470689	H16	-2.2373928303	-.4910745574	-.1074250541				
C12	.8700991018	-.0773575470	5.15192266989	Complex							
C13	-.3321538238	-.4173631352	5.7872108007	Ru1	3.6696552857	.3650040285	2.5148274614				
C14	-.3278440984	-.12820304446	6.8979275298	C12	5.0699668969	2.3413292163	2.2759192143				
C15	.8873394513	-.17860914738	7.3867677843	C13	1.7816504240	1.9014623559	2.6305949772				
C16	2.0928997507	-.14368556337	6.7602794679	P4	3.8238821767	.4409543789	4.8086569351				
C17	4.9333834471	-.12597677557	5.2828062285	C5	5.1227515300	-.7569859833	1.1909105747				
C18	6.2587698345	-.8366501652	5.5298265208	C6	4.0676187026	-.2250750618	.3433644572				
C19	7.2644673444	-.17728917793	5.8024141724	C7	2.7107050072	-.4690257203	.6295565888				
C20	6.9664189816	-.3.1474265307	5.8255205226	C8	2.3080204539	-.12682641852	1.7711267724				
C21	5.6543517881	-.3.5816507487	5.5737507988	C9	3.3483496549	-.18325715350	2.5710818613				
C22	4.6478439575	-.2.6433956227	5.3012717909	C10	4.7396494689	-.1.5921226664	2.2806228693				
C23	4.7250925178	-.1.2204022539	1.0112177127	C11	6.5703727880	-.4537970522	.8415205768				
C24	3.9253765906	-.2931578163	.2325661808	C12	8.0456871840	-.1.1444546868	-.6219759566				
C25	2.5305938770	-.1899180888	.4329819287	C13	7.0278403521	-.2.4543032123	.0460125596				
C26	1.8401395145	-.9996172822	1.4146765711	C14	.7224205246	-.1.9467734281	3.0757630365				
C27	2.6340635931	-.1.9056958378	2.1823699921	C15	.3628751646	-.2.1002315168	1.3283884220				
C28	4.0545201834	-.2.0329962939	1.9694996622	C16	7.0226125776	-.1.4027656125	-.2956618480				
C29	6.2184536482	-.1.3051902560	.7485895455	C17	6.3568897126	-.1.3353879723	-.1.1746192750				
H30	3.03078131249	-.1.8313274605	7.1633143506	C18	.8500650252	-.1.4652020017	2.0922639439				
H31	7.5212014736	-.2.1206865566	-.8087865014	C19	-.3383210488	-.4867533846	2.1165188582				
H32	6.1137830336	-.3.1570828147	-.4346571641	C20	7.5316444869	-.5138843764	2.0386795540				
H33	.0313641064	-.1.3427789825	2.5535155089	H21	8.5453508544	-.2177050093	1.7164505471				
H34	-.1964069297	-.1.3240786006	.7796348532	H22	7.2027527238	.1835270923	2.8270610874				
C35	6.4462911491	-.2.1095654633	-.5560553769	H23	7.6089354533	-.1.5331545954	2.4611149756				
H36	5.8978160656	-.1.6755213754	-.4.108752224	H24	4.3336780000	.4810370934	-.4489475047				
C37	.3549899865	-.8576904477	1.6180723705	H25	1.9386311392	.0595876642	.0618528669				
H38	.0783862355	.2102753623	1.6635297771	H26	3.0849069106	-.2.4037698831	3.4660267294				
C39	7.0335307396	-.1.8891190851	1.9119810217	H27	5.4947670278	-.1.9801192187	2.9675550912				
H40	8.1099062096	-.1.8421094658	1.6714420366	H28	6.5810030140	.5855697595	.4607180914				
H41	6.8642847424	-.1.3137683564	2.8365316455	O29	4.6312387766	1.5956425697	5.6589693321				
H42	6.7893814357	-.2.9513896345	2.1001112591	O30	2.4433994515	.4305406870	5.6881717990				
H43	8.2863283356	-.1.4326388915	5.9986865694	O31	4.4794501493	-.9892957390	5.3231326869				
H44	4.8196526743	2.1658612271	9.1115154194	C32	6.0344703696	1.8720295400	5.4185311404				
H45	-1.2775754165	-.0019311761	5.4233753862	H33	6.1299296613	2.6553410892	4.6535912968				
H46	.8723301913	.6117932498	4.2979370381	H34	6.4465935054	2.2022351133	6.3862209819				
H47	.8938669594	-.2.4452127786	8.2600323860	H35	6.5690224285	.9652099338	5.0849687090				
H48	5.4183533208	-.4.6497594634	5.5982053056	C36	4.5312810005	-.1.2926080807	6.7399823860				
H49	4.4286337275	.4093738361	-.4382112222	H37	4.9608859484	-.4510105247	7.3091919948				
H50	1.9732235383	.6029010603	-.0755412484	H38	3.5215708416	-.1.5171813849	7.1204477806				
H51	2.1515247746	-.2.4931854781	2.9715260265	H39	5.1792346993	-.2.177457469	6.8366436939				
H52	4.6337070718	-.2.6996741580	2.6137509004	C40	1.7297695959	1.6540575741	6.0203495033				
H53	6.5608063287	-.2646829355	.5883998554	H41	2.3799694060	2.3192965442	6.6115305771				
H54	4.4105905804	.2353685708	7.6145190018	H42	1.3921019815	2.1517933146	5.0991269160				
H55	4.2132755541	4.8765142272	5.7888768708	H43	.8685833838	1.3313760052	6.6257205741				
H56	3.8080601170	2.9352666340	4.2691674524	P(OPh) <sub>3</sub>							
H57	3.6282166988	-.2.9986223730	5.1160564867	Ligand							
H58	6.5042940963	.2290595193	5.5001404836	P1	-.6178350463	1.1728332697	-.0982684461				
C60	4.7657145435	4.8027680884	8.4883960079	O2	-.8506912720	.9782518206	-.1.7740036863				
F61	4.7386632718	6.0065122048	7.8534167552	C3	-.1.9293413353	1.6070780637	-.2.3943138142				
F62	3.8124404572	4.8319440516	9.4678122015	O4	.5968254179	.0085052369	.0085814331				
F63	5.9719559488	4.6947639064	9.1220512377								

C5	.2716965318	-1.3107189839	.3210450803	C46	5.8072783949	3.9474153148	6.1734556725
O6	.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	-.17291231547	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	-.17001302067	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	P(pyr) <sub>3</sub> (pyr = NC <sub>4</sub> H <sub>4</sub> )			
H27	-2.2455612608	-.1220672853	-3.6511399486	Ligand			
H28	2.0911995955	-1.4993536499	1.4693948708	P1	1.9509591153	2.8159207388	7.3142474802
H29	1.6561467816	-.39022929412	2.0609944841	N2	.4694852009	2.0032069769	6.8454193944
H30	-.4288695405	-5.0337842605	1.2488074535	C3	-.7421342743	2.7026877446	6.7518386649
H31	-2.0533209151	-3.7628176695	-.1735245013	C4	-1.7264728022	1.8139130337	6.3651912718
H32	-1.5833731797	-1.3943159130	-.8090759430	C5	-1.1075958416	.5297839926	6.2036265328
H33	1.6842153661	1.1182734456	-1.9648675225	C6	.2369373401	.6650164136	6.4989402584
H34	3.6741545569	1.9952925401	-3.1769959882	N7	3.1442655456	1.7511961108	6.5947819379
H35	4.5959512920	4.2610292605	-2.6383930232	C8	3.7206828096	2.0502913128	5.3524191133
H36	3.4969457913	5.6531219865	-.8620210937	C9	4.5480868871	1.0031033244	4.9955783127
H37	1.4844214490	4.7657021488	.3521531327	C10	4.4888885071	.0299867744	6.0478412494
			C11	3.6204966433	.5018582800	7.0159047137	
Complex			N12	2.0644006971	2.3353145294	8.9958965357	
Ru1	4.6061185194	.2866406830	2.6293352556	C13	1.5522136693	1.2112725342	9.6580143847
C12	7.0265653148	2.314603301	2.4473060028	C14	1.9549423030	1.2755102793	10.9797981486
C13	4.6695421609	2.7149278540	2.6022127644	C15	2.7396021953	2.4655630989	11.1442311901
P4	4.7837377463	.3840895260	4.9020878950	C16	2.7867536148	3.1034874227	9.9199511662
C5	4.5460607014	-.17587896674	1.6775243165	H17	-.7792267747	.37692915216	6.9711965699
C6	4.5277675136	-.7655489829	.6164677053	H18	-2.7765477025	2.0583982578	6.2042124480
C7	3.5780725870	.2728055160	.5870210095	H19	-1.5943627390	-.3932725410	5.8871341112
C8	2.5655889035	.3882522631	1.6204640528	H20	1.0601376975	-.0470295650	6.4684819143
C9	2.5413600968	-.6125208716	2.6339003928	H21	3.4863292622	2.9877665620	4.8489063581
C10	3.5229065197	-1.66694042700	2.6695045962	H22	5.1456934113	.9462399143	4.0856889754
C11	5.6174464941	-.28374478256	1.6624403809	H23	5.0407122223	-.9092279045	6.0990898955
H12	6.1099784525	-.46122883575	.4836919800	H24	3.3209814907	.0950956688	7.9804919012
H13	4.3632283903	-.4395597533	.8238927941	H25	.9221061344	.4995647502	9.1270835446
H14	9964591677	1.5682509440	2.5272984391	H26	1.6987956946	.5526573017	11.7549828004
H15	.8868155823	1.4129053822	.7447128713	H27	3.2038619840	2.8215133078	12.0640765758
C16	5.2849404950	-.38834465692	.5718092003	H28	3.2623707513	4.0330957761	9.6085502891
H17	5.1389401838	-3.4149397066	-.4181230340				
C18	1.5838555500	1.5268865936	1.5963841639	Complex			
H19	2.1251277854	2.4828887394	1.4836858298	Ru1	9.9686451757	5.5984808338	7.9479613214
C20	5.8504162121	-.3039537724	3.0277938736	C12	10.2517007665	3.3219550292	7.1474635215
H21	6.7143397994	-.41883106770	2.9623801309	C13	9.622733697	6.3497724161	5.6586512676
H22	6.0691819662	-.27511649897	3.8034794560	P4	12.2688010469	5.7842677662	7.6932499728
H23	4.9796176267	-.41072420871	3.3471637310	N5	12.8717670397	7.4267802354	7.6950173789
H24	5.3534521990	-.7560265435	-.1020183691	N6	13.1295134527	4.9865035140	6.4238549158
H25	3.6728511858	1.0739176816	-.1522280838	N7	13.1874120131	5.1673958615	9.0602935234
H26	1.8126869117	-.5263181820	3.4457969108	C8	8.9337430010	7.4348945904	8.7980243500
H27	3.5175577398	-.23677925273	3.5084674857	C9	9.9300866465	6.9533767642	9.7038976494
H28	6.5546506288	-.23169365267	1.3821044215	C10	9.9110507660	5.6063182961	10.2179140654
O29	5.1119608257	1.7242497645	5.7925149525	C11	8.9273642191	4.6786873100	9.7772310562
O30	3.4017594982	-.0438158563	5.7303925055	C12	7.9328777023	5.1471761723	8.8293502456
O31	5.7683893045	-.7929293586	5.5049816432	C13	7.9389151238	6.4810949951	8.3645097079
C33	-.1184788184	2.1641302568	6.3282644205	C14	8.8524600562	3.2407702401	10.2606093291
C34	.8726636969	2.6872036845	5.4821705419	C15	7.6153701468	3.0883524645	11.1823531068
C35	2.0713985961	1.9905801927	5.2514269351	C16	10.1244322041	2.7394513729	10.9588454046
C36	2.2649402845	.7520558017	5.8908467841	C17	8.9012106519	8.8565510401	8.3045455478
C37	1.2828125297	.2152094335	6.7406637909	C18	12.1684606813	8.4586708496	7.0457632536
C38	.0934112086	9.255594554	6.9561618125	C19	12.9775914287	9.5773047960	7.0199569131
H39	-1.0471284861	2.7185388378	6.5010860125	C20	14.2195513003	9.2344543711	7.6518032182
H40	.7218157847	3.6539407142	4.9889883478	C21	14.1473005997	7.9110835367	8.0390132404
H41	2.8353087701	2.4095773096	4.5848151907	C22	12.5772452661	4.6456460585	5.1716611918
H42	1.4720266441	-.7458854486	7.2296810152	C23	13.6119397440	4.2682644021	4.3450247852
H43	-.6679584928	.5069490053	7.6238520919	C24	14.8396432937	4.3835056735	5.0844220996
C44	8.0201677721	4.7240662708	5.5226408017	C25	14.5318968861	4.8345520549	6.3486191826
C45	6.7693116844	4.9641174184	6.1169255210	C26	13.4733249589	3.8042664340	9.2351203144

C27	13.8704492318	3.6107919412	10.5452642865	N6	13.3874622814	5.1447230672	6.4782950923
C28	13.8014261537	4.8774986141	11.2142441676	N7	13.5892509221	4.8438668666	9.0450226081
C29	13.3627468480	5.8146151869	10.2954954249	C8	9.2287865792	7.4429674108	9.0308959631
H30	10.7396089128	7.6282196831	10.0025834291	C9	10.1832727238	6.8858319129	9.9351293264
H31	10.7245504025	5.2781090956	10.8713729878	C10	10.1348038991	5.4945667938	10.3142696423
H32	7.2339938438	4.4268866053	8.3942892129	C11	9.1588874181	4.6216900464	9.7557824600
H33	7.2470531708	6.7720656896	7.5675862530	C12	8.2089134700	5.1804531173	8.8127481454
H34	8.6973345216	2.6245274237	9.3536214754	C13	8.2469225485	6.5429581113	8.4639205919
H35	7.5014979038	2.0321858295	11.4841594270	C14	9.0177070597	3.1503807580	10.1162196669
H36	6.6817748949	3.4011800392	10.6820774588	C15	7.6927989707	2.9432794690	10.8914473074
H37	7.7303016490	3.6945597469	12.0999901675	C16	10.1925798820	2.5648036460	10.9111023416
H38	10.0159033144	1.6668276265	11.1968652639	C17	9.2034668164	8.8991239867	8.6477575998
H39	10.3061616980	3.2703378145	11.9123156956	C18	12.6126944068	8.5562779040	7.8624028154
H40	11.0117964858	2.8589826506	10.3155572252	C19	13.7382147373	9.4774450699	7.3001613015
H41	8.6719165015	8.8825728260	7.2248711278	C20	15.0075796008	8.5980488327	7.2920110329
H42	9.8671199565	9.3613055528	8.4680463382	C21	14.7389111044	7.6033684323	8.4330757286
H43	8.1159209396	9.4274665497	8.8360708743	C22	12.7647479099	4.9839172517	5.1471945973
H44	11.1910820168	8.2499231618	6.6102171365	C23	13.5228045929	3.7710002408	4.5778910700
H45	12.7109648875	10.5401936716	6.5833112744	C24	14.9611350830	3.9016410940	5.1536033836
H46	15.0751986467	9.8916089634	7.8130782626	C25	14.8435785224	4.9675250524	6.2837531361
H47	14.8655170356	7.2741442386	8.5498413407	C26	13.6052281374	3.3598305078	8.9560822448
H48	11.5026654465	4.7091155377	5.0183312653	C27	14.3214433193	2.9342907565	10.2501981860
H49	13.4995022052	3.9277392414	3.3155731461	C28	13.8522471873	3.9872494964	11.2722844861
H50	15.8430257132	4.1438070221	4.7298691989	C29	13.8050155582	5.2889955853	10.4458994141
H51	15.1606506965	5.0430934252	7.2107308874	H30	10.9771427332	7.5254893100	10.3345244802
H52	13.3581184920	3.1111856730	8.4043073895	H31	10.8868682748	5.0989016135	11.0007890044
H53	14.1911200731	2.6611122914	10.9742453892	H32	7.5275081060	4.5067479534	8.2858777589
H54	14.0754703856	5.0876465790	12.2489396020	H33	7.5919037717	6.9151882462	7.6702600907
H55	13.2173611692	6.8894532892	10.3832143465	H34	8.9560708959	2.6085241814	9.1514255946
P(pyrd) <sub>3</sub> (pyrd = NC <sub>4</sub> H <sub>8</sub> )				H35	7.5355572627	1.8683084459	11.0903200421
Ligand				H36	6.8196305346	3.3160735362	10.3284715359
P1	0.2985988841	1.2021265858	-0.8710621978	H37	7.7196572377	3.4699727172	11.8635252848
N2	-1.1266063397	2.1229149011	-0.5584155766	H38	10.0278489022	1.4863157446	11.0804569052
N3	0.4533352023	-0.0430489849	0.3131732106	H39	10.2947425555	3.0413435058	11.9048067062
N4	1.4841059507	2.2960081934	-0.1266638308	H40	11.1414319975	2.6778109979	10.3626769905
C5	-2.1070718743	2.3900017199	-1.6375688936	H41	8.2524146555	9.3608489535	8.9733256778
C6	-3.3299535099	2.9592742783	-0.8895171013	H42	9.2784023304	9.0018662538	7.5496005488
C7	-2.6877860155	3.6974699187	0.3031689499	H43	10.0304453339	9.4572943969	9.1138487847
C8	-1.5555297372	2.7370550146	0.7167538913	H44	11.6850146754	4.8216144307	5.2381205676
H9	-2.3484744437	1.4729384501	-2.2062686365	H45	12.9377472512	5.8908171936	4.5296180470
H10	-1.7199584828	3.1369291980	-2.3642637164	H46	13.0403511787	2.8498635681	4.9479595344
H11	-3.9509142376	3.6108269266	-1.5286306902	H47	13.5053674739	3.7493888484	3.4745297244
H12	-3.9673461740	2.1334668241	-0.5204936053	H48	15.3259429673	2.9376705678	5.5487542257
H13	-2.2634427086	4.6628666309	-0.0327684997	H49	15.3259410940	4.2347690671	4.3886599370
H14	-3.3950945251	3.9033646198	1.1258040183	H50	15.3141757513	5.9191703979	5.9554681414
H15	-1.9442253586	1.9680794522	1.4197947045	H51	15.3246183979	4.6638710471	7.2279077447
H16	-0.707890356	3.2452463226	1.2122243222	H52	12.5785852599	2.9486593042	8.8915033910
C17	-0.0679985865	-1.3904751264	-0.0178829726	H53	14.1396679509	3.0289726016	8.0491473609
C18	0.1700473374	-2.1961861428	1.2721643208	H54	14.0748726399	1.8996331418	10.5440295087
C19	-0.0875029513	-1.1429031640	2.3685358118	H55	15.4176883625	2.9976054864	10.1149913051
C20	0.5680080805	0.1258771225	1.7858292703	H56	12.8416338333	3.7284079859	11.6375831761
H21	0.4584759369	-1.8121787376	-0.8939601778	H57	14.5146503694	4.0739134341	12.1510815820
H22	-1.1547890704	-1.3731467178	-0.2563705694	H58	14.7648390944	5.8389710642	10.5255055773
H23	-0.4854493113	-3.0812422501	1.3471180465	H59	13.0799074757	5.9799074757	10.7877456780
H24	1.2206402729	-2.5404960476	1.3156436489	H60	13.0137130032	8.0754812275	9.4150713345
H25	-1.1768102519	-0.9868798078	2.4887389627	H61	14.9593726739	6.6738750425	8.3686822681
H26	0.3259157156	-1.4215578460	3.3539282004	H62	15.0910068242	8.0487750158	6.3364979137
H27	1.6366129647	0.1827473897	2.0842200791	H63	15.9367342043	9.1779137384	7.4353461191
H28	0.0886964833	1.0558639310	2.1341359106	H64	13.4883995301	9.8641070138	6.2978407295
C29	1.5634901215	3.6395847210	-0.7380078646	H65	13.8826153039	10.3497664883	7.9633071790
C30	2.7994164966	4.2724066375	-0.0504821767	H66	11.8494178324	8.3072939725	7.1061968880
C31	3.6767114498	3.0521570031	0.3704032370	H67	12.1058956925	9.0583574818	8.7095474517
C32	2.8846884660	1.8208784745	-0.1324228825	PPh <sub>2</sub> Me			
H33	0.6300472737	4.2008423445	-0.5640556789	Ligand			
H34	1.7257280790	3.5889120635	-1.8425422201	P1	.0087356105	-.0306978477	.3367518705
H35	3.3276680925	4.9626145349	-0.7310984168	C2	-.1175907660	.0651106489	2.2037143849
H36	2.4919495466	4.8529781503	0.8365638926	H3	.8899573965	.0068294898	2.6513618440
H37	4.6915101781	3.0856721245	-0.0630815172	H4	-.6256867916	.9789632633	2.5597626229
H38	3.7851268188	3.0153474264	1.4682980492	H5	-.6899154372	-.8130263173	2.5478892398
H39	2.9960760946	0.9324842241	0.5106524770	C6	-.45202207872	.4270437144	-.7841672975
H40	3.2254106895	1.5408292839	-1.1587487612	C7	-.38451358434	-.7894310639	-.9719891504
Complex				C8	-.24829461718	-.8951884990	-.6421742190
Ru1	10.2925247644	5.6813193249	8.0649434743	C9	-.17823551207	.2093113702	-.1126532660
C12	10.4012362830	3.4961163152	6.9703200505	C10	-.24714298204	1.4289406077	.0684231776
C13	10.1525067214	6.8199612372	5.9061172468	C11	-.38301007544	1.5368539297	-.2649339361
P4	12.6820794508	5.7602706576	7.9005763635	H12	-.5807025540	.5138018543	-.10465680481
N5	13.2866616533	7.3176020136	8.3441665398	H13	-.43759378108	-.16556598193	-.13832474192
				H14	-.19534163165	-.18424784487	-.8012935819

H15	-1.9356282205	2.3010695028	.4612283756	H8	-2.3412825279	-.9259757177	-.0909510737
H16	-4.3525279598	2.4898909588	-.1216744371	H9	-2.3001142915	.8221486426	.3393778341
C17	1.8663056021	4.0925071436	-.8981459594	C10	1.5089589282	4.1912085012	-.7071546722
C18	1.3019025418	3.2267689250	-1.8521104860	C11	1.1726707204	3.3182984024	-1.7564846819
C19	.7366250835	2.0088381930	-1.4506620083	C12	.7243176392	2.0199779904	-1.4740610627
C20	.7037933525	1.6363786383	-.0853424754	C13	.5771119768	1.5724724799	-.1398257094
C21	1.2767897780	2.5128965666	.8611072570	C14	.9236365378	2.4581253584	.9028935206
C22	1.8555283102	3.7291822460	.4568646772	C15	1.3890918284	3.7543041056	.6211589950
H23	2.3148747663	5.0417435664	-1.2116113848	H16	1.8694500083	5.2027324817	-.9250910312
H24	1.3074635341	3.4995976682	-2.9136448446	H17	1.2707512084	3.6462798229	-2.7977707618
H25	.3072762024	1.3376383557	-2.2047641346	H18	.4903517749	1.3382390851	-2.3019557630
H26	1.2756836722	2.2535694822	1.9252250840	H19	.8331582832	2.1425057528	1.9478074213
H27	2.2948872535	4.3954314627	1.2083726556	H20	1.6549735931	4.4256509910	1.4460423844
<b>Complex</b>							
Ru1	3.8190972889	.5124243020	2.6155011961	Ru1	3.5168693023	.1316126455	2.4056018256
C12	6.0508435844	1.4659645293	2.8893478203	C12	5.5836294163	1.4145738983	2.6584513983
C13	2.7932949215	2.7027465039	2.9350601470	C13	2.2379725063	2.2032318847	2.6256077436
P4	3.8260831334	.3751312760	4.9683587350	P4	3.5944507809	.1416069672	4.7561456212
C5	4.2982306929	1.7800436717	6.0739461500	C5	2.1177551646	-.6426271931	5.5420158450
C6	4.8093316509	2.9970891339	5.5838427775	C6	.8537129660	-.0453903649	5.3243162896
C7	5.2013148391	3.9988408861	6.4891983446	C7	-.3034535896	-.6201237934	5.8710742119
C8	5.0905729711	3.7973858906	7.8736092539	C8	-.2199760426	-.18024608324	6.6285254054
C9	4.5699849099	2.5879654850	8.3648717271	C9	1.0289093498	-.24065047502	6.8400648487
C10	4.1739297250	1.5847801436	7.4694292537	C10	2.1929063155	-.18295960064	6.3013351905
C11	2.1667646070	-.1008409540	5.6270619458	C11	4.6101639351	-.13194839653	1.0638141094
C12	1.7848386611	-.14497425720	5.7947744194	C12	3.8668293473	-.3986721184	.2217854929
C13	.4894874710	-.17791741035	6.2290472596	C13	2.4865684324	-.1871403203	.4260468694
C14	-.4413991995	-.7620155578	6.4938228887	C14	1.7526049474	-.8896066231	1.4587165309
C15	-.0728144064	.5835007405	6.3180255745	C15	2.4845641620	-.18139915819	2.2658159105
C16	1.2197744278	.9150610041	5.8856869103	C16	3.8913902411	-.20487234506	2.0570370316
C17	4.7186912808	-.8652823192	1.0414050227	C17	6.1019222414	-.14938258582	.8227063328
C18	3.9409437349	.1585351956	.3775944947	H18	3.1595573734	-.23106226434	6.4843867813
C19	2.5948360225	.3981198458	.7534455050	H19	7.3896387684	-.4221946140	-.6854830524
C20	1.9331689810	-.3752240542	1.7777657804	H20	5.9300609607	-.3792747155	-.2973414995
C21	2.7205355061	-.13802330140	2.4283718431	H21	-.0571229669	-.10391126472	2.6341727340
C22	4.0829615830	-.16513334921	2.0471717502	H22	-.3164010657	-.10590852189	.8627561371
C23	6.1687209742	-.10692895210	.6322872951	C23	6.3131894566	-.23529616524	-.4480518825
H24	3.7549959780	.6511896780	7.8625939742	H24	5.7966251821	-.19239813897	-.3248341821
H25	7.2463292995	-.19342633923	-.10641301472	C25	.2881429092	-.6157194337	1.6767907641
H26	5.7901608630	-.28580593370	-.5922392554	H26	.1068695590	.4735189723	1.6939085534
H27	.2577589100	-.5634071297	3.1345483307	C27	6.8707996425	-.20766064260	2.0188311200
H28	-.1955337454	-.4499657759	1.4076447445	H28	7.9514644486	-.0928226698	1.7941711959
C29	6.2042852985	-.18396608044	-.7110034892	H29	6.7189304167	-.14563248721	2.9175679393
H30	5.6214736857	-.13256557255	-.14953714010	H30	6.5683624033	-.31181631360	2.2386728427
C31	.5103161096	-.0815778968	2.1759998989	H31	-.12759260037	-.1437374543	5.7027686940
H32	.3660792625	1.0071573396	2.2883969781	H32	.7878981763	.8606025168	4.7089160218
C33	7.0351418540	-.17663730859	1.6928367700	H33	-.11263003647	-.22516599969	7.0498052988
H34	8.0838981504	-.18012205161	1.349701427	H34	1.1026841682	-.3291429740	7.4270834999
H35	7.0049122143	-.12087844857	2.6436340294	H35	4.4118854125	.2252796577	-.4927021809
H36	6.7152642984	-.28116155545	1.8659523187	H36	1.9781352701	.6104934703	-.1246860403
H37	.2100960390	-.28308326784	6.3624141757	H37	1.9724043085	-.23165584731	3.0935866261
H38	5.5954685060	4.9440537018	6.1013765929	H38	4.4241981645	-.27358254308	2.7197795841
H39	4.8971700985	3.1535148902	4.5070943928	H39	6.5008223341	-.4781776527	.6359401122
H40	5.4040911080	4.5823482833	8.5706851978	C41	3.7214457115	1.7824984572	5.5849172730
H41	4.4703531561	2.4227533822	9.4437349706	H42	3.8005949456	1.6487217511	6.6779461201
H42	-.14503073526	-.10167489502	6.8352261721	H43	4.6120821881	2.2907129189	5.1827008864
H43	-.7967238425	1.3806380450	6.5191552542	H44	2.8354772712	2.3826862147	5.3309141339
H44	4.4328435198	.8270376356	-.3344370205	C45	5.0450886002	-.7633040714	5.4548845937
H45	2.0715610736	1.2639279425	.3349483192	H46	5.0568410651	-.7241812515	6.5582425304
H46	2.2811996456	-.19332380739	3.2672918035	H47	5.0563475351	-.18142198796	5.1226515172
H47	4.6547635528	-.24095611625	2.5879792158	H48	5.9423570704	-.2606476821	5.0573217357
H48	6.5869317331	-.0578568604	.4706907482				
H49	1.5017397672	1.9629712189	5.7472498975				
H50	2.4992402026	-.22533643051	5.5857338418				
C52	4.9718501299	-.9628824329	5.5513651847				
H53	4.9418991827	-.10824345197	6.6474405309				
H54	4.7365929987	-.19231547275	5.0661134730				
H55	5.9836218034	-.6534542558	5.2376079232				
<b>PPhMe<sub>2</sub></b>							
Ligand							
P1	.0035052603	-.1751721724	.1146474883	P1	.1146005261	-.3377821192	-.0909980287
C2	-.1009063461	-.2890932474	1.9783279157	C2	-.1199536937	-.1780079108	1.7729672619
H3	.9121877574	-.2823241625	2.4160500900	H3	.8912038459	-.1131316229	2.2178887180
H4	-.6990235605	.5203130174	2.4357305422	H4	-.6524894140	.7613500838	2.0160492032
H5	-.5672674624	-.12563381249	2.2348042442	C5	-.8681455318	-.13908827691	2.3509760468
C6	-.18242036190	.0333750618	-.2702920804	H6	-.9674157843	-.13023729234	3.4477788450
H7	-.19465743613	.2880791671	-.13368569488	H7	-.18840412960	-.14733715069	1.9260284251
				H8	-.3334784059	-.23327639736	2.1331223921
				C9	-.43263607140	.1377916534	-.15230325422
				C10	-.36718431479	-.1024977136	-.15854763921
				C11	-.23356493931	-.12137892393	-.11636776237
				C12	-.16403062636	-.0907974455	-.6645022753
				C13	-.23101755914	1.1519624609	-.6080097919
				C14	-.36419447562	1.2652917161	-.10351607228

H15	-5.3655735570	.2289076995	-1.8587938494	C2	2.1769121594	.2392362074	-.1396442604
H16	-4.1974825573	-1.9836741777	-1.9708698371	H3	2.4185303762	-.7807668134	-.4934026407
H17	-1.8207414803	-2.1800068668	-1.2281453370	C4	2.9429574018	.5714326749	1.1203783136
H18	-1.7794686103	2.0374432181	-1.2390569786	H5	2.4322444615	.9421966251	-.9562218333
H19	-4.1480110395	2.2366371904	-.9891800555	C6	-.2916089415	-.0981108802	-1.6017052107
C20	2.1172351958	3.7112260209	-1.3475227359	C7	-.1038092304	-1.5506975350	-1.9755344046
C21	1.6303598016	2.8035919259	-2.3051946339	H8	.2320130740	.5663205856	-2.3161933459
C22	1.0193204277	1.6101124550	-.18974126005	H9	-.13624570197	.1797035964	-1.6154892153
C23	.8622260480	1.3040422494	-.5241408932	C10	.0154843485	2.1198877724	.2216385048
C24	1.3575135404	2.2229874880	.4264271308	H11	.4247379804	2.5950302525	-.6909723201
C25	1.9821815881	3.4145577889	.0169814834	H12	.6077321503	2.4883392369	1.0804039106
H26	2.6021983485	4.6410415938	-1.6649991442	C13	-1.4496322482	2.4495887330	.3932039793
H27	1.7334435543	3.0236144900	-3.3739849671	C14	-.9277291903	-2.5511177343	-1.4135143375
H28	.6533026586	.9047191741	-2.6536438545	H15	-1.7220528593	-2.2603970446	-.7154267104
H29	1.2582897791	2.0184207836	1.4975353568	C16	-.7400118281	-3.9028792899	-1.7370929475
H30	2.3597527474	4.1141396604	.7717932614	H17	-.13938552885	-4.6626902767	-1.2938683433
Complex							
Ru1	3.6520036702	.2313012088	2.4581308245	C18	.2799544620	-4.281820291	-2.6266255847
C12	5.7779545182	1.4108686000	2.6629282186	H19	.4256081317	-5.3390923918	-2.8801778353
C13	2.4604059886	2.3153149125	2.9169354867	C20	1.1086766630	-3.2993298078	-3.1893151882
P4	3.7939420672	.0491605701	4.8177110148	H21	1.9053081885	-3.5833818065	-3.8864076729
C5	2.2682832250	-.6521532722	5.6213863770	C22	.9175166851	-1.9460928982	-2.8644840420
C6	1.0156146548	-.2488956299	5.1084996503	H23	1.5629021976	-1.1807002849	-3.3134793164
C7	-.1740186588	-.6607083320	5.7302726020	C24	3.0280172402	-.3611014194	2.1779334585
C8	-.1297460720	-1.4805101969	6.8705268995	H25	2.5477867799	-.13408655835	2.0673992323
C9	1.1118223329	-1.8674185611	7.3998141251	C26	3.7151980325	-.0475015388	3.3597155746
C10	2.3046656698	-1.4493218716	6.7861955051	H27	3.7736783134	-.7875543459	4.1660571131
C11	5.1333572003	-1.1112950776	5.3381149895	C28	4.3280429299	1.2086841403	3.5105968310
C12	6.4195923251	-.6291295006	5.6619421785	H29	4.8657004890	1.4530457560	4.4334663746
C13	7.4531293559	-.15214882424	5.9908115085	C30	4.2476746336	2.1465196432	2.4687166133
C14	7.2224513052	-.29060933500	5.9949463579	H31	4.7237787589	3.1281624924	2.5734703486
C15	5.9492194715	-.33984805459	5.6610440401	C32	3.5599999039	1.8290248116	1.2856155520
C16	4.9156010869	-.25093153687	5.3304110823	H33	3.5074065681	2.5628661658	.4715572034
C17	4.6783015633	-1.2073072816	1.0482109935	C34	-2.0941767411	2.2406571865	1.6326798601
C18	4.0363487801	-.1648422346	.2669507442	H35	-1.5138700074	1.8535113296	2.4789390209
C19	2.6681383429	.1343416652	.4310431356	C36	-3.4594031445	2.5210974298	1.7895507760
C20	1.8463045587	-.5932915926	1.3778298161	H37	-3.9388875642	2.3569300459	2.7613645559
C21	2.4748315215	-.16246098116	2.1389044281	C38	-4.2104332766	3.0122296048	.7074033452
C22	3.8717637405	-.19385726856	1.9678602739	H39	-5.2766383402	3.2324735120	.8305563605
C23	6.1553551605	-.14871074473	.8214357207	C40	-3.5830993242	3.2207811504	-.5313056249
H24	3.2648556846	-.17505059815	7.2173052844	H41	-4.1573573199	3.6061209355	-1.3814646780
H25	7.3888589551	-.24222636983	-.7275422241	C42	-2.2152063664	2.9404070043	-.6850437105
H26	5.8518878401	-.32806289742	-.4157863787	H43	-1.7283048711	3.1131976883	-1.6530469577
Complex							
Ru1	1.2503035688			Cu1	1.2503035688	1.8569542262	1.7181951307
C12	2.8650503329			C12	2.8650503329	.0137929908	1.6390699101
C13	-.2512432892			C13	-.2512432892	.5100835934	3.1004879173
P4	2.3547837670			C4	2.3547837670	2.2613079793	3.7802936443
C5	-.5490952597			C5	-.5490952597	2.9883072584	.9593644803
C6	.5063228511			C6	.5063228511	3.9109917902	1.2174247174
C7	1.8102511407			C7	1.8102511407	3.7293178787	.6321115860
C8	2.0832773327			C8	2.0832773327	2.6372580647	-.2433554773
C9	.9964167751			C9	.9964167751	1.7128896474	-.5141155082
C10	-.2801374493			C10	-.2801374493	1.8822676905	.0611726540
C11	-.19042962116			C11	-.19042962116	3.1359713206	1.5972881198
C12	3.4257064646			C12	3.4257064646	2.4054646676	-.9221280614
C13	4.5681690870			C13	4.5681690870	3.2826610918	-.3853965666
C14	3.2704172442			C14	3.2704172442	2.6070917176	-.24496305513
C15	4.1208712570			C15	4.1208712570	2.8554887779	3.4587706691
C16	5.0965621671			C16	5.0965621671	2.8788796116	4.6124341234
C17	5.9994348469			C17	5.9994348469	1.8070734588	4.7911260342
C18	6.9173017494			C18	6.9173017494	1.8047447317	5.8533707014
C19	6.9518211344			C19	6.9518211344	2.8775423938	6.7596680182
C20	6.0681350729			C20	6.0681350729	3.9555778498	6.5878028172
C21	5.1535583763			C21	5.1535583763	3.9565783028	5.5236777091
C22	1.6381160853			C22	1.6381160853	3.5004329230	5.0035811178
C23	1.1527001720			C23	1.1527001720	4.8327172400	4.4841721205
C24	2.0258602498			C24	2.0258602498	5.8152587689	3.9668737098
C25	1.5385348642			C25	1.5385348642	7.0508602220	3.5110519633
C26	.1644107732			C26	.1644107732	7.3359576937	3.5716311001
C27	-.7152965522			C27	-.7152965522	6.3757882984	4.0991798199
C28	-.2241514358			C28	-.2241514358	5.1396097119	4.5484645947
C29	2.5846154335			C29	2.5846154335	.7160386691	4.8561127973
C30	2.2290749488			C30	2.2290749488	.8435485136	6.3213554532
C31	3.2015328803			C31	3.2015328803	1.1789688411	7.2876981868
C32	2.8560815073			C32	2.8560815073	1.2890955236	8.6439593925
C33	1.5328876653			C33	1.5328876653	1.0653498210	9.0583752989
C34	.5584565180			C34	.5584565180	.7229439501	8.1054742080
P1	.3039012609	.2451094865	.1672474562	C35	.9028095949	.6123088383	6.7493272751

H36	.3362745004	4.7380557301	1.9111590607	C8	9.8867798537	5.3789697521	10.2613679412
H37	2.6088415236	4.4282569436	.8954086799	C9	8.9232403090	4.5208498778	9.6552245658
H38	1.2096319408	.8056417247	-1.0881233228	C10	7.9226845232	5.1275893655	8.7983790699
H39	-1.0436165985	1.1102920488	-.0757282703	C11	7.9043451837	6.5127431423	8.5544211603
H40	-2.6573247688	3.4215013781	.8379141818	C12	8.8254345370	3.0237671589	9.9037966419
H41	-1.8888400721	3.9118054917	2.3796802521	C13	7.8150935371	2.7884497509	11.0535140180
H42	-2.2118452813	2.1813916398	2.0592408202	C14	10.1606561850	2.3204618173	10.1798412707
H43	3.6862890977	1.3454657905	-.7282797099	C15	8.8091544010	8.8701182359	8.8952691454
H44	5.5140137410	3.0114470512	-.8863534984	C16	13.2453415877	4.0021101270	9.7037544913
H45	4.7128092398	3.1474388009	.6991383792	C17	13.8516069727	3.9927808977	10.9495232283
H46	4.3874727090	4.3562295084	-.5848795205	C18	14.1616924049	5.3485769757	11.2853400373
H47	4.2203296913	2.3713542449	-2.9620446317	C19	13.7392141254	6.1460081629	10.2343838165
H48	3.0075475374	3.6559217422	-2.6824963318	H20	10.5994615183	7.4465382432	10.4967189863
H49	2.4850840976	1.9584493186	-2.8758629104	H21	10.6968050193	4.9596807262	10.8643131098
H50	4.4615396891	2.1546250439	2.6750300140	H22	7.2482895990	4.4735345242	8.2384397296
H51	4.0234599123	3.8510237469	2.9892945935	H23	7.2221787886	6.9234194269	7.8040441220
H52	5.9852665756	.9719135336	4.0796831449	H24	8.4107697027	2.5835814116	8.9760568307
H53	7.6099992164	.9632380607	5.9693020404	H25	7.6514340902	1.7053766288	11.1980105770
H54	7.6681867989	2.8778276492	7.5890706075	H26	6.8374374882	3.2582460146	10.8429871484
H55	6.0926576039	4.8037054219	7.2819130204	H27	8.1970375804	3.2071903561	12.0029601532
H56	4.4812709477	4.8137761686	5.3981410512	H28	9.9848284603	1.2414981821	10.3385728118
H57	.8039732622	2.9595720125	5.4828644424	H29	10.6671572954	2.7104370441	11.0814059683
H58	3.1031734879	5.6199143038	3.9220143583	H30	10.8337148529	2.4376782541	9.3162715632
H59	2.2378996082	7.7960682704	3.1141986234	H31	8.9709583785	9.0534923807	7.8163716473
H60	-.2157268150	8.3018159504	3.2202928674	H32	9.5666068447	9.4289049435	9.4696257838
H61	-1.7882750802	6.5902388088	4.1661208675	H33	7.8154442708	9.2704414509	9.1689842813
H62	-.9152152548	4.3936543185	4.9592286845	H34	12.8646022279	3.1930138006	9.0842665986
H63	1.9630315181	-.0446144122	4.3586229084	H35	14.0623802270	3.1043162769	11.5454403466
H64	3.6403108305	.4231727083	4.7296752061	H36	14.6597779974	5.7021336200	12.1884697032
H65	4.2386003227	1.3474095693	6.9750639431	H37	13.8055649907	7.2206971076	10.0805329253
H66	3.6273855837	1.5478129317	9.3792423420	C38	14.0434881319	10.1398063637	7.3508169385
H67	1.2637909780	1.1519185178	10.1176361466	C39	14.7499707212	9.0531594045	6.8102063241
H68	-.4753874207	.5356675899	8.4192507558	C40	14.2412686481	7.7493329876	6.9199173564
H69	.1458777779	.3438648967	6.0013756195	C41	13.0154465998	7.5313909863	7.5802859630
H71	2.4092329087	3.6266555814	5.7876034102	C42	12.3068249286	8.6258205990	8.1075526715
PPh <sub>2</sub> pyr				C43	12.8169569370	9.9260534002	8.0017636197
Ligand				H44	14.4439281961	11.1549151555	7.2558167766
P1	-.2281912344	-.2467009439	1.5609138046	H45	15.7010021013	9.2194701044	6.2928966210
C2	1.2425048632	.8078297665	1.9691710211	H46	14.7940417253	6.9096441982	6.4891667004
N3	-1.4313202116	.9824757014	1.1481337330	H47	11.3446589724	8.4096451635	8.5724533048
C4	.2458279063	-.9102439864	-.1035369843	H48	12.2554001125	10.7719994056	8.4124996082
C5	-2.7941477757	.7853124713	1.3905816640	C50	14.4711407578	3.5705634229	4.3699204901
C6	-3.4907901684	1.8690688347	.8845162440	C51	15.0466442444	3.6035426923	5.6496802782
C7	-2.5288082718	2.7662309919	.3136170713	C52	14.3841040714	4.2521536862	6.7050988443
C8	-1.2753058367	2.2001718618	.4808385541	C53	13.1320238438	4.8634318650	6.4820080219
C9	1.2529936811	-.19024498935	-.1401979763	C54	12.5563537147	4.8340391564	5.1932168524
C10	1.6213924999	-.5001723931	-.1354215576	C55	13.2313499134	4.1909835340	4.1453470958
C11	.9741845958	-.21298813953	-.25462959198	H56	14.9883207978	3.0617810564	3.5490809678
C12	-.0411186732	-.11608120881	-.25144764296	H57	16.0145891901	3.1251308580	5.8341903147
C13	-.4062527955	-.5517563939	-.13012624820	H58	14.8409279159	4.2757710567	7.6988659222
C14	1.4303641023	1.1414474240	3.3292393414	H59	11.5897012572	5.3140992926	5.0188126568
C15	2.5248546126	1.9249481242	3.7272699549	H60	12.7769687111	4.1682620517	3.1493474302
C16	3.4533735116	2.3717232171	2.7718138761	PPh( <i>pyr</i> ) <sub>2</sub>			
C17	3.2819891671	2.0351625129	1.4183598394	Ligand			
C18	2.1844251394	1.2567205483	1.0175705441	P1	-.2074435975	-.8997182362	-1.6106095937
H19	-3.1292391198	-.1133537396	1.9076649575	N2	-1.5697076434	-1.8198787830	-.9856218877
H20	-4.5713535368	2.0095107211	.9296417958	N3	1.0664783479	-1.1103019899	-.4144351643
H21	-2.7326024077	3.7285298756	-.1584214742	C4	-.7666296225	.8160798084	-1.2118876795
H22	-.2818941787	2.5571458885	.2143028323	C5	-2.3915221005	-.15992325846	.1267008753
H23	1.7552717042	-.22076517632	.7867631640	C6	-3.3091920924	-.26308772616	.1978882503
H24	2.4103514088	-.32607835168	-.13689208927	C7	-3.0541469811	-.35202225709	-.8995785580
H25	1.2560534376	-.26017153173	-.34942624561	C8	-.19861495761	-.30056438428	-.16083179673
H26	-.5534339551	-.8720720761	-.34393355730	C9	1.0882355784	-.8451724158	.9593237188
H27	-.119040494976	.2092418800	-.12856793071	C10	2.3336781289	-.11951951517	1.4481233292
H28	.7171961001	.7776760877	4.0789338948	C11	3.1114317669	-.16918243736	.3486365669
H29	2.6594423925	2.1770848975	4.7851020937	C12	2.3145930850	-.16370310791	-.7786067621
H30	4.3139480632	2.9746067136	3.0828285431	C13	-2.0864335564	1.2116657322	-1.5305192757
H31	4.0068782143	2.3775849736	.6709479451	C14	-2.4788213493	2.5514154934	-1.3871311915
H32	2.0640531059	.9843377085	-.0368179715	C15	-1.5594356437	3.5138888121	-.9364320097
Complex				C16	-.2424673123	3.1311497306	-.6347225836
Ru1	9.9529120087	5.7528180460	8.0921217533	C17	.1561995922	1.7917599987	-.7747293955
C12	10.0070787755	3.6982349781	6.7914342429	H18	-2.2512440329	-.7196157636	.7518383022
C13	9.9184468946	7.0676072813	6.0408786560	H19	-4.0873998314	-.27358018365	.9549944449
P4	12.2967315767	5.8396047757	7.8024070384	H20	-3.599070967	-.44323497609	-1.1422039925
N5	13.1783548289	5.3210209073	9.2570004133	H21	-1.4735487681	-.3579390582	-2.5026880130
C6	8.8680436842	7.3909750864	9.1778845748	H22	.2122118032	-.4352656185	1.4577910206
C7	9.8454813827	6.8015352189	10.0332284732	H23	2.6547146581	-.1077514184	2.4869582075
				H24	4.1402449266	-.20508503523	.3851349466

H25	2.5047285269	-1.9160101882	-1.8143940271	H12	-.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	-2.848119833	H16	.0408880220	-2.7751914339	4.3682351793				
H30	1.1860936025	1.5034910118	-.5385100543	H17	2.2765261074	-1.7129897442	4.0507562130				
Complex											
Ru1	1.0645324931	-.5183265461	-1.2511317139	C20	1.0516741532	3.5776943276	-1.0199628034				
C12	-.5804530036	-.3377824550	-3.0378510306	C21	1.0088896171	2.1953403254	-.7726035278				
C13	.1634558172	-2.7143997207	-.6778133817	C22	-.1704443940	1.5815662970	-.2949204019				
P4	-.4986115960	.2765326907	.2667424095	C23	-1.3135519471	2.3837866931	-.0867858948				
C5	2.9997812853	-1.5600816110	-1.9708046981	C24	-1.2746131486	3.7635372509	-.3423722192				
C6	3.0095460259	-1.2664108559	-.5452549984	H25	-.0642499537	5.4414473770	-1.0084740086				
C7	2.8684949715	.0604492151	-.0551316127	H26	1.9757201296	4.0371264871	-1.3894415562				
C8	2.6055571012	1.1563882622	-.9586287116	H27	1.8985226038	1.5804153544	-.9561240015				
C9	2.4486439613	.8427322309	-2.3421246797	H28	-2.2455415214	1.9233300816	.2608848870				
C10	2.6988672089	-.4900058095	-2.8426381278	H29	-2.1723741360	4.3720087421	-.1819401923				
C11	3.1900432448	-2.9962813079	-2.4246973529	C30	-4.5268863922	-1.5458198619	-.8411982297				
C12	4.6869064816	-3.3766800000	-2.3175454383	C31	-3.5212743947	-1.6229243619	-1.8191602262				
C13	2.5243439676	2.5761068661	-.4579896555	C32	-2.2093523078	-1.2312374294	-1.5106241690				
C14	2.6311051292	-3.2812233365	-3.8275932727	C33	-1.8786660559	-.7378426261	-.2279756875				
N15	-1.0300214144	1.9306607140	.0312744216	C34	-2.9006845129	-.6667089054	.7453454226				
C16	-2.067762810	-.6049675042	.6323514410	C35	-4.2121317418	-1.0711077645	.4427962049				
N17	.2070927164	.4027549773	1.8889358302	H36	-5.5495473054	-.18617689328	-1.07607091952				
C18	.7242159669	1.5339568399	2.5332403845	H37	-3.7563944239	-1.9992089637	-2.8213568690				
C19	1.4797408036	1.1062874422	3.6133053122	H38	-1.4232399017	-1.3122168454	-2.2714590551				
C20	1.4555307546	-.3273495867	3.6220859339	H39	-2.6773611530	-.2985887904	1.7537874198				
C21	.6783546867	-.7382545434	2.5521913143	H40	-4.9899443177	-1.0131302413	1.2130801306				
C22	-.8920340209	2.6329112378	-1.1768596705	Complex							
C23	-1.5449821508	3.8433599639	-1.0457910264	Ru1	.1507179132	-1.8596117049	.2831353600				
C24	-2.1150947649	3.8930568160	.2702018156	C12	.1839975487	-2.0737664859	-2.1401866806				
C25	-1.8057385464	2.7074020098	.9077049098	C13	-1.7870144913	-3.3503171674	.3402781875				
C26	-2.7749253882	-1.1968859710	-.4359620510	P4	-1.2382561012	.0406095828	-.1164181282				
C27	-4.0193886498	-.17954857625	-.1919876534	C5	2.4271341385	-1.9724696381	.2164666695				
C28	-4.5563260237	-1.8203949514	1.1062368080	C6	1.9079581573	-3.2409314781	.6808888339				
C29	-3.8473323006	-1.2385288625	2.1695007749	C7	1.0027797149	-3.2965781068	1.7700848366				
C30	-2.6050581586	-.6283130471	1.9371884188	C8	.5800355017	-2.1125621163	2.4774393853				
H31	3.1090267760	-2.0923972070	.1651731913	C9	1.0962361154	-.8648650705	1.9985088820				
H32	2.8693859433	.2410054633	1.0255390637	C10	2.0346413785	-.7895240699	.9086808871				
H33	2.1484591524	1.6265786834	-3.0440572517	C11	3.3858353900	-1.9644413834	-.9634289803				
H34	2.5197924551	-.6873667503	-3.9022839829	C12	4.7607253647	-2.5017385415	-.4942157482				
H35	2.6172279035	-3.6139690158	-1.7041822834	C13	-.3808803859	-2.2044428400	3.6337257024				
H36	5.2971418286	-2.7809270798	-3.0210794305	C14	3.5321138259	-.5989109899	-.16506769639				
H37	4.8241934000	-4.4440278542	-2.5653408812	C15	-2.2877392904	.6078613116	1.3532339507				
H38	5.0821763376	-3.2100816605	-1.2994361270	C16	-.1115564683	1.4702498603	-.4582647646				
H39	2.2944687310	2.6043696793	.6193648239	C17	-2.4235772775	.0814385695	-.15329469095				
H40	3.5039146037	3.0697408910	-.6080277892	C18	-3.3413446739	-.4628773867	1.7245516557				
H41	1.7589600329	3.1597003770	-.9957685345	C19	-2.7880570162	1.3166971841	-.21170121854				
H42	3.1947020310	-.27434954443	-4.6132345275	C20	.4210593316	1.6245444254	-.17591208539				
H43	2.7125824768	-4.3598184318	-4.0475214952	C21	-2.9710260735	1.9849860866	1.1753614477				
H44	1.5668617431	-2.9967797661	-3.8938468757	C22	-3.0257738369	-1.1079666935	-.19945186433				
H45	.4516316053	2.5329787604	2.1994697988	C23	.3246869125	2.3460758912	.5610247104				
H46	1.9714706576	1.7579596813	4.3366405011	C24	-4.1020146785	-.0589608595	3.0043984047				
H47	1.9361272946	-.9864601953	4.3460624292	C25	-3.7431308793	1.3623002246	-.31443191937				
H48	.4269525040	-1.7295208064	2.1745018644	C26	1.3502084217	2.6401147980	-2.0313398814				
H49	-.4181665342	2.1449584178	-2.0272740418	C27	-3.7211349496	2.3922632387	2.4619841566				
H50	-1.6217127665	4.6072110368	-1.8200577904	C28	-3.9840172827	-1.0519016967	-3.0198531677				
H51	-2.6939220692	4.7097970103	.7036213969	C29	1.2605381883	3.3580820486	.2862489266				
H52	-2.0633526889	2.3362218861	1.8973262022	C30	-4.7564827171	1.3287505807	2.8713647573				
H53	-2.3445523413	-1.1920961599	-.14425425184	C31	-4.3443016364	.1765313980	-3.5969776371				
H54	-4.5645185599	-2.2566322034	-1.0225822016	C32	1.7732847920	3.5105279209	-1.0118001625				
H55	-5.5244214278	-2.2995479167	1.2912192550	C33	2.1255504110	-4.1490838696	.1116657444				
H56	-4.2558425680	-1.2626444983	3.1859202580	C34	.5219491570	-4.2494931589	2.0129404845				
H57	-2.0510285960	-.1868912883	2.7715680802	C35	.7624205302	.0647075177	2.4733424616				
PPh <sub>2</sub> Cy Ligand											
P1	-.1043846489	-.2506625316	.0400430130	H36	2.3619083157	.1909334466	.5553731858				
C2	.0416584425	-.2483542466	1.9312044037	H37	2.9627806593	-2.6693394748	-.17047406145				
C3	1.5768023607	.3373348914	3.8834829135	H38	5.2125751234	-1.8249721570	.2544422617				
C4	1.3942464436	.3727934507	2.3521771284	H39	5.4515965827	-2.5689230877	-1.3532292775				
C5	-.0809350106	-1.6893069031	2.4787280332	H40	4.6802978557	-3.5051064311	-.0401529464				
C6	.1041875878	-1.7299127519	4.0100133504	H41	-1.2034694803	-.2899120396	3.3924036697				
C7	1.4406434504	-1.0938784409	4.4365779444	H42	.1306141049	-2.5755023493	4.5424683851				
H8	.8114779819	.9873069695	4.3554603221	H43	-.8177746927	-1.2193221470	3.8701596918				
H9	2.5612928087	.7644732394	4.1540415969	H44	4.0095176907	.1476698421	-.9884072113				
H10	2.2168404999	-.1970627011	1.8720842715	H45	4.1714894940	-.6999307165	-2.5452384652				
H11	1.4700484054	1.4120168369	1.9829533606	H46	2.5496163957	-.2160309441	-1.9703259466				
				H47	-1.5622495985	.6771265622	2.1926575106				
				H48	-4.0584295879	-.5593988927	.8851957874				

H49	-2.8688509606	-1.4532323546	1.8381831286	C10	2.8961979718	-2.6852083626	1.4014193704
H50	-2.3148142901	2.2455624197	-1.7822327339	C11	1.7050916837	-1.1437663508	3.1411138380
H51	.1088100861	.9369782868	-2.5522567564	C12	2.7294907412	-.4179017102	4.0488323856
H52	-3.6931586255	1.9165299964	.3389980222	C13	4.4721356620	-1.9787744722	-2.0502050215
H53	-2.2397906644	2.7661699694	.9000558077	C14	1.1499521704	-2.4023567323	3.8295210411
H54	-2.7348031377	-2.0668258576	-1.5552262578	C15	-1.9264316031	-1.5664837499	-1.4382498176
H55	-.0699420154	2.2518806027	1.5788096431	C16	-.9678345604	.0426428236	.8364862475
H56	-4.8646371778	-.8254604836	3.2378615043	C17	.0332561710	.8028424620	-1.82691197826
H57	-3.3950940614	-.0480282430	3.8607720684	C18	-1.8295960483	-1.8974973241	-2.9483159661
H58	-4.0110633973	2.3264816588	-3.5913111858	C19	.8009811270	.4493450542	-3.1242659449
H59	1.7485128909	2.7484543507	-3.0462572575	C20	-.7289381168	1.3855589293	1.2047132365
H60	-4.2102118272	3.3733724135	2.3098639147	C21	-3.2767176466	-.8683461622	-1.1319869038
H61	-2.9885157950	2.5301289469	3.2846884499	C22	-1.1392768158	1.7625661328	-2.1477505086
H62	-4.4412904761	-1.9815987123	-3.3756558744	C23	-1.6245675633	-.8022659731	1.7648346767
H63	1.5803689821	4.0319390081	1.0892579890	C24	-3.0075014910	-2.8009028948	-3.3711177724
H64	-5.5503976382	1.2826924158	2.0983162829	C25	1.3360399745	1.7336969744	-3.7908311989
H65	-5.2516593696	1.6173734453	3.8180120682	C26	-1.14405046207	1.8759255040	2.4559245372
H66	-5.0871440420	.2111390156	-4.4020785523	C27	-4.4540793124	-1.7713660207	-1.5588172671
H67	2.4978073147	4.3035105922	-1.2277991454	C28	-.6117129683	3.0513331593	-2.8148176054
PPhC <sub>2</sub>				C29	-2.0478666598	-.3064358475	3.0074457480
Ligand				C30	-4.3675042361	-2.1565579138	-3.0466246101
P1	.1429295241	-.2920130635	.1341045631	C31	.2043151225	2.7384271773	-4.0834251950
C2	.2845123310	-.0139270149	4.4487503924	C32	-1.8115831119	1.0344791622	3.3584789539
C3	2.0285463515	-.2112999176	.0019383099	H33	.9834717193	.6087857560	1.0544869852
C4	-1.9565315241	-.9866042301	3.7520095788	H34	3.2666712115	.3296102191	-1.1055774137
C5	-1.6618125848	-.6130626708	2.2844440571	H35	3.9399502658	-3.8658669746	-.1081012045
C6	-1.415727695	-.5853908630	1.9985040787	H36	2.6965934584	-3.5596569198	2.0267374853
C7	.5806411475	.3602698140	2.9794943371	H37	.8617945192	-.4494463563	2.9653567086
C8	-1.2294789484	-.0445091722	4.7301818675	H38	3.6059835218	-1.0621391002	4.2476207790
H9	-1.6253704275	-2.0297372943	3.9352124553	H39	2.2663840914	-.1640553541	5.0194524655
H10	-3.0480207621	-.9664317108	3.9346724174	H40	3.0936287920	.5177895158	3.587821690
H11	-2.0877144824	.3885901941	2.0718371239	H41	5.5565557536	-2.0995649438	-1.8657097228
H12	-2.1633047458	-1.3220738902	1.5981333989	H42	4.0919737738	-2.8838699957	-2.5527045899
H13	.2433059341	-1.6156127225	2.1577907992	H43	4.3272616448	-1.1243938759	-2.7309933755
H14	1.6734281778	.3438235711	2.8054788631	H44	1.9639158359	-3.0717439088	4.1665994473
H15	.2434565121	1.3991053886	2.7926388162	H45	.5757998249	-2.1111758904	4.7268696767
H16	.7158576588	-1.0134639663	4.6641011481	H46	.4894274223	-2.9688665009	3.1511646076
H17	.7900846865	.6990967561	5.1281446743	H47	-1.8868897064	-2.5266331485	-.8842926480
H18	-1.6399303285	.9802950651	4.6203256240	H48	.7528454771	1.3528057201	-1.1803657239
H19	-1.4210895660	-.3511429281	5.7761488773	H49	-.8686180407	-2.3884412782	-3.1712256263
C20	3.9632217248	.1857447213	-1.6214750252	H50	-1.8781822788	-.9574999855	-3.5358505964
C21	2.4319192966	.1851817136	-1.4386455572	H51	1.6167429198	-.2618664265	-2.9089594113
C22	2.6451059385	-1.5819129321	.3737292137	H52	.1234507845	-.0721535242	-3.8248903517
C23	4.1771260776	-1.5844183253	.1887136705	H53	-.2207733503	2.0706306421	.5182361399
C24	4.5770170802	-1.1750343864	-1.2413290059	H54	-3.3702967981	-.6228099445	-.0604409544
H25	4.4059786643	.9783669375	-.9833896683	H55	-3.3379245603	.0904045116	-1.6829479184
H26	4.2172921446	.4462373034	-2.6666886651	H56	-1.7188052648	2.0108918102	-1.2404822296
H27	1.9782298516	-.5369461846	-2.1482221640	H57	-1.8374689574	1.2564872233	-2.8420618036
H28	2.0162004681	1.1779064644	-1.6927093637	H58	-.17697140967	-1.8602874087	1.5211808752
H29	2.4370828814	.5482070517	.7011157082	H59	-2.9196623540	-3.7712653261	-2.8426526737
H30	2.3954129520	-1.8509916277	1.4174165913	H60	-2.9322455550	-3.0218081910	-4.4528203411
H31	2.1968951863	-2.3664646996	-.2703744145	H61	2.0819999217	2.2109471199	-3.1199250290
H32	4.6301295446	-.8752040597	.9119141100	H62	1.8715172764	1.4760292898	-4.7240791551
H33	4.5836611060	-2.5844117625	.4333478305	H63	-.9484411395	2.9222773361	2.7172179910
H34	4.2190358147	-.1946572502	-.19536141419	H64	-4.4429412717	-.26913484194	-.9394885625
H35	5.6789544452	-1.1432910418	-1.3382796105	H65	-5.4101948025	-1.2560224241	-1.3440232718
C36	-1.2956488150	4.1476140726	-.3961660523	H66	.0278138989	3.5985090542	-2.0906611642
C37	-2.1244094922	3.0579399933	-.7084653387	H67	-1.4585811836	3.7222826286	-3.0544981749
C38	-1.6513387044	1.7456458477	-.5461192672	H68	-2.5582447723	-.9766214604	3.7081717477
C39	-.3516964509	1.4919530878	-.0492078628	H69	-5.1962701899	-2.8388779154	-3.3159136895
C40	.4697237841	2.6017004537	.2570308449	H70	-4.4952645931	-1.2432963851	-3.6648084788
C41	.0047058507	3.9153750498	.0820285556	H71	.6154002391	3.6707155743	-4.5151076287
H42	-1.6573948907	5.1729286324	-.5322651988	H72	-.4720631337	2.3062732372	-4.8489877341
H43	-3.1367476744	3.2287592094	-1.0921999686	H73	-2.1415997304	1.4186383298	4.3301394874
H44	-2.2928354114	.8986549446	-.8181283419				
H45	1.4852553825	2.4439738468	.6372087163				
H46	.6597655853	4.7605951850	.3234475881				
Complex				PiBu <sub>3</sub>			
Ru1	1.5412710615	-2.0292892227	-.2506713975	Ligand			
Cl2	1.3703626463	-3.1123438939	-2.4292769875	P1	0.0309321597	0.0336511008	0.0242492171
Cl3	-.0620290743	-3.6985408677	.5462719205	C2	-0.0500712502	0.1190983821	1.9106122982
P4	-.3841128772	-.6984813354	-.7622055951	C3	1.9101685299	-.0284767046	-0.1680401380
C5	2.3455845427	-1.4106235669	1.7875005808	C4	-0.2231547073	1.8697987866	-0.3450930244
C6	2.4672879693	-.3495370557	.8312724178	C5	-1.4780674212	0.1240820974	2.5077257391
C7	3.1939551489	-.5036697028	-.3999501712	C6	-2.2143231964	-1.2046201009	2.2535276596
C8	3.7541232579	-1.7700094691	-.7438355352	C7	-1.4238601155	0.4395657388	4.0163216409
C9	3.6057918593	-2.8663520831	.1838249226	C8	2.5426836037	-1.4314932663	-0.0036327456
			C9	4.0794575976	-1.3189279025	0.0589346788	
			C10	2.1104765827	-2.3946389047	-1.1251042968	
			C11	-.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	-2.43884401236	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	[RuCl <sub>2</sub> (p-cymene)] <sub>2</sub>			
H34	0.6046545265	1.8198015054	-2.3486085561	Ru1	-1.7618371670	-0.6490459919	-0.0005169187
H35	-2.4650484738	2.0421744075	-2.0819805973	Cl2	-0.7888514036	-2.8390719226	-0.0067056857
H36	-1.5694168733	0.5330249036	-2.4133388562	Cl3	0.0000000000	0.0000000000	1.6215241140
H37	-1.5530250907	1.8670404166	-3.6079137649	Cl4	0.0000000000	0.0000000000	-1.6257469185
H38	-1.1366701885	4.2362899525	-1.5352075622	C5	-3.1050264558	0.8037154015	-0.9750523699
H39	-0.2914299223	4.0440986114	-3.0962904909	C6	-3.4653533883	-0.5344135871	-1.3874141240
H40	0.6489017826	4.2067389758	-1.5840517950	H7	-3.4311774920	-0.8079396018	-2.4459317299
Complex				C8	-3.7262511394	-1.5310823304	-0.4001196042
Ru1	1.4152752978	0.5571392537	1.6692504817	H9	-3.8732711661	-2.5715575033	-0.7041139505
Cl12	0.4702449462	-0.3425738982	3.7355483454	C10	-3.6297463816	-1.2077379367	1.0005029690
Cl13	2.9280425612	-1.3584299302	1.5353525167	C11	-3.2642836622	0.1221537516	1.3867479021
P4	-0.1009218310	-0.8717195847	0.5116568895	H12	-3.0622692473	0.3361947144	2.4411927909
C5	2.8120253149	1.7686365116	0.3915770379	C13	-3.0334489736	1.1485832004	0.4036006812
C6	1.4587364618	2.1183409508	0.0945103785	H14	-2.6489078311	2.1268743568	0.7037703110
C7	0.5471870647	2.5571234602	1.1230738425	Ru15	1.7618371670	0.6490459919	-0.0005169187
C8	0.9655381567	2.6274659430	2.4840031157	Cl16	0.7888514036	2.8390719226	-0.0067056857
C9	2.3472648248	2.2986601604	2.7865664457	C17	3.1050264558	-0.8037154015	-0.9750523699
C10	3.2349430023	1.8756575517	1.7745205379	C18	3.4653533883	0.5344135871	-1.3874141240
C11	-0.7902294227	-2.3430984890	1.4346464226	C19	3.7262511394	1.5310823304	-0.4001196042
C12	0.6594357125	-1.3648279203	-1.1332545544	H20	3.4311774920	0.8079396018	-2.4459317299
C13	-1.6420351020	0.0967982242	0.0317044854	H21	3.8732711661	2.5715575033	-0.7041139505
C14	0.0542965405	3.0681059279	3.6219322477	C22	3.6297463816	1.2077379367	1.0005029690
C15	3.7774085645	1.2999685755	-0.6670469800	C23	3.2642836622	-0.1221537516	1.3867479021
C16	0.3739202606	4.5379715135	3.9898223558	H24	3.0622692473	-0.3361947144	2.4411927909
C17	-1.4451970860	2.8734100356	3.3468405917	C25	3.0334489736	-1.1485832004	0.4036006812
C18	0.1441850797	-3.3932890743	2.0884253841	H26	2.6489078311	-2.1268743568	0.7037703110
C19	0.7574844480	-4.3859654958	1.0866526856	H29	-2.7728481158	1.5262746259	-1.7262805788
C20	-0.6605326369	-4.1474175820	3.1678727315	H30	-3.7309709299	-1.9937696219	1.7530080506
C21	-2.9353059776	-0.6231636735	-0.4601386026	H31	2.7728481158	-1.5262746259	-1.7262805788
C22	-3.9111356032	-0.8982414993	0.7015293904	H32	3.7309709299	1.9937696219	1.7530080506
C23	-3.6310466084	0.2281297164	-1.5432198696				
C24	-0.1755180637	-1.9040252407	-2.3233577166	[PdL <sub>n</sub> ] complexes			
C25	0.6777028833	-1.8085262042	-3.6078747569	L = PPh <sub>3</sub>			
C26	-0.6744518504	-3.3485863675	-2.1396086672	B3LYP			
H27	1.0996873495	2.0212625858	-0.9370876896	E = -1036.28092 H			
H28	-0.4919804028	2.7727765748	0.8615024732	P1	2.2893556158	0.0002094824	0.0054962915
H29	2.6626312917	2.2564684353	3.8336090653	C2	4.3601835672	4.1815157805	0.0018481748
H30	4.2287288228	1.5078794151	2.0495426742	C3	4.9008505789	3.1668707007	0.7927601576
H31	-1.5271489029	-2.8420942428	0.7745137343	C4	4.3122287508	1.9009190076	0.8136215198
H32	-1.3555459239	-1.8460339890	2.2450638334	C5	3.1674411935	1.6329083718	0.0473370651
H33	1.1520405314	-0.4251291802	-1.4503748985	C6	2.6257722854	2.6673050755	-0.7338787373
H34	1.4912822919	-2.0483071697	-0.8832426659	C7	3.2204581251	3.9282557993	-0.7633616505
H35	-1.2814201632	0.7994708147	-0.7456803261	H8	4.8200311022	5.1662936457	-0.0132736305
H36	-1.8844952636	0.7191172548	0.9133918941	H9	5.7851622721	3.3594750775	1.3954487069
H37	0.3146176896	2.4241071076	4.4840131725	H10	4.7439311537	1.1198512619	1.4316972857
H38	4.5488244040	2.0695714655	-0.8594156040	H11	1.7269433751	2.4831293034	-1.3183954628
H39	3.2605484727	1.0905109953	-1.6190627324	H12	2.7891007811	4.7153992870	-1.3765994896
H40	4.2816334670	0.3743670126	-0.3364169816	C13	3.9965500798	-2.1463732420	3.7802076425
H41	0.1198940196	5.2199755059	3.1571299219	C14	4.6344973395	-2.3390527759	2.5540856214
H42	1.4434292537	4.6790073005	4.2283740538	C15	4.1561460731	-1.7077210261	1.4042052028
H43	-0.2145928747	4.8449051450	4.8729983731	C16	3.0265743658	-0.8772059372	1.4630053118
H44	-1.8065315401	3.5143812989	2.5200699541	C17	2.3855000420	-0.7032059355	2.7009282412
H45	-2.0268185400	3.1451131701	4.2453886217	C18	2.8698043943	-1.3250094227	3.8512983465
H46	-1.6603318272	1.8171040668	3.1117506948	H19	4.3707055414	-2.6382603471	4.6742973591
H47	0.9623151912	-2.8473095943	2.5884891519	H20	5.5091403503	-2.9818627982	2.490852177
H48	-0.0249675883	-4.9381436739	0.5298842095	H21	4.6632620328	-1.8643399739	0.4570666973
H49	1.4164352526	-3.8822676487	0.3598105117	H22	1.4951558556	-0.0810213274	2.7603819368

H23	2.3623308206	-1.1759728104	4.8010298270	C28	2.5333027729	-2.0145450233	-1.8700282609
C24	4.2253518229	-2.2693845274	-3.5808588616	C29	3.1313123796	-2.7211457157	-2.9051640916
C25	4.8616793015	-1.1293661334	-3.0880549784	H30	4.7469997871	-2.7726822691	-4.3293593700
C26	4.3141693197	-0.4265501268	-2.0130541781	H31	5.7234330380	-0.6280698844	-3.5524091537
C27	3.1153053579	-0.8504764547	-1.4194529413	H32	4.6765134049	0.6163526194	-1.6919558732
C28	2.4784046874	-1.9923008746	-1.9336380447	H33	1.6269675268	-2.4020231706	-1.4006998196
C29	3.0315932205	-2.7005596423	-2.9997430814	H34	2.6963979216	-3.6607806084	-3.2431510732
H30	4.6540567368	-2.8161792558	-4.4167625975	M06-L			
H31	5.7892183733	-0.7857111349	-3.5395572376	E=-1036.177731 H			
H32	4.8208524375	0.4569465433	-1.6369466123	P1	2.2324760707	0.0039246326	-0.0003672465
H33	1.5392885112	-2.3247557380	-1.4969832249	C2	4.4172957615	4.0971484503	0.0248078758
H34	2.5266050771	-3.5840732851	-3.3820471649	C3	4.8646238796	3.0941576966	0.8796261766
<b>BP86</b>							
E=-1036.280009 H							
P1	2.2800271649	0.0003672233	0.0058666352	C4	4.2292686765	1.8551310974	0.9032997160
C2	4.3708751937	4.1906939991	0.0042583064	C5	3.1292539490	1.6062473375	0.0746520275
C3	4.9030184724	3.1721368114	0.8101552706	C6	2.6790390721	2.6288330281	-0.7715432186
C4	4.3072208571	1.9007165374	0.8302808655	C7	3.3225577392	3.8611658782	-0.8034491350
C5	3.1638613327	1.6335307207	0.0479875728	H8	4.9183577487	5.0637164536	0.0066149210
C6	2.6288197260	2.6707522946	-0.7484339448	H9	5.7191510846	3.2743540421	1.5305963391
C7	3.2321405838	3.9362086564	-0.7776715241	H10	4.5948603617	1.0738855117	1.5690355357
H8	4.8380189756	5.1821958921	-0.0099935175	H11	1.8156070497	2.4518288580	-1.4140471309
H9	5.7892567636	3.3658582669	1.4261147187	H12	2.9644511157	4.6425579842	-1.4720364766
H10	4.7307246605	1.1107683269	1.4600445220	C13	4.0428120027	-2.1162910831	3.7092132858
H11	1.7281533260	2.4828887474	-1.3462778767	C14	4.5892124631	-2.3777556191	2.4561580814
H12	2.8068982680	4.7283972353	-1.4048542145	C15	4.0673156477	-1.7652288675	1.3195723593
C13	4.0013355684	-2.1551146716	3.7906077237	C16	2.9832784036	-0.8858483975	1.4222502931
C14	4.6346280217	-2.3558756483	2.5540493911	C17	2.4324246405	-0.6416912258	2.6876483225
C15	4.1514387425	-1.7199215467	1.3990848189	C18	2.9626546087	-1.2444135052	3.8232686152
C16	3.0211524731	-0.8780225372	1.4652312660	H19	4.4552742913	-2.5948362114	4.5961146446
C17	2.3833890032	-0.6951723946	2.7129136829	H20	5.4326972337	-0.0604303415	2.3615133983
C18	2.8742928215	-1.3205995826	3.86795546487	H21	4.5100396320	-1.9695585468	0.3451770806
H19	4.3807360716	-2.6524754617	4.6907192217	H22	1.5794051268	0.0316778292	2.7800317152
H20	5.5121863030	-3.0098530588	2.4863517898	H23	2.5270417387	-0.10385391163	4.7998398065
H21	4.6536264185	-1.8800937321	0.4387830437	C24	4.2794512320	-2.2213272530	-3.5207236494
H22	1.4907122850	-0.0602522710	2.7750947379	C25	4.8115354436	-1.0072871882	-3.0968815890
H23	2.3700198745	-1.1643264590	4.8287244100	C26	4.2198413271	-0.3075978003	-2.0480372925
C24	4.2319770771	-2.2695981090	-3.5951971483	C27	3.0787457916	-0.8118208479	-1.4137542378
C25	4.8593446087	-1.1121728546	-3.1082125459	C28	2.5439412323	-0.2086439147	-1.8587992950
C26	4.3060846151	-0.4085855338	-2.0262135092	C29	3.1435507296	-2.7324454195	-2.8973113209
C27	3.1107449672	-0.8508437259	-1.4209568431	H30	4.7468631102	-2.7675474734	-4.3385093637
C28	2.4811086898	-2.0094920285	-1.9284103375	H31	5.6988071758	-0.6025187146	-3.5820153931
C29	3.0413559861	-2.7186104191	-3.0007659940	H32	4.6522405925	0.6363202736	-1.7176754222
H30	4.6662834160	-2.8176458028	-4.4393004560	H33	1.6489159654	-2.4280617038	-1.3801254164
H31	5.7870799555	-0.7547210804	-3.5706491187	H34	2.7193103677	-3.6800412607	-3.2258191623
H32	4.8036467137	0.4920771790	-1.6503886142	[PdL <sub>2</sub> ] B3LYP			
H33	1.5411538712	-2.3538612413	-1.4792473675	E=-2199.386214 H			
H34	2.5425318751	-3.6184721472	-3.3792324773	Pd1	-0.0055093235	-0.0205084688	-0.0560172855
<b>M06</b>				P2	2.3076534625	-0.0143680842	0.0177430721
E=-1035.695557 H				C3	4.2925058228	4.1963275532	0.0978697249
P1	2.2266067184	0.0043723234	0.0001244911	C4	4.8965299477	3.1540658572	0.8019230146
C2	4.4166790230	4.0931988447	0.0159905887	C5	4.3250081045	1.8802376152	0.7982827229
C3	4.8789405200	3.0873833857	0.8566074022	C6	3.1393054894	1.6368687234	0.0900171157
C4	4.2439222328	1.8500774692	0.8854906605	C7	2.5313291798	2.6960317778	-0.6018179054
C5	3.1314242847	1.6085124914	0.0763556045	C8	3.1086098972	3.9650795370	-0.6053506944
C6	2.6666132524	2.6318185985	-0.7550460277	H9	4.7386576656	5.1877924477	0.1038005266
C7	3.3085369517	3.8627969239	-0.7926939566	H10	5.8140734638	3.3317667396	1.3577910923
H8	4.9180204851	5.0597836299	-0.0064931627	H11	4.8012129154	1.0767660195	1.3527440555
H9	5.7454777452	3.2642710112	1.4928105580	H12	1.5954737673	2.5187715337	-1.1277774636
H10	4.6208144248	1.0642942777	1.5407721707	H13	2.6288308624	4.7759464793	-1.1476493167
H11	1.7909274399	2.4561844853	-1.3828300876	C14	3.9824449820	-2.1704267117	3.7940503194
H12	2.9389058353	4.6478294159	-1.4509924026	C15	4.6433167356	-2.3307993238	2.5759960795
C13	4.0424268991	-2.1101882007	3.7084887635	C16	4.1650857856	-1.6977696009	1.4267757120
C14	4.6022178152	-2.3581449095	2.4605145819	C17	3.0142648039	-0.8982326383	1.4819550094
C15	4.0803552890	-1.7493279579	1.3239178486	C18	2.3477858013	-0.7556848003	2.7098623244
C16	2.9848488781	-0.8884620397	1.4238444101	C19	2.8328058642	-1.3796264364	3.8583373027
C17	2.4211247437	-0.6574288662	2.6820483752	H20	4.3558291642	-2.6646494586	4.6873129530
C18	2.9499739736	-1.2562542496	3.8182107762	H21	5.5341604761	-2.9515116943	2.5172473401
H19	4.4552702931	-2.5863392280	4.5967538322	H22	4.688851187	-1.8318428402	0.4846324253
H20	5.4567068823	-3.0279173710	2.3699373749	H23	1.4377113756	-0.1612440373	2.7537247084
H21	4.5333015186	-1.9425003377	0.3510232498	H24	2.3069533888	-1.2568686132	4.8020428614
H22	1.5568338483	0.037718745	2.7687323231	C25	4.2726470874	-2.2408253280	-3.5669789165
H23	2.5038200748	-1.0609384020	4.7924162255	C26	4.9134268547	-1.1195733625	-3.0387504135
C24	4.2793921570	-2.2238554591	-3.5131278781	C27	4.3484020709	-0.4271907083	-1.9659168512
C25	4.8251407565	-1.0218675582	-3.0781696311	C28	3.1309461367	-0.8480791145	-1.4117139210
C26	4.2337797908	-0.3199712236	-2.0327471012	C29	2.4866921131	-1.9688668340	-1.9608676070
C27	3.0813417666	-0.8112877128	-1.4154165730	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
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C62	-3.1940219101	0.0829886637	-1.6305247177	H69	-2.5331809163	-0.2205453537	-4.9493243597
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H65	-4.9004037377	0.6196565034	-5.0935386489				
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H67	-5.0016261628	0.9363507882	-0.8079304374				
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<b>BP86</b>							
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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				
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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				
C39	-4.3289505713	0.5516398376	1.8731931697				
C40	-3.2204069880	0.9307427169	1.1127527099				
C41	-2.7720714836	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				
C46	-2.8718054478	-1.9401359726	0.4332540261				
C47	-4.0402142169	-2.5167752645	-0.1075909644				
C48	-4.4294414823	-3.8129183687	0.2676348955				
H49	-3.9626623487	-5.5585148187	1.4722687611				
H50	-1.1650732526	-2.2521635059	1.7325713597				
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H52	-5.3372812668	-4.2530077814	-0.1626967481				
C53	-4.3584837477	0.5959786011	-4.0961887429				
C54	-4.9503541248	3.0261188660	1.0403091407				
C55	4.3363755875	1.7795131975	0.9594739275				
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C58	3.2620259741	3.9581093723	-0.4047141345				
H59	4.9000848302	5.0895970608	0.4218773465				
H100	5.8508467225	3.1480620341	1.6422687036				
H111	4.7598907109	0.9284051820	1.4959649580				
H121	1.7209388913	2.5899795045	-1.0529246594				
H131	2.8369316354	4.8098026297	-0.9356401810				
C141	3.9256424885	-2.4573434225	3.5651857431				
C151	4.5892552320	-2.5302735513	2.3441801738				
C161	4.1275806302	-1.8025590276	1.2502283178				
C171	2.9920206792	-0.9989834155	1.3702625010				
C181	2.3217053334	-0.9426563841	2.5974600983				
C191	2.7911938293	-1.6600596261	3.6915443606				
H201	4.2890996466	-3.0291534751	4.4196046959				
H211	5.4733131093	-3.1591106029	2.2405197120				
H221	4.6539678972	-1.8626956305	0.2953529002				
H231	1.4172809732	-0.3345849954	2.6797533085				
H241	2.2634840890	-1.6056978400	4.6441479117				
C251	4.2301059317	-1.9715350764	-3.7132982745				
C261	4.8747814730	-0.8881778698	-3.1250392237				
C271	4.3196607999	-0.2624552168	-2.0119844105				
C281	3.1090479323	-0.7146113996	-1.4826289802				
C291	2.4595774878	-1.7948007773	-2.0888560105				
C301	3.0216461081	-2.4259412876	-3.1924096073				
H311	4.6673681163	-2.4597260058	-4.5846311912				
H321	5.81764965						

H46	-1.8887900833	2.5418310948	0.5971075182	C53	-4.2574433800	-3.7382285624	0.7765515947
H47	-3.0763133933	4.2169694092	1.9979439970	H54	-3.6950909095	-5.2819283255	2.1707078630
C48	-3.5985264032	-4.3631921145	1.5937387887	H55	-1.6332367408	-4.1020354664	2.9060943461
C49	-2.4665980525	-3.7220798280	2.0872889881	H56	-1.0315602276	-1.9072351479	1.8986646382
C50	-2.0921359060	-2.4831538820	1.5796930556	H57	-4.5761223845	-2.0554046972	-0.5298049353
C51	-2.8550192365	-1.8640799804	0.5846361094	H58	-5.156644739	-4.2560343990	0.4449394624
C52	-3.9877974706	-2.5146671108	0.0920570668	C59	-4.4225045190	-0.0690348372	-4.1012680338
C53	-4.3550401127	-3.7604059508	0.5945121145	C60	-5.0767437035	0.4516231647	-2.9885603164
H54	-3.8871112919	-5.3400749351	1.9831725463	C61	-4.4579793428	0.4384447513	-1.7408647542
H55	-1.8654126512	-4.1951664796	2.8628632798	C62	-3.1719738068	-0.0918490506	-1.5959734594
H56	-1.1894644979	-1.9852533279	1.9425856186	C63	-2.5155256463	-0.5984094607	-2.7251495647
H57	-4.5860796614	-2.0460276185	-0.6907516268	C64	-3.1399624081	-0.5961970111	-3.9668860308
H58	-5.2373947313	-4.2636757372	0.2008979233	H65	-4.9084994546	-0.0567871416	-5.0755993676
C59	-4.3811607277	0.1280145751	-4.1091456896	H66	-6.0766125733	0.8705018126	-3.0906050473
C60	-5.0405197474	0.6144258255	-2.9850523364	H67	-4.9781389947	0.8446813665	-0.8730324294
C61	-4.4393803271	0.5364738392	-1.7312013618	H68	-1.4998755866	-0.9847841813	-2.6163083146
C62	-3.1685327917	-0.0256367781	-1.5949592619	H69	-2.6195354597	-0.9962601664	-4.8356449082
C63	-2.5064687672	-0.4991632948	-2.7319996559	[PdL <sub>3</sub> ]			
C64	-3.1130564561	-0.4309634618	-3.9810040323	B3LYP			
H65	-4.8540881281	0.1910720376	-5.0897072028	E= -3235.677136 H			
H66	-6.0307976695	1.0584080249	-3.0834235045	Pd1	6.9840965099	-1.7454600420	-0.5588489995
H67	-4.9632112495	0.9155396081	-0.8521219735	C1	6.9070277412	0.8384400827	4.8908570227
H68	-1.5014668628	-0.9149920242	-2.6253097192	C2	8.2632746253	0.9063981833	4.5703654066
H69	-2.5894875141	-0.8052200156	-4.8603503061	C3	8.6918109135	0.6574788791	3.2648511663
M06-L							
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P2	2.2806293279	0.0410433243	-0.0120383922	C5	6.4082424931	0.2458711062	2.6015513522
C3	4.5369090028	4.0496513909	0.5071311069	C6	5.9788616805	0.5089897960	3.9014318351
C4	5.0107735346	2.9221388988	1.1723829838	H7	6.5756117722	1.0329966615	5.9080165090
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C6	3.2020302369	1.6008476520	0.2496791706	H9	9.7502732231	0.7199961518	3.0292641060
C7	2.7239012025	2.7448944278	-0.4024717021	H10	5.6879135717	-0.0416282008	1.8386909249
C8	3.3919950653	3.9583502511	-0.2829718518	H11	4.9214359554	0.4414035284	4.1452694822
H9	5.0554593081	5.0018281276	0.6099075030	C12	8.2696543320	4.2643536000	-1.4026781025
H10	5.9016626375	2.9905631838	1.7957798967	C13	7.9450219940	4.1279870570	-0.0541601252
H11	4.7301862752	0.8225169712	1.5630775331	C14	7.9347437083	2.8657523631	0.5454442124
H12	1.8136987032	2.6713624634	-1.0011648914	C15	8.2421685919	1.7187513491	-0.2002022365
H13	3.0120135026	4.8388088804	-0.7990029364	C16	8.5532096752	1.8687903027	-1.5619665674
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C16	4.0490784252	-1.8539430127	1.1870374953	H19	7.7025577159	5.0059601370	0.5405669170
C17	2.9196436386	-1.0397695306	1.3215515707	H20	7.6893435746	2.7795000618	1.5992646843
C18	2.2312606594	-1.0314318036	2.5407254895	H21	8.7701128495	0.9908769587	-2.1650215131
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H21	5.3606344482	-3.2704619983	2.1371020107	C24	12.3743030293	0.2717758027	0.6888243206
H22	4.5902838512	-1.8766730136	0.2417719190	C25	11.0234877475	0.6172153297	0.6264944540
H23	1.3349365889	-0.4145379676	2.6325191644	C26	10.0321098086	-0.3761905799	0.5759104800
H24	2.1307867054	-1.7862647025	4.5511547742	C27	10.4326040046	-1.7222589465	0.5727945613
C25	4.2001512273	-1.8521177147	-3.7743084000	C28	11.7831991167	-2.0672568976	0.6403779569
C26	4.8609787832	-0.8039535466	-3.1406790070	H29	13.8111291571	-1.3370185345	0.7459923004
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C28	3.0795927673	-0.6522195101	-1.5069801031	H31	10.7396620634	1.6656787263	0.6102897684
C29	2.4150893643	-1.6980707744	-2.1607558217	H32	9.6769452204	-2.5006759104	0.4997353243
C30	2.9758241733	-2.3002079203	-3.2804155381	H33	12.0713095655	-3.1158059125	0.6369919309
H31	4.6354513152	-2.3160642013	-4.6575636745	P34	8.2170744118	-0.0029874559	0.4959592440
H32	5.8150412216	-0.4472233161	-3.5266558924	C35	10.1359100706	-2.6870369534	-5.5146408715
H33	4.8334469371	0.6090734880	-1.5164792028	C36	8.8493408752	-2.8950441200	-6.0160051392
H34	1.4444333077	-2.0246822924	-1.7800053082	C37	7.7302922204	-2.5692597924	-5.2467798059
H35	2.4512772936	-3.1152590753	-3.7763026660	C38	7.8768652129	-2.0275621440	-3.9592402243
P36	-2.2816451635	-0.1819838596	0.0021113948	C39	9.1765468361	-1.8365278768	-3.4611965379
C37	-4.6102423934	2.8696838044	2.5879425181	C40	10.2948729968	-2.1573740294	-4.2325825088
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C39	-4.3325336605	0.5931478145	1.8324355298	H42	8.7133976590	-3.3145068155	-7.0102717582
C40	-3.2298744577	0.9727803401	1.0598342553	H43	6.7366638597	-2.7442159140	-5.6496359832
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C42	-3.5110508551	3.2564410130	1.8243952406	H45	11.2904144962	-2.0007210016	-3.8240390847
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H45	-4.6575896323	-0.4477306583	1.8399412903	C48	6.3602004894	0.6475932545	-4.7276592709
H46	-1.9423878573	2.6029851066	0.4934084118	C49	5.9818725407	0.1266178395	-3.4812434576
H47	-3.1832610636	4.2951753142	1.8237190445	C50	5.1927218239	0.9218464927	-2.6349959517
C48	-3.4382566889	-4.3132352209	1.7445333392	C51	4.7736667437	2.1922002426	-3.0307751452
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C50	-1.9503457210	-2.4203818138	1.6042262065	H53	6.2593270463	2.3144518556	-6.0866997416
C51	-2.7755886222	-1.8260222394	0.6413772559	H54	6.9760836977	0.0560851527	-5.3991525757
C52	-3.9306545443	-2.5004851920	0.2280376646	H55	4.9198494409	0.5418149109	-1.6528450273
				H56	4.1630822997	2.7914556087	-2.3597574050
				C57	3.0533005219	-4.2614533646	-4.6351423498

C58	3.0247281766	-2.8902723141	-4.8827819716	H31	10.5800105787	1.7416021937	1.0881666496
C59	4.0322603720	-2.0611600606	-4.3825808635	H32	9.7144423662	-2.4291770992	0.3294852333
C60	5.0810930415	-2.5923591907	-3.6182878190	H33	12.1358359222	-2.9904830003	0.6461105002
C61	5.0886902151	-3.9738825823	-3.3628919819	P34	8.1635417495	0.0099985122	0.4880688618
C62	4.0925068708	-4.8019900205	-3.8738548029	C35	10.1213820824	-2.7610074564	-5.5655768536
H63	2.2690911301	-4.9053283092	-5.0261469613	C36	8.8193551117	-3.0052555714	-6.0326693323
H64	2.2187481046	-2.4586344127	-5.4721900877	C37	7.7064124074	-2.6736854897	-5.2417960110
H65	3.9986954913	-0.9972248132	-4.5945281262	C38	7.8790928751	-2.0902997997	-3.9671622196
H66	5.8769202385	-4.4035768409	-2.7509277477	C39	9.1939108763	-1.8636000084	-3.5010970652
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P68	6.4404113258	-1.5658094901	-2.8737069041	H41	10.9876757714	-3.0226236779	-6.1844834737
C70	2.2087402483	-5.4074539912	-0.1780291493	H42	8.6659687007	-3.4588798942	-7.0194271684
C71	3.2565360209	-6.3052017071	0.0316801727	H43	6.6955312572	-2.8745335853	-5.6145676469
C72	4.5464594965	-5.8350416333	0.2875699020	H44	9.3360966001	-1.4437581579	-2.4965846545
C73	4.8079451777	-4.4575510554	0.3274094467	H45	11.3160782686	-2.0036782477	-3.9143919910
C74	3.7483671160	-3.5651511227	0.0990784630	C46	5.1725102377	2.6598160816	-4.2936714582
C75	2.4575892384	-4.0343128832	-0.1413396134	C47	5.9774755467	1.8753779806	-5.1353729530
H76	1.2052032497	-5.7759188677	-0.3768071153	C48	6.3856082514	0.5916958816	-4.7343208316
H77	3.0708667738	-7.3765362605	-0.0005000343	C49	6.0014260340	0.0781437084	-3.4775326347
H78	5.3501078654	-6.5461028562	0.4556681605	C50	5.2087293925	0.8835520461	-2.6311501150
H79	3.9482609506	-2.4957572598	0.0958597290	C51	4.7878620358	2.1577637165	-3.0388764760
H80	1.6498095862	-3.3277582603	-0.3158460825	H52	4.8551567062	3.6606279669	-4.6088835428
C81	6.5900096072	-3.5797817089	5.3467904979	H53	6.2894671629	2.2614614547	-6.1136296421
C82	5.4402356265	-4.0457203758	4.7119541030	H54	7.0069804660	-0.0137520020	-5.4042950335
C83	5.3811379545	-4.1123942442	3.3172138457	H55	4.9372824006	0.5044230421	-1.6375517267
C84	6.4716491850	-3.7046227778	2.5358746836	H56	4.1720613565	2.7676706433	-2.3674063406
C85	7.6188886299	-3.2225878380	3.1886778105	C57	3.0311558642	-4.3098988681	-4.5790280740
C86	7.6823081594	-3.1695583727	4.5786281180	C58	3.0614045960	-2.9490588512	-4.9179340119
H87	6.6345257848	-3.5298387907	6.4321251013	C59	4.0799164823	-2.1173384202	-4.4226961137
H88	4.5830808621	-4.3650868122	5.3006821431	C60	5.0789733236	-2.6371949927	-3.5726013723
H89	4.4813020712	-4.4882884327	2.8404118986	C61	5.0284761747	-4.0052854006	-3.2257626504
H90	8.4675115421	-2.8786838356	2.6033006187	C62	4.0212185022	-4.8367776629	-3.7324251328
H91	8.5796627794	-2.7917361790	5.0620547922	H63	2.2353648944	-4.9570524682	-4.9667123017
C92	9.4313092618	-7.2079959364	-0.2745070384	H64	2.2908828381	-2.5277665777	-5.5753022614
C93	8.7549425572	-7.2037860615	0.9465012799	H65	4.0976658103	-1.0585359467	-4.7024223911
C94	7.8669761495	-6.1722291430	1.2554425943	H66	5.7821836972	-4.4179122729	-2.5448202421
C95	7.6398930084	-5.1274003793	0.3453841475	H67	3.9995468897	-5.8956119094	-3.4497234634
C96	8.3373217141	-5.1362328610	-0.8733069791	P68	6.4619344372	-1.6144740844	-2.8558938106
C97	9.2207673219	-6.1707350178	-1.1838902890	C70	2.1875665485	-5.1249637787	0.0883385024
H98	10.1241671732	-8.0117508228	-0.5120475136	C71	3.1860089569	-6.0930502804	0.2828618203
H99	8.9189619091	-8.0053457737	1.6631377691	C72	4.5242858147	-5.7048708256	0.458478862
H100	7.3523667259	-6.1778280809	2.2120603087	C73	4.8813417004	-4.3408820192	0.4276630689
H101	8.1965277845	-4.3158604665	-1.5725427856	C74	3.8718776822	-3.3774028316	0.2157867994
H102	9.7507801536	-6.1584444898	-2.1332788017	C75	2.5331521819	-3.7641740661	0.0579253359
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BP86							
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C1	6.3761406829	0.8799895402	4.7231939542	H78	5.2951334248	-6.4686151736	0.6124199335
C2	7.7712651207	0.8626031546	4.5740518695	H79	4.1563654036	-2.3185199429	0.1565128588
C3	8.3477987660	0.6063836323	3.3189574585	H80	1.7613653903	-3.0030076870	-0.1068611001
C4	7.5323086647	0.35499646838	2.1968383167	C81	7.0711794445	-3.7574005626	5.3496778253
C5	6.1292582930	0.3543745792	2.3630843824	C82	5.8134648571	-4.0054142160	4.7802443166
C6	5.5546401740	0.6260229351	3.6120077650	C83	5.6515444465	-4.0097338293	3.3837994026
H7	5.9293475437	1.0802118999	5.7042207895	C84	6.7478290387	-3.7606655574	2.5315585636
H8	8.4186108442	1.0496726424	5.4395242592	C85	8.0059253360	-3.4895041462	3.1170621549
H9	9.4386773066	0.5989020380	3.2146048431	C86	8.1682973758	-3.4991015185	4.5091335024
H10	5.4910294854	0.1238682886	1.5002710273	H87	7.1962534097	-3.7581502610	6.4387568812
H11	4.4635996979	0.6252908214	3.7219711984	H88	4.9474153205	-4.2034231524	5.4236780796
C12	8.4000641592	4.2775730812	-1.4388962182	H89	4.6648639871	-4.2174254213	2.9561048951
C13	8.0588465221	4.1625857888	-0.0830239258	H90	8.8677997744	-3.2668181543	2.4767645236
C14	7.9786434288	2.8974056631	0.5229534513	H91	9.1558239218	-3.2950340714	4.9398713350
C15	8.2316706602	1.7286694268	-0.2252551339	C92	9.2960870346	-7.3224637958	-0.6141667074
C16	8.5567627527	1.8559779173	-1.5932588863	C93	8.7046549017	-7.3300087710	0.6598675796
C17	8.6507523447	3.1185519721	-2.1929639778	C94	7.9016005233	-6.2554902396	1.0729133548
H18	8.4631407125	5.2658120130	-1.9098724542	C95	7.6753140250	-5.1587054733	0.2123449756
H19	7.8569881682	5.0617331564	0.5120839359	C96	8.2863078792	-5.1556531348	-1.0600259134
H20	7.7197881343	2.8199536507	1.5846802027	C97	9.0869793550	-6.2319809250	-1.4729817244
H21	8.7254746992	0.9544499080	-2.1945357497	H98	9.9261610760	-8.1615732124	-0.9325710161
H22	8.9028360902	3.1962094961	-3.2569690596	H99	8.8717841606	-8.1754105709	1.3382884633
C23	12.7161643735	-0.9370600225	1.0596463733	H100	7.4577994211	-6.2610314024	2.0750786347
C24	12.2727478291	0.3902580395	1.1814724344	H101	8.1380548851	-4.2899928022	-1.7187439010
C25	10.9144203978	0.7003592575	1.0117317631	H102	9.5548513478	-6.2111751907	-2.4643401973
C26	9.9769993471	-0.3171170267	0.7284997641	P103	6.6090189786	-3.7047214029	0.6709032138
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Pd1	6.8775072925	-1.7504429132	-0.5586701487				
C1	6.7780478151	0.6201502351	4.8707853911				
C2	8.0982800133	0.9056975950	4.5361851010				
C3	8.5447600925	0.7182098760	3.2328212992				

C4	7.6743462439	0.2416093836	2.2501664062	C84	6.5671816121	-3.6759549755	2.5573608154
C5	6.3526103643	-0.0479781404	2.5990431799	C85	7.7183404401	-3.1388331976	3.1482360248
C6	5.9036974273	0.1442340852	3.9000335595	C86	7.8187057238	-3.0117163450	4.5262818402
H7	6.4328851232	0.7609019259	5.8944206117	H87	6.8311786382	-3.2873683925	6.4248258441
H8	8.7859946807	1.2746545081	5.2965422671	H88	4.7713868926	-4.2237606902	5.3969002723
H9	9.5817884100	0.9412641671	2.9782264711	H89	4.6018609540	-4.4770926099	2.9499942402
H10	5.6827071326	-0.4536357854	1.8359588136	H90	8.5473731778	-2.8091622776	2.5175324756
H11	4.8743447376	-0.0983898078	4.1602029447	H91	8.7227342728	-2.5892144305	4.9631751512
C12	8.2458245034	4.1764864065	-1.4070586645	C92	9.6825810281	-6.8090278210	-0.5431586649
C13	7.7883145140	4.0395067605	-0.1026728240	C93	9.2557246955	-6.7877118576	0.7806353721
C14	7.7813037384	2.7896974403	0.5132322230	C94	8.2881551950	-5.8754381931	1.1913258748
C15	8.2233187223	1.6601536781	-0.1772340844	C95	7.7360767302	-4.9714010173	0.2792284836
C16	8.6678024551	1.8079220794	-1.4974081999	C96	8.1758481271	-5.0000032838	-1.0496030754
C17	8.6899317185	3.0547689387	-2.1038595612	C97	9.1390953467	-5.9127676368	-1.4600812989
H18	8.2509356375	5.1552865734	-1.8857896848	H98	10.4444846388	-7.5209622062	-0.8591994595
H19	7.4376822985	4.9123414481	0.4477455871	H99	9.6803636323	-7.4860472690	1.5019180813
H20	7.4274328775	2.6966376953	1.5405927734	H100	7.9617156649	-5.8618376939	2.2324001569
H21	8.9900079459	0.9286077009	-2.0605737450	H101	7.7691760157	-4.2766981558	-1.7609920476
H22	9.0355911070	3.1493215918	-3.1329225133	H102	9.4718724856	-5.9117361966	-2.4978944827
C23	12.6178583433	-1.2914635155	0.7209375846	P103	6.4760380729	-3.7030253170	0.7172911383
M06-L							
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C27	10.2817681427	-1.8323965450	0.4941183181	Pd1	6.7919300101	-1.7130873075	-0.5481324549
C28	11.6102367730	-2.2374945580	0.5619535048	C1	6.8352269586	0.6127103406	4.9196132347
H29	13.6603826430	-1.6028059448	0.7691172194	C2	8.1365772379	0.9213753095	4.5314014514
H30	13.0729286899	0.8056695133	0.9169308013	C3	8.5325449009	0.7425486431	3.2093760177
H31	10.7122998237	1.5257063851	0.7855043014	C4	7.6325304257	0.2484518601	2.2592053330
H32	9.4911650134	-2.5711549903	0.3369995381	C5	6.3299610627	-0.0649105427	2.6638483624
H33	11.8526489956	-3.2969161538	0.4787981796	C6	5.9302207320	0.1222687555	3.9827585405
P34	8.1481033765	-0.0473311685	0.4988999741	H7	6.5307262308	0.7443241723	5.9571528537
C35	10.0692852919	-3.0017534793	-5.3245238918	H8	8.8488319318	1.3004743071	5.2635351962
C36	8.7914654547	-3.1792886700	-5.8477282929	H9	9.5543179704	0.9823280714	2.9135741730
C37	7.6734074942	-2.7558907327	-5.1346364966	H10	5.6409391521	-0.4903988668	1.9293425878
C38	7.8191127959	-2.1484396438	-3.8843407393	H11	4.9172041641	-0.1404390289	4.2842489531
C39	9.1080800359	-1.9863134342	-3.3616463722	C12	8.3349808986	4.1689137376	-1.3955418160
C40	10.2245024548	-2.4029310995	-4.0766819998	C13	7.8339547990	4.0442433831	-0.1043082771
H41	10.9416629379	-3.3354404431	-5.8850000630	C14	7.7670119920	2.7937975817	0.5086208116
H42	8.6614523519	-3.6521743833	-6.8209767812	C15	8.1915937933	1.6476683981	-0.1715803706
H43	6.6763512041	-2.9006802479	-5.5545484579	C16	8.6795447932	1.7849989530	-1.4801526577
H44	9.2266867732	-1.5433459468	-2.3694172237	C17	8.7619314826	3.0322733315	-2.0822996284
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C48	6.6280841915	0.6371809441	-4.7027481336	H21	8.9843749474	0.8943190628	-2.0355451802
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C50	5.4850811004	1.0442250141	-2.6220728291	C23	12.4838536142	-1.4491107678	0.5579000739
C51	5.2370655869	2.3553202106	-3.0078472409	C24	12.2005944829	-0.0932654023	0.7102526798
H52	5.5050885421	3.8431578673	-4.5429988047	C25	10.8828521438	0.3549457914	0.6974893244
H53	6.7474592380	2.3109328154	-6.0505149622	C26	9.8250856369	-0.5499511348	0.5406070302
H54	7.1729133002	-0.0321409470	-5.3709875785	C27	10.1265112626	-1.9083811319	0.3713707073
H55	5.1639778703	0.6886130337	-1.6398525019	C28	11.4432123090	-2.3575455935	0.3845639163
H56	4.7104646450	3.0299454361	-2.3332662338	H29	13.5171622409	-1.7936336754	0.5635352622
C57	2.8580159278	-3.8968991552	-4.7131148667	H30	13.0125489695	0.6219855394	0.8349861109
C58	3.1082883637	-2.6037086847	-5.1613977042	H31	10.6710737108	1.4205164958	0.7958296977
C59	4.1661279393	-1.8701511815	-4.6320547413	H32	9.3088331067	-2.6135184552	0.2013346925
C60	4.9836194791	-2.4231713998	-3.6421792022	H33	11.6497950879	-3.4187114224	0.2456004525
C61	4.7140204172	-3.7194158572	-3.1910488288	P34	8.0579868597	-0.0511374358	0.5014394044
C62	3.6654984539	-4.4557583400	-3.7259011174	C35	10.2253779018	-2.9352646727	-5.0686999112
H63	2.0268885999	-4.4665533422	-5.1275800654	C36	8.9826276325	-3.1412169834	-5.6643942835
H64	2.4752654086	-2.1600830989	-5.9302332204	C37	7.8159517664	-2.7270055378	-5.0245509916
H65	4.3550275479	-0.8581365674	-4.9937371168	C38	7.8764046051	-0.2099161159	-3.7738339565
H66	5.3256893489	-4.1466884043	-2.3922551407	C39	9.1323907848	-1.9077018847	-3.1798115902
H67	3.4693548461	-5.4615118682	-3.3533871442	C40	10.2964476662	-2.3159265330	-3.8211167237
P68	6.4059902632	-1.5503563852	-2.8643985258	H41	11.1341653071	-3.2636368169	-5.5711488105
C70	2.4101110896	-5.7953704486	0.0022177766	H42	8.9186659524	-3.6300811723	-6.6362109663
C71	3.5224353382	-6.5777972578	0.2971079326	H43	6.8483511954	-2.8986383431	-5.4978993768
C72	4.7571973715	-5.9783250597	0.5175735738	H44	9.1835573046	-1.4503056764	-2.1880869225
C73	4.8931310133	-4.5898920765	0.4332341893	H45	11.2599966849	-2.1592170515	-3.3367536199
C74	3.7728377159	-3.8136193159	0.1259614576	C46	5.6585578588	2.8010073726	-4.2892657389
C75	2.5351435087	-4.4112731650	-0.0803086780	C47	6.3420177258	1.9224668422	-5.1262712423
H76	1.4442009895	-6.2678403071	-0.171772177	C48	6.5776761852	0.6116678661	-4.7221922993
H77	3.4274797083	-7.6621683000	0.3588466671	C49	6.1341750668	0.1663334404	-3.4720879359
H78	5.6249711968	-6.5948275534	0.7565252225	C50	5.4643343216	1.0643991115	-2.6319909156
H79	3.8891124021	-2.7306629548	0.0256583763	C51	5.2190433046	2.3693271755	-3.0400928261
H80	1.6706596421	-3.7968126535	-0.3277598540	H52	5.4804606914	3.8280861271	-4.6046098107
C81	6.7588670334	-3.3983959194	5.3437014950	H53	6.6958331997	2.2603107375	-6.0998662276
C82	5.6069746463	-3.9189279000	4.7675729029	H54	7.1135399434	-0.0723959903	-5.3823421162
C83	5.5108649177	-4.0607137005	3.3847589475	H55	5.1620299892	0.7299271227	-1.6365793755

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
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C82	5.7464663781	-3.9706283456	4.7670223650	H54	5.8629533884	-0.4582008943	-4.7934304020
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	0.9131773380	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
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C94	8.2407238094	-5.8238174427	1.0709043523	H66	-0.5291550704	3.4955767575	0.5105578160
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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
<b>[PdL<sub>4</sub>] B3LYP</b>							
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P2	1.7395685183	1.7409593461	0.9799314961	H78	-5.3723029636	-4.1763401268	-1.6038628752
P3	-1.1923745564	1.6979450356	-1.9830983178	C79	-4.2879270690	-2.3126247232	-1.4860739657
C4	3.0022938091	2.8373817247	0.1481288039	H80	-4.8463040323	-1.8321872588	-2.2854261184
C5	-0.3676711357	3.0035722073	-3.0290903016	C81	-3.2622397259	-1.6132551235	-0.8519678541
C6	-2.4999221692	2.7468859513	-1.1627642844	H82	-3.0357797348	-0.6041137565	-1.1763610543
C7	-3.8697112085	4.7498542253	-0.9652189366	C83	-2.8106133117	-3.5207098392	0.5478867872
C8	-2.8453591783	4.0384295579	-1.5937581759	H84	-2.2529523484	-4.0045547804	1.3427328784
H9	-4.1217252430	5.7484582457	-1.3158500778	C85	-3.8313457449	-4.2267710637	-0.0935704046
H10	-2.3192374080	4.4928337778	-2.4271960110	H86	-4.0449574261	-5.2502887254	0.2071648862
P11	-1.1967765088	-1.1613212383	1.0046967170	C87	0.8711489324	-4.5689918902	3.4607592941
P12	1.7448493748	-1.1986294967	-1.9671219564	H88	1.3506565956	-5.3781141669	4.0067966973
C13	0.8816934967	2.9961954965	2.0652444630	C89	1.2998085290	-4.2365310133	2.1745585112
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C15	-2.2293384983	-0.3250149236	2.3220465487	C91	-3.6716124107	-0.4835634856	-5.3185703340
C16	-0.3765404936	-2.4726229637	2.0482784538	H92	-4.2272433782	-0.9982089834	-6.0986609537
C17	-2.5140132379	-2.1975949200	0.1817860325	C93	-4.2755715554	0.5322973648	-4.5755289623
C18	3.0361745715	-2.2625354505	-1.1424244603	H94	-5.3063298584	0.8164660054	-4.7768518198
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C25	4.7100725554	3.0545967968	-1.5789816334	C101	4.2854268036	0.9269550063	-5.2941330021
H26	5.2477104513	2.6149785655	-2.4151780187	H102	4.8549804748	1.4255292200	-6.0746361508
C27	4.2673255795	4.9047326810	-0.1001202770	C103	2.9856779109	1.3393709639	-4.9939793780
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				H107	-0.5112082593	-4.0973344624	5.0488091693

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C112	4.3457396694	-0.4279708840	4.2258741015	C51	4.0788071197	-0.8242248179	-3.5296664133
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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
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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
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C126	-4.2320308243	2.9046089608	0.5438005614	C65	-0.2424111847	3.6603342523	1.5912236834
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C132	-0.0618385156	4.2765197725	-5.0820486725	C71	-3.6367265864	0.9544399828	4.3928687184
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P11	-1.1946035237	-1.1187790125	0.9363754162	H88	1.2641728114	-5.4075833647	3.9706747361
P12	1.7155076238	-1.1888521705	-1.8822241432	C89	1.2653368967	-4.2415962638	2.1354218270
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C18	3.0412615240	-2.2210777367	-1.0541088050	C95	-3.4881160961	1.2263985054	-3.5807971517
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C23	3.6294238713	2.3823983591	-1.0184016480	H100	-0.5609232124	-0.5277973549	-3.7800649780
H24	3.4189637771	1.3798970531	-1.4048925250	C101	4.2225942664	0.8261615403	-5.3168428450
C25	4.5824939144	3.1818626964	-1.6675263888	H102	4.7842922289	1.2955069617	-6.1335853520
H26	5.1118059367	2.7825320594	-2.5403798579	C103	2.9296603111	1.2719090359	-4.9990701569
C27	4.1307209668	4.9792735526	-0.1052785837	H104	2.4706820282	2.0973217778	-5.5555502895
H28	4.3181294081	5.9969063719	0.2595549457	C105	-2.1577707154	0.8576182203	-3.2810908225
C29	3.1840910435	4.1740701864	0.5522085148	H106	-0.2567596380	-3.8552102951	3.9843265817
H30	2.6505829878	4.5723172542	1.4219835113	H107	-0.6241620921	-4.1097656420	4.9862897908
C31	5.1489007326	-3.6466702860	0.2053659314	C108	-0.8559376244	-2.8016334979	3.2753402403
H32	5.9627903320	-4.1979116549	0.6908919796	H109	-1.6867443522	-2.2515623265	3.7295799227
C33	-0.8385180623	-4.2462507794	-3.0714869590	C110	0.6735251071	-3.1817357766	1.4330615756
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C35	-0.1906626528	-3.2266444612	-2.3577513232	C112	4.4744968357	-0.4901695595	4.0407213326
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C37	1.2914829940	-2.8405144748	-4.2350210519	C114	4.9684771716	0.6280016028	3.3489185985
H38	2.1273788828	-2.3072640949	-4.699985810	H115	5.9898076901	0.9834743889	3.5347680324
C39	0.6351360489	-3.8540265506	-4.9550281007	C116	4.1624407882	1.3028235707	2.4154366066
H40	0.9659621871	-4.0904639733	-5.9740905542	H117	4.5631946737	2.1773751741	1.8914607994
C41	-0.4312511269	-4.5629125072	-4.3778509711	C118	4.8361079565	4.4876859165	-1.2158672588
H42	-0.9408142649	-5.3529842799	-4.9420651999	H119	5.5746475015	5.1175667839	-1.7258143759
C43	3.2404099583	-3.5946207747	-1.3141167850	C120	-0.9033509119	4.6025979646	2.3931303496
H44	2.5835405671	-4.1181676713	-2.0168463065	H121	-1.7574709621	5.1519991124	1.9808813211
C45	4.2831964774	-4.2994062068	-0.6866497998	C122	-0.4874327214	4.8210310747	3.7170413299
H46	4.4198279865	-5.3657886711	-0.9056311358	H123	-1.0068513208	5.5513483588	4.3487531162
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H127	-4.7592868563	2.4934616075	1.3448711281	H66	-0.5003494365	3.4802423629	0.4029624834				
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C130	-0.5851166746	3.2185761974	-4.3876418010	C69	-1.6300717701	0.7140011267	2.9219083792				
H131	-1.3025283721	2.5658837835	-4.8963171149	H70	-0.6026982581	1.0127122404	2.7142617842				
C132	0.0359482451	4.2556132778	-5.1062829249	C71	-3.6839903871	1.0702730463	4.1229211782				
H133	-0.2024246853	4.3918144326	-6.1685704594	H72	-4.2633855373	1.6199172076	4.8638272070				
C134	2.3629916531	-0.2618282512	2.8511887331	C73	-4.2693877802	0.0267531382	3.4128116836				
H135	1.3567335882	-0.6388283738	2.6415872395	H74	-5.3074344256	-0.2467009576	3.6002958860				
C136	3.1631630065	-0.9278848576	3.7912377208	C75	-3.5360846911	-0.6759343573	2.4597064304				
H137	2.7612209654	-1.8049227394	4.3115782697	H76	-4.0093267497	-1.4904417425	1.9101727594				
M06											
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Pd1	0.2544589535	0.2718702993	-0.4959603124	H77	-4.3771835656	-3.6818243642	-1.2771820426				
P2	1.6925995495	1.7031194704	0.9430407709	H78	-5.1369285251	-4.2488828183	-1.8143147715				
P3	-1.1889560574	1.7085020647	-1.9174958551	C79	-4.1011769702	-2.3653585506	-1.6358077402				
C4	2.9620872449	2.7557882675	0.1075620451	H80	-4.6295410790	-1.8879942774	-2.4618614003				
C5	-0.3457548193	2.9748174825	-2.9666788059	C81	-3.1253377774	-1.6539198522	-0.9506085346				
C6	-2.4539609401	2.7679077136	-1.0773954310	H82	-2.8967223401	-0.6331158743	-1.2558581234				
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H10	-2.1626240916	4.5692731139	-2.2338786448	H86	-3.8842274871	-5.3039091341	0.0522536961				
P11	-1.1475936460	-1.1833122571	0.9428788537	C87	1.0846011637	-4.3895021040	3.4804377364				
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C13	0.8605112259	2.9748302079	1.9958337017	C89	1.4714496743	-4.0929629691	2.1754171241				
C14	2.7461161644	0.8746751898	2.2160648299	H90	2.3246669228	-4.5943667459	1.7177354221				
C15	-2.2032747860	-0.3402760217	2.2041724757	C91	-3.6906623943	-0.5205678005	-5.1506673886				
C16	-0.3074167095	-2.4494145761	2.0003095224	H92	-4.2581766769	-1.0590569821	-5.9079549243				
C17	-2.4156753582	-2.2327385726	0.1051028529	C93	-4.2850761442	0.5141328137	-4.4345990587				
C18	2.9811505448	-2.1895802618	-1.1048768454	H94	-5.3200049330	0.7908515578	-4.6337855849				
C19	2.7520140030	-0.3101569380	-3.2128449781	C95	-3.5663126940	1.2057361747	-3.4615918800				
C20	0.8627749187	-2.4117888010	-2.9794464353	H96	-4.0465371064	2.0162387822	-2.9123477778				
C21	-3.1822319343	2.1963815569	-0.0299831315	C97	-2.3672759883	-0.8632128035	-4.8866711516				
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C23	3.6769332247	2.1853748954	-0.9488289765	C99	-1.6536866006	-0.1741502272	-3.9149305821				
H24	3.4533555339	1.1662940855	-1.2626652565	H100	-0.6271337166	-0.4705371403	-3.6999286039				
C25	4.6505966359	2.9043581368	-1.6285376192	C101	4.2078002889	1.0401856844	-5.1918171566				
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C27	4.2114766271	4.8042351048	-0.2189216694	C103	2.9022045938	1.4253438536	-4.9010482476				
H28	4.4171778211	5.8342888092	0.0717705119	H104	2.4362841538	2.2599955476	-5.4249901615				
C29	3.2382047735	4.0792059191	0.4637405417	C105	-2.2369564400	0.8703679983	-3.1916600804				
H30	2.6929077055	4.5494492696	1.2826365350	C106	0.0030368561	-3.7165691686	4.0429224012				
C31	4.9355018947	-3.6583530576	0.2684956664	H107	-0.3089171608	-3.9412527739	5.0633624757				
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C33	-0.8539569693	-4.1160243272	-3.1002662612	H109	-1.5340300764	-2.2361138353	3.7669091256				
H34	-1.6665920180	-4.6630163787	-2.6132363083	C110	0.7810165952	-3.1308380692	1.4486708251				
C35	-0.1676373453	-3.1462428791	-2.3870019153	H111	1.1161725375	-2.8822143042	0.4412685461				
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C39	0.4884993074	-3.6371615872	-5.0347293231	H115	5.8230830995	0.8538782614	3.6746023426				
H40	0.7503965652	-3.8259874494	-6.0758768584	C116	4.0682278009	1.2361578744	2.4918295687				
C41	-0.5320694663	-4.3634712745	-4.4305942045	H117	4.5361904563	2.0555231896	1.9441736187				
H42	-1.0758639788	-5.1176781980	-4.9987510881	C118	4.9209166229	4.2199097723	-1.2632144658				
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H44	2.6972086469	-3.9877192055	-2.2691787291	C120	-0.8688167151	4.6703594313	2.1454949087				
C45	4.2197876307	-4.2436445566	-0.7710890493	H121	-1.6912476906	5.2083749010	1.6733339770				
H46	4.4169105127	-5.2769940849	-1.0560236916	C122	-0.5077225916	4.9330414929	3.4638763410				
C47	4.6756770879	-2.3386399228	0.6263458455	H123	-1.0394959628	5.6909859764	4.0378038699				
H48	5.2130521858	-1.8666670130	1.4494511395	C124	1.3974455165	4.6571900761	-3.1035821907				
C49	3.7045204545	-1.6171024709	-0.0548397769	H125	2.2231922783	5.1866432341	-2.6271064578				
H50	3.4900170918	-0.5944484123	0.2539128114	C126	-4.1506199345	2.9214658754	0.6533296104				
C51	4.0654567439	-0.6861608889	-3.5087639138	H127	-4.6917936558	2.4479135189	1.4723938761				
H52	4.5313435460	-1.5114800836	-2.9698242532	C128	-4.4043216712	4.2447968790	0.3032473600				
C53	4.7869326213	-0.0132754802	-4.4917138301	H129	-5.1561531740	4.8222892855	0.8393096610				
H54	5.8098088717	-0.3184911282	-4.7124115935	C130	-0.6921095672	3.2511593464	-4.2927661099				
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H56	1.1754233568	1.0829994062	-3.6764202606	C132	0.0007680064	4.2197579652	-5.0144091817				
C57	1.0440507320	4.9251978932	-4.4235524003	H133	-0.2803605416	4.4241903716	-6.0477665046				
H58	1.5853387064	5.6789997784	-4.9938938177	C134	2.1775573617	-0.1810215578	2.9346164504				
C59	0.7079661307	3.6884613092	-2.3878660317	H135	1.1584205923	-0.4964761662	2.7126060199				
H60	1.0133093394	3.4668000251	-1.3648341049	C136	2.8979756443	-0.8561233759	3.9113439292				
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C63	1.2131481376	3.2442558925	3.3214827359	E= -4271.678999 H							
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				P2	1.6746878865	1.6934125194	0.9286759243				
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C4	2.9540496668	2.7437723398	0.1149192253	C83	-2.8151888371	-3.4312370394	0.3947186669
C5	-0.3278618614	2.9847256500	-2.9348708275	H84	-2.2603917184	-3.9694720525	1.1626810515
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H9	-4.1577218872	5.6497741324	-1.3249658719	H88	1.4435237059	-5.3977718612	3.8151082977
H10	-2.3672246812	4.3949673791	-2.4697594508	C89	1.3780182194	-4.2060800239	2.0156281908
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P12	1.7100047897	-1.1407632099	-1.8983434711	C91	-3.5432443265	-0.5572289426	-5.2544858401
C13	0.8426040272	2.9650377197	1.9733379229	H92	-4.0870373567	-1.0972665039	-6.0281794624
C14	2.7056307164	0.8517617035	2.2048930604	C93	-4.1557861927	0.4866229546	-4.5647294985
C15	-2.1123283555	-0.3203937321	2.2665081353	H94	-5.1814916253	0.7696822766	-4.8011671606
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C18	3.0398562371	-2.1117646024	-1.0699687801	C97	-2.2311493936	-0.9073906184	-4.9396550437
C19	2.6985301244	-0.3342696240	-3.2293357067	H98	-1.7363551485	-1.7283667907	-5.4575982726
C20	0.8880039627	-2.4715063770	-2.8724736092	C99	-1.5480582828	-0.2205979551	-3.9424767774
C21	-3.1093478730	2.1709214304	-0.0098388321	H100	-0.5330572208	-0.5207139782	-3.6837692199
H22	-2.7811681847	1.2118208647	0.3873496579	C101	4.0644509856	0.9645317329	-5.3111888397
C23	3.6450958485	2.2041459144	-0.9753002166	H102	4.5985996505	1.4696048198	-6.1151158040
H24	3.3882664806	1.2062479115	-1.3256560633	C103	2.7702385868	1.3554140651	-4.9743058718
C25	4.6300249089	2.9294050692	-1.6354905924	H104	2.2812648915	2.1729842594	-5.5035661648
H26	5.1457134956	2.4830295102	-2.48467676913	C105	-2.1473517598	0.8353879854	-3.2465011042
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C29	3.2614667968	4.0503391657	0.5166167590	C108	-0.7738467979	-2.8881710536	3.1931925346
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C33	-0.8374429118	-4.1807283901	-2.9343153430	C112	4.1451939648	-0.5357216580	4.1761712252
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C35	-0.1666810008	-3.1632700027	-2.2668368695	C114	4.7221270131	0.5461575828	3.5167350761
H36	-0.4783640128	-2.8826750817	-1.2615123887	H115	5.7364473513	0.8583409580	3.7644461339
C37	1.2480734796	-2.8172942649	-4.1808473234	C116	4.0103607870	1.2366490796	2.5385144346
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C39	0.5742676533	-3.8340676097	-4.8537692873	C118	4.9330668368	4.2248602353	-1.2213931032
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C41	-0.4672943609	-4.5192610872	-4.2340978234	C120	-0.8982189124	4.6532769979	2.1300525133
H42	-0.9950198147	-5.3091502292	-4.7667420430	H121	-1.7308181126	5.1819280705	1.6670666109
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C70	5.3449183213	2.9312041394	19.8743896690	C68	5.2970826660	4.7346237399	21.6455469351
C71	4.6616983045	1.9798911391	19.0425541685	C69	4.6202523918	3.8433728285	20.8260455164
C72	3.1570129233	1.9809362248	19.0081353116	C70	5.3300662243	2.9342915509	19.9827787593
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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
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			P5 2.8448732463	3.1999713308	16.2774148975	C81 2.2974058846	2.2837566501	17.8058310750
			C6 4.3000543971	4.4650035496	12.0279384129	C82 3.6788206074	4.7167823699	16.9656602554
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			C18 5.5566213996	1.8920389877	11.4055340908	H94 3.2054811011	4.9922398372	13.8077230691
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			C20 7.4004151413	0.6654864253	10.3625615367	H96 4.2970828344	6.3262565774	9.1642847511
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P3	2.8894791818	0.2304326384	13.1031584683	C81	2.2936270167	2.3214294831	17.7582181476
P4	5.0753561845	0.5083561539	16.4466862905	C82	3.7244027417	4.7254085451	16.9267160735
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C35	0.3536610015	2.1331194495	10.4615863694	H113	0.2384402480	1.0302527057	12.2871702304
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C73	2.6145156090	1.0653632694	19.8568901219	H151	10.1412767116	5.2939232401	14.4503123904
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P2	5.1048736987	2.9257697635	12.8596040726	C80	0.9584610526	1.7614341137	17.8408777654
P3	2.8290044117	0.2785432798	13.0481373201	C81	2.3047237340	2.2157254515	17.7973377708
P4	5.1291096838	0.5628149549	16.4893151240	C82	3.6944218382	4.6319430730	16.9675655363
P5	2.8178692569	3.1572795470	16.2918404671	C83	4.7896522462	5.1096920813	16.2471188545
C6	4.2775699567	4.3254252173	12.0018951388	C84	5.4883309095	6.2383265023	16.6653817778
C7	3.2556231875	4.9839946622	12.6853267573	C85	5.0943944243	6.9110664192	17.8170092624
C8	2.5971043636	6.0677838473	12.1149243482	C86	4.0063948776	6.4411269933	18.5495353043
C9	2.9606103552	6.5107502152	10.8485804327	C87	3.3161485827	5.3095622738	18.1318004208
C10	3.9815747662	5.8655375050	10.1572198302	C88	1.2208101297	3.9154185099	15.7408817258
C11	4.6328247387	4.7794155913	10.7278879516	C89	0.7578053694	3.5536819253	14.4754020264
C12	6.7364261703	3.6957919033	13.2890042588	C90	-0.4243165352	4.0800856697	13.9649492657
C13	7.2704569989	3.3873468235	14.5411813202	C91	-1.1660775578	4.9765599958	14.7228080924
C14	8.4929484020	3.9087005043	14.9511583362	C92	-0.7160802061	5.3492012872	15.9872193025
C15	9.1982863059	4.7601757478	14.1098452062	C93	0.4651111153	4.8220850292	16.4921728108
C16	8.6715085869	5.0892832181	12.8632512806	C94	2.9666210055	4.6339992365	13.6763946772
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C18	5.5568573708	1.7923121732	11.4661238435	C96	4.2583047496	6.1950551909	9.1558329356
C19	6.8985216663	1.3253742519	11.4303514797	C97	5.4058261820	4.2582173370	10.1611684333
C20	7.3081057369	0.3862761972	10.5272393526	C98	6.6982633774	2.7361083049	15.2053566251
C21	6.4091018577	-0.1330331932	9.5718897194	C99	8.8847326258	3.6550927700	15.9366185061
C22	6.8354960552	-1.0698747634	8.6024570781	H100	9.2154111195	5.7631878414	12.2019532269
C23	5.9688771347	-1.5464894115	7.6540707378	H101	7.0512840023	4.8411084846	11.4825516515
C24	4.6305338745	-1.1040372612	7.6515496182	H102	7.6211188040	1.7310238279	12.1383751986
C25	4.1871950162	-0.2104602004	8.5933672283	H103	8.3432841998	0.0431293031	10.5154540223
C26	5.0589622129	0.3142632586	9.5843833936	H104	7.8755788830	-1.3970647168	8.6241492098
C27	4.6268912456	1.2646943626	10.5684119662	H105	6.3091619082	-2.2604489764	6.9056188466
C28	3.1829173236	1.6679098818	10.5703863932	H106	3.9389897025	-1.4792565298	6.8980419562
C29	2.6973456049	2.4932435910	9.5022907073	H107	3.1472220241	0.1089468675	8.5799805324
C30	3.5241214160	2.9086682359	8.4250176035	H108	4.5665547035	2.5973076384	8.4076665858
C31	3.0319409811	3.6770676415	7.4012179756	H109	3.6891436906	3.9682017707	6.5828341689
C32	1.6880010041	4.1015839932	7.4035622788	H110	1.3092591198	4.7175058092	6.5893411705
C33	0.8627903956	3.7287649501	8.4323545340	H111	-0.1813071117	4.0424391040	8.4526232226
C34	1.3380870452	2.9170216950	9.4881307358	H112	-0.5629448529	2.8019628438	10.5073541279
C35	0.4817834680	2.4868037271	10.5239401635	H113	0.2511521024	1.3163490889	12.2779424429
C36	0.9421798895	1.6595041890	11.5087309618	H114	5.0336572719	-1.2767972866	13.9978143232
C37	2.2953895286	1.2263827755	11.5506515087	H115	6.2229210518	-3.2880803147	13.1984975870
C38	3.6678885780	-1.2029321206	12.3404705012	H116	3.6485498337	-3.4177638926	9.7517483229
C39	4.7260690191	-1.7519513202	13.0663326432	H117	2.4909320652	-1.3925986762	10.5374779189
C40	5.3933132986	-2.8872630864	12.6158378896	H118	1.3177891618	0.6804426533	15.4235892155
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C42	3.9483312046	-2.9605747060	10.6946319619	H120	-1.2508102529	-2.6651199906	12.8267707317
C43	3.2885621398	-1.8234407824	11.1449509308	H121	0.8674476331	-1.7852716180	11.9406685446
C44	1.2301365522	-0.4677136055	13.6154921780	H122	5.4732085699	-0.7822806511	19.1805564455
C45	0.7352450817	-0.0432939335	14.8491000835	H123	4.3509950106	-2.7267086242	20.1899799380
C46	-0.4586770563	-0.5459827529	15.3563623487	H124	1.7921241044	-3.0437238008	16.7399026046
C47	-1.1792085142	-1.4849793281	14.6290084952	H125	2.9489054244	-1.1143071160	15.7177123657
C48	-0.6941924070	-1.9240840888	13.3996124997	H126	7.2241604661	-1.0968928373	17.9788663713
C49	0.4992294926	-1.4211030147	12.8982365360	H127	9.3497017734	-2.0842873634	17.2384122804
C50	4.3050282847	-0.8312197235	17.3605856971	H128	8.7171397379	-0.5026379903	13.2887367188
C51	4.6896752608	-1.2977511991	18.6227617539	H129	6.5808648336	0.4989483729	14.0451683064
C52	4.0490352102	-2.3866135938	19.1990119996	H130	7.6387685335	1.7820839018	17.2112544019
C53	3.0081507810	-3.0218973080	18.5267614307	H131	8.3381270523	3.4922895174	18.8238177340
C54	2.6126697824	-2.5640184141	17.2741893680	H132	7.8453633993	4.9356906093	20.7095744733
C55	3.2621203663	-1.4779633574	16.6969867844	H133	6.2594157780	5.7920943943	22.4141197815
C56	6.7564344794	-0.2147415382	16.0614126442	H134	3.8985898929	4.9826056182	22.4160802211
C57	7.5460565405	-0.9542585506	16.9488317989	H135	3.1356229147	3.3670065335	20.7457272019
C58	8.7461959915	-1.5144204496	16.5326971091	H136	4.6010570169	0.8784259934	20.9362546089
C59	9.1775076851	-1.3516232925	15.2183777598	H137	3.7464583223	-0.5100571162	22.7612956414
C60	8.4013156221	-0.6263446425	14.3241623133	H138	1.3794546698	-1.2985511008	22.7560294177
C61	7.2019311361	-0.0621582784	14.7477856143	H139	-0.1245464202	-0.6425859798	20.8953086052
C62	5.5753330018	1.6988175023	17.8800765486	H140	-0.5264275279	0.5935706598	18.8430824074
C63	6.9098394365	2.1856529186	17.9139324183	H141	0.2613954871	2.0955716439	17.0725310885
C64	7.3075141670	3.1333424763	18.8136265595	H142	5.1024747914	4.5796822861	15.3472759942
C65	6.3992304903	3.6448134490	19.7649514118	H143	6.3448980903	6.5829103291	16.0855327888
C66	6.8091522786	4.5954013094	20.7285920630	H144	3.7058547407	6.9455849582	19.4679247266
C67	5.9319868943	5.0673461224	21.6701952807	H145	2.4956344831	4.9297994789	18.7422104584
C68	4.5989701973	4.6082199045	21.6702531704	H146	1.3570441839	2.8636981651	13.8765710981
C69	4.1716325551	3.7004766730	20.7345756632	H147	-0.7539872494	3.7917372689	12.9666258584
C70	5.05533369601	3.1778254798	19.7530501875	H148	-1.2923292729	6.0540107912	16.5857930285
C71	4.6384256094	2.2141702681	18.7765455255	H149	0.8037307176	5.1303810891	17.4803382344
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H153	-2.1140596248	-1.8846191310	15.0207619528	C72	3.2051751552	1.7844981161	18.7583632594
H154	2.5003287834	-3.8684823321	18.9870447152	C73	2.7327014220	0.9775810448	19.8453451299
H155	10.1177361665	-1.7959385272	14.8950049237	C74	3.5772569386	0.5676339205	20.9102020536
H156	5.6391633848	7.7927424321	18.1529968133	C75	3.1003393964	-0.1925087646	21.9520350975
H157	-2.0913432436	5.3953196238	14.3280106169	C76	1.7535641107	-0.6042923237	21.9823496702
M06-L							
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Pd1	3.9786829395	1.7146732614	14.6675489177	C78	1.3658578860	0.5601468556	19.8881748950
P2	5.1105250585	2.8787573036	12.8821118012	C79	0.4982551250	0.9761443795	18.8555627831
P3	2.8335774452	0.3150601881	13.0694268411	C80	0.9513782514	1.7777055821	17.8425987670
P4	5.1172548244	0.5744829037	16.4567237543	C81	2.3055869600	2.2053100332	17.7709079347
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C6	4.2750987254	4.2866075753	12.0582730269	C83	4.7530919448	5.1140966325	16.1672166446
C7	3.2864346651	4.9635035175	12.7784330868	C84	5.4332504630	6.2562036831	16.5780147618
C8	2.6304119587	6.0628678941	12.2338470166	C85	5.0553266954	6.9035229220	17.7505852908
C9	2.9605819514	6.5038856379	10.9554319618	C86	4.0030155775	6.3980073324	18.5126633058
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C12	6.7315343559	3.6547327562	13.3063693551	C89	0.7412346195	3.4321849490	14.4530624444
C13	7.2731346331	3.3869799049	14.5662540930	C90	-0.4608376224	3.9228598786	13.9517678374
C14	8.4957860783	3.9278645915	14.9535739295	C91	-1.1890303253	4.8529058687	14.6857005551
C15	9.1937315110	4.7572960758	14.0827260412	C92	-0.7031765414	5.2969795372	15.9145264322
C16	8.6604725184	5.0447944168	12.8275994983	C93	0.4964092959	4.8021379414	16.4132021437
C17	7.4403522017	4.5003705716	12.4436500294	H94	3.0266371564	4.6099562114	13.7771703083
C18	5.5729150376	1.7703001892	11.4854435519	H95	1.8544843439	6.5658588310	12.8117568989
C19	6.9147432993	1.3027850956	11.4372960090	H96	4.1947668218	6.1663524314	9.2173270214
C20	7.3266889267	0.3832734502	10.5108372719	H97	5.3421956056	4.2029164541	10.1819583590
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C22	6.8500114362	-1.0381322127	8.5566735886	H99	8.8939580837	3.7088055220	15.9440589422
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C25	4.1986357948	-0.1798289400	8.5709737779	H102	7.6352798128	1.6925424557	12.1551818897
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C27	4.6421232064	1.2642159800	10.5686257705	H104	7.8900595177	-1.3658006560	8.5669997474
C28	3.2040765783	1.6735525872	10.5758860359	H105	6.3151955336	-2.2065812355	6.8433547237
C29	2.7236475948	2.4901096126	9.4978793303	H106	3.9427031626	-1.4314574494	6.8614021576
C30	3.5588966390	2.9070603310	8.4276170376	H107	3.1572250351	0.1341570300	8.5683375997
C31	3.0746563368	3.6780421446	7.3972221426	H108	4.6037311986	2.6037877946	8.4233024988
C32	1.7301085008	4.0976529742	7.3852234475	H109	3.7409772238	3.9741890239	6.5878601126
C33	0.8940660347	3.7232852562	8.4093799564	H110	1.3574972467	4.7129601413	6.5676678666
C34	1.3591206238	2.9164931254	9.4730533099	H111	-0.1499593465	4.0376287767	8.4187040572
C35	0.5012341272	2.5007702355	10.5134124438	H112	-0.5423838008	2.8180633597	10.4938946198
C36	0.9600439030	1.6889532082	11.5152792823	H113	0.2680568848	1.3646010630	12.2909878522
C37	2.3117252257	1.2491586803	11.5692574197	H114	4.9701237460	-1.2671367554	14.1212202133
C38	3.6759416384	-1.1776863667	12.4087023711	H115	6.1462606504	-3.3158329222	13.3826489751
C39	4.6922723120	-1.7465888048	13.1816149543	H116	3.7257126099	-3.3992529644	9.8232145441
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C41	5.0019973189	-3.5044643105	11.5597290232	H118	1.3091542669	0.7706675305	15.4331124715
C42	3.9912518553	-2.9470094208	10.7785288913	H119	-0.8631587164	-0.0641779707	16.3089226938
C43	3.3348789931	-1.7944586632	11.1984691147	H120	-1.2627651631	-2.5792788881	12.8395808677
C44	1.2336586942	-0.4027272323	13.6398937144	H121	0.8883282573	-1.7395018424	11.9769601586
C45	0.7217710579	0.0495716137	14.8592341306	H122	5.4347618866	-0.7699123248	19.1406272539
C46	-0.4907709571	-0.4256910275	15.3499133535	H123	4.3307974793	-2.7426199534	20.1300975887
C47	-1.2112736418	-1.3663672139	14.6218266858	H124	1.8341965006	-3.0934070088	16.6378417632
C48	-0.7069247384	-1.8362798348	13.4100811090	H125	2.9683940248	-1.1296136060	15.6439068010
C49	0.5039121473	-1.3585061274	12.9224433132	H126	7.1924830694	-1.0913452998	17.9194427936
C50	4.2985530351	-0.8349824379	17.3039890208	H127	9.3407969387	-2.0491263167	17.1875267100
C51	4.6712950894	-1.3022589599	18.5710871212	H128	8.7481814291	-0.3939685928	13.2595051150
C52	4.0401739071	-2.4063111751	19.1345243176	H129	6.5817815739	0.5648678254	14.0056832135
C53	3.0219349257	-3.0616364920	18.4438215840	H130	7.6319270192	1.7912452494	17.1669206848
C54	2.6375773498	-2.6017305464	17.1863759907	H131	8.3477897769	3.4614506734	18.8108676629
C55	3.2737438005	-1.4982387242	16.6243498592	H132	7.8686053819	4.8813950693	20.7257925986
C56	6.7435275984	-0.1793672102	16.0114071137	H133	6.2904199846	5.7254497247	22.4451994066
C57	7.5290445658	-0.9298198343	16.8963985977	H134	3.9238398658	4.9329979908	22.4371383887
C58	8.7415163927	-1.4711645924	16.4850739398	H135	3.1473974149	3.3452426931	20.7464318510
C59	9.1904616583	-1.2767771155	15.1790474858	H136	4.6238347475	0.8650393407	20.8987901800
C60	8.4175705941	-0.5411469211	14.2874138151	H137	3.7734418156	-0.4842685806	22.7573381682
C61	7.2052262170	0.0012469132	14.7043880466	H138	1.3868665946	-1.2107438511	22.8091847648
C62	5.5735653566	1.6962696913	17.8440700594	H139	-0.1375494102	-0.5436779825	20.9688455657
C63	6.9097231809	2.1793854837	17.8832577837	H140	-0.5478019568	0.6678204753	18.8897222515
C64	7.3159984034	3.1089643593	18.8015108057	H141	0.2528596723	2.1039097248	17.0735622617
C65	6.4165678542	3.6097582940	19.7667337940	H142	5.0497694161	4.5974462199	15.2537289487
C66	6.8315843930	4.5447433353	20.7422364959	H143	6.2638414123	6.6313091752	15.9797417086
C67	5.9570678677	5.0115343719	21.6934531944	H144	3.7208281148	6.8834801136	19.4463248245
C68	4.6222043138	4.5615513612	21.6882301786	H145	2.5387820753	4.8382580958	18.7288185646
C69	4.1868294449	3.6652966551	20.7402458025	H146	1.3359958396	2.7216835297	13.8734096810
C70	5.0646981186	3.1480805301	19.7506307453	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	14.380847431
H152	5.5207698572	-4.4009790500	11.2233015483
H153	-2.1602044971	-1.7437916696	15.0006924391
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H155	10.1398374086	-1.7047436074	14.8591748160
H156	5.5873885272	7.7947691020	18.0810648684
H157	-2.1291923742	5.2433161745	14.2980252297