Electronic Supplementary Material (ESI) for Dalton Transactions

The inhibition of iridium-promoted water oxidation catalysis (WOC) by cucurbit[*n*]urils.

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Electronic Supporting Information

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$Cp^*Ir(H_2O)_3^{2+}$, gas phase *33*

CB7, gas phase. *37*

host-guest complex gas phase *45*

$CB[7]\bullet[Cp^*Ir(H_2O)]^{2+}$ 55

H_2O *58*

CB7, COSMO *60*

$Cp^*Ir(H_2O)_3Cl_2$ – 1, COSMO *63*

$Cp^*Ir(H_2O)_3Cl_2$ – 2, COSMO *66*

$Cp^*Ir(H_2O)_3Cl_2$ –3, COSMO *70*

host-guest, Cl_2, COSMO *73*

$Cp^*Ir(H_2O)_2(O)^{2+}$, gas phase *77*

host-guest $Cp^*Ir(H_2O)_2(O)^{2+}$, gas phase *82*

host-guest $Cp^*Ir(H_2O)_2(O)^{2+}$, gas phase *86*

Experimental setup for the production of O_2

Figure 1. The volumetric glass vessel used in this study. The O_2 galvanometric probe was fixed to the top ground joint via a Teflon adaptor.

1. Relationship between the measured saturation and the molar amount of produced O_2 gas.

n_{O2} : number of moles of O_2 gas released in the overhead volume v or pure Ar gas.
V_{tot} , the total isotherm volume of the overhead gas mixture at any t time is always defined by $V_{tot} = v + V_{O_2}$. Isobaric conditions were checked by using a light silicon oil to fill the U-shaped glass part.
The isotherm and isobaric molar fraction of O_2 gas x of the gas mixture is defined by
$x = V_{O_2}/V_{tot} = V_{O2}/(v+V_{O_2})$
which leads to $V_{O_2}(1-x) = vx$ and hence to $V_{O_2} = vx/(1-x)$
Assuming an idealized behaviour of the gas mixture (that also applies to the volumetric method) one obtains the number of O_2 moles in the gas overhead mixture as a function of x.

$$n_{O_2} = (P/RT)[vx/(1-x)]$$

2. Relationship between n_{O2} (probe) and n_{O2}(volumetry)

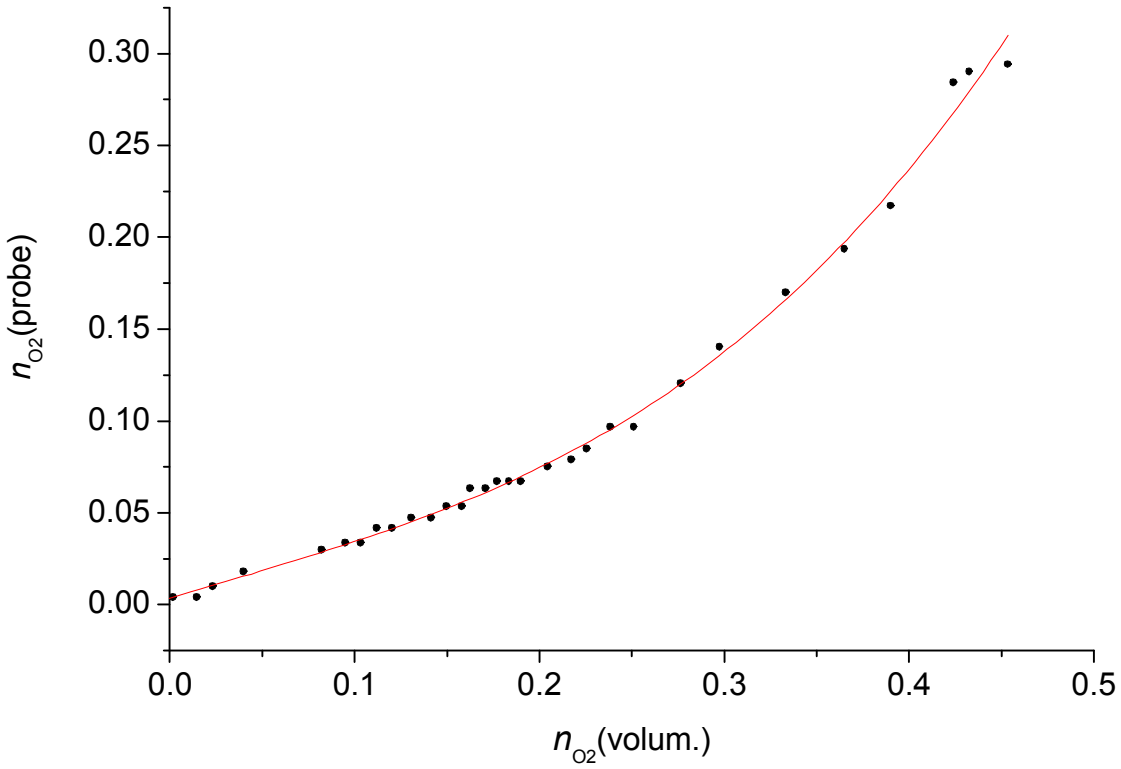

Figure 2. This curve was established by carrying out a typical WOC reaction using complex **1b**. The values of n_{O2} determined by the volumetric method and by conversion of oxygen saturation x readout were subsequently fitted against a polynomial 3rd order function (n_{O2}(probe) = a + $b \times n_{O2}$(volum.) + $c \times n_{O2}$(volum)^2 + $d \times n_{O2}$(volum.)^3; a= 0.003(3), b= 0.30(6), c= – 0.2(3), d= 2.2(5); R^2= 0.99) to demonstrate the non-linearity of probe's measures.

3. Effect of acetonitrile on WOC efficiency.

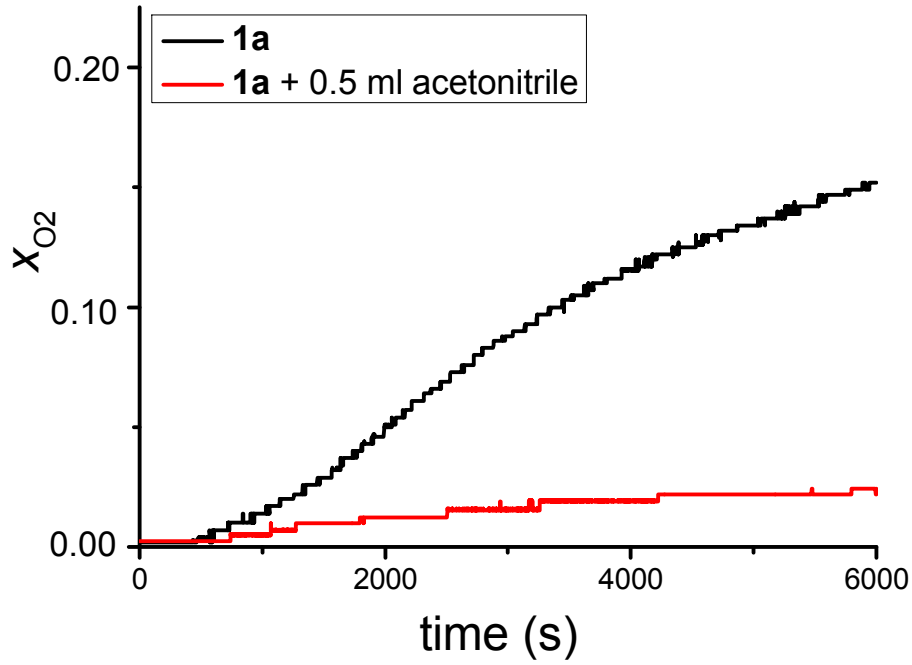

Figure 3. Oxygen evolution traces recorded for a typical WOC experiment carried out without (black plot) and with (red plot) acetonitrile (0.5 mL) in the presence of metallacycle **1a**. Under the latter condition the maximum saturation in O_2 reaches barely 2 %.

4. $KMnO_4$ as a sacrificial oxidant

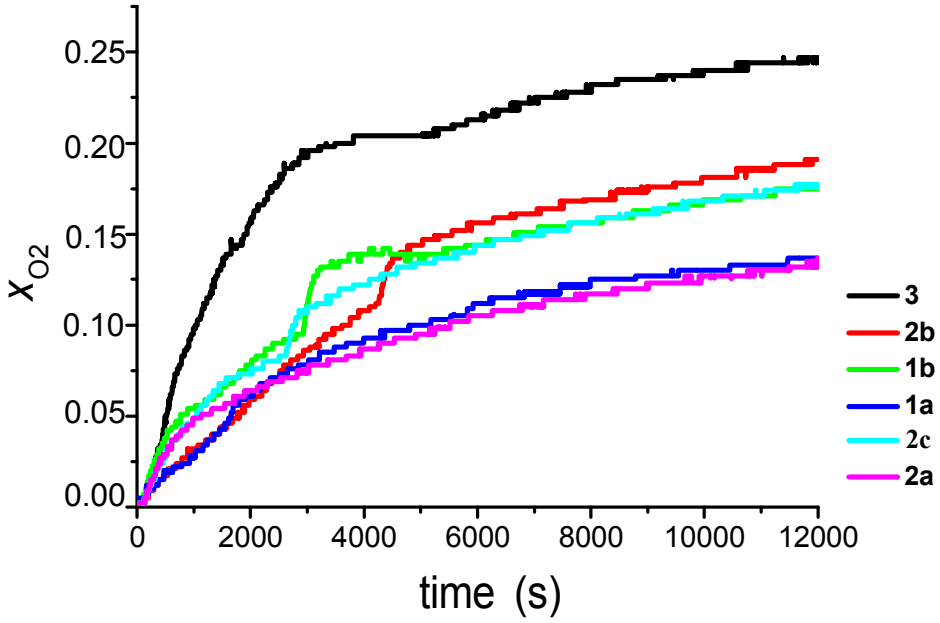

Figure 4. Oxygen evolution traces for complex **1a-3** as measured by sensor oxygen; [$KMnO_4$] = 0.166 M, V = 5 ml, $n(H^+)$ = 3 M, n(Ir) = 0.0125 mmol

5. Lack of interaction between CB[7] and 1c

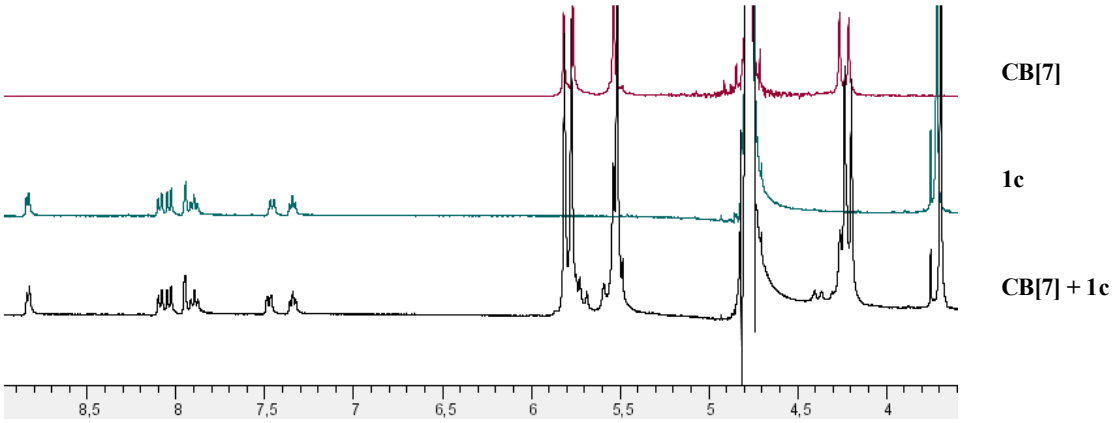

Figure 5: ^{1}H NMR (400 MHz) in D_2O for **1c** + **CB**[7] at room temperature.

6. ^{1}H NMR spectrum in D_2O of the WOC reaction medium after 30 min of reaction time with 1a as catalyst.

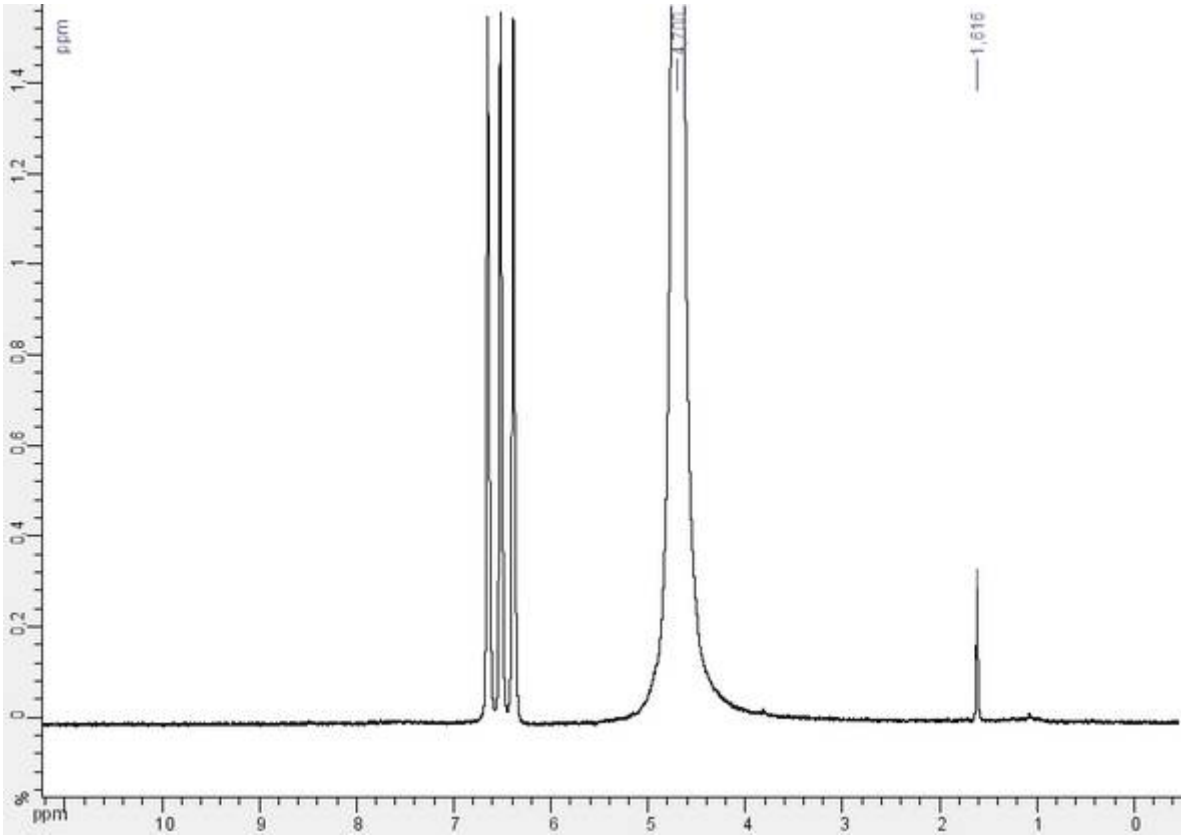

Figure 5. The signal at 1.64 ppm is indicative of the presence of a dissolved "Cp*Ir" moiety.

7. Infrared spectroscopy on CB[7] under exposure to Ir catalysts.

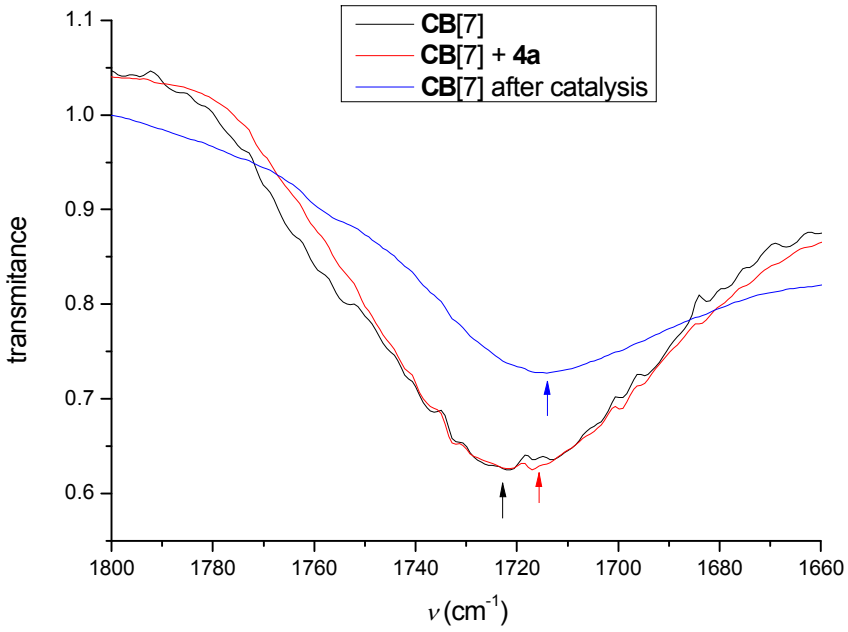

Figure 6. Plot of the elongation vibrational band for the C=O function in **CB**[7] in three situations: in the neat solid material, upon exposure to **4a** and upon WOC run initiated with complex **3**. In the latter situation, the initial dark blue solution was first treated with $nBu_3P(O)$ in toluene to remove cerium salts and the resulting aqueous solution was treated with acetone to precipitate the unsoluble material containing **CB**[7] and other inorganic salts. Spectra were measure on an ATR cell.

8. WOC

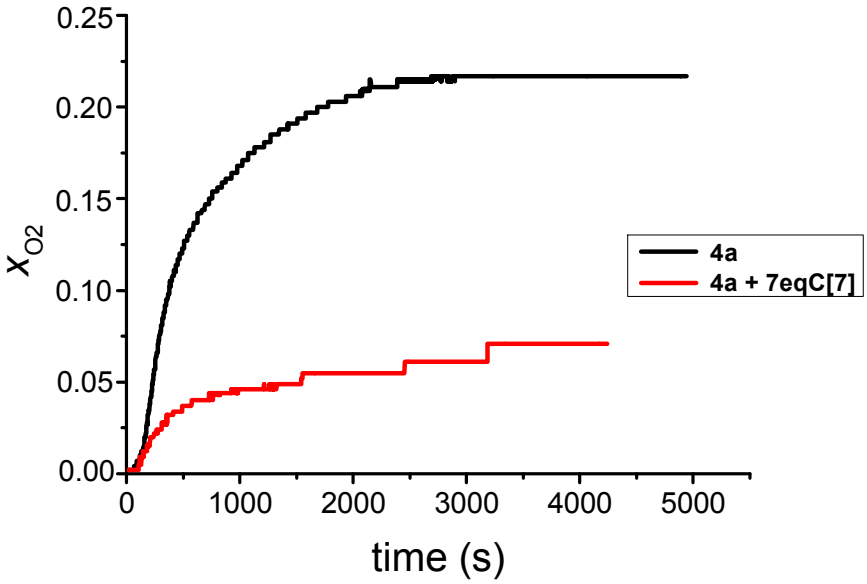

Figure 6. The effect of **CB**[7] on the production of oxygen catalysis by **4a** ; the oxygen evolution was monitored with gas galvanometric sensor; [CAN] = 0.5 M V = 5 ml, *n*(Ir) = 0.0125 mmol, *n*(**CB**[7]) = 0.0875 mmol

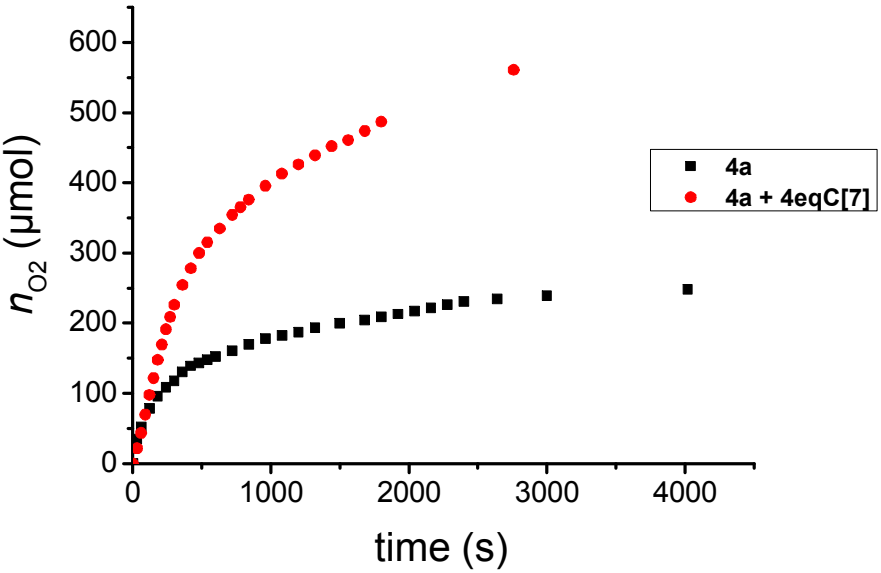

Figure 7. The effect of CB[7] on the production of O_2 catalysed by **4a** ; oxygen evolution was determined by the volumetric method; [CAN] = 0.5 M V = 5 ml, *n*(Ir) = 0.0125 mmol, *n*(CB[7]) = 0.05 mmol

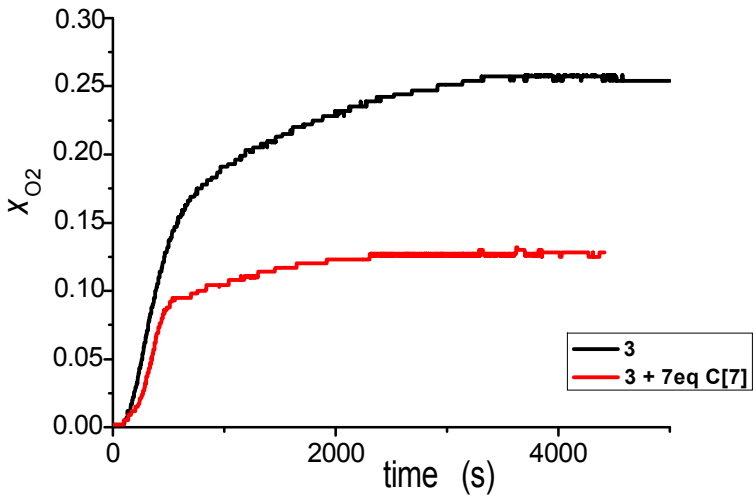

Figure 9. The effect of **CB**[7] on the production of oxygen catalysed by **3**; O_2 sensor monitoring; [CAN] = 0.5 M, V = 5 ml, *n*(Ir) = 0.0125 mmol, *n*(**CB**[7]) = 0.0875 mmol

9. Partial structure of complex 1c

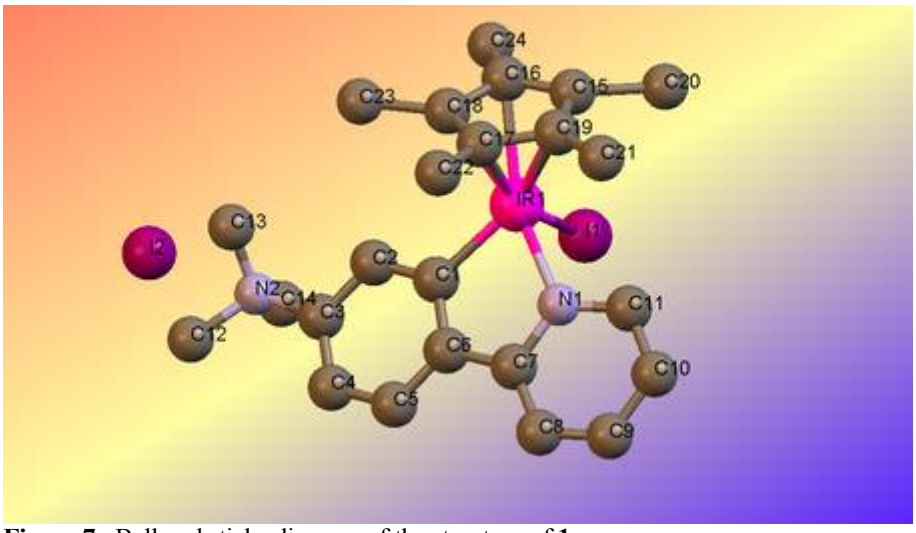

Figure 7. Ball and sticks diagram of the structure of **1c.**

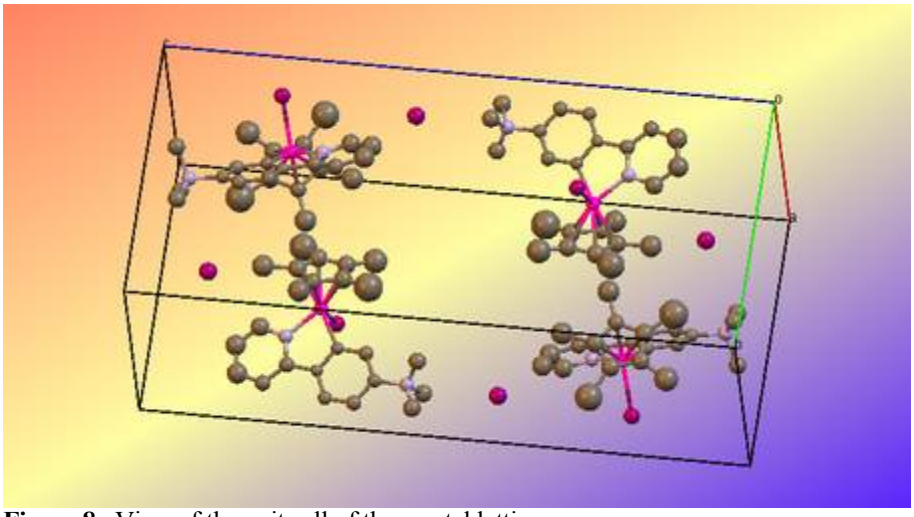

Figure 8. View of the unit cell of the crystal lattice.

List of geometrical parameters for the partial structure of 1c.

Atomic coordinates (lacking the H atoms at aromatic rings)

Number	Label	Charge	SybylType	Xfrac + ESD	Yfrac + ESD	Zfrac + ESD	Symm. op.
1	IR1	0	Ir	0.62457	0.798	0.212526	x,y,z
2	I1	0	I	0.922365	0.880405	0.199739	x,y,z
3	N2	0	N.4	0.763516	0.587828	0.061749	x,y,z
4	C1	0	C.3	0.730057	0.692886	0.181673	x,y,z
5	C2	0	C.2	0.711769	0.674556	0.133035	x,y,z
6	C3	0	C.2	0.78014	0.599773	0.116664	x,y,z
7	C4	0	C.2	0.866799	0.543321	0.148931	x,y,z
8	C5	0	C.2	0.885089	0.561651	0.197569	x,y,z
9	C6	0	C.2	0.816719	0.636433	0.213941	x,y,z
10	C7	0	C.2	0.836809	0.658352	0.264872	x,y,z
11	C8	0	C.2	0.922763	0.616161	0.303946	x,y,z
12	C9	0	C.2	0.940545	0.654447	0.348721	x,y,z
13	C10	0	C.2	0.872375	0.734922	0.354421	x,y,z
14	C11	0	C.2	0.786421	0.777113	0.315347	x,y,z
15	N1	0	N.2	0.768637	0.738829	0.270573	x,y,z
16	C12	0	C.3	0.769198	0.499279	0.047953	x,y,z
17	H12A	0	H	0.650745	0.475217	0.046194	x,y,z
18	H12B	0	H	0.847002	0.468185	0.071759	x,y,z
19	H12C	0	H	0.813679	0.494731	0.016605	x,y,z
20	C13	0	C.3	0.604032	0.611458	0.042442	x,y,z
21	H13A	0	H	0.61324	0.637696	0.011208	x,y,z
22	H13B	0	H	0.554456	0.652293	0.063576	x,y,z
23	H13C	0	H	0.527468	0.561711	0.038386	x,y,z
24	C14	0	C.3	0.925703	0.635397	0.04227	x,y,z
25	H14A	0	H	0.919647	0.628592	0.007478	x,y,z
26	H14B	0	H	1.03576	0.611063	0.057217	x,y,z
27	H14C	0	H	0.921241	0.69573	0.050159	x,y,z
28	C15	0	C.3	0.44528	0.91474	0.220554	x,y,z
29	C16	0	C.3	0.423826	0.888461	0.171977	x,y,z
30	C18	0	C.3	0.36813	0.802682	0.170618	x,y,z
31	C17	0	C.3	0.355162	0.775945	0.218356	x,y,z
32	C19	0	C.3	0.402844	0.8452	0.249218	x,y,z
33	C20	0	C.3	0.541886	0.998089	0.252927	x,y,z
34	H20A	0	H	0.618474	1.02916	0.233201	x,y,z
35	H20B	0	H	0.611561	0.976396	0.281575	x,y,z
36	H20C	0	H	0.450576	1.03613	0.26242	x,y,z
37	C21	0	C.3	0.375666	0.830051	0.303724	x,y,z
38	H21A	0	H	0.429715	0.876549	0.323105	x,y,z
39	H21B	0	H	0.4307	0.776421	0.3145	x,y,z
40	H21C	0	H	0.249786	0.827819	0.307253	x,y,z
41	C22	0	C.3	0.268908	0.694183	0.23347	x,y,z
42	H22A	0	H	0.159121	0.684751	0.212937	x,y,z
43	H22B	0	H	0.243815	0.699022	0.266844	x,y,z
44	H22C	0	H	0.348575	0.64644	0.230304	x,y,z
45	C23	0	C.3	0.299884	0.748165	0.123879	x,y,z
46	H23A	0	H	0.286836	0.78531	0.095805	x,y,z
47	H23B	0	H	0.186207	0.722526	0.128331	x,y,z
48	H23C	0	H	0.385105	0.703505	0.119075	x,y,z
49	C24	0	C.3	0.464779	0.933164	0.128653	x,y,z
50	H24A	0	H	0.545163	0.980124	0.137628	x,y,z
51	H24B	0	H	0.356199	0.955328	0.11159	x,y,z
52	H24C	0	H	0.520285	0.893848	0.10785	x,y,z
53	IR1	0	Ir	0.37543	0.298	0.287474	1-x,-1/2+y,1/2-z
54	I1	0	I	0.077635	0.380405	0.300261	1-x,-1/2+y,1/2-z
55	N2	0	N.4	0.236484	0.087828	0.438251	1-x,-1/2+y,1/2-z
56	C1	0	C.3	0.269943	0.192886	0.318327	1-x,-1/2+y,1/2-z
57	C2	0	C.2	0.288231	0.174556	0.366965	1-x,-1/2+y,1/2-z
58	C3	0	C.2	0.21986	0.099773	0.383336	1-x,-1/2+y,1/2-z
59	C4	0	C.2	0.133201	0.043321	0.351069	1-x,-1/2+y,1/2-z
60	C5	0	C.2	0.114911	0.061651	0.302431	1-x,-1/2+y,1/2-z
61	C6	0	C.2	0.183281	0.136433	0.286059	1-x,-1/2+y,1/2-z
62	C7	0	C.2	0.163191	0.158352	0.235128	1-x,-1/2+y,1/2-z
63	C8	0	C.2	0.077237	0.116161	0.196054	1-x,-1/2+y,1/2-z
64	C9	0	C.2	0.059455	0.154447	0.151279	1-x,-1/2+y,1/2-z
65	C10	0	C.2	0.127625	0.234922	0.145579	1-x,-1/2+y,1/2-z
66	C11	0	C.2	0.213579	0.277113	0.184653	1-x,-1/2+y,1/2-z
67	N1	0	N.2	0.231363	0.238829	0.229427	1-x,-1/2+y,1/2-z
68	C12	0	C.3	0.230802	-0.000721	0.452047	1-x,-1/2+y,1/2-z
69	H12A	0	H	0.349255	-0.024783	0.453806	1-x,-1/2+y,1/2-z
70	H12B	0	H	0.152998	-0.031815	0.428241	1-x,-1/2+y,1/2-z
71	H12C	0	H	0.186321	-0.005269	0.483395	1-x,-1/2+y,1/2-z
72	C13	0	C.3	0.395968	0.111458	0.457558	1-x,-1/2+y,1/2-z
73	H13A	0	H	0.38676	0.137696	0.488792	1-x,-1/2+y,1/2-z
74	H13B	0	H	0.445544	0.152293	0.436424	1-x,-1/2+y,1/2-z
75	H13C	0	H	0.472532	0.061711	0.461614	1-x,-1/2+y,1/2-z
76	C14	0	C.3	0.074297	0.135397	0.45773	1-x,-1/2+y,1/2-z
77	H14A	0	H	0.080353	0.128592	0.492522	1-x,-1/2+y,1/2-z
78	H14B	0	H	-0.035761	0.111063	0.442783	1-x,-1/2+y,1/2-z
79	H14C	0	H	0.078759	0.19573	0.449841	1-x,-1/2+y,1/2-z
80	C15	0	C.3	0.55472	0.41474	0.279446	1-x,-1/2+y,1/2-z
81	C16	0	C.3	0.576174	0.388461	0.328023	1-x,-1/2+y,1/2-z
82	C18	0	C.3	0.63187	0.302682	0.329382	1-x,-1/2+y,1/2-z
83	C17	0	C.3	0.644838	0.275945	0.281644	1-x,-1/2+y,1/2-z
84	C19	0	C.3	0.597156	0.3452	0.250782	1-x,-1/2+y,1/2-z
85	C20	0	C.3	0.458114	0.498089	0.247073	1-x,-1/2+y,1/2-z
86	H20A	0	H	0.381526	0.529155	0.266799	1-x,-1/2+y,1/2-z
87	H20B	0	H	0.388439	0.476396	0.218425	1-x,-1/2+y,1/2-z
88	H20C	0	H	0.549424	0.536129	0.23758	1-x,-1/2+y,1/2-z
89	C21	0	C.3	0.624334	0.330051	0.196276	1-x,-1/2+y,1/2-z
90	H21A	0	H	0.570285	0.376549	0.176895	1-x,-1/2+y,1/2-z
91	H21B	0	H	0.5693	0.276421	0.1855	1-x,-1/2+y,1/2-z
92	H21C	0	H	0.750214	0.327819	0.192747	1-x,-1/2+y,1/2-z
93	C22	0	C.3	0.731092	0.194183	0.26653	1-x,-1/2+y,1/2-z
94	H22A	0	H	0.840879	0.184751	0.287063	1-x,-1/2+y,1/2-z
95	H22B	0	H	0.756185	0.199022	0.233156	1-x,-1/2+y,1/2-z
96	H22C	0	H	0.651425	0.14644	0.269696	1-x,-1/2+y,1/2-z
97	C23	0	C.3	0.700116	0.248165	0.376121	1-x,-1/2+y,1/2-z
98	H23A	0	H	0.713164	0.28531	0.404195	1-x,-1/2+y,1/2-z
99	H23B	0	H	0.813793	0.222526	0.371669	1-x,-1/2+y,1/2-z
100	H23C	0	H	0.614895	0.203505	0.380925	1-x,-1/2+y,1/2-z
101	C24	0	C.3	0.535221	0.433164	0.371347	1-x,-1/2+y,1/2-z
102	H24A	0	H	0.454837	0.480124	0.362372	1-x,-1/2+y,1/2-z
103	H24B	0	H	0.643801	0.455328	0.38841	1-x,-1/2+y,1/2-z
104	H24C	0	H	0.479715	0.393848	0.39215	1-x,-1/2+y,1/2-z
105	IR1	0	Ir	0.37543	0.202	0.787474	1-x,1-y,1-z
106	I1	0	I	0.077635	0.119595	0.800261	1-x,1-y,1-z
107	N2	0	N.4	0.236484	0.412172	0.938251	1-x,1-y,1-z
108	C1	0	C.3	0.269943	0.307114	0.818327	1-x,1-y,1-z
109	C2	0	C.2	0.288231	0.325444	0.866965	1-x,1-y,1-z

110	C3	0	C.2	0.21986	0.400227	0.883336	1-x,1-y,1-z
111	C4	0	C.2	0.133201	0.456679	0.851069	1-x,1-y,1-z
112	C5	0	C.2	0.114911	0.438349	0.802431	1-x,1-y,1-z
113	C6	0	C.2	0.183281	0.363567	0.786059	1-x,1-y,1-z
114	C7	0	C.2	0.163191	0.341648	0.735128	1-x,1-y,1-z
115	C8	0	C.2	0.077237	0.383839	0.696054	1-x,1-y,1-z
116	C9	0	C.2	0.059455	0.345553	0.651279	1-x,1-y,1-z
117	C10	0	C.2	0.127625	0.265078	0.645579	1-x,1-y,1-z
118	C11	0	C.2	0.213579	0.222887	0.684653	1-x,1-y,1-z
119	N1	0	N.2	0.231363	0.261171	0.729427	1-x,1-y,1-z
120	C12	0	C.3	0.230802	0.500721	0.952047	1-x,1-y,1-z
121	H12A	0	H	0.349255	0.524783	0.953806	1-x,1-y,1-z
122	H12B	0	H	0.152998	0.531815	0.928241	1-x,1-y,1-z
123	H12C	0	H	0.186321	0.505269	0.983395	1-x,1-y,1-z
124	C13	0	C.3	0.395968	0.388542	0.957558	1-x,1-y,1-z
125	H13A	0	H	0.38676	0.362304	0.988792	1-x,1-y,1-z
126	H13B	0	H	0.445544	0.347707	0.936424	1-x,1-y,1-z
127	H13C	0	H	0.472532	0.438289	0.961614	1-x,1-y,1-z
128	C14	0	C.3	0.074297	0.364603	0.95773	1-x,1-y,1-z
129	H14A	0	H	0.080353	0.371408	0.992522	1-x,1-y,1-z
130	H14B	0	H	-0.035761	0.388937	0.942783	1-x,1-y,1-z
131	H14C	0	H	0.078759	0.30427	0.949841	1-x,1-y,1-z
132	C15	0	C.3	0.55472	0.08526	0.779446	1-x,1-y,1-z
133	C16	0	C.3	0.576174	0.111539	0.828023	1-x,1-y,1-z
134	C18	0	C.3	0.63187	0.197318	0.829382	1-x,1-y,1-z
135	C17	0	C.3	0.644838	0.224055	0.781644	1-x,1-y,1-z
136	C19	0	C.3	0.597156	0.1548	0.750782	1-x,1-y,1-z
137	C20	0	C.3	0.458114	0.001911	0.747073	1-x,1-y,1-z
138	H20A	0	H	0.381526	-0.029155	0.766799	1-x,1-y,1-z
139	H20B	0	H	0.388439	0.023604	0.718425	1-x,1-y,1-z
140	H20C	0	H	0.549424	-0.036129	0.73758	1-x,1-y,1-z
141	C21	0	C.3	0.624334	0.169949	0.696276	1-x,1-y,1-z
142	H21A	0	H	0.570285	0.123451	0.676895	1-x,1-y,1-z
143	H21B	0	H	0.5693	0.223579	0.6855	1-x,1-y,1-z
144	H21C	0	H	0.750214	0.172181	0.692747	1-x,1-y,1-z
145	C22	0	C.3	0.731092	0.305817	0.76653	1-x,1-y,1-z
146	H22A	0	H	0.840879	0.315249	0.787063	1-x,1-y,1-z
147	H22B	0	H	0.756185	0.300978	0.733156	1-x,1-y,1-z
148	H22C	0	H	0.651425	0.35356	0.769696	1-x,1-y,1-z
149	C23	0	C.3	0.700116	0.251835	0.876121	1-x,1-y,1-z
150	H23A	0	H	0.713164	0.21469	0.904195	1-x,1-y,1-z
151	H23B	0	H	0.813793	0.277474	0.871669	1-x,1-y,1-z
152	H23C	0	H	0.614895	0.296495	0.880925	1-x,1-y,1-z
153	C24	0	C.3	0.535221	0.066836	0.871347	1-x,1-y,1-z
154	H24A	0	H	0.454837	0.019876	0.862372	1-x,1-y,1-z
155	H24B	0	H	0.643801	0.044672	0.88841	1-x,1-y,1-z
156	H24C	0	H	0.479715	0.106152	0.89215	1-x,1-y,1-z
157	IR1	0	Ir	0.62457	0.702	0.712526	x,1.5-y,1/2+z
158	I1	0	I	0.922365	0.619595	0.699739	x,1.5-y,1/2+z
159	N2	0	N.4	0.763516	0.912172	0.561749	x,1.5-y,1/2+z
160	C1	0	C.3	0.730057	0.807114	0.681673	x,1.5-y,1/2+z
161	C2	0	C.2	0.711769	0.825444	0.633035	x,1.5-y,1/2+z
162	C3	0	C.2	0.78014	0.900227	0.616664	x,1.5-y,1/2+z
163	C4	0	C.2	0.866799	0.956679	0.648931	x,1.5-y,1/2+z
164	C5	0	C.2	0.885089	0.938349	0.697569	x,1.5-y,1/2+z
165	C6	0	C.2	0.816719	0.863567	0.713941	x,1.5-y,1/2+z
166	C7	0	C.2	0.836809	0.841648	0.764872	x,1.5-y,1/2+z
167	C8	0	C.2	0.922763	0.883839	0.803946	x,1.5-y,1/2+z
168	C9	0	C.2	0.940545	0.845553	0.848721	x,1.5-y,1/2+z
169	C10	0	C.2	0.872375	0.765078	0.854421	x,1.5-y,1/2+z
170	C11	0	C.2	0.786421	0.722887	0.815347	x,1.5-y,1/2+z
171	N1	0	N.2	0.768637	0.761171	0.770573	x,1.5-y,1/2+z
172	C12	0	C.3	0.769198	1.00072	0.547953	x,1.5-y,1/2+z
173	H12A	0	H	0.650745	1.02478	0.546194	x,1.5-y,1/2+z
174	H12B	0	H	0.847002	1.03181	0.571759	x,1.5-y,1/2+z
175	H12C	0	H	0.813679	1.00527	0.516605	x,1.5-y,1/2+z
176	C13	0	C.3	0.604032	0.888542	0.542442	x,1.5-y,1/2+z
177	H13A	0	H	0.61324	0.862304	0.511208	x,1.5-y,1/2+z
178	H13B	0	H	0.554456	0.847707	0.563576	x,1.5-y,1/2+z
179	H13C	0	H	0.527468	0.938289	0.538386	x,1.5-y,1/2+z
180	C14	0	C.3	0.925703	0.864603	0.54227	x,1.5-y,1/2+z
181	H14A	0	H	0.919647	0.871408	0.507478	x,1.5-y,1/2+z
182	H14B	0	H	1.03576	0.888937	0.557217	x,1.5-y,1/2+z
183	H14C	0	H	0.921241	0.80427	0.550159	x,1.5-y,1/2+z
184	C15	0	C.3	0.44528	0.58526	0.720554	x,1.5-y,1/2+z
185	C16	0	C.3	0.423826	0.611539	0.671977	x,1.5-y,1/2+z
186	C18	0	C.3	0.36813	0.697318	0.670618	x,1.5-y,1/2+z
187	C17	0	C.3	0.355162	0.724055	0.718356	x,1.5-y,1/2+z
188	C19	0	C.3	0.402844	0.6548	0.749218	x,1.5-y,1/2+z
189	C20	0	C.3	0.541886	0.501911	0.752927	x,1.5-y,1/2+z
190	H20A	0	H	0.618474	0.470845	0.733201	x,1.5-y,1/2+z
191	H20B	0	H	0.611561	0.523604	0.781575	x,1.5-y,1/2+z
192	H20C	0	H	0.450576	0.463871	0.76242	x,1.5-y,1/2+z
193	C21	0	C.3	0.375666	0.669949	0.803724	x,1.5-y,1/2+z
194	H21A	0	H	0.429715	0.623451	0.823105	x,1.5-y,1/2+z
195	H21B	0	H	0.4307	0.723579	0.8145	x,1.5-y,1/2+z
196	H21C	0	H	0.249786	0.672181	0.807253	x,1.5-y,1/2+z
197	C22	0	C.3	0.268908	0.805817	0.73347	x,1.5-y,1/2+z
198	H22A	0	H	0.159121	0.815249	0.712937	x,1.5-y,1/2+z
199	H22B	0	H	0.243815	0.800978	0.766844	x,1.5-y,1/2+z
200	H22C	0	H	0.348575	0.85356	0.730304	x,1.5-y,1/2+z
201	C23	0	C.3	0.299884	0.751835	0.623879	x,1.5-y,1/2+z
202	H23A	0	H	0.286836	0.71469	0.595805	x,1.5-y,1/2+z
203	H23B	0	H	0.186207	0.777474	0.628331	x,1.5-y,1/2+z
204	H23C	0	H	0.385105	0.796495	0.619075	x,1.5-y,1/2+z
205	C24	0	C.3	0.464779	0.566836	0.628653	x,1.5-y,1/2+z
206	H24A	0	H	0.545163	0.519876	0.637628	x,1.5-y,1/2+z
207	H24B	0	H	0.356199	0.544672	0.61159	x,1.5-y,1/2+z
208	H24C	0	H	0.520285	0.606152	0.60785	x,1.5-y,1/2+z
209	I2	0	I	0.28546	0.446029	0.090468	x,y,z
210	I2	0	I	0.71454	0.946029	0.409532	1-x,1/2+y,1/2-z
211	I2	0	I	0.71454	0.553971	0.909532	1-x,1-y,1-z
212	I2	0	I	0.28546	0.053971	0.590468	x,1/2-y,1/2+z

Interatomic distances

Number	Object1	Object2	Length
26	C1	IR1	2.0758(1)
27	C1	C2	1.3900(1)
20	C10	C9	1.3900(1)
19	C11	C10	1.3900(1)
4	C15	C19	1.4200(1)
3	C15	C20	1.7228(1)
2	C16	C15	1.4200(1)
7	C17	C22	1.5310(1)
8	C17	C18	1.4200(1)

10	C18	C16	1.4200(1)
9	C18	C23	1.6114(1)
6	C19	C17	1.4200(1)
5	C19	C21	1.5856(1)
28	C2	C3	1.3900(1)
1	C24	C16	1.4696(1)
29	C3	C4	1.3900(1)
32	C3	N2	1.5469(1)
30	C4	C5	1.3900(1)
25	C6	C1	1.3900(1)
31	C6	C3	2.7800(2)
24	C7	C6	1.4651(1)
23	C7	N1	1.3900(1)
22	C8	C7	1.3900(1)
21	C9	C8	1.3900(1)
11	IR1	C17	2.1156(3)
16	IR1	I1	2.6826(3)
17	IR1	N1	2.0917(1)
12	IR1	C18	2.1828(2)
13	IR1	C16	2.3102(1)
15	IR1	C19	2.2067(2)
14	IR1	C15	2.3243(1)
18	N1	C11	1.3900(1)
34	N2	C14	1.5968(1)
35	N2	C12	1.4535(1)
36	N2	I2	4.4375(4)
33	N2	C13	1.3366(1)

Interatomic angles.

Number	Atom1	Atom2	Atom3	Angle
1	C1	IR1	I1	87.64
1	I1	IR1	C1	87.64
2	N1	IR1	I1	86.28
2	I1	IR1	N1	86.28
3	C15	IR1	I1	98.46
3	I1	IR1	C15	98.46
4	C16	IR1	I1	99.49
4	I1	IR1	C16	99.49
5	I1	IR1	C18	129.84
5	C18	IR1	I1	129.84
6	C17	IR1	I1	160.04
6	I1	IR1	C17	160.04
7	C19	IR1	I1	127.24
7	I1	IR1	C19	127.24
8	N1	IR1	C1	76.81
8	C1	IR1	N1	76.81
9	C1	IR1	C15	159.23
9	C15	IR1	C1	159.23
10	C16	IR1	C1	123.83
10	C1	IR1	C16	123.83
11	C18	IR1	C1	99.74
11	C1	IR1	C18	99.74
12	C17	IR1	C1	109.02
12	C1	IR1	C17	109.02
13	C1	IR1	C19	144.86
13	C19	IR1	C1	144.86
14	C15	IR1	N1	123.20
14	N1	IR1	C15	123.20
15	C16	IR1	N1	158.51
15	N1	IR1	C16	158.51
16	C18	IR1	N1	143.82
16	N1	IR1	C18	143.82
17	N1	IR1	C17	107.75
17	C17	IR1	N1	107.75
18	C19	IR1	N1	98.93
18	N1	IR1	C19	98.93
19	C16	IR1	C15	35.68
19	C15	IR1	C16	35.68
20	C18	IR1	C15	61.20
20	C15	IR1	C18	61.20
21	C17	IR1	C15	62.12
21	C15	IR1	C17	62.12
22	C15	IR1	C19	36.41
22	C19	IR1	C15	36.41
23	C18	IR1	C16	36.71
23	C16	IR1	C18	36.71
24	C17	IR1	C16	62.37
24	C16	IR1	C17	62.37
25	C19	IR1	C16	61.10
25	C16	IR1	C19	61.10
26	C18	IR1	C17	38.54
26	C17	IR1	C18	38.54
27	C19	IR1	C18	63.12
27	C18	IR1	C19	63.12
28	C19	IR1	C17	38.29
28	C17	IR1	C19	38.29
29	C12	N2	C3	112.45
29	C3	N2	C12	112.45
30	C3	N2	C13	110.31
30	C13	N2	C3	110.31
31	C14	N2	C3	107.40
31	C3	N2	C14	107.40
32	C13	N2	C12	102.25
32	C12	N2	C13	102.25
33	C14	N2	C12	108.38
33	C12	N2	C14	108.38
34	C13	N2	C14	116.09
34	C14	N2	C13	116.09
35	C2	C1	IR1	125.03
35	IR1	C1	C2	125.03
36	C6	C1	IR1	114.89
36	IR1	C1	C6	114.89
37	C6	C1	C2	120.00
37	C2	C1	C6	120.00
38	C3	C2	C1	120.00
38	C1	C2	C3	120.00
39	N2	C3	C2	116.07
39	C2	C3	N2	116.07
40	C4	C3	N2	123.81
40	N2	C3	C4	123.81
41	C4	C3	C2	120.00
41	C2	C3	C4	120.00
42	C5	C4	C3	120.00
42	C3	C4	C5	120.00
43	C4	C5	C6	120.00

43	C6	C5	C4	120.00
44	C5	C6	C1	120.00
44	C1	C6	C5	120.00
45	C7	C6	C1	118.68
45	C1	C6	C7	118.68
46	C7	C6	C5	121.31
46	C5	C6	C7	121.31
47	C6	C7	C8	130.63
47	C8	C7	C6	130.63
48	N1	C7	C6	109.06
48	C6	C7	N1	109.06
49	N1	C7	C8	120.00
49	C8	C7	N1	120.00
50	C9	C8	C7	120.00
50	C7	C8	C9	120.00
51	C8	C9	C10	120.00
51	C10	C9	C8	120.00
52	C11	C10	C9	120.00
52	C9	C10	C11	120.00
53	N1	C11	C10	120.00
53	C10	C11	N1	120.00
54	C7	N1	IR1	119.51
54	IR1	N1	C7	119.51
55	C11	N1	IR1	120.35
55	IR1	N1	C11	120.35
56	C7	N1	C11	120.00
56	C11	N1	C7	120.00
57	H12A	C12	N2	109.47
57	N2	C12	H12A	109.47
58	H12B	C12	N2	109.47
58	N2	C12	H12B	109.47
59	H12C	C12	N2	109.47
59	N2	C12	H12C	109.47
60	H12A	C12	H12B	109.47
60	H12B	C12	H12A	109.47
61	H12C	C12	H12A	109.47
61	H12A	C12	H12C	109.47
62	H12C	C12	H12B	109.47
62	H12B	C12	H12C	109.47
63	H13A	C13	N2	109.47
63	N2	C13	H13A	109.47
64	N2	C13	H13B	109.47
64	H13B	C13	N2	109.47
65	H13C	C13	N2	109.47
65	N2	C13	H13C	109.47
66	H13B	C13	H13A	109.47
66	H13A	C13	H13B	109.47
67	H13C	C13	H13A	109.47
67	H13A	C13	H13C	109.47
68	H13B	C13	H13C	109.47
68	H13C	C13	H13B	109.47
69	H14A	C14	N2	109.47
69	N2	C14	H14A	109.47
70	H14B	C14	N2	109.47
70	N2	C14	H14B	109.47
71	H14C	C14	N2	109.47
71	N2	C14	H14C	109.47
72	H14B	C14	H14A	109.47
72	H14A	C14	H14B	109.47
73	H14A	C14	H14C	109.47
73	H14C	C14	H14A	109.47
74	H14C	C14	H14B	109.47
74	H14B	C14	H14C	109.47
75	C16	C15	IR1	71.62
75	IR1	C15	C16	71.62
76	C19	C15	IR1	67.28
76	IR1	C15	C19	67.28
77	IR1	C15	C20	115.62
77	C20	C15	IR1	115.62
78	C19	C15	C16	108.00
78	C16	C15	C19	108.00
79	C20	C15	C16	136.99
79	C16	C15	C20	136.99
80	C20	C15	C19	113.75
80	C19	C15	C20	113.75
81	IR1	C16	C15	72.70
81	C15	C16	IR1	72.70
82	C18	C16	IR1	66.76
82	IR1	C16	C18	66.76
83	C24	C16	IR1	121.15
83	IR1	C16	C24	121.15
84	C18	C16	C15	108.00
84	C15	C16	C18	108.00
85	C15	C16	C24	130.01
85	C24	C16	C15	130.01
86	C24	C16	C18	121.73
86	C18	C16	C24	121.73
87	C16	C18	IR1	76.53
87	IR1	C18	C16	76.53
88	C17	C18	IR1	68.17
88	IR1	C18	C17	68.17
89	C23	C18	IR1	128.20
89	IR1	C18	C23	128.20
90	C16	C18	C17	108.00
90	C17	C18	C16	108.00
91	C23	C18	C16	127.07
91	C16	C18	C23	127.07
92	C23	C18	C17	124.23
92	C17	C18	C23	124.23
93	C18	C17	IR1	73.29
93	IR1	C17	C18	73.29
94	IR1	C17	C19	74.34
94	C19	C17	IR1	74.34
95	C22	C17	IR1	127.81
95	IR1	C17	C22	127.81
96	C19	C17	C18	108.00
96	C18	C17	C19	108.00
97	C22	C17	C18	126.02
97	C18	C17	C22	126.02
98	C19	C17	C22	124.84
98	C22	C17	C19	124.84
99	C15	C19	IR1	76.30
99	IR1	C19	C15	76.30
100	C17	C19	IR1	67.38
100	IR1	C19	C17	67.38
101	C21	C19	IR1	125.86
101	IR1	C19	C21	125.86
102	C15	C19	C17	108.00
102	C17	C19	C15	108.00

103	C21	C19	C15	136.54
103	C15	C19	C21	136.54
104	C21	C19	C17	114.99
104	C17	C19	C21	114.99
105	H20A	C20	C15	109.47
105	C15	C20	H20A	109.47
106	H20B	C20	C15	109.47
106	C15	C20	H20B	109.47
107	C15	C20	H20C	109.47
107	H20C	C20	C15	109.47
108	H20B	C20	H20A	109.47
108	H20A	C20	H20B	109.47
109	H20C	C20	H20A	109.47
109	H20A	C20	H20C	109.47
110	H20C	C20	H20B	109.47
110	H20B	C20	H20C	109.47
111	C19	C21	H21A	109.47
111	H21A	C21	C19	109.47
112	H21B	C21	C19	109.47
112	C19	C21	H21B	109.47
113	H21C	C21	C19	109.47
113	C19	C21	H21C	109.47
114	H21B	C21	H21A	109.47
114	H21A	C21	H21B	109.47
115	H21A	C21	H21C	109.47
115	H21C	C21	H21A	109.47
116	H21C	C21	H21B	109.47
116	H21B	C21	H21C	109.47
117	H22A	C22	C17	109.47
117	C17	C22	H22A	109.47
118	H22B	C22	C17	109.47
118	C17	C22	H22B	109.47
119	C17	C22	H22C	109.47
119	H22C	C22	C17	109.47
120	H22B	C22	H22A	109.47
120	H22A	C22	H22B	109.47
121	H22C	C22	H22A	109.47
121	H22A	C22	H22C	109.47
122	H22C	C22	H22B	109.47
122	H22B	C22	H22C	109.47
123	C18	C23	H23A	109.47
123	H23A	C23	C18	109.47
124	H23B	C23	C18	109.47
124	C18	C23	H23B	109.47
125	H23C	C23	C18	109.47
125	C18	C23	H23C	109.47
126	H23B	C23	H23A	109.47
126	H23A	C23	H23B	109.47
127	H23A	C23	H23C	109.47
127	H23C	C23	H23A	109.47
128	H23C	C23	H23B	109.47
128	H23B	C23	H23C	109.47
129	H24A	C24	C16	109.47
129	C16	C24	H24A	109.47
130	H24B	C24	C16	109.47
130	C16	C24	H24B	109.47
131	C16	C24	H24C	109.47
131	H24C	C24	C16	109.47
132	H24B	C24	H24A	109.47
132	H24A	C24	H24B	109.47
133	H24C	C24	H24A	109.47
133	H24A	C24	H24C	109.47
134	H24C	C24	H24B	109.47
134	H24B	C24	H24C	109.47

Torsion angles

Number	Atom1	Atom2	Atom3	Atom4	Torsion
1	C2	C1	IR1	I1	-89.47
1	I1	IR1	C1	C2	-89.47
2	C6	C1	IR1	I1	93.90
2	I1	IR1	C1	C6	93.90
3	C2	C1	IR1	N1	-176.20
3	N1	IR1	C1	C2	-176.20
4	C6	C1	IR1	N1	7.17
4	N1	IR1	C1	C6	7.17
5	C15	IR1	C1	C2	18.36
5	C2	C1	IR1	C15	18.36
6	C6	C1	IR1	C15	-158.27
6	C15	IR1	C1	C6	-158.27
7	C2	C1	IR1	C16	10.37
7	C16	IR1	C1	C2	10.37
8	C6	C1	IR1	C16	-166.26
8	C16	IR1	C1	C6	-166.26
9	C18	IR1	C1	C2	40.58
9	C2	C1	IR1	C18	40.58
10	C6	C1	IR1	C18	-136.05
10	C18	IR1	C1	C6	-136.05
11	C2	C1	IR1	C17	79.29
11	C17	IR1	C1	C2	79.29
12	C6	C1	IR1	C17	-97.33
12	C17	IR1	C1	C6	-97.33
13	C19	IR1	C1	C2	97.00
13	C2	C1	IR1	C19	97.00
14	C6	C1	IR1	C19	-79.62
14	C19	IR1	C1	C6	-79.62
15	C7	N1	IR1	I1	-98.31
15	I1	IR1	N1	C7	-98.31
16	C11	N1	IR1	I1	85.93
16	I1	IR1	N1	C11	85.93
17	C1	IR1	N1	C7	-9.87
17	C7	N1	IR1	C1	-9.87
18	C11	N1	IR1	C1	174.37
18	C1	IR1	N1	C11	174.37
19	C7	N1	IR1	C15	164.01
19	C15	IR1	N1	C7	164.01
20	C11	N1	IR1	C15	-11.74
20	C15	IR1	N1	C11	-11.74
21	C7	N1	IR1	C16	155.09
21	C16	IR1	N1	C7	155.09
22	C16	IR1	N1	C11	-20.66
22	C11	N1	IR1	C16	-20.66
23	C7	N1	IR1	C18	78.63
23	C18	IR1	N1	C7	78.63
24	C11	N1	IR1	C18	-97.12

24	C18	IR1	N1	C11	-97.12
25	C7	N1	IR1	C17	96.18
25	C17	IR1	N1	C7	96.18
26	C17	IR1	N1	C11	-79.57
26	C11	N1	IR1	C17	-79.57
27	C7	N1	IR1	C19	134.55
27	C19	IR1	N1	C7	134.55
28	C11	N1	IR1	C19	-41.20
28	C19	IR1	N1	C11	-41.20
29	C16	C15	IR1	I1	94.51
29	I1	IR1	C15	C16	94.51
30	I1	IR1	C15	C19	-146.01
30	C19	C15	IR1	I1	-146.01
31	C20	C15	IR1	I1	-39.54
31	I1	IR1	C15	C20	-39.54
32	C16	C15	IR1	C1	-11.42
32	C1	IR1	C15	C16	-11.42
33	C19	C15	IR1	C1	108.06
33	C1	IR1	C15	C19	108.06
34	C1	IR1	C15	C20	-145.47
34	C20	C15	IR1	C1	-145.47
35	C16	C15	IR1	N1	-174.41
35	N1	IR1	C15	C16	-174.41
36	C19	C15	IR1	N1	-54.94
36	N1	IR1	C15	C19	-54.94
37	C20	C15	IR1	N1	51.54
37	N1	IR1	C15	C20	51.54
38	C19	C15	IR1	C16	119.48
38	C16	IR1	C15	C19	119.48
39	C16	IR1	C15	C20	-134.05
39	C20	C15	IR1	C16	-134.05
40	C16	C15	IR1	C18	-36.59
40	C18	IR1	C15	C16	-36.59
41	C19	C15	IR1	C18	82.89
41	C18	IR1	C15	C19	82.89
42	C20	C15	IR1	C18	-170.64
42	C18	IR1	C15	C20	-170.64
43	C17	IR1	C15	C16	-80.63
43	C16	C15	IR1	C17	-80.63
44	C19	C15	IR1	C17	38.85
44	C17	IR1	C15	C19	38.85
45	C20	C15	IR1	C17	145.33
45	C17	IR1	C15	C20	145.33
46	C16	C15	IR1	C19	-119.48
46	C19	IR1	C15	C16	-119.48
47	C19	IR1	C15	C20	106.47
47	C20	C15	IR1	C19	106.47
48	C15	C16	IR1	I1	-91.32
48	I1	IR1	C16	C15	-91.32
49	C18	C16	IR1	I1	149.60
49	I1	IR1	C16	C18	149.60
50	C24	C16	IR1	I1	35.45
50	I1	IR1	C16	C24	35.45
51	C1	IR1	C16	C15	175.15
51	C15	C16	IR1	C1	175.15
52	C18	C16	IR1	C1	56.07
52	C1	IR1	C16	C18	56.07
53	C24	C16	IR1	C1	-58.08
53	C1	IR1	C16	C24	-58.08
54	C15	C16	IR1	N1	12.85
54	N1	IR1	C16	C15	12.85
55	C18	C16	IR1	N1	-106.23
55	N1	IR1	C16	C18	-106.23
56	N1	IR1	C16	C24	139.62
56	C24	C16	IR1	N1	139.62
57	C18	C16	IR1	C15	-119.08
57	C15	IR1	C16	C18	-119.08
58	C24	C16	IR1	C15	126.77
58	C15	IR1	C16	C24	126.77
59	C15	C16	IR1	C18	119.08
59	C18	IR1	C16	C15	119.08
60	C18	IR1	C16	C24	-114.15
60	C24	C16	IR1	C18	-114.15
61	C15	C16	IR1	C17	79.87
61	C17	IR1	C16	C15	79.87
62	C18	C16	IR1	C17	-39.21
62	C17	IR1	C16	C18	-39.21
63	C24	C16	IR1	C17	-153.36
63	C17	IR1	C16	C24	-153.36
64	C19	IR1	C16	C15	36.17
64	C15	C16	IR1	C19	36.17
65	C18	C16	IR1	C19	-82.91
65	C19	IR1	C16	C18	-82.91
66	C24	C16	IR1	C19	162.94
66	C19	IR1	C16	C24	162.94
67	C16	C18	IR1	I1	-40.54
67	I1	IR1	C18	C16	-40.54
68	I1	IR1	C18	C17	-156.53
68	C17	C18	IR1	I1	-156.53
69	C23	C18	IR1	I1	86.35
69	I1	IR1	C18	C23	86.35
70	C16	C18	IR1	C1	-135.63
70	C1	IR1	C18	C16	-135.63
71	C17	C18	IR1	C1	108.38
71	C1	IR1	C18	C17	108.38
72	C23	C18	IR1	C1	-8.73
72	C1	IR1	C18	C23	-8.73
73	N1	IR1	C18	C16	143.44
73	C16	C18	IR1	N1	143.44
74	C17	C18	IR1	N1	27.44
74	N1	IR1	C18	C17	27.44
75	C23	C18	IR1	N1	-89.67
75	N1	IR1	C18	C23	-89.67
76	C16	C18	IR1	C15	35.57
76	C15	IR1	C18	C16	35.57
77	C15	IR1	C18	C17	-80.42
77	C17	C18	IR1	C15	-80.42
78	C23	C18	IR1	C15	162.46
78	C15	IR1	C18	C23	162.46
79	C17	C18	IR1	C16	-115.99
79	C16	IR1	C18	C17	-115.99
80	C23	C18	IR1	C16	126.89
80	C16	IR1	C18	C23	126.89
81	C17	IR1	C18	C16	115.99
81	C16	C18	IR1	C17	115.99
82	C23	C18	IR1	C17	-117.11
82	C17	IR1	C18	C23	-117.11
83	C16	C18	IR1	C19	76.90
83	C19	IR1	C18	C16	76.90

84	C17	C18	IR1	C19	-39.10
84	C19	IR1	C18	C17	-39.10
85	C19	IR1	C18	C23	-156.21
85	C23	C18	IR1	C19	-156.21
86	C18	C17	IR1	I1	63.61
86	I1	IR1	C17	C18	63.61
87	C19	C17	IR1	I1	-51.18
87	I1	IR1	C17	C19	-51.18
88	C22	C17	IR1	I1	-173.42
88	I1	IR1	C17	C22	-173.42
89	C18	C17	IR1	C1	-81.63
89	C1	IR1	C17	C18	-81.63
90	C1	IR1	C17	C19	163.58
90	C19	C17	IR1	C1	163.58
91	C22	C17	IR1	C1	41.34
91	C1	IR1	C17	C22	41.34
92	C18	C17	IR1	N1	-163.40
92	N1	IR1	C17	C18	-163.40
93	C19	C17	IR1	N1	81.81
93	N1	IR1	C17	C19	81.81
94	N1	IR1	C17	C22	-40.43
94	C22	C17	IR1	N1	-40.43
95	C18	C17	IR1	C15	77.85
95	C15	IR1	C17	C18	77.85
96	C19	C17	IR1	C15	-36.94
96	C15	IR1	C17	C19	-36.94
97	C22	C17	IR1	C15	-159.18
97	C15	IR1	C17	C22	-159.18
98	C16	IR1	C17	C18	37.33
98	C18	C17	IR1	C16	37.33
99	C19	C17	IR1	C16	-77.45
99	C16	IR1	C17	C19	-77.45
100	C22	C17	IR1	C16	160.30
100	C16	IR1	C17	C22	160.30
101	C19	C17	IR1	C18	-114.79
101	C18	IR1	C17	C19	-114.79
102	C18	IR1	C17	C22	122.97
102	C22	C17	IR1	C18	122.97
103	C18	C17	IR1	C19	114.79
103	C19	IR1	C17	C18	114.79
104	C22	C17	IR1	C19	-122.24
104	C19	IR1	C17	C22	-122.24
105	C15	C19	IR1	I1	43.99
105	I1	IR1	C19	C15	43.99
106	C17	C19	IR1	I1	160.48
106	I1	IR1	C19	C17	160.48
107	I1	IR1	C19	C21	-94.23
107	C21	C19	IR1	I1	-94.23
108	C15	C19	IR1	C1	-144.15
108	C1	IR1	C19	C15	-144.15
109	C17	C19	IR1	C1	-27.66
109	C1	IR1	C19	C17	-27.66
110	C21	C19	IR1	C1	77.63
110	C1	IR1	C19	C21	77.63
111	N1	IR1	C19	C15	136.11
111	C15	C19	IR1	N1	136.11
112	C17	C19	IR1	N1	-107.40
112	N1	IR1	C19	C17	-107.40
113	C21	C19	IR1	N1	-2.12
113	N1	IR1	C19	C21	-2.12
114	C17	C19	IR1	C15	116.49
114	C15	IR1	C19	C17	116.49
115	C15	IR1	C19	C21	-138.22
115	C21	C19	IR1	C15	-138.22
116	C15	C19	IR1	C16	-35.45
116	C16	IR1	C19	C15	-35.45
117	C17	C19	IR1	C16	81.04
117	C16	IR1	C19	C17	81.04
118	C21	C19	IR1	C16	-173.68
118	C16	IR1	C19	C21	-173.68
119	C18	IR1	C19	C15	-77.14
119	C15	C19	IR1	C18	-77.14
120	C17	C19	IR1	C18	39.36
120	C18	IR1	C19	C17	39.36
121	C21	C19	IR1	C18	144.64
121	C18	IR1	C19	C21	144.64
122	C15	C19	IR1	C17	-116.49
122	C17	IR1	C19	C15	-116.49
123	C17	IR1	C19	C21	105.28
123	C21	C19	IR1	C17	105.28
124	C2	C3	N2	C12	-156.50
124	C12	N2	C3	C2	-156.50
125	C4	C3	N2	C12	27.42
125	C12	N2	C3	C4	27.42
126	C2	C3	N2	C13	-43.06
126	C13	N2	C3	C2	-43.06
127	C13	N2	C3	C4	140.86
127	C4	C3	N2	C13	140.86
128	C2	C3	N2	C14	84.35
128	C14	N2	C3	C2	84.35
129	C4	C3	N2	C14	-91.73
129	C14	N2	C3	C4	-91.73
130	H12A	C12	N2	C3	86.66
130	C3	N2	C12	H12A	86.66
131	C3	N2	C12	H12B	-33.34
131	H12B	C12	N2	C3	-33.34
132	H12C	C12	N2	C3	-153.34
132	C3	N2	C12	H12C	-153.34
133	H12A	C12	N2	C13	-31.64
133	C13	N2	C12	H12A	-31.64
134	H12B	C12	N2	C13	-151.64
134	C13	N2	C12	H12B	-151.64
135	C13	N2	C12	H12C	88.36
135	H12C	C12	N2	C13	88.36
136	H12A	C12	N2	C14	-154.76
136	C14	N2	C12	H12A	-154.76
137	H12B	C12	N2	C14	85.24
137	C14	N2	C12	H12B	85.24
138	H12C	C12	N2	C14	-34.76
138	C14	N2	C12	H12C	-34.76
139	H13A	C13	N2	C3	144.56
139	C3	N2	C13	H13A	144.56
140	C3	N2	C13	H13B	24.56
140	H13B	C13	N2	C3	24.56
141	H13C	C13	N2	C3	-95.44
141	C3	N2	C13	H13C	-95.44
142	H13A	C13	N2	C12	-95.63
142	C12	N2	C13	H13A	-95.63
143	H13B	C13	N2	C12	144.37

143	C12	N2	C13	H13B	144.37
144	C12	N2	C13	H13C	24.37
144	H13C	C13	N2	C12	24.37
145	H13A	C13	N2	C14	22.12
145	C14	N2	C13	H13A	22.12
146	H13B	C13	N2	C14	-97.88
146	C14	N2	C13	H13B	-97.88
147	H13C	C13	N2	C14	142.12
147	C14	N2	C13	H13C	142.12
148	C3	N2	C14	H14A	179.49
148	H14A	C14	N2	C3	179.49
149	H14B	C14	N2	C3	59.49
149	C3	N2	C14	H14B	59.49
150	H14C	C14	N2	C3	-60.51
150	C3	N2	C14	H14C	-60.51
151	H14A	C14	N2	C12	57.76
151	C12	N2	C14	H14A	57.76
152	C12	N2	C14	H14B	-62.24
152	H14B	C14	N2	C12	-62.24
153	H14C	C14	N2	C12	177.76
153	C12	N2	C14	H14C	177.76
154	H14A	C14	N2	C13	-56.55
154	C13	N2	C14	H14A	-56.55
155	H14B	C14	N2	C13	-176.55
155	C13	N2	C14	H14B	-176.55
156	H14C	C14	N2	C13	63.45
156	C13	N2	C14	H14C	63.45
157	IR1	C1	C2	C3	-176.46
157	C3	C2	C1	IR1	-176.46
158	C3	C2	C1	C6	0.00
158	C6	C1	C2	C3	0.00
159	C5	C6	C1	IR1	176.81
159	IR1	C1	C6	C5	176.81
160	C7	C6	C1	IR1	-4.36
160	IR1	C1	C6	C7	-4.36
161	C2	C1	C6	C5	-0.00
161	C5	C6	C1	C2	-0.00
162	C7	C6	C1	C2	178.83
162	C2	C1	C6	C7	178.83
163	N2	C3	C2	C1	-176.23
163	C1	C2	C3	N2	-176.23
164	C4	C3	C2	C1	-0.00
164	C1	C2	C3	C4	-0.00
165	N2	C3	C4	C5	175.93
165	C5	C4	C3	N2	175.93
166	C5	C4	C3	C2	-0.00
166	C2	C3	C4	C5	-0.00
167	C6	C5	C4	C3	0.00
167	C3	C4	C5	C6	0.00
168	C1	C6	C5	C4	-0.00
168	C4	C5	C6	C1	-0.00
169	C4	C5	C6	C7	-178.80
169	C7	C6	C5	C4	-178.80
170	C8	C7	C6	C1	-176.86
170	C1	C6	C7	C8	-176.86
171	N1	C7	C6	C1	-3.43
171	C1	C6	C7	N1	-3.43
172	C8	C7	C6	C5	1.95
172	C5	C6	C7	C8	1.95
173	N1	C7	C6	C5	175.38
173	C5	C6	C7	N1	175.38
174	C6	C7	C8	C9	172.83
174	C9	C8	C7	C6	172.83
175	C9	C8	C7	N1	-0.00
175	N1	C7	C8	C9	-0.00
176	IR1	N1	C7	C6	9.99
176	C6	C7	N1	IR1	9.99
177	C11	N1	C7	C6	-174.25
177	C6	C7	N1	C11	-174.25
178	C8	C7	N1	IR1	-175.77
178	IR1	N1	C7	C8	-175.77
179	C11	N1	C7	C8	0.00
179	C8	C7	N1	C11	0.00
180	C10	C9	C8	C7	-0.00
180	C7	C8	C9	C10	-0.00
181	C11	C10	C9	C8	0.00
181	C8	C9	C10	C11	0.00
182	C9	C10	C11	N1	0.00
182	N1	C11	C10	C9	0.00
183	IR1	N1	C11	C10	175.73
183	C10	C11	N1	IR1	175.73
184	C7	N1	C11	C10	-0.00
184	C10	C11	N1	C7	-0.00
185	C18	C16	C15	IR1	57.60
185	IR1	C15	C16	C18	57.60
186	IR1	C15	C16	C24	-116.48
186	C24	C16	C15	IR1	-116.48
187	IR1	C16	C15	C19	-57.60
187	C19	C15	C16	IR1	-57.60
188	C18	C16	C15	C19	0.00
188	C19	C15	C16	C18	0.00
189	C24	C16	C15	C19	-174.08
189	C19	C15	C16	C24	-174.08
190	IR1	C16	C15	C20	108.17
190	C20	C15	C16	IR1	108.17
191	C20	C15	C16	C18	165.77
191	C18	C16	C15	C20	165.77
192	C24	C16	C15	C20	-8.31
192	C20	C15	C16	C24	-8.31
193	C17	C19	C15	IR1	-60.30
193	IR1	C15	C19	C17	-60.30
194	C21	C19	C15	IR1	128.28
194	IR1	C15	C19	C21	128.28
195	C16	C15	C19	IR1	60.30
195	IR1	C19	C15	C16	60.30
196	C17	C19	C15	C16	-0.00
196	C16	C15	C19	C17	-0.00
197	C21	C19	C15	C16	-171.42
197	C16	C15	C19	C21	-171.42
198	IR1	C19	C15	C20	-109.14
198	C20	C15	C19	IR1	-109.14
199	C20	C15	C19	C17	-169.44
199	C17	C19	C15	C20	-169.44
200	C21	C19	C15	C20	19.14
200	C20	C15	C19	C21	19.14
201	H20A	C20	C15	IR1	76.65
201	IR1	C15	C20	H20A	76.65
202	H20B	C20	C15	IR1	-43.35
202	IR1	C15	C20	H20B	-43.35

203	IR1	C15	C20	H20C	-163.35
203	H20C	C20	C15	IR1	-163.35
204	H20A	C20	C15	C16	-13.43
204	C16	C15	C20	H20A	-13.43
205	H20B	C20	C15	C16	-133.43
205	C16	C15	C20	H20B	-133.43
206	H20C	C20	C15	C16	106.57
206	C16	C15	C20	H20C	106.57
207	H20A	C20	C15	C19	151.76
207	C19	C15	C20	H20A	151.76
208	C19	C15	C20	H20B	31.76
208	H20B	C20	C15	C19	31.76
209	H20C	C20	C15	C19	-88.24
209	C19	C15	C20	H20C	-88.24
210	C17	C18	C16	IR1	61.32
210	IR1	C16	C18	C17	61.32
211	C23	C18	C16	IR1	-128.03
211	IR1	C16	C18	C23	-128.03
212	C15	C16	C18	IR1	-61.32
212	IR1	C18	C16	C15	-61.32
213	C17	C18	C16	C15	-0.00
213	C15	C16	C18	C17	-0.00
214	C23	C18	C16	C15	170.65
214	C15	C16	C18	C23	170.65
215	IR1	C18	C16	C24	113.35
215	C24	C16	C18	IR1	113.35
216	C24	C16	C18	C17	174.67
216	C17	C18	C16	C24	174.67
217	C23	C18	C16	C24	-14.68
217	C24	C16	C18	C23	-14.68
218	H24A	C24	C16	IR1	-75.75
218	IR1	C16	C24	H24A	-75.75
219	H24B	C24	C16	IR1	164.25
219	IR1	C16	C24	H24B	164.25
220	IR1	C16	C24	H24C	44.25
220	H24C	C24	C16	IR1	44.25
221	H24A	C24	C16	C15	17.32
221	C15	C16	C24	H24A	17.32
222	H24B	C24	C16	C15	-102.68
222	C15	C16	C24	H24B	-102.68
223	H24C	C24	C16	C15	137.32
223	C15	C16	C24	H24C	137.32
224	H24A	C24	C16	C18	-156.05
224	C18	C16	C24	H24A	-156.05
225	C18	C16	C24	H24B	83.95
225	H24B	C24	C16	C18	83.95
226	H24C	C24	C16	C18	-36.05
226	C18	C16	C24	H24C	-36.05
227	C19	C17	C18	IR1	66.80
227	IR1	C18	C17	C19	66.80
228	C22	C17	C18	IR1	-124.97
228	IR1	C18	C17	C22	-124.97
229	C16	C18	C17	IR1	-66.80
229	IR1	C17	C18	C16	-66.80
230	C19	C17	C18	C16	-0.00
230	C16	C18	C17	C19	-0.00
231	C22	C17	C18	C16	168.23
231	C16	C18	C17	C22	168.23
232	IR1	C17	C18	C23	122.22
232	C23	C18	C17	IR1	122.22
233	C23	C18	C17	C19	-170.98
233	C19	C17	C18	C23	-170.98
234	C22	C17	C18	C23	-2.75
234	C23	C18	C17	C22	-2.75
235	H23A	C23	C18	IR1	-110.43
235	IR1	C18	C23	H23A	-110.43
236	H23B	C23	C18	IR1	129.57
236	IR1	C18	C23	H23B	129.57
237	IR1	C18	C23	H23C	9.57
237	H23C	C23	C18	IR1	9.57
238	H23A	C23	C18	C16	-7.54
238	C16	C18	C23	H23A	-7.54
239	H23B	C23	C18	C16	-127.54
239	C16	C18	C23	H23B	-127.54
240	H23C	C23	C18	C16	112.46
240	C16	C18	C23	H23C	112.46
241	H23A	C23	C18	C17	161.69
241	C17	C18	C23	H23A	161.69
242	C17	C18	C23	H23B	41.69
242	H23B	C23	C18	C17	41.69
243	H23C	C23	C18	C17	-78.31
243	C17	C18	C23	H23C	-78.31
244	C15	C19	C17	IR1	66.10
244	IR1	C17	C19	C15	66.10
245	C21	C19	C17	IR1	-120.40
245	IR1	C17	C19	C21	-120.40
246	C18	C17	C19	IR1	-66.10
246	IR1	C19	C17	C18	-66.10
247	C15	C19	C17	C18	0.00
247	C18	C17	C19	C15	0.00
248	C21	C19	C17	C18	173.50
248	C18	C17	C19	C21	173.50
249	IR1	C19	C17	C22	125.49
249	C22	C17	C19	IR1	125.49
250	C22	C17	C19	C15	-168.41
250	C15	C19	C17	C22	-168.41
251	C21	C19	C17	C22	5.09
251	C22	C17	C19	C21	5.09
252	H22A	C22	C17	IR1	-138.57
252	IR1	C17	C22	H22A	-138.57
253	H22B	C22	C17	IR1	101.43
253	IR1	C17	C22	H22B	101.43
254	IR1	C17	C22	H22C	-18.57
254	H22C	C22	C17	IR1	-18.57
255	H22A	C22	C17	C18	-42.01
255	C18	C17	C22	H22A	-42.01
256	H22B	C22	C17	C18	-162.01
256	C18	C17	C22	H22B	-162.01
257	H22C	C22	C17	C18	77.99
257	C18	C17	C22	H22C	77.99
258	C19	C17	C22	H22A	124.32
258	H22A	C22	C17	C19	124.32
259	H22B	C22	C17	C19	4.32
259	C19	C17	C22	H22B	4.32
260	H22C	C22	C17	C19	-115.68
260	C19	C17	C22	H22C	-115.68
261	H21A	C21	C19	IR1	91.27
261	IR1	C19	C21	H21A	91.27
262	IR1	C19	C21	H21B	-28.73

262	H21B	C21	C19	IR1	-28.73
263	H21C	C21	C19	IR1	-148.73
263	IR1	C19	C21	H21C	-148.73
264	H21A	C21	C19	C15	-18.50
264	C15	C19	C21	H21A	-18.50
265	H21B	C21	C19	C15	-138.50
265	C15	C19	C21	H21B	-138.50
266	C15	C19	C21	H21C	101.50
266	H21C	C21	C19	C15	101.50
267	H21A	C21	C19	C17	170.51
267	C17	C19	C21	H21A	170.51
268	H21B	C21	C19	C17	50.51
268	C17	C19	C21	H21B	50.51
269	H21C	C21	C19	C17	-69.49
269	C17	C19	C21	H21C	-69.49

10. UV-vis spectroscopic monitoring of exposure of CB[6] and CB[7] to CAN

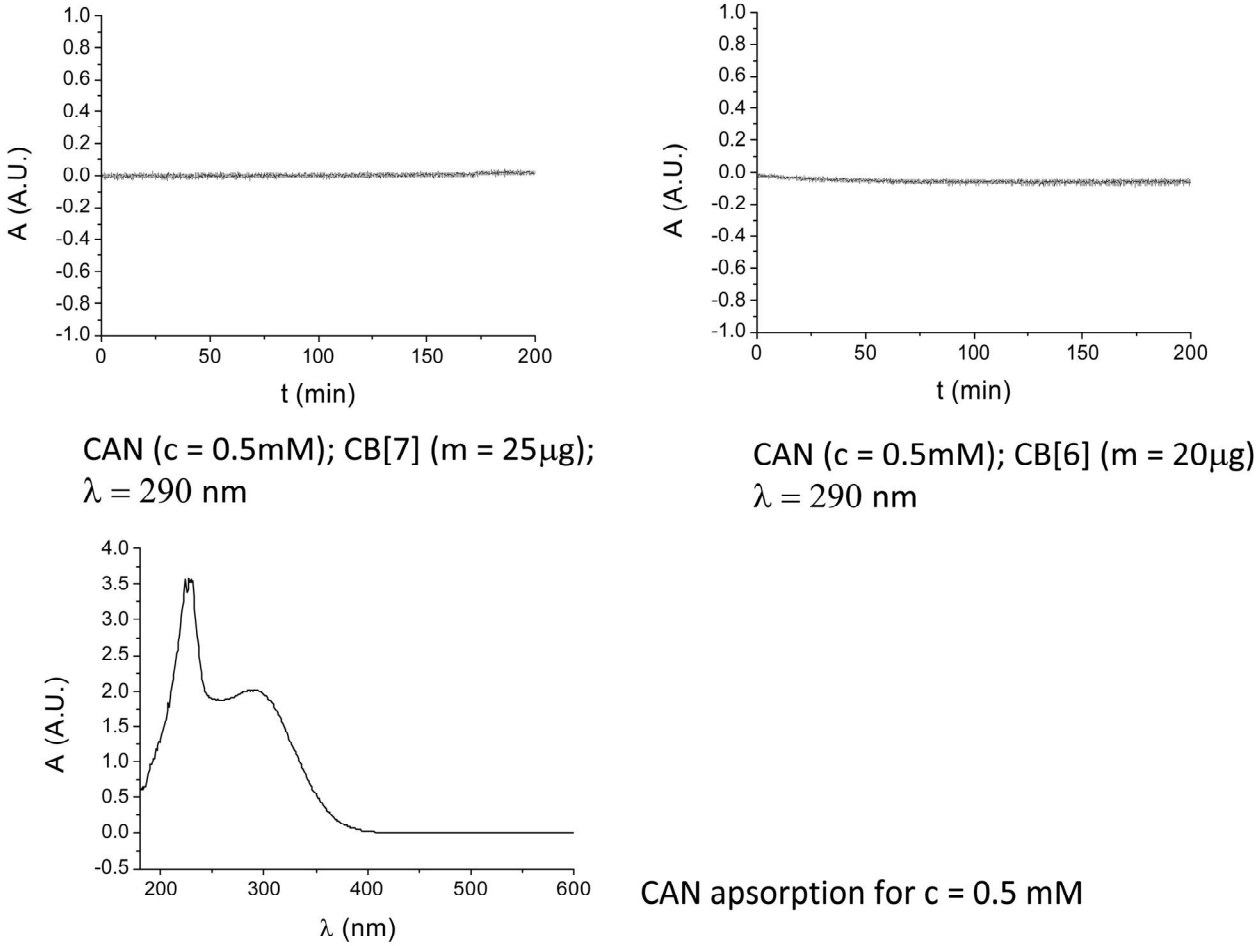

Figure 9. In a conventional wavelength scanning UV-vis spectrometer, the reference quartz cell (1cm optical path) was loaded with a stock solution of CAN whereas the sample cell was loaded with same solution of CAN added with CB[*n*] and stirred. The absorption band at 290 nm was monitored over 500 min (only a segment of 200 min corresponding to the typical time frame of a WOC experiment is shown here in two upper traces). The lower plot displays the UV-vis spectrum of the studied CAN stock solution.

11. ^{1}H NMR spectrum of CB[6] after treatment with CAN and catalyst 3 in the conditions of WOC.

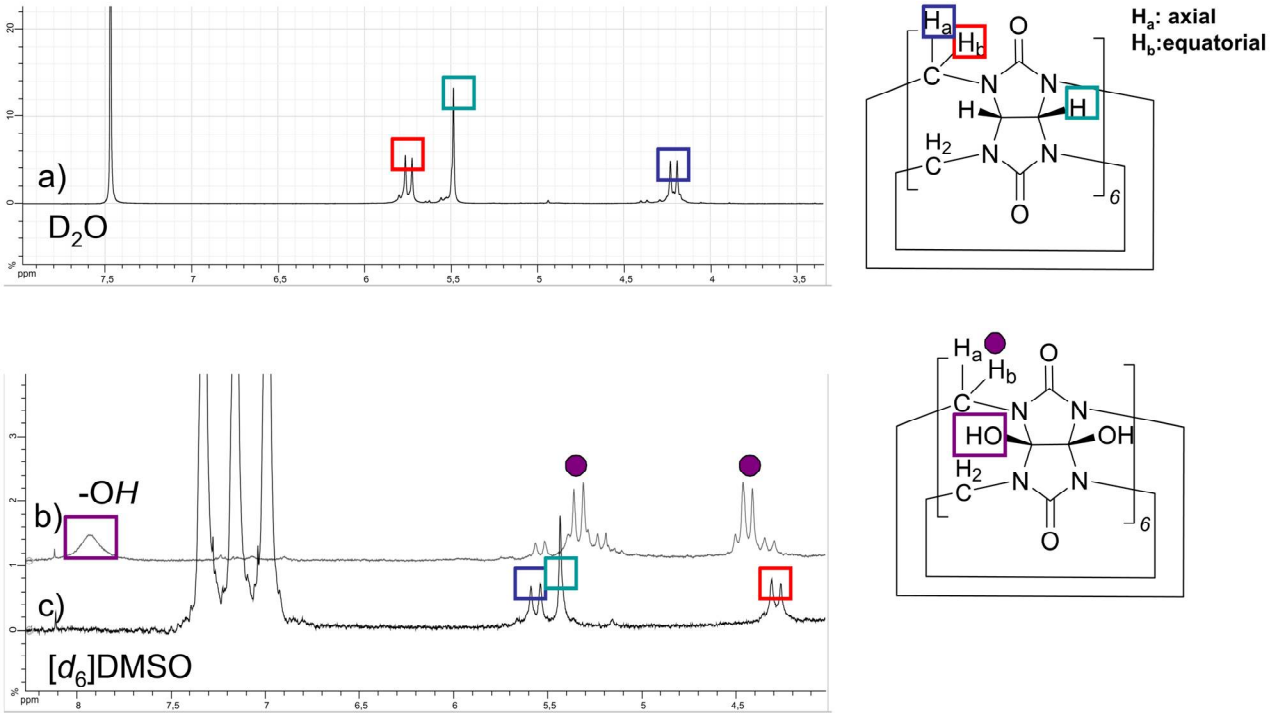

Figure 10. a) ^{1}H NMR spectrum of a solution of CB[6] in D_2O. b) ^{1}H NMR spectrum of a solution of $(OH)_6$CB[6] in [d_6]DMSO contaminated with CB[6]. c) ^{1}H NMR spectrum of the solid material recovered after a WOC experiment and upon extraction of the Ce(III) salts with a toluene solution of nBu$_3$P(O).

12. Calorimetric titrations

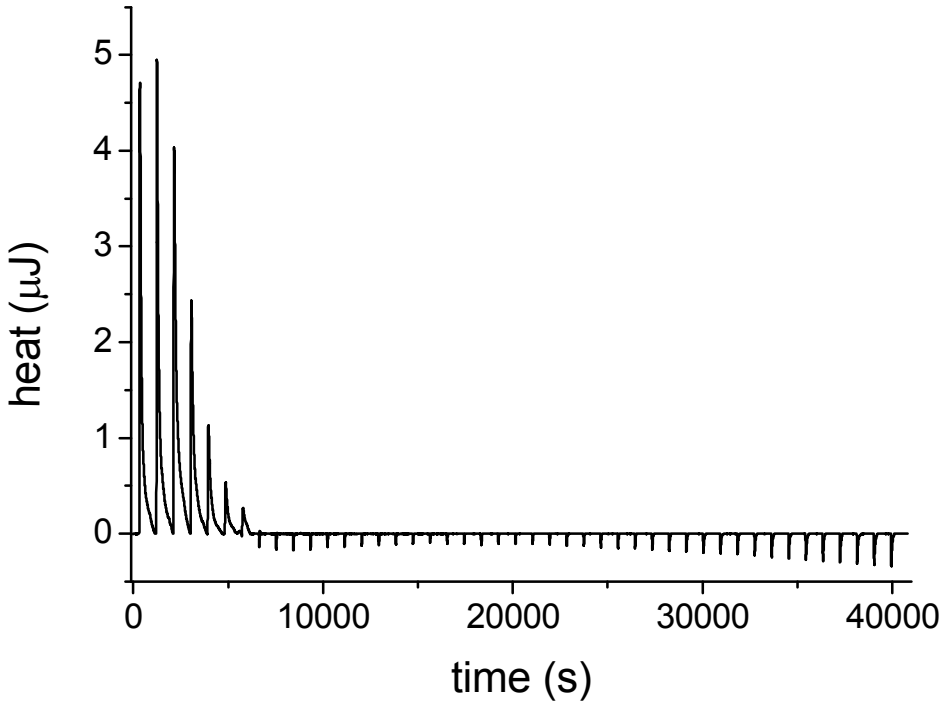

Figure 11. Heat released in the reaction : titration of cucurbit[7]uril water solution (c = 2 mM) with $IrCp^*(H_2O)_3(PF_6)_2$ complex water solution (c=10mM). Reaction was preformed on 25°C. Interval between injections was 900 seconds: $IrCp^*(H_2O)_3(PF_6)_2$: c=10mM injected into **CB**[7] : c =2mM There were 45 injections (of 2.03 μl each). Table shows the ΔH calculated for measurments of PF_6^{2-} salt :

ΔH(kcal/mol)	Statistical analysis
-3.722	Mean = -3.697
-3.612	Standard deviation = -0.07234
-3.782	
-3.672	Median = -3.697

NOTE : Raw values for the released heat were corrected for the heat values of the dilution of Ir complex (c =10mM) in pure water, enthalpies were calculated by dividing the sum of all the corrected heats for the first 11 injections divided by the number of moles of Ir complex that was used in these 11 injections. Due to the well established molarity-dependence of the enthalpy of dilution, the determination of the enthalpy and constant of inclusion was not possible by using conventional ITC models.

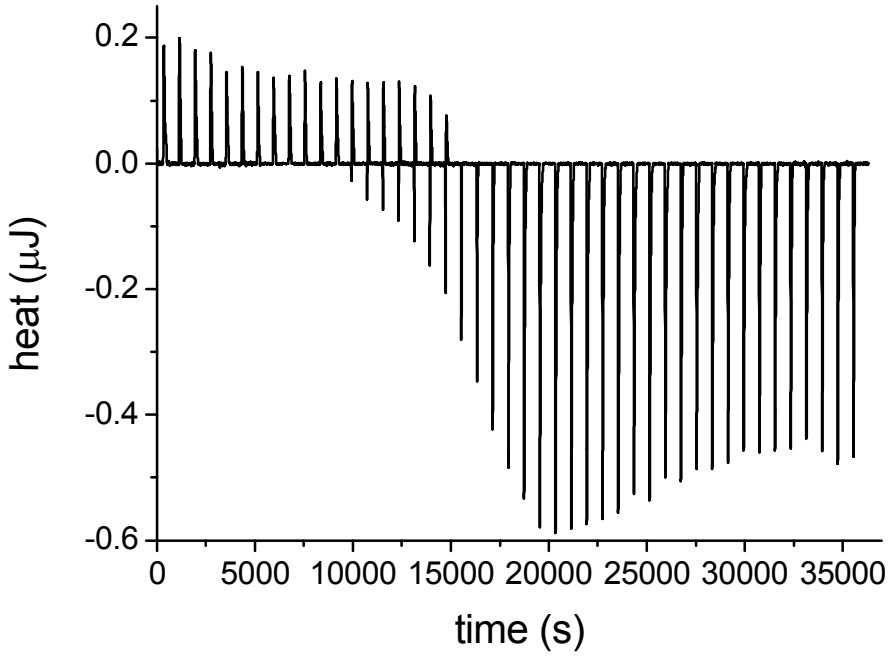

Figure 12. $IrCp^*(H_2O)_3(NO_3)_2$: *c*= 3 mM, injected into **CB**[7] : *c* =0.25mM

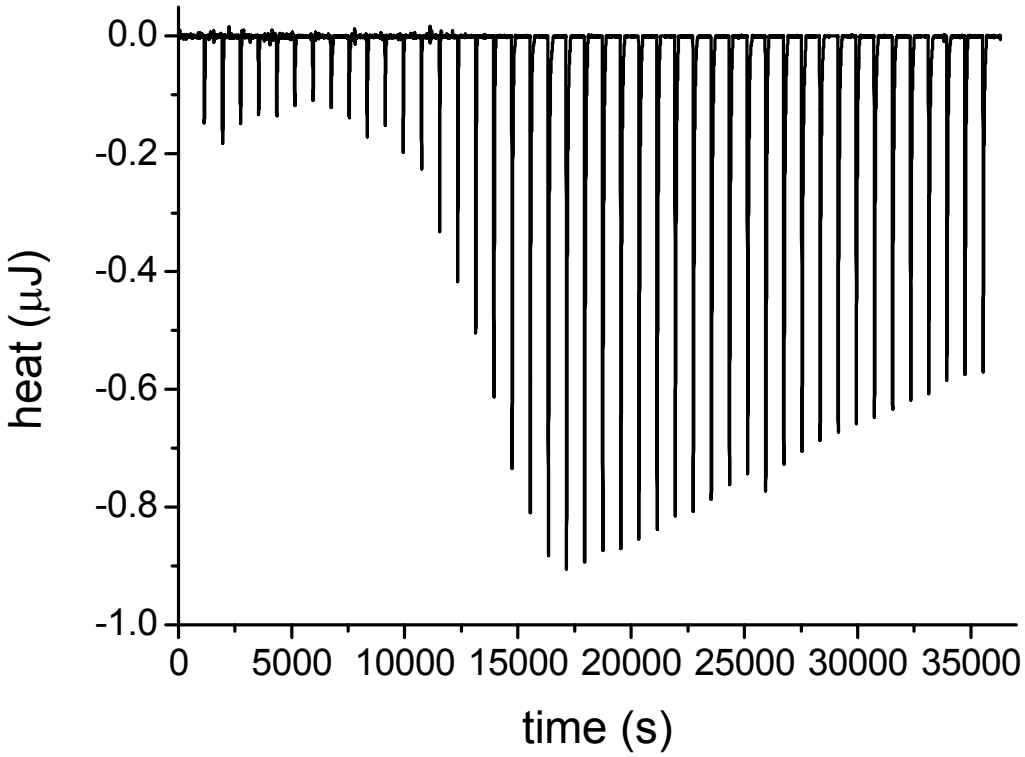

Figure 13. $IrCp^*(H_2O)_3(NO_3)_2$: *c*= 3 mM, injected into pure water.

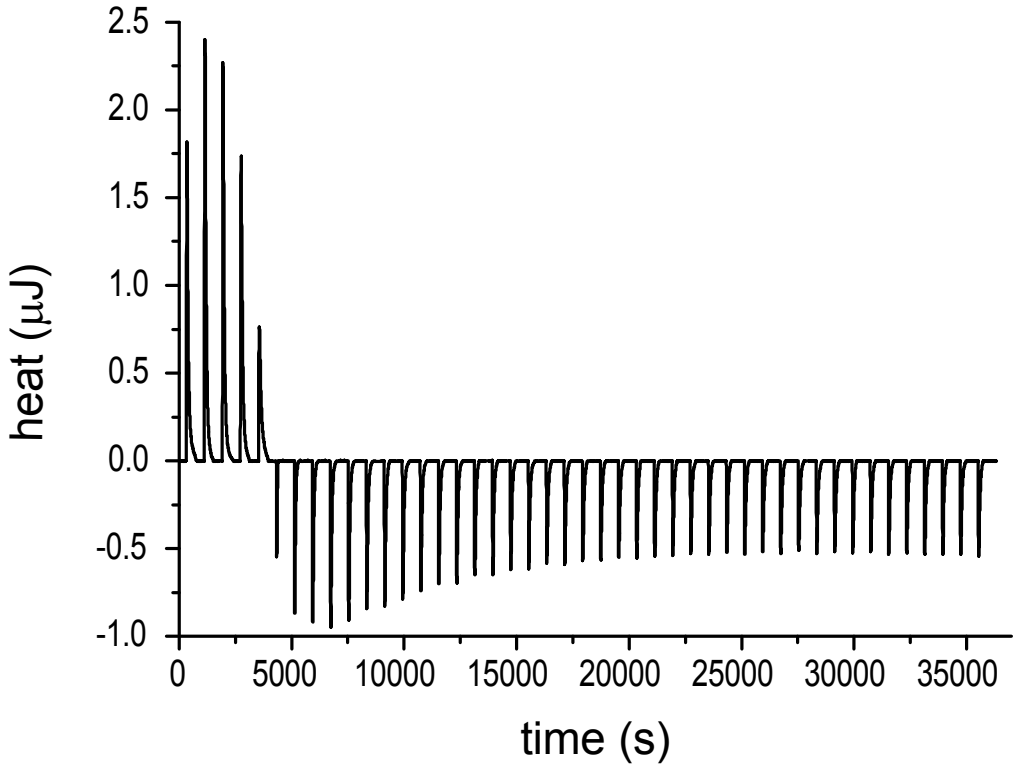

Figure 14. Thermograph: $IrCp^*(H_2O)_3(PF_6)_2$: *c*= 10 mM injected into **CB**[7] : *c*= 0.5 mM

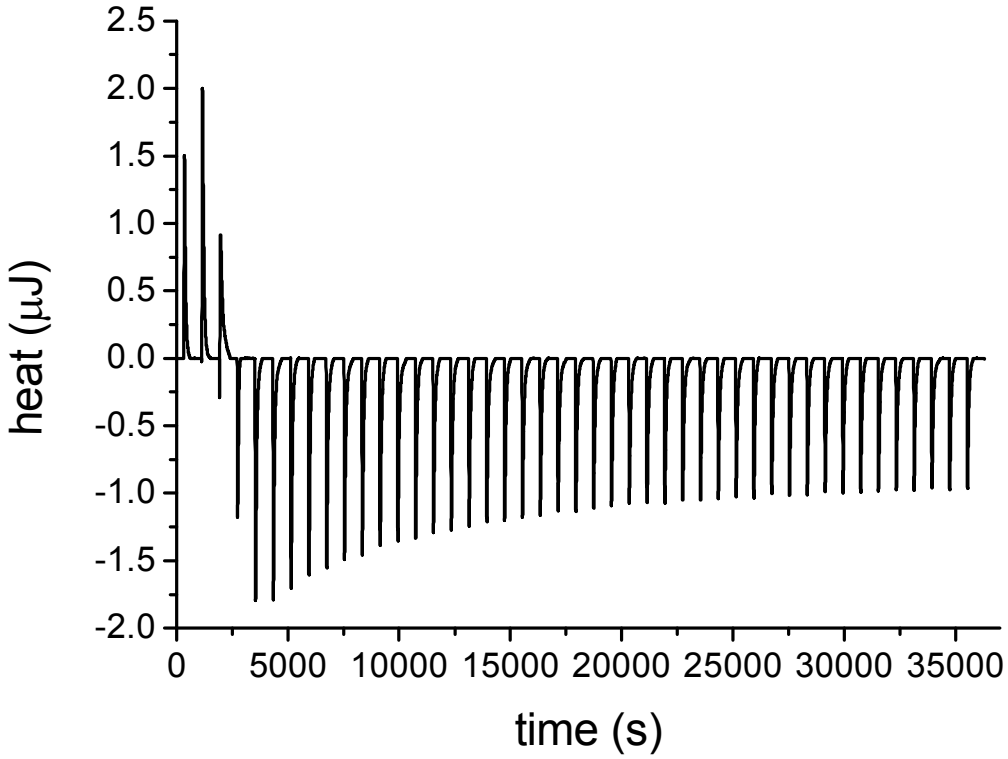

Figure 15. Dilution Thermograph : $IrCp^*(H_2O)_3(PF_6)_2$: c = 10 mM injected into water

13. Interaction of $IrCp^*(H_2O)_3(PF_6)_2$ with CB[7] in water

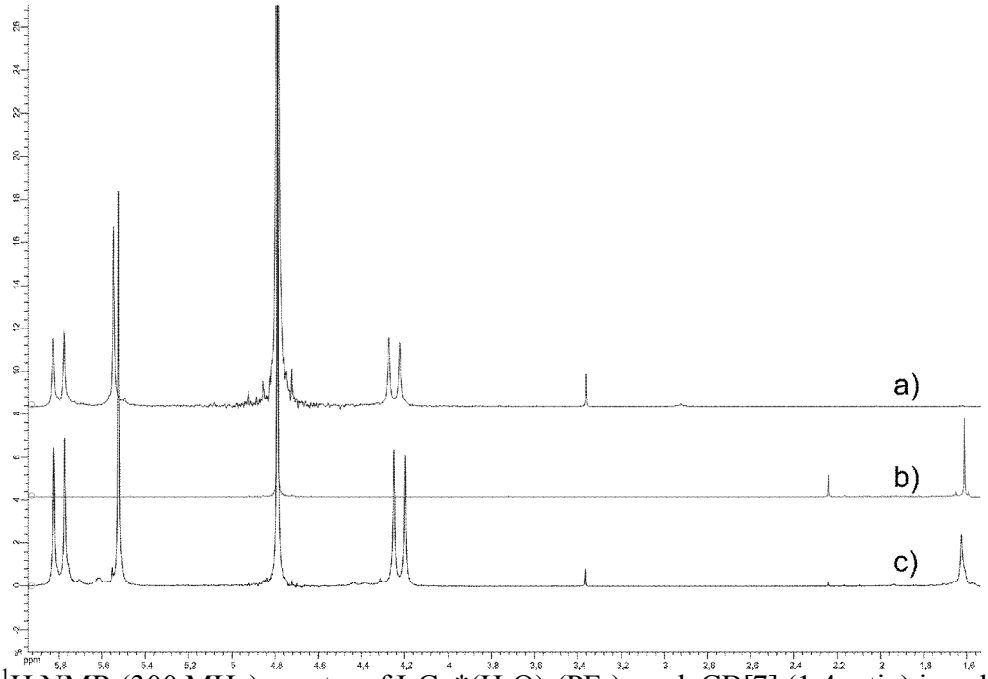

Figure 16. ^{1}H NMR (300 MHz) spectra of $IrCp^*(H_2O)_3(PF_6)_2$ and CB[7] (1:4 ratio) in solution in D_2O; a) spectrum of cucurbit[7]uril ; b) spectrum of $IrCp^*(H_2O)_3(PF_6)_2$; c) spectrum of $IrCp^*(H_2O)_3(PF_6)_2$ with CB[7]

Comments to Figure 11:

a) δ (ppm) : 4.25 (d, 2 H, *J*=15 Hz, CH_2); 5.55 (s, 2 H, CH); 5.8 (d, 2 H, *J*=15 Hz, CH_2)
b) δ (ppm) :1.61 (s, 15 H, CpCH_3)
c) δ (ppm) :1.63 (s, 15 H, CpCH_3); 4.23 (d, 2 H, J=15 Hz, CH_2); 5.52 (s, 2 H, CH); 5.8 (d, 2 H, J=15 Hz, CH_2)

14. Computational material

The method is (ZORA) B-LYP-D3(0)/all electron TZP when not specified.

$Cp^*Ir(H_2O)_3^{2+}$, gas phase

```
 Geometry CYCLE 33
 ==============

 Energy gradients wrt nuclear displacements
 ==========================================

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 H     0.000091  0.000042  0.000000
     2 H     0.000044  0.000063 -0.000049
     3 H     0.000120  0.000133  0.000016
     4 Ir   -0.000269 -0.000158  0.000369
     5 H    -0.000019  0.000298  0.000439
     6 C     0.000294  0.000241  0.000010
     7 C     0.000134 -0.000402 -0.000281
     8 C     0.000315 -0.000036  0.000102
     9 C    -0.000276  0.000189  0.000272
    10 C     0.000146  0.000166 -0.000348
    11 H    -0.000514  0.000251 -0.000158
    12 H    -0.000036 -0.000062  0.000032
    13 H     0.000073  0.000129 -0.000057
    14 H     0.000023 -0.000003 -0.000016
    15 O     0.000984 -0.000832 -0.000032
    16 H    -0.000982  0.000571 -0.000336
    17 O    -0.000062 -0.000107 -0.000334
    18 H    -0.000137  0.000030  0.000168
    19 O     0.000532 -0.000734  0.000819
    20 H    -0.000032  0.000288 -0.000547
    21 C    -0.000170 -0.000043  0.000086
    22 H     0.000030  0.000050 -0.000008
    23 H    -0.000033 -0.000107 -0.000048
    24 C    -0.000145  0.000104 -0.000026
    25 H    -0.000001 -0.000050 -0.000023
    26 H     0.000013 -0.000049  0.000003
    27 C    -0.000021 -0.000032 -0.000255
    28 H    -0.000048  0.000036  0.000056
    29 H     0.000006 -0.000043  0.000063
    30 C    -0.000264 -0.000464  0.000094
    31 H     0.000022  0.000061 -0.000013
    32 H     0.000200  0.000292  0.000038
    33 C     0.000031  0.000175 -0.000087
    34 H    -0.000027  0.000008  0.000012
    35 H    -0.000021 -0.000007  0.000039
 ----------------------------------------

 dE(predicted):    -0.51291E-05, dE(actual):    -0.34405E-05, Trust radius:    0.784141, all in a.u.

-------------------------------------------------------
Geometry Convergence after Step  33       ** CONVERGED **
-------------------------------------------------------
current energy                          -6.30479409 Hartree
energy change                -0.00000344     0.00100000    T
constrained gradient max      0.00098412     0.00100000    T
constrained gradient rms      0.00026864     0.00066667    T
gradient max                  0.00098412
gradient rms                  0.00026864
cart. step max                0.00587000     0.01000000    T
cart. step rms                0.00145086     0.00666667    T

                                    hartree              eV         kcal/mol           kJ/mol
                              ---------------------  -----------  -----------  -----------

Pauli Repulsion
  Kinetic (Delta T^0):          69.525027959984286     1891.8723     43627.62      182537.94
  Delta V^Pauli Coulomb:       -36.003876643687320     -979.7153    -22592.78      -94528.16
  Delta V^Pauli LDA-XC:         -8.442151637512678     -229.7226     -5297.53      -22164.87
  Delta V^Pauli GGA-Exchange:    0.557562632729155       15.1721       349.88        1463.88
  Delta V^Pauli GGA-Correlation: -0.646488352305294      -17.5918      -405.68       -1697.35
                              ---------------------  -----------  -----------  -----------
  Total Pauli Repulsion:        24.990073959208146      680.0145     15681.51      65611.43
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  24.990073959208146      680.0145     15681.51      65611.43
  Electrostatic Interaction:        -5.222233987366392     -142.1042     -3277.00      -13710.97
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
```

Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	19.767839971841752	537.9103	12404.51	51900.46
Orbital Interactions				
A:	-26.020640314579254	-708.0576	-16328.20	-68317.18
Total Orbital Interactions:	-26.024570317066310	-708.1646	-16330.67	-68327.50
Alternative Decomposition Orb.Int.				
Kinetic:	-62.486107787974220	-1700.3335	-39210.63	-164057.25
Coulomb:	33.612813364329057	914.6512	21092.36	88250.43
XC:	2.848724106578846	77.5177	1787.60	7479.32
Total Orbital Interactions:	-26.024570317066317	-708.1646	-16330.67	-68327.50
Residu (E=Steric+OrbInt+Res):	-0.000000536243675	0.0000	0.00	0.00
Dispersion Energy:	-0.048063187698335	-1.3079	-30.16	-126.19
Total Bonding Energy:	-6.304794069166568	-171.5622	-3956.32	-16553.23

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-5.222233987366392	-142.1042	-3277.00	-13710.97
Kinetic Energy:	7.038920172010066	191.5388	4416.99	18480.68
Coulomb (Steric+OrbInt) Energy:	-2.391063815601939	-65.0642	-1500.42	-6277.74
XC Energy:	-5.682353250509971	-154.6247	-3565.73	-14919.02
Dispersion Energy:	-0.048063187698335	-1.3079	-30.16	-126.19
Total Bonding Energy:	-6.304794069166571	-171.5622	-3956.32	-16553.23

List of All Frequencies:

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
83.271686	116.434125	2.430277
89.089438	72.216118	1.612644
118.691066	30.980081	0.921677
121.957030	40.783896	1.246733
124.260094	85.210445	2.654010
128.072901	20.647197	0.662821
132.227711	19.935374	0.660731
132.957220	29.048063	0.968071
136.358152	55.575501	1.899514
138.001753	76.788959	2.656204
141.625216	22.016681	0.781575
148.225145	20.721879	0.769891
169.136631	194.498146	8.245770
189.327422	227.121280	10.778279
193.789894	290.856140	14.128219
209.547331	197.675610	10.382771
213.713455	219.306397	11.747927
254.671763	377.144407	24.075013
262.580021	349.791239	23.022298
301.179607	32.129988	2.425572
302.697924	23.851730	1.809703
303.624603	127.163671	9.677832
304.719864	53.250312	4.067251
305.378300	44.840287	3.432295
352.431300	7.860829	0.694418
437.560678	192.854686	21.151762
439.397792	202.294910	22.280293
440.168360	181.507725	20.025898
488.784975	603.354085	73.921058
490.420381	650.750978	79.994736
515.047318	665.654284	85.935762
515.334034	202.244300	26.124211
516.538547	1910.099870	247.307269
547.301389	0.505319	0.069322
567.708494	18.304087	2.604663
584.072729	2.317542	0.339291
586.744635	5.153018	0.757860
597.345178	35.592441	5.329190
601.239324	27.200726	4.099265
612.232524	19.327687	2.966022
770.464166	0.862572	0.166581

774.880919	1.409408	0.273747
936.191208	0.124642	0.029249
936.615381	0.229282	0.053828
998.543168	129.862427	32.503373
1000.561142	98.298236	24.652867
1004.838003	38.198519	9.621010
1005.971746	58.224870	14.681566
1014.038812	45.977461	11.686316
1067.623021	34.511659	9.235530
1068.736540	33.347807	8.933384
1101.966880	0.007126	0.001968
1138.397050	0.849814	0.242491
1139.074412	0.784159	0.223890
1345.293819	8.247690	2.781170
1347.612249	3.687650	1.245640
1364.978064	42.493126	14.538594
1372.980497	31.964679	11.000509
1380.017798	70.274283	24.308557
1383.079265	28.737345	9.962579
1384.657473	14.187636	4.924141
1388.435440	51.447723	17.904818
1388.920910	44.837786	15.609887
1392.583165	19.958875	6.966831
1430.450043	0.171738	0.061577
1446.096515	77.724017	28.172837
1446.798362	15.793184	5.727377
1448.249495	36.913093	13.399910
1450.188766	100.282611	36.452577
1461.794545	0.271208	0.099373
1462.647027	4.655738	1.706892
1466.266934	32.372512	11.897823
1469.331422	52.948326	19.500694
1479.600670	62.012871	22.998760
1598.088469	65.468266	26.224651
1601.602556	296.297469	118.948992
1602.967660	306.085199	122.983022
2951.002748	14.897469	11.019457
2953.241203	4.487171	3.321618
2954.302427	14.725293	10.904279
2955.919020	11.049307	8.186639
2956.316945	23.961487	17.755906
3018.902339	4.210739	3.186291
3019.157492	5.706906	4.318814
3023.261175	3.005851	2.277829
3026.815222	10.846736	8.229303
3028.044388	5.984946	4.542559
3054.904568	0.132282	0.101292
3056.813116	4.062151	3.112454
3060.566204	4.675579	3.586867
3062.439659	0.471256	0.361745
3063.144321	1.043841	0.801456
3556.324893	204.175712	182.005109
3559.751500	112.170559	100.086761
3563.232635	122.492172	109.403341
3659.425192	156.782722	143.810019
3659.735022	90.540056	83.055514
3663.003251	111.677734	102.537322

Statistical Thermal Analysis *** ideal gas assumed ***

Pressure: 1.000000 atm.
Temperature: 298.150000 K

Moments of Inertia (and direction vectors)
==========

3045.5131	3508.9488	3512.4547
-0.0770	0.8705	0.4861
-0.8496	-0.3124	0.4248
0.5217	-0.3803	0.7637

The rotational contribution to the molecular entropy includes
a term, dependent on the symmetry number sigma. The results
reported below were computed using sigma = 1, determined
from the point group symmetry of the input geometry (NOSYM).
If this is not the correct symmetry, please contact SCM to
report a bug.

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	43.714	31.996	69.981	145.691
	Internal Energy (Kcal/mole):	0.889	0.889	192.649	194.426
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	71.288	77.250

****

*** DONE CALCULATING ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ***

CB7, gas phase.

```
Geometry CYCLE 8
==============

Energy gradients wrt nuclear displacements
==========================================

    Atom      Cartesian (a.u./angstrom)
                X         Y         Z
----------------------------------------
    1 H    -0.000010  0.000133 -0.000015
    2 C    -0.000147  0.000009  0.000013
    3 C     0.000053  0.000090  0.000275
    4 H    -0.000005  0.000019  0.000010
    5 H     0.000038  0.000049 -0.000118
    6 C    -0.000338  0.000153 -0.000330
    7 C    -0.000179 -0.000080  0.000251
    8 H     0.000077  0.000112 -0.000020
    9 H    -0.000025  0.000009  0.000024
   10 C     0.000187 -0.000072  0.000047
   11 C     0.000092  0.000057  0.000146
   12 H     0.000140 -0.000059  0.000066
   13 H     0.000139 -0.000126 -0.000052
   14 C    -0.000136  0.000236 -0.000199
   15 C    -0.000066 -0.000076  0.000011
   16 H    -0.000127 -0.000060 -0.000144
   17 H    -0.000060 -0.000026 -0.000111
   18 C    -0.000006  0.000339 -0.000019
   19 C     0.000176  0.000018  0.000075
   20 H    -0.000050  0.000038 -0.000033
   21 H    -0.000026 -0.000018 -0.000063
   22 C     0.000140  0.000178 -0.000017
   23 C    -0.000108 -0.000054  0.000135
   24 H    -0.000046 -0.000029  0.000155
   25 H    -0.000130  0.000005  0.000119
   26 C    -0.000090 -0.000059  0.000135
   27 C     0.000117 -0.000114  0.000126
   28 H    -0.000016  0.000023 -0.000080
   29 H     0.000038  0.000120 -0.000060
   30 O    -0.000007  0.000109 -0.000013
   31 O     0.000098  0.000031 -0.000043
   32 O    -0.000007  0.000052 -0.000183
   33 O     0.000013  0.000294 -0.000733
   34 O     0.000042  0.000326 -0.000402
   35 O     0.000124 -0.000134 -0.000104
   36 O    -0.000177  0.000124 -0.000142
   37 O     0.000093  0.000095  0.000143
   38 O     0.000017 -0.000098  0.000202
   39 O     0.000084 -0.000065  0.000078
   40 O     0.000158 -0.000156  0.000109
   41 O     0.000070 -0.000104  0.000174
   42 O    -0.000130  0.000032  0.000020
   43 O     0.000044  0.000002  0.000168
   44 N    -0.000328 -0.000370  0.000106
   45 N     0.000357  0.000353 -0.000199
   46 N    -0.000176  0.000516  0.000213
   47 N    -0.000012 -0.000497  0.000141
   48 N     0.000201 -0.000130 -0.000059
   49 N     0.000016  0.000111 -0.000184
   50 N    -0.000572 -0.000256  0.000080
   51 N    -0.000156  0.000089  0.000092
   52 N     0.000147  0.000271 -0.000275
   53 N     0.000084  0.000192 -0.000042
   54 N     0.000054 -0.000430 -0.000814
   55 N     0.000037 -0.000179 -0.000355
   56 N     0.000127  0.000062 -0.000267
   57 N    -0.000383  0.000023  0.000193
   58 N     0.000506  0.000337  0.000132
   59 N    -0.000141 -0.000128 -0.000144
   60 N     0.000174 -0.000190 -0.000032
   61 N     0.000377  0.000254  0.000386
   62 N     0.000058 -0.000088 -0.000112
   63 N     0.000119 -0.000338  0.000230
   64 N     0.000319 -0.000191 -0.000074
   65 N    -0.000281 -0.000066  0.000343
   66 N    -0.000205 -0.000385 -0.000001
   67 N    -0.000352 -0.000660 -0.000035
   68 N     0.000005 -0.000110  0.000211
   69 N     0.000250 -0.000011  0.000327
   70 N    -0.000165  0.000194  0.000245
   71 N    -0.000022  0.000004  0.000043
   72 C    -0.000127 -0.000109  0.000231
```

```
    73 C     0.000157 -0.000159 -0.000163
    74 H    -0.000025  0.000037  0.000120
    75 H     0.000008  0.000037 -0.000018
    76 C     0.000049 -0.000175 -0.000085
    77 C    -0.000159  0.000267 -0.000171
    78 H     0.000029 -0.000075  0.000118
    79 H     0.000083 -0.000028 -0.000025
    80 C     0.000156 -0.000058 -0.000127
    81 C     0.000007  0.000038 -0.000039
    82 H     0.000053  0.000013  0.000056
    83 H    -0.000009  0.000065  0.000096
    84 C     0.000275 -0.000289  0.000427
    85 C    -0.000115 -0.000044 -0.000194
    86 H     0.000134  0.000055 -0.000114
    87 H     0.000010  0.000098 -0.000092
    88 C    -0.000315 -0.000258  0.000366
    89 C    -0.000221  0.000050  0.000085
    90 H     0.000029 -0.000029 -0.000082
    91 H    -0.000058 -0.000068  0.000050
    92 C     0.000101  0.000443  0.000525
    93 C    -0.000073  0.000002  0.000001
    94 H    -0.000003 -0.000124  0.000022
    95 H     0.000080 -0.000213  0.000071
    96 C     0.000237 -0.000034  0.000143
    97 C     0.000040  0.000154 -0.000202
    98 H    -0.000179 -0.000034 -0.000019
    99 H    -0.000116  0.000000 -0.000114
   100 C    -0.000015 -0.000026 -0.000222
   101 H     0.000011  0.000052 -0.000120
   102 C    -0.000104  0.000141 -0.000347
   103 H    -0.000006  0.000071  0.000061
   104 C    -0.000169  0.000100  0.000131
   105 H     0.000082  0.000050 -0.000010
   106 C     0.000136  0.000215 -0.000192
   107 H    -0.000040  0.000042 -0.000011
   108 C    -0.000389 -0.000015  0.000139
   109 H     0.000096 -0.000009 -0.000011
   110 C     0.000178  0.000485  0.000428
   111 H     0.000066 -0.000200 -0.000046
   112 C    -0.000067  0.000040 -0.000256
   113 H     0.000052  0.000021  0.000107
   114 C     0.000088 -0.000082  0.000081
   115 H    -0.000019 -0.000029 -0.000166
   116 C     0.000082 -0.000154 -0.000138
   117 H    -0.000126  0.000086 -0.000047
   118 C    -0.000085  0.000097  0.000047
   119 H     0.000015 -0.000083 -0.000021
   120 C     0.000162  0.000001  0.000104
   121 H    -0.000130 -0.000046  0.000009
   122 C    -0.000335  0.000091 -0.000032
   123 H     0.000145 -0.000033  0.000029
   124 C     0.000230  0.000236 -0.000033
   125 H    -0.000036 -0.000129  0.000115
   126 C     0.000041 -0.000189 -0.000216
 ----------------------------------------

----------------------------------------
Geometry Convergence after Step   8
----------------------------------------
current energy                          -29.92083518 Hartree
energy change                 -0.00009261     0.00100000    T
constrained gradient max       0.00081435     0.00100000    T
constrained gradient rms       0.00017859     0.00066667    T
gradient max                   0.00081435
gradient rms                   0.00017859
cart. step max                 0.00968254     0.01000000    T
cart. step rms                 0.00272179     0.00666667    T


                                    hartree             eV        kcal/mol          kJ/mol
                                ---------------     ----------     ----------     ----------

Pauli Repulsion
  Kinetic (Delta T^0):          391.573919567982500    10655.2685      245716.37      1028077.18
  Delta V^Pauli Coulomb:       -203.720493469521585    -5543.5167     -127836.55      -534868.08
  Delta V^Pauli LDA-XC:         -47.522622248611412    -1293.1563      -29820.90      -124770.63
  Delta V^Pauli GGA-Exchange:     2.862158965663355       77.8833        1796.03        7514.60
  Delta V^Pauli GGA-Correlation:  -3.369642246255633      -91.6926        -2114.48       -8846.99
                                ---------------     ----------     ----------     ----------
  Total Pauli Repulsion:        139.823320569257220     3804.7861       87740.47       367106.08
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli): 139.823320569257220     3804.7861       87740.47       367106.08
```

Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-30.819827397483877	-838.6502	-19339.74	-80917.45
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	109.003493171773343	2966.1360	68400.73	286188.63
Orbital Interactions				
A:	-138.670266228749483	-3773.4099	-87016.91	-364078.73
Total Orbital Interactions:	-138.670266228749369	-3773.4099	-87016.91	-364078.73
Alternative Decomposition Orb.Int.				
Kinetic:	-362.345625644161714	-9859.9262	-227375.34	-951338.31
Coulomb:	204.509300593479992	5564.9812	128331.54	536939.09
XC:	19.166058821932271	521.5350	12026.88	50320.48
Total Orbital Interactions:	-138.670266228749455	-3773.4099	-87016.91	-364078.73
Residu (E=Steric+OrbInt+Res):	-0.000058107784269	-0.0016	-0.04	-0.15
Dispersion Energy:	-0.253801186119520	-6.9063	-159.26	-666.35
Total Bonding Energy:	-29.920632350879817	-814.1818	-18775.48	-78556.61

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-30.819827397483877	-838.6502	-19339.74	-80917.45
Kinetic Energy:	29.228293923820786	795.3423	18341.03	76738.87
Coulomb (Steric+OrbInt) Energy:	0.788749016174137	21.4630	494.95	2070.86
XC Energy:	-28.864046707271424	-785.4307	-18112.46	-75782.54
Dispersion Energy:	-0.253801186119520	-6.9063	-159.26	-666.35
Total Bonding Energy:	-29.920632350879899	-814.1818	-18775.48	-78556.61

List of All Frequencies:

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
12.805815	0.000000	0.000000
17.141498	0.000000	0.000000
18.794241	0.000000	0.000000
27.639151	0.389790	0.002700
34.189983	4.825554	0.041355
35.827793	3.968126	0.035636
40.457208	6.474989	0.065662
49.918136	21.241109	0.265775
53.525446	15.113332	0.202768
58.470630	7.065432	0.103551
59.947674	4.315832	0.064851
65.331503	13.797259	0.225940
66.647641	1.905922	0.031840
80.527441	131.883086	2.662018
82.154411	476.348605	9.809206
83.219182	91.579400	1.910290
84.892541	70.854323	1.507697
88.152814	279.298392	6.171386
91.029990	92.243154	2.104732
91.684920	320.297261	7.360871
94.776990	176.533289	4.193799
97.786247	129.055974	3.163253
99.236835	277.405570	6.900271
100.712787	23.691075	0.598064
108.091194	89.234479	2.417693
120.608865	69.921946	2.113834
136.219962	0.830567	0.028359
136.793104	21.238712	0.728233
138.884997	93.237678	3.245823
141.501711	1.270085	0.045048
145.082132	3.896292	0.141691
146.445663	3.102227	0.113875
154.631327	0.377216	0.014621
155.975988	4.558124	0.178206
167.272167	19.467577	0.816232
171.398111	28.360203	1.218410
174.494195	29.597871	1.294552
176.342265	8.170679	0.361154

180.085311	12.697557	0.573161
180.708207	18.000774	0.815356
185.130028	1.328588	0.061652
198.161725	0.259998	0.012914
207.470858	0.011416	0.000594
217.104343	26.146107	1.422832
219.744663	18.652538	1.027388
225.999817	15.716281	0.890299
226.339386	33.040110	1.874475
229.738310	22.267588	1.282285
250.556455	25.616094	1.608780
251.708243	14.239204	0.898382
254.203890	37.637800	2.398195
254.843137	12.870418	0.822136
278.024599	1.767493	0.123174
281.040355	9.158670	0.645177
281.641949	4.625259	0.326521
282.607317	2.260876	0.160154
310.805360	10.973597	0.854900
316.198823	2.284772	0.181084
319.250290	56.306433	4.505753
320.633363	38.041292	3.057328
331.627826	0.069492	0.005777
339.685655	0.811458	0.069091
340.586008	18.223716	1.555757
346.156290	3.708399	0.321764
354.952007	818.144863	72.791038
356.491085	861.733288	77.001576
359.074018	8.809114	0.792856
359.703055	15.656151	1.411585
359.914965	17.763749	1.602554
363.533247	2.835490	0.258375
364.924253	4.953239	0.453075
368.466014	7.952960	0.734521
369.206555	14.527953	1.344472
373.317097	1.580008	0.147848
374.137488	3.734010	0.350175
403.253749	0.706806	0.071442
403.984650	2.646890	0.268027
407.994681	0.115564	0.011818
411.098280	24.817762	2.557327
412.464288	156.178189	16.146738
414.819628	206.101258	21.429795
424.897326	0.977228	0.104078
425.656324	1.838645	0.196171
426.974496	0.301903	0.032311
431.002228	1.003601	0.108422
441.993000	3.416798	0.378541
442.676874	2.481351	0.275330
499.504137	0.506532	0.063420
499.630837	0.426252	0.053382
557.657866	9.838712	1.375258
558.210487	29.098336	4.071404
586.470487	4.866882	0.715443
586.774994	7.195807	1.058350
593.982389	60.980223	9.079055
596.066432	75.258410	11.244180
601.216716	9.653895	1.454828
601.876317	20.566414	3.102729
602.618279	117.544599	17.755097
606.342818	94.749863	14.400411
608.366482	9.094317	1.386799
611.040627	11.656748	1.785359
627.399536	0.808299	0.127114
628.392677	0.261549	0.041197
629.046885	1.408224	0.222041
632.960940	44.832960	7.112993
634.105791	1.982569	0.315114
640.671395	554.190955	88.996482
642.060823	127.373465	20.499025
647.887382	0.684807	0.111211
651.040412	197.583609	32.243110
651.580359	158.211871	25.839560
656.662789	1.477285	0.243156
662.788329	4.348818	0.722477
671.410018	258.683952	43.534682
671.989081	270.253991	45.521064
684.966394	4.612482	0.791921
685.691273	1.231628	0.211683
686.427304	3.786596	0.651511
688.586887	0.448262	0.077369
697.397311	3.738506	0.653516
699.436825	0.135164	0.023697
702.905370	0.159235	0.028055
703.497767	0.474881	0.083739

704.036839	0.348085	0.061427
705.423642	1.920407	0.339564
706.728961	0.802434	0.142148
706.916684	1.393268	0.246877
709.856011	4.001816	0.712042
710.810335	4.017354	0.715767
713.222863	24.040388	4.297786
713.488572	21.901980	3.916954
714.964983	9.882955	1.771127
718.595538	349.813104	63.008430
746.929686	29.967430	5.610574
748.351936	4.128398	0.774400
753.462267	3.233884	0.610751
754.466181	3.045891	0.576013
759.129588	30.078079	5.723268
761.691233	337.497177	64.435792
763.091477	61.471440	11.757854
768.885183	4753.325327	916.087804
770.548874	4451.019423	859.681835
772.378793	1114.883199	215.842907
773.668385	84.903491	16.464876
789.502338	138.825603	27.472682
789.864790	85.152250	16.858811
794.173483	12.039088	2.396553
805.102990	70.335898	14.194057
806.049549	13.863611	2.801020
806.242004	197.713818	39.955863
807.845189	26.210726	5.307442
809.554328	113.601726	23.052021
811.384957	154.612285	31.444813
812.759209	100.021742	20.376725
872.305655	4.523202	0.988992
873.341610	33.209410	7.269815
875.924648	41.997160	9.220718
885.418878	0.283341	0.062884
886.461918	0.432806	0.096168
901.570700	0.497228	0.112366
901.718763	0.516450	0.116729
923.918959	0.701281	0.162407
925.117030	0.559366	0.129709
934.290770	36.019065	8.435145
935.346412	1.250267	0.293125
944.029719	11.680427	2.763901
944.139087	34.975184	8.277021
945.395791	13.092888	3.102610
946.246084	281.253353	66.708300
948.509153	1421.369987	337.929992
949.120497	1277.156488	303.839013
949.589348	164.757278	39.215568
951.575350	176.264004	42.042147
951.859264	31.117077	7.424199
960.716220	28.023475	6.748312
963.524295	4.475629	1.080923
963.939411	30.172601	7.290219
964.717708	0.282041	0.068201
971.571406	0.671194	0.163456
974.647768	1.737213	0.424403
984.006086	0.068193	0.016820
984.518177	0.122795	0.030303
992.335871	0.083126	0.020676
993.685431	0.045663	0.011373
994.211624	0.191296	0.047672
1006.180379	4.255344	1.073219
1008.079447	0.049170	0.012424
1011.159255	0.073243	0.018564
1011.760348	0.126787	0.032154
1044.310540	0.062318	0.016312
1044.680393	0.245464	0.064276
1059.898926	9.910845	2.633014
1063.536967	10.206910	2.720977
1065.763243	9.734780	2.600548
1073.203106	100.205403	26.955732
1076.467841	20.831902	5.620928
1080.741357	35.249931	9.549005
1081.349832	7.489362	2.029968
1085.567171	41.121523	11.189327
1090.022116	13.483795	3.684050
1104.200098	5.439741	1.505581
1105.804531	57.323571	15.888748
1115.706894	6.843291	1.913785
1137.353693	1.729173	0.492960
1143.225544	7.823099	2.241758
1144.284825	1469.298009	421.426750
1144.597657	1909.287677	547.775107
1146.804620	1355.152801	389.543329

1147.311507	1622.162386	466.502254
1148.650424	1163.817965	335.081927
1160.441741	340.991883	99.184876
1163.777171	14.437030	4.211393
1164.744821	3.279383	0.957417
1165.695644	12.861936	3.758111
1179.735685	123.959524	36.655799
1180.460303	491.847936	145.532607
1181.437753	32.762642	9.702146
1182.594134	583.656779	173.010047
1184.588933	3157.565626	937.557963
1185.194426	3304.557924	981.705083
1191.130104	481.501516	143.758963
1191.723783	675.819299	201.875803
1193.911692	916.534149	274.283022
1194.381492	804.761723	240.928650
1197.745029	822.536416	246.943490
1198.351565	568.867319	170.872944
1202.854166	1134.195797	341.962970
1205.374056	111.086104	33.562913
1208.375732	184.497446	55.881805
1211.303318	176.200326	53.498017
1215.155575	873.311948	265.998603
1228.932081	25.503829	7.856178
1230.065210	14.168202	4.368385
1232.254674	28.672941	8.856269
1235.448926	77.139809	23.888090
1239.037325	402.870393	125.120310
1239.838508	401.489291	124.772006
1241.907189	480.586250	149.602397
1243.142510	403.537198	125.742636
1243.695064	246.499779	76.843744
1245.050932	99.763998	31.134295
1250.015498	106.113869	33.248007
1250.669384	2.850003	0.893441
1251.706282	5.276613	1.655525
1252.412716	66.608974	20.910204
1274.576691	31.483121	10.058236
1275.347874	5.158568	1.649058
1281.997449	9.006467	2.894141
1282.820414	46.607249	14.986403
1285.878798	243.058338	78.340913
1289.039588	2733.418725	883.182573
1290.644634	3073.925430	994.438840
1304.861015	45.265884	14.805168
1305.262628	16.299656	5.332789
1305.707923	25.552113	8.362785
1306.180541	236.288916	77.361455
1306.641925	12.783418	4.186794
1307.792822	37.390247	12.256751
1308.071536	43.582977	14.289810
1340.604960	192.351531	64.636010
1343.390168	2101.005958	707.469171
1344.761783	1902.827988	641.391144
1360.300399	64.607387	22.029015
1360.478602	13.408914	4.572602
1368.339681	85.229506	29.232231
1368.643560	469.541484	161.080288
1370.493311	269.196199	92.474909
1372.813128	36.243454	12.471511
1373.244610	9.677149	3.330991
1375.695915	17.800942	6.138235
1376.324354	185.141858	63.870966
1377.350019	20.664705	7.134304
1377.603249	9.031355	3.118568
1379.317695	165.323746	57.158078
1379.364806	104.248754	36.043594
1380.189243	36.645776	12.677705
1380.635842	10.665504	3.690954
1384.628344	248.141949	86.121478
1385.327496	23.011830	7.990642
1385.675699	36.503471	12.678674
1386.018247	188.604991	65.523970
1388.122234	1.936237	0.673696
1389.275616	33.751664	11.753350
1390.220157	15.191200	5.293632
1390.605259	27.245035	9.496625
1392.714789	5.642507	1.969756
1393.598103	3.733199	1.304058
1401.416884	1.991402	0.699527
1402.240992	117.962947	41.461627
1402.661224	5.872353	2.064634
1404.172846	44.498987	15.662056
1407.384288	108.543288	38.290738
1409.393853	32.872566	11.612990

1409.552159	413.192966	145.986313
1410.490518	631.942780	223.422032
1411.186544	893.630418	316.097048
1413.104876	92.838808	32.883802
1414.461015	44.794370	15.881535
1419.920464	74.421172	26.487355
1420.451048	35.565686	12.662969
1423.894051	0.564791	0.201578
1428.435454	284.698222	101.935028
1429.609523	159.423682	57.127910
1430.325039	219.201103	78.587875
1431.066574	122.709355	44.016508
1431.274563	36.325102	13.031904
1432.200080	94.290974	33.849471
1432.902044	66.777985	23.984346
1433.552898	85.489817	30.718937
1433.702568	69.611971	25.016184
1434.133838	3.733074	1.341944
1435.388846	15.537605	5.590256
1435.641787	11.043573	3.974054
1437.918378	34.532438	12.446279
1438.887619	24.317708	8.770565
1700.882381	7.553156	3.220185
1701.315782	0.953286	0.406524
1704.361908	0.766999	0.327668
1704.645235	3.493264	1.492600
1710.948684	7.141489	3.062696
1711.469823	23.771624	10.197793
1717.082958	8.721790	3.753833
1717.674989	1.152747	0.496310
1724.579041	123.545889	53.405929
1726.890316	165.225278	71.518651
1733.849963	349.461982	151.876129
1735.886992	382.941828	166.621993
1740.034603	8752.382664	3817.352388
1745.488634	5.918092	2.589267
2861.484432	63.793935	45.756084
2864.032530	15.399050	11.054776
2864.142814	51.083624	36.673675
2865.313289	15.459083	11.102836
2868.427855	37.406005	26.894491
2869.048326	6.303101	4.532838
2870.623654	6.533779	4.701308
2875.005976	32.533043	23.444529
2875.811677	11.633742	8.386060
2877.469328	9.909741	7.147450
2878.626206	2.542800	1.834744
2880.615252	14.634279	10.566585
2882.154777	37.254490	26.913736
2883.558598	43.002909	31.081694
2884.623182	93.422057	67.548636
2884.875254	77.497495	56.039309
2886.489473	50.035098	36.201187
2887.024908	167.799132	121.427852
2890.420671	33.084019	23.969413
2892.329790	171.434015	124.286191
2893.535865	123.860787	89.834007
2897.599052	274.322714	199.240732
2898.314159	157.785158	114.627726
2903.999151	151.665964	110.398376
2920.775615	97.663625	71.500504
2926.220601	29.458082	21.606758
2926.761181	166.203263	121.928408
2927.236224	60.824392	44.628636
3034.406411	12.806635	9.740625
3034.465062	6.934018	5.274062
3035.543071	11.742245	8.934404
3035.877228	3.070945	2.336869
3036.753449	12.210079	9.294073
3037.313265	7.618750	5.800312
3037.881580	15.460468	11.772577
3038.659111	13.603522	10.361233
3041.038722	8.554402	6.520632
3041.277425	10.974680	8.366156
3043.235000	8.768734	6.688834
3043.441229	7.717377	5.887253
3044.095687	8.892284	6.784998
3044.406108	8.883285	6.778823

Statistical Thermal Analysis *** ideal gas assumed ***

```
Pressure:                  1.000000 atm.
Temperature:             298.150000 K


Moments of Inertia (and direction vectors)
==========================================

      71272.7527      74194.2649     115510.1859
-------------------------------------------------
          0.9388          0.2117          0.2718
         -0.0751          0.8958         -0.4382
         -0.3362          0.3909          0.8568


The rotational contribution to the molecular entropy includes
a term, dependent on the symmetry number sigma. The results
reported below were computed using sigma = 1, determined
from the point group symmetry of the input geometry (NOSYM).
If this is not the correct symmetry, please contact SCM to
report a bug.

    Temp                                                    Transl     Rotat    Vibrat     Total
    ----                                                    ------     -----    ------     -----

    298.15   Entropy (cal/mole-K):                          47.030    41.631   224.865   313.526
             Internal Energy (Kcal/mole):                    0.889     0.889   619.205   620.983
             Constant Volume Heat Capacity (cal/mole-K):     2.981     2.981   241.295   247.257

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


*** DONE CALCULATING ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ***
```

host-guest complex gas phase

```
G E O M E T R Y   U P D A T E  ***  23  ***

*** Using NEW gradient routines ***

Energy gradients wrt nuclear displacements
==========================================

    Atom      Cartesian (a.u./angstrom)
                X         Y         Z
------------------------------------------
    1 H    -0.000053 -0.000041  0.000052
    2 C     0.000009 -0.000001  0.000048
    3 C     0.000030  0.000005 -0.000091
    4 H    -0.000004  0.000043 -0.000048
    5 H     0.000050  0.000077  0.000010
    6 C    -0.000015  0.000025  0.000013
    7 C    -0.000115 -0.000025 -0.000080
    8 H     0.000011 -0.000003  0.000016
    9 H     0.000005  0.000015 -0.000023
   10 C     0.000004  0.000003 -0.000072
   11 C    -0.000049 -0.000066  0.000056
   12 H     0.000062 -0.000020  0.000014
   13 H     0.000027 -0.000014 -0.000046
   14 C     0.000003 -0.000012 -0.000005
   15 C    -0.000048  0.000001  0.000108
   16 H    -0.000036 -0.000010 -0.000028
   17 H    -0.000032 -0.000023 -0.000012
   18 C    -0.000101  0.000023 -0.000202
   19 C     0.000049  0.000000  0.000105
   20 H    -0.000029  0.000034 -0.000029
   21 H    -0.000048  0.000005 -0.000035
   22 C    -0.000054 -0.000007  0.000051
   23 C    -0.000082 -0.000041  0.000004
   24 H    -0.000002 -0.000011 -0.000005
   25 H    -0.000003 -0.000005  0.000002
   26 C    -0.000015 -0.000071  0.000037
   27 C     0.000027 -0.000087 -0.000083
   28 H    -0.000019 -0.000016  0.000061
   29 H    -0.000031 -0.000008  0.000032
   30 O     0.000027 -0.000090  0.000012
   31 O    -0.000009 -0.000040 -0.000044
   32 O    -0.000057  0.000032  0.000108
   33 O    -0.000042 -0.000056  0.000073
   34 O    -0.000079 -0.000037  0.000074
   35 O    -0.000022  0.000098 -0.000010
   36 O     0.000209 -0.000060  0.000105
   37 O     0.000028  0.000080 -0.000011
   38 O     0.000031  0.000145  0.000010
   39 O     0.000029  0.000036 -0.000070
   40 O     0.000010 -0.000014 -0.000017
   41 O     0.000047  0.000021  0.000099
   42 O    -0.000005  0.000013 -0.000006
   43 O    -0.000008  0.000016 -0.000020
   44 N     0.000037 -0.000019  0.000040
   45 N    -0.000085  0.000022 -0.000145
   46 N     0.000069 -0.000181 -0.000025
   47 N     0.000123 -0.000063  0.000071
   48 N     0.000089  0.000064 -0.000105
   49 N     0.000004  0.000027  0.000238
   50 N    -0.000053 -0.000031  0.000079
   51 N    -0.000021 -0.000161  0.000159
   52 N    -0.000152 -0.000176  0.000036
   53 N    -0.000031 -0.000130 -0.000006
   54 N     0.000025  0.000076  0.000360
   55 N    -0.000086  0.000026 -0.000158
   56 N    -0.000057  0.000047  0.000092
   57 N    -0.000046  0.000125 -0.000008
   58 N     0.000043  0.000017  0.000046
   59 N    -0.000010  0.000072  0.000007
   60 N     0.000026  0.000171  0.000080
   61 N     0.000090 -0.000113  0.000027
   62 N     0.000124 -0.000063  0.000172
   63 N     0.000064  0.000064  0.000008
   64 N     0.000048 -0.000041  0.000012
   65 N    -0.000090  0.000010 -0.000035
   66 N     0.000087  0.000017 -0.000006
   67 N    -0.000090  0.000031  0.000085
   68 N     0.000083 -0.000043 -0.000287
   69 N     0.000015  0.000123  0.000097
```

70	N	0.000128	0.000035	-0.000086
71	N	-0.000070	0.000130	0.000043
72	C	-0.000002	-0.000047	0.000043
73	C	-0.000068	-0.000071	0.000051
74	H	-0.000042	-0.000101	-0.000038
75	H	-0.000084	-0.000048	-0.000076
76	C	-0.000078	-0.000035	-0.000016
77	C	-0.000147	-0.000077	0.000032
78	H	-0.000025	0.000012	-0.000002
79	H	0.000010	0.000003	0.000003
80	C	-0.000017	0.000006	-0.000118
81	C	-0.000021	-0.000034	-0.000155
82	H	-0.000013	-0.000023	0.000028
83	H	-0.000033	-0.000021	0.000046
84	C	0.000008	0.000160	-0.000139
85	C	0.000014	-0.000021	-0.000104
86	H	-0.000076	-0.000056	0.000034
87	H	-0.000064	-0.000023	0.000027
88	C	0.000017	0.000131	-0.000041
89	C	-0.000176	0.000067	-0.000084
90	H	0.000020	0.000054	-0.000018
91	H	0.000001	0.000005	0.000060
92	C	0.000163	-0.000032	0.000000
93	C	-0.000039	-0.000048	0.000027
94	H	-0.000002	-0.000011	0.000016
95	H	0.000005	0.000008	-0.000009
96	C	-0.000050	0.000049	-0.000157
97	C	0.000103	-0.000087	-0.000015
98	H	0.000079	-0.000008	0.000003
99	H	0.000016	-0.000011	0.000050
100	C	-0.000058	0.000014	-0.000051
101	H	0.000024	0.000002	0.000023
102	C	0.000081	-0.000057	0.000118
103	H	-0.000022	0.000005	-0.000046
104	C	0.000028	-0.000018	0.000009
105	H	-0.000069	-0.000065	-0.000116
106	C	-0.000062	0.000058	-0.000203
107	H	0.000009	0.000006	0.000005
108	C	-0.000113	0.000097	0.000053
109	H	0.000009	-0.000045	-0.000024
110	C	0.000040	-0.000051	-0.000257
111	H	-0.000035	-0.000018	0.000050
112	C	-0.000091	0.000027	-0.000048
113	H	0.000016	0.000000	0.000020
114	C	0.000095	-0.000001	0.000040
115	H	-0.000078	-0.000018	0.000009
116	C	-0.000099	0.000148	-0.000057
117	H	-0.000016	-0.000047	0.000010
118	C	0.000051	0.000052	-0.000138
119	H	-0.000014	-0.000010	0.000014
120	C	-0.000095	0.000125	0.000247
121	H	-0.000036	-0.000007	-0.000050
122	C	0.000020	-0.000074	-0.000086
123	H	-0.000039	0.000025	0.000038
124	C	-0.000033	-0.000021	0.000158
125	H	0.000043	-0.000028	-0.000019
126	C	0.000198	-0.000091	0.000016
127	H	0.000024	-0.000108	0.000253
128	H	0.000014	0.000034	0.000032
129	H	-0.000036	-0.000041	-0.000125
130	Ir	0.000050	-0.000510	0.000318
131	H	0.000080	0.000066	-0.000067
132	C	0.000226	-0.000066	0.000093
133	C	-0.000031	0.000260	-0.000245
134	C	0.000065	-0.000247	-0.000031
135	C	-0.000252	0.000292	0.000127
136	C	0.000002	0.000133	-0.000026
137	H	0.000045	-0.000012	0.000021
138	H	0.000017	0.000031	-0.000016
139	H	0.000046	0.000024	-0.000122
140	H	-0.000001	-0.000031	-0.000052
141	O	0.000006	-0.000268	0.000205
142	H	0.000008	0.000075	-0.000055
143	O	0.000216	0.000480	-0.000384
144	H	0.000005	-0.000075	0.000026
145	O	-0.000173	0.000240	-0.000013
146	H	0.000050	0.000071	-0.000021
147	C	0.000000	0.000075	-0.000128
148	H	0.000020	0.000022	-0.000094
149	H	-0.000002	-0.000019	-0.000046
150	C	0.000035	0.000069	-0.000054
151	H	-0.000004	-0.000023	-0.000039
152	H	-0.000015	0.000009	-0.000044
153	C	0.000073	-0.000244	0.000247
154	H	0.000042	0.000022	0.000054

```
  155 H     0.000190 -0.000122  0.000014
  156 C    -0.000025  0.000015  0.000031
  157 H     0.000027  0.000004  0.000076
  158 H     0.000000  0.000011  0.000061
  159 C    -0.000008  0.000063 -0.000041
  160 H     0.000054  0.000057 -0.000022
  161 H     0.000031  0.000010 -0.000040
---------------------------------------
```

Geometry Convergence Tests

Energy old :   -36.42874206
        new :   -36.42875614

Convergence tests:
(Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

Item	Value	Criterion	Conv.	Ratio
change in energy	-0.00001407	0.00100000	YES	0.35852525
gradient max	0.00051035	0.00100000	YES	0.18089671
gradient rms	0.00008991	0.00066667	YES	0.22243903
cart. step max	0.00498935	0.01000000	YES	0.90041204
cart. step rms	0.00080693	0.00666667	YES	0.93023529

prediction dE :   -0.00001145

****
Geometry CONVERGED
****

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	467.685345681582021	12726.3658	293477.02	1227907.70
Delta V^Pauli Coulomb:	-243.722090862730710	-6632.0155	-152937.94	-639892.26
Delta V^Pauli LDA-XC:	-57.264001648711677	-1558.2328	-35933.71	-150346.62
Delta V^Pauli GGA-Exchange:	3.599372473983408	97.9439	2258.64	9450.15
Delta V^Pauli GGA-Correlation:	-4.160827277065724	-113.2219	-2610.96	-10924.25
Total Pauli Repulsion:	166.137798367057314	4520.8395	104253.05	436194.73
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	166.137798367057314	4520.8395	104253.05	436194.73
Electrostatic Interaction:	-36.319889135431310	-988.3145	-22791.08	-95357.86
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	129.817909231626004	3532.5250	81461.98	340836.87
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-165.762432459095777	-4510.6253	-104017.51	-435209.20
Total Orbital Interactions:	-165.807209896583828	-4511.8437	-104045.61	-435326.77
Alternative Decomposition Orb.Int.				
Kinetic:	-430.396951241144905	-11711.6969	-270078.19	-1130007.04
Coulomb:	241.599758025071111	6574.2639	151606.15	634320.07
XC:	22.989983319490047	625.5893	14426.43	60360.19
Total Orbital Interactions:	-165.807209896583743	-4511.8437	-104045.61	-435326.77
Residu (E=Steric+OrbInt+Res):	0.000000747198398	0.0000	0.00	0.00
Dispersion Energy:	-0.439463574571615	-11.9584	-275.77	-1153.81
Total Bonding Energy:	-36.428763492331043	-991.2771	-22859.40	-95643.71

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-36.319889135431310	-988.3145	-22791.08	-95357.86
Kinetic Energy:	37.288394440437116	1014.6688	23398.82	97900.67
Coulomb (Steric+OrbInt) Energy:	-2.122332090461214	-57.7516	-1331.78	-5572.18

XC Energy:	-34.835473132303946	-947.9215	-21859.59	-91460.52
Dispersion Energy:	-0.439463574571615	-11.9584	-275.77	-1153.81
Total Bonding Energy:	-36.428763492330972	-991.2771	-22859.40	-95643.71

List of All Frequencies:

Intensities
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Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
36.977504	3.077742	0.028526
38.789649	10.134845	0.098540
47.933899	6.248688	0.075077
50.285717	32.042415	0.403876
51.393310	11.687401	0.150558
54.129749	31.907605	0.432921
62.507114	75.742862	1.186723
65.439139	21.545732	0.353408
66.780348	10.960914	0.183474
72.178327	46.779534	0.846332
74.362537	41.073637	0.765589
79.301507	8.102036	0.161047
82.137925	91.050707	1.874585
82.538031	107.160899	2.217014
86.481757	179.726051	3.895952
86.698132	28.720065	0.624127
90.060556	4.434212	0.100099
91.595757	19.915168	0.457233
94.765495	3.749514	0.089064
97.868975	61.593402	1.510975
101.279133	186.691194	4.739384
111.597155	311.091770	8.702013
118.298185	252.587430	7.489760
119.446452	427.574066	12.801554
121.165854	71.575664	2.173821
125.139634	112.656225	3.533688
129.970189	14.979408	0.487996
132.289908	22.240714	0.737486
133.597511	38.988936	1.305623
137.153195	58.805984	2.021648
141.891720	7.003351	0.249081
145.229873	57.192392	2.081960
148.386460	6.494473	0.241555
149.792333	50.473992	1.895114
153.406407	21.158753	0.813601
155.885966	13.263063	0.518238
161.980533	57.842056	2.348468
163.515310	15.382267	0.630459
164.218197	45.426049	1.869839
167.533688	151.863998	6.377274
172.323456	138.999320	6.003923
174.105909	88.479151	3.861291
176.363446	51.764939	2.288349
181.981093	49.287451	2.248230
184.061030	106.633306	4.919634
185.377782	8.409754	0.390768
187.445718	33.964065	1.595781
189.123461	14.372944	0.681348
192.743605	41.085235	1.984924
195.987818	8.077095	0.396791
196.822343	47.456956	2.341275
197.620661	88.802572	4.398818
204.642585	9.964259	0.511116
204.901408	53.979126	2.772355
208.432421	6.609219	0.345298
210.413287	12.465531	0.657449
211.062966	5.120504	0.270896
220.820368	97.328814	5.387145
224.008950	3.645700	0.204703
229.296415	19.773476	1.136471
229.573435	28.153982	1.620091
231.345540	26.360594	1.528602
233.432660	83.498192	4.885587
236.625953	139.550641	8.276987
239.448465	5.117265	0.307134
241.303818	41.870231	2.532489
249.707042	72.416194	4.532570
256.280583	53.297683	3.423750
261.940329	1.902646	0.124922

264.806044	2.146019	0.142443
265.360462	1.028968	0.068441
268.127236	10.980020	0.737942
278.472329	0.276396	0.019293
278.545029	0.312848	0.021843
279.086063	0.970042	0.067859
280.789664	12.824808	0.902631
287.238747	2.166377	0.155975
287.441035	1.911137	0.137695
292.948016	11.679190	0.857593
324.264188	2.878417	0.233954
324.921609	2.364599	0.192581
327.899634	1.054856	0.086699
328.017861	7.288436	0.599253
329.815716	7.410164	0.612600
332.664385	33.402859	2.785275
335.446926	27.778229	2.335643
337.901858	0.316461	0.026803
343.828391	10.981010	0.946372
346.630621	12.910114	1.121696
347.078732	130.723366	11.372588
351.971451	188.858697	16.661822
354.282459	146.992709	13.053396
355.237259	24.956720	2.222205
355.705488	91.242893	8.135190
357.580658	43.900953	3.934831
358.729607	43.557766	3.916615
358.831100	39.292091	3.534055
360.706899	246.405296	22.278326
361.038302	85.619676	7.748273
364.153860	322.345339	29.422826
366.186442	278.360462	25.549822
367.877444	35.881972	3.308701
372.145243	29.539962	2.755500
375.254649	49.041155	4.612802
388.320382	134.663338	13.107433
392.335788	2.555064	0.251268
399.790261	4.523512	0.453300
400.299342	1.229231	0.123338
406.575526	1.163432	0.118566
412.051353	167.688684	17.319413
420.846504	33.192926	3.501445
424.799208	3.219641	0.342822
427.533744	39.106015	4.190753
428.325879	75.716750	8.129135
430.468428	64.172196	6.924147
433.999898	108.017134	11.750608
436.819249	151.476643	16.585383
439.541961	5.887171	0.648612
440.353819	7.093209	0.782929
444.406558	13.964495	1.555549
446.131234	6.545306	0.731932
462.259033	232.391420	26.926727
482.819638	200.078607	24.213839
486.751785	1.482567	0.180884
487.950116	8.799072	1.076193
549.768652	4.177953	0.575734
550.266978	2.204954	0.304124
562.843382	3.015732	0.425460
569.407749	4.969331	0.709250
574.241270	6.027545	0.867587
585.432535	1.811789	0.265866
587.672438	4.539818	0.668732
588.839393	1.167459	0.172312
590.604839	1.526311	0.225953
597.858376	9.276513	1.390148
598.779332	19.021434	2.854882
600.059161	3.258857	0.490160
601.354201	8.558055	1.289981
605.512059	220.547272	33.473610
606.071341	166.109876	25.234649
608.184884	3.558476	0.542472
611.335462	27.811926	4.261757
616.187538	8.024658	1.239417
618.085654	4.782042	0.740867
624.030962	61.157612	9.566096
629.169548	72.257441	11.395368
633.216674	154.682946	24.551207
638.428724	0.467800	0.074860
644.223393	22.986306	3.711793
646.024635	3.792591	0.614134
648.947571	5.490936	0.893170
651.831378	747.679662	122.159965
652.750178	134.202109	21.957577
655.064660	202.064692	33.178189

662.182037	1.283850	0.213093
663.615573	446.155749	74.213196
667.510916	350.326864	58.615150
672.528515	6.459930	1.088972
673.130384	8.183406	1.380738
680.827231	7.500427	1.279974
681.531255	43.057398	7.355490
699.707970	19.069103	3.344453
700.398412	2.552758	0.448160
701.614349	5.700270	1.002471
703.072057	5.256900	0.926419
704.423573	15.964606	2.818838
706.745094	45.415218	8.045301
707.428157	35.970174	6.378271
710.622125	292.599953	52.118397
713.186266	0.977214	0.174691
713.994019	0.203617	0.036441
714.965351	0.551311	0.098801
716.478325	6.094333	1.094479
716.879099	5.101926	0.916765
718.257760	30.834264	5.551265
739.632590	9.856758	1.827377
741.369272	5.619580	1.044279
749.568347	21.109288	3.966093
749.816690	35.249811	6.625062
751.914034	2.081501	0.392304
752.908355	30.924634	5.836127
753.815683	100.343765	18.959795
761.523887	4580.630855	874.353182
762.150706	4661.105887	890.446632
764.654404	352.637841	67.588402
764.951136	60.509627	11.602090
778.646248	677.345734	132.199151
779.796677	1420.465073	277.645098
785.912150	31.338654	6.173514
788.466023	23.505013	4.645383
788.805139	17.225175	3.405740
789.082053	9.467306	1.872521
790.303688	39.124970	7.750435
790.815345	30.341182	6.014308
790.913068	2.606157	0.516663
791.747371	26.722672	5.303280
812.186103	40.728538	8.291487
835.904418	91.026249	19.072224
840.493099	14.914732	3.142156
847.153162	9.599490	2.038394
851.984719	101.753640	21.730005
856.179851	31.580908	6.777471
862.563386	13.310070	2.877726
866.481689	264.907501	57.534947
867.814850	75.478933	16.418403
869.954358	1064.700923	232.167898
872.971091	41.007060	8.972977
881.026066	0.134598	0.029724
881.951517	0.288372	0.063749
896.340035	1.416327	0.318211
897.175666	1.572873	0.353712
913.607224	38.108980	8.726999
916.220359	0.713856	0.163941
919.985070	3.720501	0.857947
920.572968	89.273550	20.599615
921.059937	2.923938	0.675047
921.554347	2.932991	0.677501
923.737111	1811.806997	419.506210
924.674536	26.910317	6.237144
925.949359	229.369695	53.235501
927.984076	37.601717	8.746338
928.147102	152.134527	35.393432
934.042822	230.504277	53.966449
938.339180	77.399845	18.204469
938.870177	164.617009	38.739885
939.281386	51.979171	12.237794
940.803046	81.753055	19.278835
943.545303	27.365828	6.472163
946.722731	9.256123	2.196494
951.329760	13.802554	3.291309
955.594656	2.036776	0.487860
957.752917	18.801987	4.513727
970.685451	1.955954	0.475900
978.843480	3.739910	0.917598
983.316236	26.632935	6.564329
990.252375	13.099446	3.251448
991.705192	1.524667	0.378997
996.741968	6.658779	1.663625
997.373732	11.240109	2.810001

1012.114443	1.027072	0.260561
1018.555029	0.853584	0.217926
1044.532057	12.072712	3.160856
1047.127900	119.666866	31.408827
1047.941878	107.219960	28.163778
1049.890078	4.719696	1.242041
1052.774449	10.454187	2.758695
1053.194063	249.518607	65.870265
1055.500910	102.839475	27.207995
1059.558606	43.622041	11.585347
1060.088606	3.625868	0.963457
1060.539493	4.912311	1.305842
1062.253104	12.894727	3.433351
1065.574549	14.443252	3.857686
1066.246257	3.345882	0.894224
1067.972888	16.331751	4.371908
1070.397874	7.362209	1.975293
1072.405322	5.759559	1.548197
1085.573369	101.348167	27.577389
1087.990361	39.070460	10.654955
1089.944358	79.227622	21.645071
1103.859962	735.511166	203.507923
1108.824608	2036.485556	566.007596
1110.829776	2262.739035	630.028291
1122.297432	6.420003	1.806015
1124.458172	78.137123	22.023117
1132.196437	514.679115	146.061716
1134.727950	514.797873	146.422078
1135.502133	788.355925	224.382179
1137.368998	91.496170	26.084491
1138.739127	318.965181	91.042797
1141.118497	102.896232	29.431221
1145.212344	116.357668	33.400972
1150.241093	6.889176	1.986252
1152.135234	0.625685	0.180691
1156.115142	7.603644	2.203438
1162.015261	82.809371	24.119560
1165.359403	10.166012	2.969536
1170.106369	22.125578	6.489303
1175.300056	66.910668	19.711614
1177.074887	55.413631	16.349285
1181.219318	567.143547	167.919683
1183.692179	1388.125445	411.856158
1184.312529	1293.978459	384.123998
1186.268943	2044.811012	608.015157
1191.055928	54.579285	16.294389
1191.419215	57.743230	17.244228
1193.555253	1003.069077	300.089943
1195.334235	849.125911	254.413130
1196.581317	1305.719588	391.624819
1199.433810	54.403348	16.356109
1200.800995	51.470676	15.492053
1211.740536	1399.026252	424.926260
1215.305934	389.290674	118.587165
1216.231233	65.666611	20.018836
1217.033603	319.094297	97.341869
1217.977711	398.409385	121.631755
1218.282652	57.838394	17.662101
1219.681625	35.555589	10.870072
1221.566722	71.648665	21.938320
1222.745579	82.451147	25.270328
1225.958271	20.663263	6.349692
1226.374373	24.125681	7.416188
1226.929618	23.492805	7.224912
1230.757924	16.010040	4.939047
1234.578846	6.487998	2.007741
1242.781304	4.479040	1.395268
1245.171001	6.877872	2.146650
1266.434928	0.082559	0.026208
1267.175285	0.648116	0.205858
1278.803438	1.041812	0.333942
1279.492228	6.344339	2.034708
1283.584410	1.706254	0.548967
1287.200614	1407.779028	454.212205
1287.903441	1496.053907	482.957168
1302.521150	1.512883	0.493933
1302.716434	9.217700	3.009889
1303.750411	7.626310	2.492224
1305.501988	3.594157	1.176123
1305.606432	0.122282	0.040018
1307.653757	2.899157	0.950260
1308.678738	1.767339	0.579737
1336.937165	56.320306	18.873571
1340.048089	1569.113389	527.051170
1340.719688	1654.577977	556.036494

1355.503926	9.606977	3.264116
1355.840710	6.776651	2.303042
1364.562195	108.161675	36.995152
1364.987266	246.545681	84.353687
1367.319967	33.070080	11.334007
1369.297219	1.088572	0.373623
1371.624904	0.807863	0.277748
1372.918262	6.116558	2.104892
1374.070901	10.394426	3.580039
1377.659604	28.618236	9.882410
1380.491481	73.480512	25.426347
1381.784859	51.550058	17.854499
1382.173355	20.325668	7.041828
1383.016480	8.815934	3.056143
1383.677814	2.554295	0.885899
1384.344711	36.982704	12.832787
1385.496357	25.693574	8.922940
1386.046864	5.438424	1.889422
1387.203577	45.627060	15.865025
1387.545522	93.550753	32.536632
1388.681616	119.000422	41.421828
1390.850837	185.953094	64.827912
1393.665251	4.943262	1.726832
1394.430613	22.608210	7.902075
1396.555936	1.155084	0.404343
1397.286313	21.826436	7.644451
1398.427398	2.555602	0.895800
1398.491002	1.109248	0.388836
1402.498115	4.436170	1.559511
1404.514030	7.981806	2.809994
1405.717155	21.294281	7.503070
1406.023906	7.963194	2.806455
1407.922834	141.048513	49.776624
1409.778672	121.793150	43.037979
1410.801282	193.493312	68.424223
1411.689068	29.137514	10.310260
1412.550890	182.215244	64.515918
1414.685288	0.093615	0.033196
1415.603142	3.441474	1.221136
1417.596129	3.121771	1.109256
1419.772909	10.647280	3.789096
1423.204222	105.290613	37.560810
1423.993872	178.245524	63.621635
1426.137254	590.102717	210.943919
1427.073298	136.570583	48.851906
1427.861671	58.378566	20.893809
1428.180629	157.768224	56.478187
1428.799821	103.541259	37.081978
1429.243017	26.070639	9.339762
1429.861593	132.297493	47.415866
1430.275710	11.154369	3.998921
1430.410688	46.236844	16.577804
1431.989656	9.821025	3.525127
1433.388724	122.735579	44.097354
1434.721081	169.306676	60.886307
1434.923549	429.000681	154.299605
1436.463388	349.372256	125.794324
1438.248891	44.145085	15.914554
1439.095188	16.119506	5.814593
1440.578456	8.721995	3.149422
1446.947433	0.372780	0.135202
1448.679075	6.697402	2.431961
1452.733343	0.746956	0.271994
1468.129145	4.279023	1.574660
1469.945018	9.109059	3.356237
1484.793915	35.592526	13.246559
1487.768584	7.191193	2.681726
1489.165224	12.653146	4.723017
1497.962857	9.964986	3.741587
1506.827106	44.970084	16.984986
1515.337588	21.451486	8.147884
1519.916775	58.967789	22.465326
1529.021284	96.470624	36.973170
1617.163950	765.547050	310.315886
1631.126829	973.658087	398.081758
1644.268225	164.795284	67.919662
1646.317583	3.505164	1.446439
1665.137231	608.626133	254.026309
1670.601979	660.883034	276.742376
1688.462493	72.208809	30.560445
1693.218625	361.106982	153.259355
1699.486857	1307.968663	557.177050
1714.149944	77.851510	33.449830
1717.640627	13.529655	5.825016
1721.979877	1486.699607	641.696054

1726.378026	144.187809	62.393955
1727.265337	111.033286	48.071793
1741.277939	380.882537	166.240650
1742.758390	160.096712	69.935497
1752.432835	2620.814746	1151.213240
2922.822181	9.363419	6.859855
2932.438683	8.829630	6.490072
2934.410909	10.129987	7.450886
2935.213550	2.532974	1.863582
2935.916995	39.162742	28.820064
2936.359765	7.398887	5.445700
2939.600696	5.697165	4.197834
2940.648269	4.447637	3.278314
2940.994002	42.742349	31.508708
2942.711309	6.185967	4.562820
2943.053027	18.301246	13.500716
2943.217677	1.924172	1.419529
2944.708451	12.264371	9.052440
2945.761725	25.742233	19.007365
2946.043459	34.889300	25.763773
2946.368127	19.834958	14.648608
2947.227084	76.351882	56.404197
2947.369554	67.178083	49.629542
2948.937554	126.572247	93.558260
2949.000021	11.816155	8.734318
2950.437656	58.159542	43.011590
2951.502371	101.941009	75.417153
2952.451892	69.276361	51.267952
2956.827784	68.980139	51.124393
2959.021122	39.568485	29.347801
2959.878262	70.479616	52.289615
2960.369406	67.938461	50.412668
2961.055309	52.919159	39.276929
2961.535075	6.151590	4.566488
2969.706059	3.173436	2.362225
2979.587340	9.479161	7.079525
2983.177310	8.617937	6.444073
2996.614911	11.978402	8.997211
3049.104998	7.240527	5.533764
3049.352333	0.434134	0.331825
3049.905478	17.412811	13.311694
3050.498165	14.400189	11.010753
3051.020030	17.153623	13.118343
3052.256722	17.982336	13.757681
3053.467643	17.080838	13.073160
3053.806356	6.691007	5.121663
3054.424871	6.720453	5.145245
3056.033095	6.011105	4.604584
3056.153314	4.009467	3.071425
3056.734564	15.945815	12.217505
3058.628125	9.406811	7.211858
3058.860933	11.599266	8.893410
3075.605603	16.713456	12.884720
3089.363641	21.742673	16.836819
3090.327825	4.878552	3.778971
3107.017611	29.357465	22.863374
3124.115218	29.218737	22.880555
3130.696786	6.341216	4.976129
3143.286273	3.644413	2.871373
3148.097338	5.637651	4.448611
3153.646400	6.694654	5.291993
3175.436178	9.475927	7.542289
3318.431643	592.215682	492.595965
3326.652220	362.461435	302.236754
3343.998056	1704.763733	1428.921215
3356.547809	553.298036	465.511095
3373.796007	188.388632	159.313135
3382.949724	703.625530	596.643896

```
Statistical Thermal Analysis  ***  ideal gas assumed  ***

Pressure:                  1.000000 atm.
Temperature:             298.150000 K


Moments of Inertia (and direction vectors)
==========================================

      77308.3644      78439.8719     119606.4908
-------------------------------------------------
```

```
          -0.0119          0.9612          0.2756
          -0.8977          0.1111         -0.4264
          -0.4404         -0.2525          0.8616


 The rotational contribution to the molecular entropy includes
 a term, dependent on the symmetry number sigma. The results
 reported below were computed using sigma = 1, determined
 from the point group symmetry of the input geometry (NOSYM).
 If this is not the correct symmetry, please contact SCM to
 report a bug.

     Temp                                                  Transl     Rotat    Vibrat     Total
     ----                                                  ------     -----    ------     -----

     298.15   Entropy (cal/mole-K):                        47.877    41.802   298.355   388.034
              Internal Energy (Kcal/mole):                  0.889     0.889   824.136   825.914
              Constant Volume Heat Capacity (cal/mole-K):   2.981     2.981   326.139   332.100

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


*** DONE CALCULATING ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ***
```

CB[7]•[Cp*Ir(H_2O)]$^{2+}$

Geometry CYCLE 65
==========

Energy gradients wrt nuclear displacements
==========

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	-0.000010	-0.000012	0.000028
2	C	-0.000131	0.000138	-0.000097
3	C	0.000095	-0.000026	-0.000037
4	H	0.000012	0.000034	-0.000020
5	H	-0.000015	0.000005	-0.000030
6	C	-0.000071	-0.000268	0.000182
7	C	0.000181	-0.000135	-0.000261
8	H	-0.000005	0.000035	0.000058
9	H	-0.000017	-0.000024	-0.000062
10	C	0.000124	-0.000124	-0.000150
11	C	-0.000014	0.000016	-0.000053
12	H	-0.000005	-0.000002	0.000013
13	H	-0.000020	0.000005	0.000007
14	C	-0.000056	0.000156	-0.000066
15	C	0.000009	0.000074	0.000035
16	H	-0.000031	0.000031	0.000022
17	H	0.000018	0.000020	-0.000015
18	C	0.000176	0.000158	0.000133
19	C	-0.000128	0.000025	-0.000040
20	H	-0.000010	0.000038	-0.000011
21	H	0.000020	0.000019	-0.000022
22	C	-0.000199	0.000326	-0.000030
23	C	0.000052	-0.000082	0.000001
24	H	-0.000027	0.000048	-0.000002
25	H	-0.000006	-0.000019	0.000008
26	C	-0.000083	-0.000021	-0.000047
27	C	0.000132	0.000013	0.000108
28	H	-0.000013	-0.000011	-0.000002
29	H	-0.000020	0.000011	-0.000047
30	O	0.000211	0.000021	-0.000074
31	O	-0.000010	0.000059	0.000002
32	O	0.000059	0.000011	-0.000021
33	O	-0.000130	-0.000419	-0.000056
34	O	0.000002	-0.000100	-0.000040
35	O	-0.000077	-0.000031	0.000038
36	O	-0.000015	-0.000154	0.000146
37	O	-0.000128	-0.000038	0.000070
38	O	-0.000172	0.000276	-0.000151
39	O	-0.000024	0.000190	0.000164
40	O	0.000241	0.000080	-0.000151
41	O	0.000129	-0.000100	-0.000022
42	O	0.000182	-0.000283	0.000217
43	O	-0.000226	0.000152	-0.000317
44	N	0.000209	0.000269	0.000104
45	N	-0.000108	-0.000168	0.000135
46	N	-0.000238	-0.000094	-0.000108
47	N	0.000654	0.000083	0.000603
48	N	0.000113	0.000147	-0.000224
49	N	0.000004	0.000159	0.000085
50	N	0.000074	-0.000071	0.000066
51	N	-0.000099	-0.000060	-0.000022
52	N	-0.000012	-0.000097	0.000041
53	N	-0.000138	-0.000005	-0.000254
54	N	-0.000041	-0.000065	0.000064
55	N	-0.000064	-0.000007	0.000052
56	N	-0.000137	0.000033	0.000285
57	N	0.000047	-0.000008	0.000025
58	N	-0.000619	-0.000310	-0.000211
59	N	0.000007	0.000158	0.000096
60	N	-0.000018	-0.000054	-0.000017
61	N	0.000179	-0.000021	0.000053
62	N	-0.000292	0.000030	-0.000002
63	N	0.000183	-0.000122	-0.000061
64	N	0.000058	0.000057	0.000026
65	N	-0.000005	0.000202	-0.000372
66	N	0.000184	0.000010	-0.000046
67	N	-0.000086	-0.000001	-0.000032
68	N	0.000284	-0.000239	-0.000101
69	N	-0.000054	0.000144	-0.000086
70	N	-0.000083	0.000088	-0.000069
71	N	0.000013	-0.000041	0.000062
72	C	0.000121	-0.000067	-0.000017
73	C	0.000065	0.000091	-0.000004
74	H	-0.000015	-0.000014	-0.000018
75	H	0.000024	0.000060	-0.000043
76	C	-0.000173	0.000041	0.000228
77	C	0.000119	0.000032	0.000035
78	H	-0.000117	0.000065	0.000043
79	H	-0.000025	0.000047	0.000008
80	C	0.000043	-0.000231	0.000012
81	C	-0.000006	-0.000024	0.000092
82	H	-0.000034	-0.000004	0.000013
83	H	-0.000003	0.000010	0.000014
84	C	0.000055	-0.000007	0.000112
85	C	0.000067	-0.000043	-0.000054

```
    86 H    -0.000010  0.000008  0.000041
    87 H    -0.000045 -0.000006  0.000024
    88 C     0.000147  0.000192  0.000243
    89 C     0.000003 -0.000027 -0.000104
    90 H    -0.000028  0.000010  0.000027
    91 H    -0.000021 -0.000022  0.000018
    92 C     0.000097  0.000019 -0.000043
    93 C    -0.000012  0.000009  0.000007
    94 H    -0.000019  0.000010 -0.000009
    95 H    -0.000060  0.000013  0.000004
    96 C     0.000153 -0.000068 -0.000164
    97 C    -0.000099 -0.000053  0.000022
    98 H     0.000011 -0.000016 -0.000037
    99 H    -0.000040 -0.000022  0.000041
   100 C    -0.000109  0.000053 -0.000116
   101 H    -0.000020 -0.000011  0.000017
   102 C    -0.000062  0.000010  0.000227
   103 H    -0.000015  0.000044 -0.000044
   104 C    -0.000096  0.000005  0.000213
   105 H     0.000017  0.000024 -0.000044
   106 C     0.000069  0.000169 -0.000026
   107 H     0.000015  0.000029  0.000002
   108 C     0.000001  0.000135  0.000119
   109 H    -0.000007  0.000014 -0.000046
   110 C    -0.000132  0.000100 -0.000057
   111 H     0.000002 -0.000023  0.000001
   112 C    -0.000057  0.000022 -0.000045
   113 H    -0.000021  0.000014  0.000059
   114 C    -0.000053 -0.000138 -0.000056
   115 H    -0.000019 -0.000012  0.000012
   116 C    -0.000023  0.000078 -0.000099
   117 H    -0.000044 -0.000010 -0.000014
   118 C     0.000072 -0.000120  0.000132
   119 H    -0.000062 -0.000012  0.000001
   120 C     0.000067 -0.000171 -0.000246
   121 H    -0.000009  0.000017 -0.000020
   122 C     0.000216 -0.000300  0.000159
   123 H    -0.000032 -0.000053 -0.000027
   124 C     0.000064 -0.000126  0.000164
   125 H    -0.000031  0.000026 -0.000027
   126 C    -0.000039  0.000009 -0.000017
   127 H    -0.000054  0.000036  0.000009
   128 H     0.000019  0.000001  0.000002
   129 C    -0.000025  0.000051  0.000003
   130 Ir   -0.000087  0.000211 -0.000326
   131 H     0.000017  0.000028 -0.000010
   132 C     0.000224 -0.000332  0.000248
   133 C     0.000119 -0.000175  0.000055
   134 C    -0.000227  0.000082 -0.000029
   135 C    -0.000010  0.000264  0.000235
   136 C     0.000119 -0.000251 -0.000145
   137 H     0.000003  0.000023  0.000087
   138 H     0.000001  0.000024  0.000024
   139 H     0.000051 -0.000037  0.000017
   140 H    -0.000043  0.000009 -0.000043
   141 H    -0.000006  0.000008 -0.000025
   142 C     0.000170 -0.000078  0.000092
   143 H     0.000003  0.000003  0.000012
   144 H     0.000014 -0.000052 -0.000039
   145 O     0.000035  0.000032  0.000028
   146 H    -0.000045  0.000107 -0.000109
   147 C    -0.000165 -0.000054 -0.000129
   148 H    -0.000025  0.000031 -0.000110
   149 H    -0.000084  0.000139 -0.000047
   150 C     0.000083 -0.000142  0.000061
   151 H     0.000011  0.000064 -0.000047
   152 H     0.000038  0.000031 -0.000056
   153 C    -0.000051  0.000051  0.000000
   154 H     0.000019  0.000031  0.000008
   155 H    -0.000005  0.000007  0.000016
 ----------------------------------------

 dE(predicted):    -0.38831E-04, dE(actual):    -0.31377E-03, Trust radius:    0.155000, all in a.u.

-----------------------------------------------------
Geometry Convergence after Step  65       ** CONVERGED **
-----------------------------------------------------
current energy                          -35.37025203 Hartree
energy change                -0.00031377     0.00100000    T
constrained gradient max      0.00065447     0.00100000    T
constrained gradient rms      0.00011692     0.00066667    T
gradient max                  0.00065447
gradient rms                  0.00011692
cart. step max                0.00858424     0.01000000    T
cart. step rms                0.00205164     0.00666667    T



                                    hartree             eV        kcal/mol          kJ/mol
                              ---------------     ----------      ---------     ----------

Pauli Repulsion
  Kinetic (Delta T^0):          455.351543763564905      12390.7460        285737.44       1195525.31
  Delta V^Pauli Coulomb:       -236.706143717617465      -6441.1019       -148535.36       -621471.89
  Delta V^Pauli LDA-XC:         -55.403491696626610      -1507.6057        -34766.22       -145461.85
  Delta V^Pauli GGA-Exchange:     3.408910707569135         92.7612          2139.12          8950.09
  Delta V^Pauli GGA-Correlation:   -3.987396625964635       -108.5026         -2502.13        -10468.91
```

Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	162.663422430925323	4426.2969	102072.85	427072.76
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	162.663422430925323	4426.2969	102072.85	427072.76
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-35.602991227129280	-968.8067	-22341.22	-93475.64
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	127.060431203796043	3457.4903	79731.63	333597.11
Orbital Interactions				
A:	-162.049522298440507	-4409.5919	-101687.62	-425460.96
Total Orbital Interactions:	-162.092837773449645	-4410.7705	-101714.80	-425574.69
Alternative Decomposition Orb.Int.				
Kinetic:	-419.384461900994097	-11412.0319	-263167.75	-1101093.75
Coulomb:	235.119454249333359	6397.9259	147539.70	617306.04
XC:	22.172169878211228	603.3354	13913.25	58213.02
Total Orbital Interactions:	-162.092837773449503	-4410.7705	-101714.80	-425574.69
Residu (E=Steric+OrbInt+Res):	-0.000153006722488	-0.0042	-0.10	-0.40
Dispersion Energy:	-0.337691839290378	-9.1891	-211.90	-886.61
Total Bonding Energy:	-35.370251415666466	-962.4735	-22195.17	-92864.58

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-35.602991227129280	-968.8067	-22341.22	-93475.64
Kinetic Energy:	35.967081862570808	978.7141	22569.69	94431.56
Coulomb (Steric+OrbInt) Energy:	-1.586842475006591	-43.1802	-995.76	-4166.25
XC Energy:	-33.809807736810882	-920.0117	-21215.98	-88767.64
Dispersion Energy:	-0.337691839290378	-9.1891	-211.90	-886.61
Total Bonding Energy:	-35.370251415666324	-962.4735	-22195.17	-92864.58

H_2O

```
 Geometry CYCLE 3
 ==============

 Energy gradients wrt nuclear displacements
 ==========================================

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ------------------------------------------
     1 H    -0.000152  0.000000  0.000077
     2 O     0.000000  0.000000 -0.000154
     3 H     0.000152  0.000000  0.000077
 ------------------------------------------

 dE(predicted):    -0.46664E-06, dE(actual):     0.18875E-04, Trust radius:    0.020000, all in a.u.

------------------------------------------------------------
Geometry Convergence after Step   3       ** CONVERGED **
------------------------------------------------------------
current energy                          -0.50240820 Hartree
energy change                0.00001887     0.00100000    T
constrained gradient max     0.00015420     0.00100000    T
constrained gradient rms     0.00009538     0.00066667    T
gradient max                 0.00015420
gradient rms                 0.00009538
cart. step max               0.00012156     0.01000000    T
cart. step rms               0.00005794     0.00666667    T
```

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	3.771264929886803	102.6213	2366.50	9901.45
Delta V^Pauli Coulomb:	-2.033238899598766	-55.3272	-1275.88	-5338.27
Delta V^Pauli LDA-XC:	-0.435698484851745	-11.8560	-273.40	-1143.93
Delta V^Pauli GGA-Exchange:	0.025567569450018	0.6957	16.04	67.13
Delta V^Pauli GGA-Correlation:	-0.030609805585458	-0.8329	-19.21	-80.37
Total Pauli Repulsion:	1.297285309300852	35.3009	814.06	3406.02
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	1.297285309300852	35.3009	814.06	3406.02
Electrostatic Interaction:	-0.245357246934792	-6.6765	-153.96	-644.19
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	1.051928062366060	28.6244	660.09	2761.84
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A1:	-0.688824214901492	-18.7439	-432.24	-1808.51
A2:	0.000000000000000	0.0000	0.00	0.00
B1:	-0.646794635673532	-17.6002	-405.87	-1698.16
B2:	-0.218564591200139	-5.9474	-137.15	-573.84
Total Orbital Interactions:	-1.554327083423971	-42.2954	-975.36	-4080.89
Alternative Decomposition Orb.Int.				
Kinetic:	-3.289813044948764	-89.5204	-2064.39	-8637.40
Coulomb:	1.731774202710198	47.1240	1086.70	4546.77
XC:	0.003711758814596	0.1010	2.33	9.75
Total Orbital Interactions:	-1.554327083423971	-42.2954	-975.36	-4080.89
Residu (E=Steric+OrbInt+Res):	-0.000000006240068	0.0000	0.00	0.00
Dispersion Energy:	-0.000010396830522	-0.0003	-0.01	-0.03
Total Bonding Energy:	-0.502409424128501	-13.6713	-315.27	-1319.08

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-0.245357246934792	-6.6765	-153.96	-644.19
Kinetic Energy:	0.481451884938039	13.1010	302.12	1264.05
Coulomb (Steric+OrbInt) Energy:	-0.301464703128636	-8.2033	-189.17	-791.50
XC Energy:	-0.437028962172590	-11.8922	-274.24	-1147.42
Dispersion Energy:	-0.000010396830522	-0.0003	-0.01	-0.03
Total Bonding Energy:	-0.502409424128501	-13.6713	-315.27	-1319.08

```
 Intensities
 ===========

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1          1e-40 esu2 cm2           km/mole
             ----------         ----------         ----------
```

```
          1603.158271          191.322582           76.881297
          3641.921997            4.729584            4.317493
          3737.508644           54.463441           51.022925


 ============================
 Statistical Thermal Analysis  ***  ideal gas assumed  ***
 ============================

 Pressure:                  1.000000 atm.
 Temperature:             298.150000 K


 Moments of Inertia (and direction vectors)
 ==========================================

          2.3127          4.2392          6.5520
 -------------------------------------------------
          1.0000          0.0000          0.0000
          0.0000          0.0000          1.0000
          0.0000          1.0000          0.0000


 The rotational contribution to the molecular entropy includes
 a term, dependent on the symmetry number sigma. The results
 reported below were computed using sigma = 2, determined
 from the point group symmetry of the input geometry (C(2V)).
 If this is not the correct symmetry, please contact SCM to
 report a bug.

     Temp                                                  Transl     Rotat    Vibrat     Total
     ----                                                  ------     -----    ------     -----

     298.15   Entropy (cal/mole-K):                        34.608    10.561     0.008    45.177
              Internal Energy (Kcal/mole):                  0.889     0.889    12.843    14.621
              Constant Volume Heat Capacity (cal/mole-K):   2.981     2.981     0.052     6.014


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


=====================================================================
*** DONE CALCULATING ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ***
=====================================================================
```

CB7, COSMO

```
Geometry CYCLE 41
==============

Energy gradients wrt nuclear displacements
==========================================

    Atom      Cartesian (a.u./angstrom)
                X         Y         Z
-----------------------------------------
    1 H     0.000827  0.000121 -0.000225
    2 C     0.000142 -0.000083 -0.000012
    3 C     0.000030  0.000213  0.000216
    4 H    -0.000156 -0.000112 -0.000036
    5 H     0.000000  0.000154 -0.000126
    6 C    -0.000178  0.000683 -0.000386
    7 C    -0.000100  0.000412  0.000062
    8 H     0.000093 -0.000143  0.000091
    9 H     0.000092  0.000017 -0.000024
   10 C    -0.000075  0.000308  0.000015
   11 C    -0.000085  0.000055  0.000078
   12 H    -0.000225  0.000109  0.000125
   13 H     0.000024 -0.000205  0.000120
   14 C    -0.000308  0.000158 -0.000412
   15 C    -0.000444 -0.000261  0.000257
   16 H    -0.000174  0.000094 -0.000270
   17 H     0.000540  0.000293 -0.000022
   18 C    -0.000036 -0.000177 -0.000159
   19 C    -0.000018 -0.000080 -0.000218
   20 H     0.000018 -0.000002  0.000043
   21 H     0.000044 -0.000068  0.000156
   22 C    -0.000008  0.000296 -0.000749
   23 C     0.000002  0.000004  0.000190
   24 H    -0.000191  0.000251  0.000122
   25 H     0.000074  0.000223 -0.000072
   26 C    -0.000044 -0.000446 -0.000374
   27 C     0.000401 -0.000173 -0.000119
   28 H    -0.000192 -0.000114  0.000031
   29 H     0.000023 -0.000116  0.000155
   30 O    -0.000176 -0.000378 -0.000184
   31 O     0.000193  0.000160 -0.000103
   32 O    -0.000175  0.000063  0.000044
   33 O     0.000057 -0.000193  0.000286
   34 O     0.000137 -0.000436  0.000675
   35 O    -0.000285  0.000087 -0.000066
   36 O    -0.000270  0.000330 -0.000389
   37 O    -0.000347  0.000145 -0.000266
   38 O     0.000194 -0.000724  0.000657
   39 O     0.000736 -0.000408  0.000305
   40 O     0.000085 -0.000216  0.000570
   41 O    -0.000134  0.000062 -0.000220
   42 O    -0.000174 -0.000094  0.000889
   43 O     0.000176 -0.000481  0.000565
   44 N    -0.000387 -0.000316  0.000695
   45 N     0.000146  0.000057 -0.000158
   46 N     0.000072 -0.000189 -0.000101
   47 N    -0.000127 -0.000079 -0.000008
   48 N     0.000151 -0.000027 -0.000179
   49 N     0.000371 -0.000340 -0.000358
   50 N    -0.000288  0.000308 -0.000002
   51 N     0.000193 -0.000408 -0.000197
   52 N     0.000146  0.000189 -0.000090
   53 N    -0.000361  0.000167 -0.000189
   54 N     0.000093  0.000259  0.000113
   55 N    -0.000540  0.000459 -0.000447
   56 N    -0.000455 -0.000350 -0.000190
   57 N     0.000563  0.000528 -0.000537
   58 N    -0.000210 -0.000129  0.000379
   59 N    -0.000414  0.000471 -0.000016
   60 N     0.000396  0.000217  0.000331
   61 N    -0.000220 -0.000534 -0.000135
   62 N     0.000164  0.000152 -0.000346
   63 N    -0.000104  0.000256 -0.000875
   64 N     0.000120  0.000083  0.000148
   65 N     0.000426 -0.000529  0.000051
   66 N    -0.000162  0.000407 -0.000023
   67 N     0.000356  0.000601  0.000294
   68 N    -0.000224 -0.000464 -0.000159
   69 N     0.000021 -0.000034  0.000452
   70 N     0.000327 -0.000783  0.000370
   71 N    -0.000039  0.000695  0.000710
   72 C     0.000161  0.000577  0.000040
```

```
    73 C    -0.000021  0.000088  0.000170
    74 H    -0.000158  0.000111  0.000001
    75 H    -0.000053 -0.000035 -0.000051
    76 C     0.000041 -0.000077 -0.000001
    77 C    -0.000154  0.000039  0.000107
    78 H    -0.000146  0.000049 -0.000036
    79 H     0.000043 -0.000108 -0.000041
    80 C    -0.000283  0.000119  0.000116
    81 C    -0.000135  0.000038  0.000107
    82 H     0.000072 -0.000035 -0.000025
    83 H    -0.000008  0.000015  0.000075
    84 C     0.000127  0.000311 -0.000167
    85 C     0.000004  0.000020  0.000042
    86 H    -0.000014  0.000019 -0.000005
    87 H     0.000099 -0.000001  0.000070
    88 C     0.000100  0.000113 -0.000145
    89 C     0.000183 -0.000079  0.000187
    90 H     0.000041 -0.000077 -0.000042
    91 H    -0.000025  0.000184 -0.000172
    92 C     0.000127 -0.000246  0.000039
    93 C     0.000226 -0.000154 -0.000114
    94 H     0.000028 -0.000083 -0.000065
    95 H    -0.000143  0.000035 -0.000067
    96 C    -0.000225 -0.000410  0.000230
    97 C     0.000050  0.000130 -0.000065
    98 H    -0.000022  0.000031 -0.000193
    99 H     0.000002 -0.000081 -0.000024
   100 C     0.000205  0.000214 -0.000176
   101 H     0.000099 -0.000062  0.000026
   102 C    -0.000310  0.000092 -0.000220
   103 H    -0.000130 -0.000016 -0.000041
   104 C     0.000084 -0.000219  0.000420
   105 H     0.000026  0.000091  0.000009
   106 C     0.000113  0.000254 -0.000003
   107 H    -0.000005  0.000144  0.000165
   108 C    -0.000165  0.000036 -0.000127
   109 H    -0.000024  0.000042  0.000073
   110 C    -0.000113 -0.000011  0.000384
   111 H    -0.000105 -0.000002  0.000089
   112 C     0.000162  0.000239 -0.000228
   113 H     0.000028  0.000121  0.000067
   114 C     0.000205 -0.000018  0.000000
   115 H    -0.000188 -0.000303 -0.000020
   116 C     0.000098 -0.000160 -0.000055
   117 H    -0.000144  0.000006 -0.000059
   118 C    -0.000226  0.000013 -0.000145
   119 H     0.000040 -0.000034 -0.000007
   120 C    -0.000092 -0.000112 -0.000196
   121 H    -0.000016  0.000022  0.000010
   122 C    -0.000164 -0.000071 -0.000015
   123 H     0.000556 -0.000604 -0.000360
   124 C     0.000317  0.000214 -0.000072
   125 H    -0.000039 -0.000090 -0.000001
   126 C    -0.000234 -0.000276 -0.000240
 ----------------------------------------

 dE(predicted):    -0.26415E-04, dE(actual):     0.32288E-03, Trust radius:    0.126000, all in a.u.

------------------------------------------------------------
Geometry Convergence after Step  41       ** CONVERGED **
------------------------------------------------------------
current energy                          -30.14406883 Hartree
energy change                0.00032288     0.00100000    T
constrained gradient max     0.00088874     0.00100000    T
constrained gradient rms     0.00025362     0.00066667    T
gradient max                 0.00088874
gradient rms                 0.00025362
cart. step max               0.00557700     0.01000000    T
cart. step rms               0.00173116     0.00666667    T


                                      hartree             eV        kcal/mol           kJ/mol
                                   --------------     ----------     ----------     ----------

Pauli Repulsion
  Kinetic (Delta T^0):          390.524685494696200    10626.7174      245057.97      1025322.42
  Delta V^Pauli Coulomb:       -203.136813372561363    -5527.6339     -127470.29      -533335.63
  Delta V^Pauli LDA-XC:         -47.424237791662144    -1290.4792      -29759.16      -124512.32
  Delta V^Pauli GGA-Exchange:     2.855004534680653       77.6886        1791.54         7495.81
  Delta V^Pauli GGA-Correlation:  -3.364318767834600      -91.5478        -2111.14        -8833.02
                                   --------------     ----------     ----------     ----------
  Total Pauli Repulsion:        139.454320097318742     3794.7451       87508.92       366137.27
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)
```

Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	139.454320097318742	3794.7451	87508.92	366137.27
Electrostatic Interaction:	-30.683020827985935	-834.9275	-19253.89	-80558.26
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	108.771299269332815	2959.8176	68255.03	285579.01
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-138.312527881360381	-3763.6754	-86792.43	-363139.49
Total Orbital Interactions:	-138.339006185243136	-3764.3959	-86809.05	-363209.01
Alternative Decomposition Orb.Int.				
Kinetic:	-361.386382765712426	-9833.8238	-226773.40	-948819.81
Coulomb:	204.060451099841117	5552.7674	128049.88	535760.64
XC:	18.986925480628212	516.6605	11914.48	49850.17
Total Orbital Interactions:	-138.339006185243107	-3764.3959	-86809.05	-363209.01
Residu (E=Steric+OrbInt+Res):	-0.000092327623535	-0.0025	-0.06	-0.24
Solvation Energy (el):	-0.321024833840324	-8.7355	-201.45	-842.85
Dispersion Energy:	-0.255207134994591	-6.9445	-160.14	-670.05
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.000000000000000	0.0000	0.00	0.00
Total Bonding Energy:	-30.144031212368770	-820.2608	-18915.67	-79143.14

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-30.683020827985935	-834.9275	-19253.89	-80558.26
Kinetic Energy:	29.138302728983774	792.8936	18284.56	76502.60
Coulomb (Steric+OrbInt) Energy:	0.923545399656206	25.1309	579.53	2424.77
XC Energy:	-28.946626544187879	-787.6778	-18164.28	-75999.36
Solvation:	-0.321024833840324	-8.7355	-201.45	-842.85
Dispersion Energy:	-0.255207134994591	-6.9445	-160.14	-670.05
Total Bonding Energy:	-30.144031212368748	-820.2608	-18915.67	-79143.14

$Cp^*Ir(H_2O)_3Cl_2$ – 1, COSMO

```
 Geometry CYCLE 65
 ==============

 Energy gradients wrt nuclear displacements
 ==========================================

     Atom      Cartesian (a.u./angstrom)
                  X         Y         Z
 ------------------------------------------
     1 H    -0.000043  0.000010 -0.000055
     2 H     0.000037  0.000059 -0.000015
     3 H    -0.000163 -0.000349 -0.000479
     4 Ir   -0.000309  0.000019 -0.000438
     5 H    -0.000422 -0.000940 -0.000271
     6 C     0.000117  0.000173 -0.000398
     7 C    -0.000072 -0.000210  0.000297
     8 C     0.000068 -0.000265  0.000325
     9 C     0.000051 -0.000014  0.000235
    10 C     0.000158  0.000488 -0.000429
    11 H     0.000166 -0.000252  0.000102
    12 H     0.000094 -0.000088  0.000096
    13 H    -0.000008 -0.000018  0.000017
    14 H     0.000024 -0.000006  0.000028
    15 O     0.000405  0.000879  0.000336
    16 H    -0.000123  0.000247  0.000083
    17 O    -0.000037  0.000472  0.000981
    18 H     0.000627 -0.000057 -0.000538
    19 O    -0.000382 -0.000144  0.000197
    20 H     0.000706 -0.000604  0.000557
    21 C    -0.000021  0.000043  0.000008
    22 H     0.000021 -0.000048  0.000012
    23 H    -0.000020 -0.000064  0.000029
    24 C     0.000031  0.000037 -0.000037
    25 H    -0.000001  0.000025  0.000022
    26 H    -0.000010  0.000036  0.000008
    27 C     0.000152  0.000017 -0.000024
    28 H    -0.000155  0.000134  0.000036
    29 H     0.000014 -0.000024  0.000004
    30 C    -0.000063 -0.000048  0.000085
    31 H    -0.000019  0.000019 -0.000035
    32 H    -0.000023 -0.000055  0.000054
    33 C    -0.000083 -0.000009  0.000140
    34 H    -0.000027  0.000052  0.000012
    35 H     0.000025 -0.000044 -0.000067
    36 Cl   -0.000407  0.000694 -0.000902
    37 Cl   -0.000307 -0.000165  0.000024
 ------------------------------------------

 dE(predicted):    -0.64971E-05, dE(actual):     0.87504E-06, Trust radius:    0.037000, all in a.u.

-----------------------------------------------------------
Geometry Convergence after Step  65       ** CONVERGED **
-----------------------------------------------------------
current energy                              -7.09954167 Hartree
energy change                    0.00000088     0.00100000    T
constrained gradient max         0.00098114     0.00100000    T
constrained gradient rms         0.00028591     0.00066667    T
gradient max                     0.00098114
gradient rms                     0.00028591
cart. step max                   0.00548764     0.01000000    T
cart. step rms                   0.00185841     0.00666667    T


                                        hartree            eV        kcal/mol          kJ/mol
                                  ---------------    ----------    ----------    ----------

Pauli Repulsion
  Kinetic (Delta T^0):             72.262089706671148     1966.3515       45345.15       189724.09
  Delta V^Pauli Coulomb:          -37.998758253898167    -1033.9988      -23844.58       -99765.73
  Delta V^Pauli LDA-XC:            -8.774032872173851     -238.7536       -5505.79       -23036.22
  Delta V^Pauli GGA-Exchange:       0.597087242477190       16.2476         374.68         1567.65
  Delta V^Pauli GGA-Correlation:   -0.677190722200267      -18.4273        -424.94        -1777.96
                                  ---------------    ----------    ----------    ----------
  Total Pauli Repulsion:           25.409195100876055      691.4194       15944.51       66711.83
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli): 25.409195100876055      691.4194       15944.51       66711.83
```

Electrostatic Interaction:	-5.372791238592933	-146.2011	-3371.48	-14106.26
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	20.036403862283123	545.2183	12573.03	52605.57
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-26.966417656317603	-733.7936	-16921.68	-70800.32
Total Orbital Interactions:	-26.971205996684429	-733.9239	-16924.69	-70812.89
Alternative Decomposition Orb.Int.				
Kinetic:	-64.434255771106891	-1753.3453	-40433.11	-169172.11
Coulomb:	34.963333635566599	951.4007	21939.83	91796.22
XC:	2.499716138855844	68.0207	1568.60	6563.00
Total Orbital Interactions:	-26.971205996684446	-733.9239	-16924.69	-70812.89
Residu (E=Steric+OrbInt+Res):	-0.000003072897645	-0.0001	0.00	-0.01
Solvation Energy (el):	-0.110952906966446	-3.0192	-69.62	-291.31
Dispersion Energy:	-0.059116808814555	-1.6087	-37.10	-155.21
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.005332960874095	0.1451	3.35	14.00
Total Bonding Energy:	-7.099541962205857	-193.1884	-4455.03	-18639.84

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-5.372791238592933	-146.2011	-3371.48	-14106.26
Kinetic Energy:	7.827833935564257	213.0062	4912.04	20551.98
Coulomb (Steric+OrbInt) Energy:	-3.035427691229216	-82.5982	-1904.76	-7969.51
XC Energy:	-6.354420213041084	-172.9126	-3987.46	-16683.53
Solvation:	-0.105619946092351	-2.8741	-66.28	-277.31
Dispersion Energy:	-0.059116808814555	-1.6087	-37.10	-155.21
Total Bonding Energy:	-7.099541962205882	-193.1884	-4455.03	-18639.84

Single point energy in the gas phase of the COSMO geometry:

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	72.262083217430671	1966.3513	45345.15	189724.07
Delta V^Pauli Coulomb:	-37.998765178439768	-1033.9990	-23844.59	-99765.74
Delta V^Pauli LDA-XC:	-8.774032125416332	-238.7536	-5505.79	-23036.22
Delta V^Pauli GGA-Exchange:	0.597088717948498	16.2476	374.68	1567.66
Delta V^Pauli GGA-Correlation:	-0.677190955645576	-18.4273	-424.94	-1777.96
Total Pauli Repulsion:	25.409183675877493	691.4191	15944.51	66711.80
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	25.409183675877493	691.4191	15944.51	66711.80
Electrostatic Interaction:	-5.372791238469266	-146.2011	-3371.48	-14106.26
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	20.036392437408228	545.2180	12573.03	52605.54
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-26.993205189365639	-734.5225	-16938.49	-70870.65
Total Orbital Interactions:	-26.993205189368446	-734.5225	-16938.49	-70870.65
Alternative Decomposition Orb.Int.				
Kinetic:	-64.454392155588110	-1753.8932	-40445.75	-169224.98
Coulomb:	34.933342810991824	950.5846	21921.01	91717.48
XC:	2.527844155227831	68.7861	1586.25	6636.85
Total Orbital Interactions:	-26.993205189368453	-734.5225	-16938.49	-70870.65

Residu (E=Steric+OrbInt+Res):	-0.000003869159086	-0.0001	0.00	-0.01
Dispersion Energy:	-0.059116808813129	-1.6087	-37.10	-155.21
Total Bonding Energy:	-7.015933429932432	-190.9133	-4402.57	-18420.33

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-5.372791238469266	-146.2011	-3371.48	-14106.26
Kinetic Energy:	7.807691061842561	212.4581	4899.40	20499.09
Coulomb (Steric+OrbInt) Energy:	-3.065426236607031	-83.4145	-1923.58	-8048.28
XC Energy:	-6.326290207885579	-172.1471	-3969.81	-16609.67
Dispersion Energy:	-0.059116808813129	-1.6087	-37.10	-155.21
Total Bonding Energy:	-7.015933429932444	-190.9133	-4402.57	-18420.33

$Cp^*Ir(H_2O)_3Cl_2$ – 2, COSMO

```
 Geometry CYCLE 2
 ==============

 Energy gradients wrt nuclear displacements
 ==========================================

     Atom      Cartesian (a.u./angstrom)
                  X         Y         Z
 ----------------------------------------
     1 H    -0.000055  0.000199  0.000039
     2 H     0.000000  0.000027 -0.000060
     3 H     0.000044  0.000056 -0.000625
     4 Ir   -0.000306  0.001917  0.003007
     5 H    -0.000103  0.000074  0.000054
     6 C    -0.000139  0.000206  0.000070
     7 C    -0.000831 -0.000379 -0.001082
     8 C     0.000009 -0.000166  0.000792
     9 C     0.002004 -0.000997  0.002356
    10 C     0.000379 -0.000799  0.000076
    11 H     0.000163  0.000028  0.000115
    12 H     0.000026  0.000005 -0.000002
    13 H     0.000030  0.000021 -0.000054
    14 H     0.000104  0.000269 -0.000023
    15 O     0.000328 -0.001244 -0.000481
    16 H    -0.000058 -0.000002 -0.000003
    17 O    -0.001295 -0.000089 -0.001197
    18 H     0.000289  0.000010  0.000272
    19 O    -0.000105  0.000413 -0.000089
    20 H    -0.000001 -0.000302  0.000139
    21 C    -0.000081 -0.000076 -0.000234
    22 H    -0.000084  0.000008  0.000078
    23 H    -0.000025  0.000020 -0.000024
    24 C     0.000231  0.000010 -0.000579
    25 H     0.000026 -0.000054  0.000099
    26 H     0.000042 -0.000029 -0.000039
    27 C     0.000378  0.000885 -0.000576
    28 H     0.000016 -0.000010  0.000087
    29 H    -0.000197 -0.000198  0.000023
    30 C     0.000181  0.000144  0.000074
    31 H     0.000063 -0.000056 -0.000020
    32 H     0.000065 -0.000031  0.000053
    33 C    -0.000063  0.000088 -0.000157
    34 H     0.000004  0.000017 -0.000018
    35 H     0.000029 -0.000074  0.000109
    36 Cl   -0.000096 -0.000261  0.000262
    37 Cl   -0.000972  0.000371 -0.002441
 ----------------------------------------

 dE(predicted):    -0.83649E-04, dE(actual):     0.21220E-03, Trust radius:    0.037000, all in a.u.
 Residual max backtransformation error  0.1320E-02

-----------------------------------------------------------
Geometry Convergence after Step   2       ** CONVERGED **
-----------------------------------------------------------
current energy                              -7.09776887 Hartree
energy change                  0.00021220     0.00100000    T
constrained gradient max       0.00300652     0.01000000    T
constrained gradient rms       0.00061577     0.00666667    T
gradient max                   0.00300652
gradient rms                   0.00061577
cart. step max                 0.01812398     0.02000000    T
cart. step rms                 0.00487340     0.01333333    T


                                      hartree              eV         kcal/mol           kJ/mol
                                ---------------------  -----------  ----------  -----------

Pauli Repulsion
  Kinetic (Delta T^0):           71.504887592261099     1945.7470     44870.00      187736.06
  Delta V^Pauli Coulomb:        -37.399873993165826    -1017.7024    -23468.78      -98193.36
  Delta V^Pauli LDA-XC:          -8.694668411037181     -236.5940     -5455.99      -22827.85
  Delta V^Pauli GGA-Exchange:     0.591656958943663       16.0998       371.27        1553.40
  Delta V^Pauli GGA-Correlation: -0.671697696212592      -18.2778      -421.50       -1763.54
                                ---------------------  -----------  ----------  -----------
  Total Pauli Repulsion:        25.330304450789164      689.2727     15895.01      66504.70
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli): 25.330304450789164     689.2727     15895.01      66504.70
```

Electrostatic Interaction:	-5.337777566826345	-145.2483	-3349.51	-14014.33
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	19.992526883962817	544.0243	12545.50	52490.37
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-26.879816001376792	-731.4370	-16867.34	-70572.95
Total Orbital Interactions:	-26.881474042496048	-731.4821	-16868.38	-70577.30
Alternative Decomposition Orb.Int.				
Kinetic:	-63.773791170685321	-1735.3732	-40018.66	-167438.07
Coulomb:	34.454194517950739	937.5463	21620.34	90459.47
XC:	2.438122610238524	66.3447	1529.95	6401.29
Total Orbital Interactions:	-26.881474042496059	-731.4821	-16868.38	-70577.30
Residu (E=Steric+OrbInt+Res):	-0.000009406513380	-0.0003	-0.01	-0.02
Solvation Energy (el):	-0.153978835357109	-4.1900	-96.62	-404.27
Dispersion Energy:	-0.060106674715891	-1.6356	-37.72	-157.81
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.005337242839705	0.1452	3.35	14.01
Total Bonding Energy:	-7.097704832279907	-193.1384	-4453.88	-18635.02

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-5.337777566826345	-145.2483	-3349.51	-14014.33
Kinetic Energy:	7.731096421575778	210.3738	4851.34	20297.99
Coulomb (Steric+OrbInt) Energy:	-2.945688881728465	-80.1563	-1848.45	-7733.91
XC Energy:	-6.336586538067586	-172.4273	-3976.27	-16636.71
Solvation:	-0.148641592517404	-4.0447	-93.27	-390.26
Dispersion Energy:	-0.060106674715891	-1.6356	-37.72	-157.81
Total Bonding Energy:	-7.097704832279913	-193.1384	-4453.88	-18635.02

Single point gas phase energies from COSMO geometries:

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	71.504612419518395	1945.7395	44869.83	187735.33
Delta V^Pauli Coulomb:	-37.399693388037164	-1017.6974	-23468.66	-98192.88
Delta V^Pauli LDA-XC:	-8.694619059591060	-236.5926	-5455.96	-22827.72
Delta V^Pauli GGA-Exchange:	0.591658771739848	16.0999	371.27	1553.40
Delta V^Pauli GGA-Correlation:	-0.671690897714553	-18.2776	-421.49	-1763.52
Total Pauli Repulsion:	25.330267845915465	689.2717	15894.98	66504.61
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	25.330267845915465	689.2717	15894.98	66504.61
Electrostatic Interaction:	-5.337777566794422	-145.2483	-3349.51	-14014.33
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	19.992490279121043	544.0233	12545.48	52490.28
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-26.914035289440864	-732.3682	-16888.81	-70662.79
Total Orbital Interactions:	-26.914035289442953	-732.3682	-16888.81	-70662.79
Alternative Decomposition Orb.Int.				
Kinetic:	-63.685215895466357	-1732.9629	-39963.08	-167205.51
Coulomb:	34.319119811329472	933.8708	21535.58	90104.84
XC:	2.452060794693948	66.7240	1538.69	6437.88
Total Orbital Interactions:	-26.914035289442936	-732.3682	-16888.81	-70662.79
Residu (E=Steric+OrbInt+Res):	-0.000013272513979	-0.0004	-0.01	-0.03

Dispersion Energy:	-0.060106674714863	-1.6356	-37.72	-157.81
Total Bonding Energy:	-6.981664957550752	-189.9808	-4381.06	-18330.36

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-5.337777566794422	-145.2483	-3349.51	-14014.33
Kinetic Energy:	7.819396524052038	212.7766	4906.75	20529.82
Coulomb (Steric+OrbInt) Energy:	-3.080586849221675	-83.8270	-1933.10	-8088.08
XC Energy:	-6.322590390871817	-172.0464	-3967.49	-16599.96
Dispersion Energy:	-0.060106674714863	-1.6356	-37.72	-157.81
Total Bonding Energy:	-6.981664957550738	-189.9808	-4381.06	-18330.36

Cp*Ir(H_2O)$_3$$Cl_2$ –3, COSMO

```
 Geometry CYCLE 3
 ==============

 Energy gradients wrt nuclear displacements
 ==========================================

    Atom      Cartesian (a.u./angstrom)
                X          Y          Z
 ----------------------------------------
     1 H    -0.000666 -0.000656  0.000592
     2 H     0.000423 -0.000566 -0.000284
     3 H     0.000192 -0.000733 -0.000637
     4 Ir   -0.003990 -0.002557  0.005755
     5 H     0.000437 -0.000754  0.000034
     6 C     0.004179 -0.001892 -0.005139
     7 C    -0.006926  0.000067 -0.000391
     8 C    -0.000207  0.002580  0.002801
     9 C     0.005030 -0.000351 -0.004775
    10 C    -0.000425  0.001756 -0.000864
    11 H     0.000262  0.000191 -0.001371
    12 H    -0.005300  0.000576 -0.006757
    13 H     0.000106  0.000512  0.000298
    14 H    -0.000947  0.001221  0.001787
    15 O    -0.000900 -0.000578  0.001491
    16 H     0.000678 -0.000084  0.000770
    17 O    -0.002242 -0.001878  0.000347
    18 H    -0.000023 -0.000364 -0.000051
    19 O     0.005554 -0.000879 -0.000269
    20 H    -0.001563  0.001124  0.000695
    21 C    -0.000863 -0.000302  0.001040
    22 H    -0.000860  0.000817 -0.000279
    23 H    -0.000480  0.001170  0.000065
    24 C     0.002292  0.001355 -0.000206
    25 H    -0.000988 -0.001485 -0.000393
    26 H    -0.000634  0.001826 -0.000396
    27 C    -0.000950 -0.006565  0.002709
    28 H    -0.000650 -0.000983 -0.001272
    29 H     0.004246  0.006304  0.005780
    30 C     0.000691 -0.000675  0.000714
    31 H     0.000213 -0.000174  0.000219
    32 H     0.000483  0.000896 -0.001077
    33 C    -0.001239 -0.003470  0.002943
    34 H     0.002597 -0.001150 -0.000196
    35 H     0.000554  0.000815  0.002131
    36 Cl    0.002829  0.003849  0.000332
    37 Cl   -0.000914  0.001037 -0.006146
 ----------------------------------------

 dE(predicted):    -0.12519E-02, dE(actual):    -0.30292E-03, Trust radius:    0.037000, all in a.u.
 Residual max backtransformation error  0.6071E-01

---------------------------------------------------------
Geometry Convergence after Step   3       ** CONVERGED **
---------------------------------------------------------
current energy                              -7.08074322 Hartree
energy change                     -0.00030292     0.00100000    T
constrained gradient max           0.00692570     0.01000000    T
constrained gradient rms           0.00236283     0.00666667    T
gradient max                       0.00692570
gradient rms                       0.00236283
cart. step max                     0.00891802     0.02000000    T
cart. step rms                     0.00289789     0.01333333    T

                                           hartree             eV         kcal/mol          kJ/mol
                                    --------------------     -----------     ----------      -----------

Pauli Repulsion
  Kinetic (Delta T^0):                71.153757065800946       1936.1922       44649.66        186814.16
  Delta V^Pauli Coulomb:             -37.120579586130980      -1010.1024      -23293.52        -97460.07
  Delta V^Pauli LDA-XC:               -8.640327292185013       -235.1153       -5421.89        -22685.18
  Delta V^Pauli GGA-Exchange:          0.582680640660179         15.8555         365.64          1529.83
  Delta V^Pauli GGA-Correlation:      -0.665324181573860        -18.1044        -417.50         -1746.81
                                    --------------------     -----------     ----------      -----------
  Total Pauli Repulsion:              25.310206646571274        688.7258       15882.40         66451.94
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):   25.310206646571274        688.7258       15882.40         66451.94
  Electrostatic Interaction:         -5.331659516089392       -145.0818       -3345.67        -13998.27
```

(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	19.978547130481882	543.6439	12536.73	52453.67
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-26.759256726212381	-728.1564	-16791.69	-70256.42
Total Orbital Interactions:	-26.760021421835265	-728.1772	-16792.17	-70258.43
Alternative Decomposition Orb.Int.				
Kinetic:	-63.398015768544816	-1725.1478	-39782.86	-166451.47
Coulomb:	34.253365197798821	932.0815	21494.31	89932.20
XC:	2.384629148910746	64.8891	1496.38	6260.84
Total Orbital Interactions:	-26.760021421835248	-728.1772	-16792.17	-70258.43
Residu (E=Steric+OrbInt+Res):	-0.000001776927524	0.0000	0.00	0.00
Solvation Energy (el):	-0.249185601322561	-6.7807	-156.37	-654.24
Dispersion Energy:	-0.055152974514315	-1.5008	-34.61	-144.80
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.005576425333467	0.1517	3.50	14.64
Total Bonding Energy:	-7.080238218784316	-192.6631	-4442.92	-18589.16

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-5.331659516089392	-145.0818	-3345.67	-13998.27
Kinetic Energy:	7.755741297256129	211.0445	4866.80	20362.70
Coulomb (Steric+OrbInt) Energy:	-2.867216165259684	-78.0209	-1799.21	-7527.87
XC Energy:	-6.338341684187947	-172.4751	-3977.37	-16641.31
Solvation:	-0.243609175989094	-6.6289	-152.87	-639.60
Dispersion Energy:	-0.055152974514315	-1.5008	-34.61	-144.80
Total Bonding Energy:	-7.080238218784302	-192.6631	-4442.92	-18589.16

Single point gas phase energy from the COSMO geometry

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	71.153755595825956	1936.1922	44649.66	186814.16
Delta V^Pauli Coulomb:	-37.120582933805970	-1010.1025	-23293.52	-97460.08
Delta V^Pauli LDA-XC:	-8.640329033827005	-235.1153	-5421.89	-22685.18
Delta V^Pauli GGA-Exchange:	0.582678622964330	15.8555	365.64	1529.82
Delta V^Pauli GGA-Correlation:	-0.665324981370622	-18.1044	-417.50	-1746.81
Total Pauli Repulsion:	25.310197269786691	688.7255	15882.39	66451.91
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	25.310197269786691	688.7255	15882.39	66451.91
Electrostatic Interaction:	-5.331659515663390	-145.0818	-3345.67	-13998.27
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	19.978537754123302	543.6437	12536.72	52453.64
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-26.823596068781040	-729.9072	-16832.06	-70425.34
Total Orbital Interactions:	-26.823596068779221	-729.9072	-16832.06	-70425.34
Alternative Decomposition Orb.Int.				
Kinetic:	-63.178436082674018	-1719.1727	-39645.07	-165874.96
Coulomb:	33.952841012689284	923.9038	21305.73	89143.17
XC:	2.401999001205529	65.3617	1507.28	6306.45
Total Orbital Interactions:	-26.823596068779207	-729.9072	-16832.06	-70425.34
Residu (E=Steric+OrbInt+Res):	-0.000000536638935	0.0000	0.00	0.00
Dispersion Energy:	-0.055152974512969	-1.5008	-34.61	-144.80
Total Bonding Energy:	-6.900211825807824	-187.7643	-4329.95	-18116.50

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-5.331659515663390	-145.0818	-3345.67	-13998.27
Kinetic Energy:	7.975319513151938	217.0195	5004.59	20939.20
Coulomb (Steric+OrbInt) Energy:	-3.167742457755622	-86.1987	-1987.79	-8316.91
XC Energy:	-6.320976391027768	-172.0025	-3966.47	-16595.72
Dispersion Energy:	-0.055152974512969	-1.5008	-34.61	-144.80
Total Bonding Energy:	-6.900211825807813	-187.7643	-4329.95	-18116.50

host-guest, Cl_2, COSMO

```
G E O M E T R Y   U P D A T E  ***  13  ***

*** Using NEW gradient routines ***

Energy gradients wrt nuclear displacements
==========================================

    Atom      Cartesian (a.u./angstrom)
                X         Y         Z
------------------------------------------
    1 H    -0.000176 -0.000178  0.000185
    2 C     0.000042 -0.000275  0.000414
    3 C     0.000063  0.000668  0.000026
    4 H     0.000182 -0.000351 -0.000180
    5 H     0.000008  0.000142  0.000031
    6 C    -0.000058 -0.000150  0.000294
    7 C     0.000145 -0.000145 -0.000066
    8 H     0.000018  0.000022 -0.000045
    9 H    -0.000067  0.000119  0.000106
   10 C     0.000119 -0.000050  0.000139
   11 C     0.000128 -0.000095  0.000011
   12 H     0.000069  0.000025 -0.000040
   13 H    -0.000058  0.000026  0.000006
   14 C    -0.000064 -0.000034  0.000030
   15 C    -0.000101  0.000067  0.000016
   16 H     0.000027 -0.000014 -0.000038
   17 H     0.000029 -0.000013 -0.000014
   18 C    -0.000017 -0.000060 -0.000050
   19 C    -0.000424  0.000093 -0.000115
   20 H     0.000448  0.000021 -0.000267
   21 H    -0.000094 -0.000104 -0.000033
   22 C    -0.000117 -0.000068 -0.000009
   23 C     0.000007  0.000372  0.000049
   24 H     0.000068 -0.000070 -0.000071
   25 H    -0.000037 -0.000106 -0.000004
   26 C     0.000091  0.000033 -0.000086
   27 C    -0.000599 -0.000243 -0.000037
   28 H     0.000315  0.000036 -0.000086
   29 H     0.000003  0.000019  0.000109
   30 O     0.000112 -0.000208  0.000009
   31 O    -0.000182 -0.000167  0.000050
   32 O    -0.000092  0.000078  0.000028
   33 O     0.000015  0.000006  0.000110
   34 O    -0.000052  0.000366 -0.000230
   35 O     0.000351 -0.000627  0.000425
   36 O    -0.000251  0.000279 -0.000420
   37 O     0.000017  0.000357 -0.000346
   38 O     0.000072  0.000351 -0.000008
   39 O     0.000003  0.000021 -0.000107
   40 O    -0.000003 -0.000056  0.000117
   41 O    -0.000046 -0.000005 -0.000150
   42 O     0.000001 -0.000065 -0.000222
   43 O    -0.000124 -0.000185  0.000526
   44 N    -0.000121  0.000068 -0.000209
   45 N    -0.000243 -0.000161 -0.000146
   46 N    -0.000076 -0.000581 -0.000077
   47 N     0.000111  0.000176 -0.000097
   48 N    -0.000153  0.000294 -0.000005
   49 N     0.000122 -0.000134 -0.000106
   50 N     0.000018  0.000020  0.000172
   51 N    -0.000015 -0.000172  0.000103
   52 N    -0.000023  0.000049 -0.000326
   53 N    -0.000113  0.000215 -0.000197
   54 N    -0.000048  0.000210  0.000261
   55 N    -0.000081 -0.000048 -0.000142
   56 N     0.000103 -0.000562  0.000121
   57 N     0.000732  0.000137 -0.000004
   58 N     0.000181 -0.000180  0.000131
   59 N    -0.000031 -0.000048 -0.000181
   60 N    -0.000048  0.000340 -0.000080
   61 N    -0.000074 -0.000077 -0.000039
   62 N     0.000055  0.000077 -0.000047
   63 N    -0.000111  0.000010 -0.000053
   64 N    -0.000116  0.000076  0.000062
   65 N    -0.000014 -0.000098 -0.000020
   66 N     0.000076  0.000064 -0.000090
   67 N    -0.000063  0.000064 -0.000093
   68 N     0.000147 -0.000173  0.000025
   69 N    -0.000107  0.000166  0.000207
```

70	N	0.000115	-0.000378	-0.000466
71	N	0.000041	0.000488	-0.000181
72	C	0.000112	-0.000144	-0.000052
73	C	-0.000086	0.000160	-0.000268
74	H	-0.000040	-0.000258	0.000111
75	H	-0.000228	-0.000160	-0.000270
76	C	-0.000322	0.000008	0.000050
77	C	-0.000063	-0.000332	0.000156
78	H	-0.000120	0.000149	-0.000024
79	H	0.000026	0.000009	0.000089
80	C	-0.000002	0.000097	0.000099
81	C	-0.000165	0.000032	0.000136
82	H	-0.000148	0.000012	0.000067
83	H	0.000009	0.000002	0.000013
84	C	0.000028	0.000140	-0.000219
85	C	-0.000011	0.000167	0.000076
86	H	-0.000070	0.000012	0.000028
87	H	-0.000068	0.000036	0.000033
88	C	-0.000086	-0.000442	0.000389
89	C	-0.000017	-0.000215	0.000036
90	H	0.000018	0.000256	-0.000110
91	H	-0.000026	0.000207	-0.000086
92	C	-0.000238	0.000800	-0.000586
93	C	0.000014	0.000494	0.000185
94	H	0.000128	-0.000150	-0.000034
95	H	0.000068	-0.000043	-0.000009
96	C	0.000167	0.000040	0.000180
97	C	-0.000128	-0.000481	0.000380
98	H	0.000168	0.000084	-0.000172
99	H	0.000242	-0.000010	0.000067
100	C	-0.000174	0.000269	-0.000059
101	H	0.000048	0.000025	0.000037
102	C	0.000222	-0.000128	0.000140
103	H	-0.000144	-0.000030	-0.000130
104	C	0.000142	0.000060	0.000205
105	H	-0.000126	-0.000065	-0.000235
106	C	0.000057	-0.000127	-0.000323
107	H	-0.000003	0.000154	0.000085
108	C	0.000015	-0.000082	-0.000126
109	H	-0.000053	0.000033	0.000148
110	C	-0.000142	-0.000042	0.000313
111	H	0.000034	-0.000013	-0.000008
112	C	-0.000087	0.000063	0.000188
113	H	0.000051	0.000000	-0.000022
114	C	-0.000033	-0.000028	-0.000122
115	H	-0.000005	0.000013	0.000024
116	C	-0.000021	-0.000124	-0.000089
117	H	-0.000023	0.000018	0.000007
118	C	0.000028	0.000225	0.000248
119	H	-0.000083	-0.000102	-0.000183
120	C	0.000139	0.000300	0.000146
121	H	-0.000064	-0.000078	-0.000188
122	C	-0.000029	-0.000270	-0.000272
123	H	-0.000099	0.000130	0.000050
124	C	0.000034	-0.000711	-0.000260
125	H	-0.000220	0.000188	0.000208
126	C	0.000278	0.000590	0.000071
127	H	0.000550	-0.000394	0.000472
128	H	0.000072	0.000990	0.000349
129	H	0.000072	0.000061	0.000053
130	Ir	0.000799	0.001639	0.000342
131	H	0.000018	-0.000422	-0.000047
132	C	0.000176	0.000037	0.000032
133	C	-0.000094	0.000241	-0.000242
134	C	-0.000024	-0.000078	0.000008
135	C	-0.000005	0.000020	0.000442
136	C	0.000059	-0.000290	0.000070
137	H	0.000115	0.000036	0.000066
138	H	0.000165	-0.000109	0.000246
139	H	0.000038	0.000070	-0.000261
140	H	-0.000026	-0.000178	0.000040
141	O	0.001729	0.000751	-0.000071
142	H	-0.001257	-0.000050	0.000204
143	O	-0.000586	-0.000402	0.000025
144	H	0.000161	-0.000169	0.000000
145	O	-0.000191	-0.001010	-0.000282
146	H	0.000090	0.000675	0.000149
147	C	-0.001289	0.000127	-0.000659
148	H	0.000938	-0.000116	0.000012
149	H	0.000183	-0.000304	0.000074
150	C	0.000142	0.000165	0.000063
151	H	0.000019	-0.000133	-0.000040
152	H	-0.000002	0.000057	-0.000007
153	C	-0.001133	-0.000433	0.000760
154	H	0.000563	0.000249	0.000106

```
  155 H     0.000214 -0.000216 -0.000112
  156 C     0.000439 -0.001716 -0.000649
  157 H    -0.000338  0.000067  0.000753
  158 H    -0.000147  0.000186 -0.000118
  159 C     0.000002 -0.000055 -0.000959
  160 H    -0.000257 -0.000127  0.000389
  161 H     0.000313  0.000277  0.000228
  162 Cl   -0.000218  0.000166  0.000052
  163 Cl   -0.000233 -0.000024 -0.000187
----------------------------------------


 Geometry Convergence Tests


 Energy  old :        -37.24787769
         new :        -37.24795977

 Convergence tests:
 (Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

      Item               Value         Criterion    Conv.        Ratio
-------------------------------------------------------------------------
change in energy      -0.00008208     0.00100000    YES        0.05231289
gradient max           0.00172938     0.01000000    YES        0.20580535
gradient rms           0.00028121     0.00666667    YES        0.27911633
cart. step max         0.00461067     0.01000000    YES        0.98964599
cart. step rms         0.00092816     0.00666667    YES        0.72065266

prediction dE :       -0.00003363


*************************************************************************************************
                           Geometry CONVERGED
*************************************************************************************************


                                        hartree             eV         kcal/mol           kJ/mol
                                   --------------------  -----------  ----------  -----------

Pauli Repulsion
  Kinetic (Delta T^0):              468.082554333671453    12737.1744    293726.27     1228950.57
  Delta V^Pauli Coulomb:           -244.056742412101670    -6641.1219   -153147.93     -640770.89
  Delta V^Pauli LDA-XC:             -57.399114758354919    -1561.9094    -36018.49     -150701.35
  Delta V^Pauli GGA-Exchange:         3.629061729394522       98.7518      2277.27        9528.10
  Delta V^Pauli GGA-Correlation:     -4.182095250307558     -113.8006     -2624.30      -10980.09
                                   --------------------  -----------  ----------  -----------
  Total Pauli Repulsion:            166.073663642301824     4519.0943    104212.81      436026.34
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli): 166.073663642301824     4519.0943    104212.81      436026.34
  Electrostatic Interaction:       -36.312463403259670     -988.1124    -22786.42      -95338.36
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                   --------------------  -----------  ----------  -----------
  Total Steric Interaction:         129.761200239042154     3530.9819     81426.39      340687.98
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -166.228842670734508    -4523.3170   -104310.18     -436433.76
                                   --------------------  -----------  ----------  -----------
  Total Orbital Interactions:      -166.283171034974629    -4524.7953   -104344.28     -436576.40

Alternative Decomposition Orb.Int.
  Kinetic:                         -430.243364345855412   -11707.5176   -269981.82    -1129603.79
  Coulomb:                          241.535455694499632     6572.5142    151565.80      634151.25
  XC:                                22.424737616381194      610.2082     14071.74       58876.14
                                   --------------------  -----------  ----------  -----------
  Total Orbital Interactions:      -166.283171034974600    -4524.7953   -104344.28     -436576.40

  Residu (E=Steric+OrbInt+Res):      -0.000314053712023       -0.0085        -0.20          -0.82


  Solvation Energy (el):             -0.270589402249712       -7.3631       -169.80        -710.43
  Dispersion Energy:                 -0.455108907349421      -12.3841       -285.59       -1194.89

Post-SCF Solvation Energies
  Solvation Energy (cd):              0.000000000000000        0.0000         0.00           0.00

Total Bonding Energy:               -37.247983159243631    -1013.5692    -23373.46      -97794.57
```

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-36.312463403259670	-988.1124	-22786.42	-95338.36
Kinetic Energy:	37.839189987816042	1029.6567	23744.45	99346.78
Coulomb (Steric+OrbInt) Energy:	-2.521600771314070	-68.6162	-1582.33	-6620.46
XC Energy:	-35.527410662886766	-966.7500	-22293.79	-93277.20
Solvation:	-0.270589402249712	-7.3631	-169.80	-710.43
Dispersion Energy:	-0.455108907349421	-12.3841	-285.59	-1194.89
Total Bonding Energy:	-37.247983159243596	-1013.5692	-23373.46	-97794.57

Single point gas phase energy from COSMO geometry

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	468.081985133382716	12737.1589	293725.91	1228949.08
Delta V^Pauli Coulomb:	-244.056780659319600	-6641.1229	-153147.96	-640770.99
Delta V^Pauli LDA-XC:	-57.398989932503824	-1561.9060	-36018.41	-150701.03
Delta V^Pauli GGA-Exchange:	3.629042293154953	98.7513	2277.26	9528.05
Delta V^Pauli GGA-Correlation:	-4.182079483084973	-113.8002	-2624.29	-10980.05
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	166.073177351629283	4519.0811	104212.50	436025.07
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	166.073177351629283	4519.0811	104212.50	436025.07
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-36.312457433853830	-988.1122	-22786.41	-95338.34
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	129.760719917775447	3530.9688	81426.09	340686.72
Orbital Interactions				
A:	-166.341955184928224	-4526.3949	-104381.16	-436730.74
Total Orbital Interactions:	-166.341955184931265	-4526.3949	-104381.16	-436730.74
Alternative Decomposition Orb.Int.				
Kinetic:	-430.238120440469970	-11707.3749	-269978.53	-1129590.03
Coulomb:	241.397328797180222	6568.7555	151479.13	633788.60
XC:	22.498836458358575	612.2245	14118.23	59070.69
Total Orbital Interactions:	-166.341955184931180	-4526.3949	-104381.16	-436730.74
Residu (E=Steric+OrbInt+Res):	-0.000339107095341	-0.0092	-0.21	-0.89
Dispersion Energy:	-0.455108703660145	-12.3841	-285.59	-1194.89
Total Bonding Energy:	-37.036683077911306	-1007.8194	-23240.87	-97239.80

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-36.312457433853830	-988.1122	-22786.41	-95338.34
Kinetic Energy:	37.843864692912746	1029.7840	23747.39	99359.05
Coulomb (Steric+OrbInt) Energy:	-2.659790969234706	-72.3766	-1669.04	-6983.28
XC Energy:	-35.453190664075265	-964.7304	-22247.22	-93082.34
Dispersion Energy:	-0.455108703660145	-12.3841	-285.59	-1194.89
Total Bonding Energy:	-37.036683077911199	-1007.8194	-23240.87	-97239.80

$Cp^*Ir(H_2O)_2(O)^{2+}$, gas phase

Triplet state
B-LYPD3

Geometry CYCLE 52
==========

Energy gradients wrt nuclear displacements
==========

Atom	Cartesian (a.u./angstrom) X	Y	Z
1 H	0.000010	-0.000015	-0.000021
2 H	0.000017	-0.000071	-0.000016
3 H	-0.000576	-0.000607	0.000395
4 Ir	0.000340	-0.000796	-0.000878
5 H	0.000463	-0.000576	-0.000569
6 C	-0.000187	-0.000327	0.000501
7 C	-0.000063	-0.000204	0.000180
8 C	-0.000483	-0.000132	0.000033
9 C	0.000030	0.000395	-0.000303
10 C	-0.000086	0.000120	0.000024
11 H	-0.000019	-0.000004	0.000096
12 H	0.000001	0.000131	-0.000041
13 H	-0.000011	-0.000003	-0.000019
14 H	0.000008	0.000041	-0.000016
15 O	-0.000090	0.000461	0.000961
16 H	-0.000160	0.000446	-0.000203
17 O	0.000199	0.000537	0.000379
18 H	0.000490	-0.000086	-0.000792
19 O	-0.000474	0.000414	0.000376
20 H	0.000091	-0.000055	-0.000004
21 C	-0.000062	0.000163	-0.000006
22 H	0.000028	0.000022	-0.000007
23 H	0.000033	-0.000032	-0.000010
24 C	0.000050	0.000093	-0.000068
25 H	0.000011	0.000005	-0.000031
26 H	0.000053	0.000015	0.000024
27 C	0.000099	-0.000048	0.000087
28 H	0.000049	-0.000009	-0.000012
29 H	0.000032	0.000011	-0.000016
30 C	0.000086	-0.000050	-0.000024
31 H	0.000018	0.000006	0.000051
32 H	0.000029	0.000028	-0.000024
33 C	0.000073	0.000127	-0.000044

dE(predicted): -0.83979E-05, dE(actual): -0.20916E-04, Trust radius: 0.132000, all in a.u.

Geometry Convergence after Step 52 ** CONVERGED **
---

current energy	-5.94056548 Hartree		
energy change	-0.00002092	0.00100000	T
constrained gradient max	0.00096131	0.00100000	T
constrained gradient rms	0.00027890	0.00066667	T
gradient max	0.00096131		
gradient rms	0.00027890		
cart. step max	0.00520825	0.01000000	T
cart. step rms	0.00176331	0.00666667	T

S**2 value *** see also R. Bulo et al., J.Am.Chem.Soc., 124 (2002) 13903-13910, note (29) ***

	exact	expectation value
Total S2 (S squared)	2.00000	2.01455

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	66.548694625290011	1810.8821	41759.94	174723.57
Delta V^Pauli Coulomb:	-34.598297926051785	-941.4676	-21710.76	-90837.82
Delta V^Pauli LDA-XC:	-8.050746212002835	-219.0720	-5051.92	-21137.23
Delta V^Pauli GGA-Exchange:	0.534462698774508	14.5435	335.38	1403.23
Delta V^Pauli GGA-Correlation:	-0.617431171965225	-16.8012	-387.44	-1621.07
Total Pauli Repulsion:	23.816682014044673	648.0849	14945.20	62530.69

```
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  23.816682014044673        648.0849         14945.20         62530.69
  Electrostatic Interaction:        -5.001860003736566       -136.1075         -3138.71        -13132.38
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                    --------------------     -----------      ----------      -----------
  Total Steric Interaction:         18.814822010308106        511.9774         11806.48         49398.31
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -24.704339070335038       -672.2393        -15502.21        -64861.23
                                   --------------------      -----------      ----------       -----------
  Total Orbital Interactions:      -24.709674365597007       -672.3845        -15505.56        -64875.24

Alternative Decomposition Orb.Int.
  Kinetic:                         -59.920662551624687      -1630.5242        -37600.79       -157321.68
  Coulomb:                          32.384261543440722        881.2206         20321.43         85024.87
  XC:                                2.826726642586958         76.9191          1773.80          7421.57
                                   --------------------      -----------      ----------       -----------
  Total Orbital Interactions:      -24.709674365597007       -672.3845        -15505.56        -64875.24

  Residu (E=Steric+OrbInt+Res):      0.000005771956325          0.0002            0.00             0.02
  Dispersion Energy:                -0.045718885363717         -1.2441          -28.69           -120.03

Total Bonding Energy:               -5.940565468696292       -161.6510         -3727.76        -15596.95


Summary of Bonding Energy (energy terms are taken from the energy decomposition above)
================================================================================

  Electrostatic Energy:             -5.001860003736566       -136.1075         -3138.71        -13132.38
  Kinetic Energy:                    6.628032073665324        180.3579          4159.15         17401.90
  Coulomb (Steric+OrbInt) Energy:   -2.214030610654738        -60.2468         -1389.33         -5812.94
  XC Energy:                        -5.306988042606593       -144.4105         -3330.19        -13933.50
  Dispersion Energy:                -0.045718885363717         -1.2441          -28.69           -120.03
                                   --------------------      -----------      ----------       -----------
  Total Bonding Energy:             -5.940565468696291       -161.6510         -3727.76        -15596.95


Single point PBE0:


 S**2 value  ***  see also R. Bulo et al., J.Am.Chem.Soc., 124 (2002) 13903-13910, note (29)  ***

                                      exact      expectation value

 Total S2 (S squared)                 2.00000             2.04052

                                                hartree              eV         kcal/mol           kJ/mol
                                   --------------------      -----------      ----------       -----------

Pauli Repulsion
  Kinetic (Delta T^0):               65.421461138622931       1780.2085         41052.59        171764.02
  Delta V^Pauli Coulomb:            -33.675898858718590       -916.3678        -21131.95        -88416.06
  Delta V^Pauli Hybrid-X:            -5.656148085247537       -153.9116         -3549.29        -14850.21
  Delta V^Pauli Hybrid-C:            -0.639512349311500        -17.4020          -401.30         -1679.04
  Delta V^Pauli HF-Exchange:         -1.390342301180027        -37.8331          -872.45         -3650.34
                                   --------------------      -----------      ----------       -----------
  Total Pauli Repulsion:             24.059559544165282        654.6939         15097.60         63168.36
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  24.059559544165282        654.6939         15097.60         63168.36
  Electrostatic Interaction:        -5.105234943616575       -138.9205         -3203.58        -13403.79
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                    --------------------     -----------      ----------      -----------
  Total Steric Interaction:         18.954324600548706        515.7734         11894.02         49764.57
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -26.748168455706359       -727.8547        -16784.73        -70227.31
                                   --------------------      -----------      ----------       -----------
  Total Orbital Interactions:      -26.748168455705848       -727.8547        -16784.73        -70227.31

Alternative Decomposition Orb.Int.
  Kinetic:                         -58.297879557903251      -1586.3660        -36582.48       -153061.06
```

Coulomb:	31.330125356180851	852.5361	19659.95	82257.23
XC:	0.219585746016543	5.9752	137.79	576.52
Total Orbital Interactions:	-26.748168455705859	-727.8547	-16784.73	-70227.31
Residu (E=Steric+OrbInt+Res):	0.000032534927562	0.0009	0.02	0.09
Total Bonding Energy:	-7.793811320229580	-212.0804	-4890.69	-20462.65

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-5.105234943616575	-138.9205	-3203.58	-13403.79
Kinetic Energy:	7.123581580719680	193.8425	4470.12	18702.96
Coulomb (Steric+OrbInt) Energy:	-2.345740967610176	-63.8309	-1471.97	-6158.74
XC Energy:	-7.466416989722521	-203.1715	-4685.25	-19603.08
Total Bonding Energy:	-7.793811320229592	-212.0804	-4890.69	-20462.65

$Cp^*Ir(H_2O)_2(O)^{2+}$, gas phase

Singlet state (Broken symmetry)
B-LYPD3

S**2 value *** see also R. Bulo et al., J.Am.Chem.Soc., 124 (2002) 13903-13910, note (29) ***

	exact	expectation value
Total S2 (S squared)	0.00000	0.99489

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	66.548928020530980	1810.8885	41760.09	174724.19
Delta V^Pauli Coulomb:	-34.598509417435523	-941.4733	-21710.89	-90838.37
Delta V^Pauli LDA-XC:	-8.050825153046002	-219.0741	-5051.97	-21137.44
Delta V^Pauli GGA-Exchange:	0.534462863536703	14.5435	335.38	1403.23
Delta V^Pauli GGA-Correlation:	-0.617437065143322	-16.8013	-387.45	-1621.08
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	23.816619248442837	648.0832	14945.16	62530.52
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	23.816619248442837	648.0832	14945.16	62530.52
Electrostatic Interaction:	-5.001860003736567	-136.1075	-3138.71	-13132.38
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	18.814759244706270	511.9756	11806.44	49398.14
Orbital Interactions				
A:	-24.699526871620392	-672.1083	-15499.19	-64848.60
Total Orbital Interactions:	-24.699526871620701	-672.1083	-15499.19	-64848.60
Alternative Decomposition Orb.Int.				
Kinetic:	-59.940222670307087	-1631.0564	-37613.06	-157373.03
Coulomb:	32.397748123490118	881.5876	20329.90	85060.28
XC:	2.842947675196254	77.3605	1783.98	7464.16
Total Orbital Interactions:	-24.699526871620716	-672.1083	-15499.19	-64848.60
Residu (E=Steric+OrbInt+Res):	0.000004537328184	0.0001	0.00	0.01
Dispersion Energy:	-0.045718885363717	-1.2441	-28.69	-120.03
Total Bonding Energy:	-5.930481974949965	-161.3766	-3721.43	-15570.48

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-5.001860003736567	-136.1075	-3138.71	-13132.38
Kinetic Energy:	6.608705350223889	179.8320	4147.03	17351.15
Coulomb (Steric+OrbInt) Energy:	-2.200756756617224	-59.8856	-1381.00	-5778.09
XC Energy:	-5.290851679456368	-143.9714	-3320.06	-13891.13
Dispersion Energy:	-0.045718885363717	-1.2441	-28.69	-120.03
Total Bonding Energy:	-5.930481974949986	-161.3766	-3721.43	-15570.48

--PBE0 broken symmetry--

S**2 value *** see also R. Bulo et al., J.Am.Chem.Soc., 124 (2002) 13903-13910, note (29) ***

	exact	expectation value
Total S2 (S squared)	0.00000	1.00258

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	65.421461138622931	1780.2085	41052.59	171764.02
Delta V^Pauli Coulomb:	-33.675898858776549	-916.3678	-21131.95	-88416.06

Delta V^Pauli Hybrid-X:	-5.656148085247537	-153.9116	-3549.29	-14850.21
Delta V^Pauli Hybrid-C:	-0.639512349311500	-17.4020	-401.30	-1679.04
Delta V^Pauli HF-Exchange:	-1.390342301180027	-37.8331	-872.45	-3650.34
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	24.059559544107319	654.6939	15097.60	63168.36
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	24.059559544107319	654.6939	15097.60	63168.36
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-5.105234943616575	-138.9205	-3203.58	-13403.79
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	18.954324600490743	515.7734	11894.02	49764.57
Orbital Interactions				
A:	-26.734752650718313	-727.4896	-16776.31	-70192.08
Total Orbital Interactions:	-26.734752650717933	-727.4896	-16776.31	-70192.08
Alternative Decomposition Orb.Int.				
Kinetic:	-58.320782934464020	-1586.9893	-36596.85	-153121.19
Coulomb:	31.346907485699802	852.9928	19670.48	82301.29
XC:	0.239122798046278	6.5069	150.05	627.82
Total Orbital Interactions:	-26.734752650717940	-727.4896	-16776.31	-70192.08
Residu (E=Steric+OrbInt+Res):	0.000034830640532	0.0009	0.02	0.09
Total Bonding Energy:	-7.780393219586658	-211.7153	-4882.27	-20427.42

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-5.105234943616575	-138.9205	-3203.58	-13403.79
Kinetic Energy:	7.100678204158910	193.2193	4455.74	18642.83
Coulomb (Steric+OrbInt) Energy:	-2.328956542436213	-63.3741	-1461.44	-6114.67
XC Energy:	-7.446879937692786	-202.6399	-4672.99	-19551.78
Total Bonding Energy:	-7.780393219586664	-211.7153	-4882.27	-20427.42

host-guest $Cp^*Ir(H_2O)_2(O)^{2+}$, gas phase

triplet
B-LYPD3

Geometry CYCLE 59
==========

Energy gradients wrt nuclear displacements
==========

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	-0.000012	0.000043	-0.000010
2	C	-0.000070	-0.000071	0.000072
3	C	0.000051	-0.000081	-0.000093
4	H	0.000011	0.000029	-0.000022
5	H	-0.000020	0.000026	0.000031
6	C	0.000009	-0.000026	0.000041
7	C	-0.000073	-0.000065	0.000008
8	H	0.000009	-0.000012	-0.000018
9	H	-0.000030	-0.000018	-0.000001
10	C	-0.000322	0.000190	0.000258
11	C	0.000005	-0.000126	0.000012
12	H	0.000043	0.000053	-0.000015
13	H	0.000032	-0.000005	-0.000020
14	C	-0.000072	-0.000139	0.000097
15	C	-0.000022	0.000176	0.000102
16	H	0.000017	-0.000003	0.000011
17	H	0.000021	0.000058	-0.000055
18	C	0.000022	-0.000235	0.000126
19	C	-0.000010	-0.000144	-0.000029
20	H	0.000012	-0.000023	0.000029
21	H	0.000026	0.000064	0.000015
22	C	0.000129	-0.000223	0.000002
23	C	0.000091	-0.000063	-0.000020
24	H	-0.000009	0.000018	0.000000
25	H	-0.000030	-0.000002	0.000008
26	C	-0.000342	0.000224	-0.000099
27	C	-0.000083	0.000039	-0.000041
28	H	-0.000006	-0.000001	-0.000007
29	H	-0.000022	-0.000011	0.000016
30	O	-0.000122	0.000090	-0.000047
31	O	-0.000148	-0.000275	-0.000543
32	O	-0.000181	0.000224	-0.000032
33	O	-0.000056	-0.000023	0.000033
34	O	0.000046	0.000004	-0.000087
35	O	0.000035	0.000055	-0.000082
36	O	0.000461	-0.000056	-0.000050
37	O	-0.000031	0.000023	-0.000023
38	O	-0.000054	-0.000058	0.000016
39	O	0.000322	-0.000571	-0.000255
40	O	0.000079	-0.000187	-0.000084
41	O	-0.000087	0.000114	-0.000066
42	O	-0.000133	0.000180	0.000004
43	O	0.000163	-0.000114	0.000073
44	N	0.000023	-0.000083	0.000004
45	N	-0.000169	0.000017	-0.000006
46	N	-0.000010	0.000130	-0.000049
47	N	-0.000054	-0.000080	0.000020
48	N	-0.000073	0.000090	0.000040
49	N	0.000037	0.000047	-0.000062
50	N	0.000011	0.000015	0.000027
51	N	-0.000074	0.000095	-0.000040
52	N	0.000005	-0.000112	-0.000083
53	N	0.000059	-0.000196	0.000071
54	N	0.000122	0.000272	0.000128
55	N	-0.000104	-0.000095	0.000028
56	N	0.000030	-0.000052	-0.000015
57	N	0.000027	-0.000014	0.000002
58	N	0.000062	-0.000021	-0.000076
59	N	0.000059	0.000043	0.000053
60	N	-0.000052	0.000038	-0.000092
61	N	-0.000004	-0.000139	-0.000247
62	N	-0.000012	0.000051	0.000083
63	N	0.000065	-0.000009	-0.000094
64	N	-0.000026	-0.000032	-0.000032
65	N	-0.000029	0.000066	0.000156
66	N	-0.000027	0.000431	-0.000010
67	N	0.000042	0.000177	0.000076
68	N	-0.000109	0.000112	0.000027
69	N	0.000048	-0.000152	-0.000108
70	N	0.000056	0.000075	0.000066

71	N	0.000259	-0.000143	0.000061
72	C	-0.000077	-0.000027	0.000069
73	C	0.000002	0.000077	-0.000026
74	H	0.000007	-0.000021	-0.000022
75	H	-0.000024	0.000003	-0.000037
76	C	-0.000023	-0.000369	-0.000006
77	C	-0.000014	0.000073	-0.000003
78	H	-0.000004	0.000023	0.000008
79	H	-0.000023	0.000070	-0.000016
80	C	0.000522	-0.000561	-0.000096
81	C	-0.000115	0.000010	-0.000003
82	H	-0.000020	-0.000004	-0.000012
83	H	-0.000030	0.000002	0.000010
84	C	0.000117	0.000018	-0.000066
85	C	0.000025	0.000043	-0.000041
86	H	-0.000025	-0.000004	-0.000009
87	H	0.000056	-0.000014	0.000061
88	C	-0.000133	0.000075	0.000186
89	C	-0.000035	-0.000044	-0.000033
90	H	-0.000020	-0.000011	-0.000008
91	H	0.000002	-0.000002	0.000006
92	C	-0.000046	0.000002	0.000176
93	C	0.000044	0.000167	0.000020
94	H	0.000018	-0.000056	0.000038
95	H	0.000045	-0.000037	-0.000021
96	C	-0.000276	-0.000060	-0.000081
97	C	0.000075	0.000041	-0.000046
98	H	-0.000021	0.000006	0.000001
99	H	-0.000013	-0.000006	-0.000019
100	C	-0.000073	0.000036	0.000060
101	H	-0.000018	0.000006	0.000025
102	C	0.000110	-0.000110	-0.000008
103	H	-0.000004	0.000009	-0.000016
104	C	-0.000042	0.000003	0.000080
105	H	-0.000003	0.000063	0.000010
106	C	0.000022	0.000035	0.000064
107	H	0.000077	0.000039	0.000027
108	C	-0.000057	0.000037	-0.000056
109	H	0.000041	-0.000011	0.000012
110	C	0.000003	0.000010	0.000032
111	H	0.000005	-0.000035	0.000027
112	C	0.000038	0.000027	0.000004
113	H	0.000011	-0.000019	0.000017
114	C	0.000058	0.000044	-0.000117
115	H	0.000011	-0.000019	0.000005
116	C	-0.000135	0.000132	-0.000044
117	H	-0.000006	0.000007	-0.000005
118	C	0.000091	-0.000009	-0.000213
119	H	0.000027	-0.000007	0.000071
120	C	0.000114	-0.000048	-0.000093
121	H	-0.000010	-0.000049	0.000005
122	C	-0.000017	0.000079	0.000107
123	H	0.000002	-0.000052	0.000007
124	C	-0.000054	-0.000044	-0.000072
125	H	0.000002	0.000007	0.000034
126	C	-0.000014	-0.000010	-0.000007
127	H	-0.000035	-0.000041	-0.000011
128	H	0.000009	0.000082	-0.000036
129	H	0.000720	0.000467	0.000872
130	Ir	-0.000731	-0.000377	0.000093
131	H	-0.000176	-0.000027	-0.000371
132	C	0.000199	0.000210	0.000246
133	C	-0.000115	0.000032	0.000289
134	C	0.000100	0.000406	-0.000313
135	C	0.000170	-0.000171	0.000095
136	C	-0.000059	-0.000146	-0.000338
137	H	-0.000059	0.000132	0.000064
138	H	-0.000088	0.000085	-0.000026
139	H	-0.000051	0.000010	0.000002
140	H	-0.000108	-0.000090	-0.000098
141	O	0.000420	-0.000328	0.000020
142	H	-0.000496	0.000112	0.000211
143	O	-0.000198	0.000338	-0.000035
144	H	0.000057	-0.000148	-0.000158
145	O	0.000196	-0.000046	-0.000050
146	H	-0.000086	0.000080	0.000087
147	C	0.000044	-0.000053	0.000030
148	H	-0.000014	0.000000	-0.000033
149	H	0.000034	-0.000001	-0.000022
150	C	0.000045	0.000076	0.000282
151	H	0.000054	-0.000005	-0.000005
152	H	0.000064	-0.000049	-0.000065
153	C	0.000043	0.000245	-0.000066
154	H	-0.000063	0.000005	0.000033
155	H	0.000066	0.000006	0.000070

```
   156 C     0.000020  0.000037  0.000318
   157 H    -0.000017  0.000000 -0.000051
   158 H    -0.000069  0.000118  0.000040
   159 C     0.000116 -0.000082 -0.000242
 ----------------------------------------

 dE(predicted):    -0.15947E-04, dE(actual):     0.11066E-03, Trust radius:    0.159000, all in a.u.
 Residual max backtransformation error  0.1838E-02

-----------------------------------------------------------
Geometry Convergence after Step  59       ** CONVERGED **
-----------------------------------------------------------
current energy                          -36.05044253 Hartree
energy change                0.00011066     0.00100000    T
constrained gradient max     0.00087154     0.00100000    T
constrained gradient rms     0.00013514     0.00066667    T
gradient max                 0.00087154
gradient rms                 0.00013514
cart. step max               0.00594886     0.01000000    T
cart. step rms               0.00181381     0.00666667    T



 S**2 value  ***  see also R. Bulo et al., J.Am.Chem.Soc., 124 (2002) 13903-13910, note (29)  ***

                                    exact      expectation value

 Total S2 (S squared)               2.00000            2.01342


                                          hartree            eV        kcal/mol          kJ/mol
                                   --------------------  ----------  ----------  ----------

Pauli Repulsion
  Kinetic (Delta T^0):              463.721449112626885   12618.5027   290989.63   1217500.49
  Delta V^Pauli Coulomb:           -241.738750505443164   -6578.0461  -151693.37   -634685.00
  Delta V^Pauli LDA-XC:             -56.724622420931318   -1543.5555   -35595.24   -148930.48
  Delta V^Pauli GGA-Exchange:         3.564729044154916      97.0012     2236.90      9359.19
  Delta V^Pauli GGA-Correlation:     -4.119447655115756    -112.0959    -2584.99    -10815.61
                                   --------------------  ----------  ----------  ----------
  Total Pauli Repulsion:            164.703357575291562    4481.8064   103352.93    432428.60
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli): 164.703357575291562    4481.8064   103352.93    432428.60
  Electrostatic Interaction:       -36.044847607837021    -980.8302   -22618.49    -94635.73
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                   --------------------  ----------  ----------  ----------
  Total Steric Interaction:         128.658509967454535    3500.9762    80734.44    337792.87
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -164.230035140451093    -4468.9266  -103055.91   -431185.90
                                   --------------------  ----------  ----------  ----------
  Total Orbital Interactions:      -164.277580641230799    -4470.2204  -103085.75   -431310.73

Alternative Decomposition Orb.Int.
  Kinetic:                         -426.920589576740781   -11617.1003  -267896.74  -1120879.85
  Coulomb:                          239.801113522116452     6525.3203   150477.49    629597.73
  XC:                                22.841895413393662      621.5596    14333.51     59971.39
                                   --------------------  ----------  ----------  ----------
  Total Orbital Interactions:      -164.277580641230657    -4470.2204  -103085.75   -431310.73

  Residu (E=Steric+OrbInt+Res):      -0.000006663845606       -0.0002        0.00        -0.02
  Dispersion Energy:                 -0.431364817230081      -11.7380     -270.69     -1132.55

Total Bonding Energy:               -36.050442154851950     -980.9824   -22622.00    -94650.42


Summary of Bonding Energy (energy terms are taken from the energy decomposition above)
================================================================================

  Electrostatic Energy:             -36.044847607837021     -980.8302   -22618.49    -94635.73
  Kinetic Energy:                    36.800859535886104     1001.4023    23092.89     96620.64
  Coulomb (Steric+OrbInt) Energy:    -1.937643647172308      -52.7260    -1215.89     -5087.28
  XC Energy:                        -34.437445618498501     -937.0906   -21609.83    -90415.50
  Dispersion Energy:                 -0.431364817230081      -11.7380     -270.69     -1132.55
                                   --------------------  ----------  ----------  ----------
  Total Bonding Energy:             -36.050442154851808     -980.9824   -22622.00    -94650.42
```

host-guest $Cp^*Ir(H_2O)_2(O)^{2+}$, gas phase

Broken symmetry singlet
B-LYPD3

S**2 value *** see also R. Bulo et al., J.Am.Chem.Soc., 124 (2002) 13903-13910, note (29) ***

	exact	expectation value
Total S2 (S squared)	0.00000	1.00219

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	463.721470345604871	12618.5032	290989.65	1217500.55
Delta V^Pauli Coulomb:	-241.738801482909537	-6578.0475	-151693.40	-634685.13
Delta V^Pauli LDA-XC:	-56.724651555483469	-1543.5563	-35595.26	-148930.55
Delta V^Pauli GGA-Exchange:	3.564568370725851	96.9968	2236.80	9358.77
Delta V^Pauli GGA-Correlation:	-4.119455939330638	-112.0961	-2585.00	-10815.63
Total Pauli Repulsion:	164.703129738607089	4481.8002	103352.79	432428.01
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	164.703129738607089	4481.8002	103352.79	432428.01
Electrostatic Interaction:	-36.044847607837021	-980.8302	-22618.49	-94635.73
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	128.658282130770061	3500.9700	80734.30	337792.27
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-164.267147634955052	-4469.9365	-103079.20	-431283.34
Total Orbital Interactions:	-164.267147634956729	-4469.9365	-103079.20	-431283.34
Alternative Decomposition Orb.Int.				
Kinetic:	-426.934746704264171	-11617.4856	-267905.63	-1120917.02
Coulomb:	239.810514081739257	6525.5761	150483.39	629622.42
XC:	22.857084987567962	621.9729	14343.04	60011.27
Total Orbital Interactions:	-164.267147634956956	-4469.9365	-103079.20	-431283.34
Residu (E=Steric+OrbInt+Res):	-0.000006242299423	-0.0002	0.00	-0.02
Dispersion Energy:	-0.431364817230082	-11.7380	-270.69	-1132.55
Total Bonding Energy:	-36.040236563716171	-980.7047	-22615.59	-94623.63

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-36.044847607837021	-980.8302	-22618.49	-94635.73
Kinetic Energy:	36.786723641340700	1001.0177	23084.02	96583.53
Coulomb (Steric+OrbInt) Energy:	-1.928293643469715	-52.4715	-1210.02	-5062.73
XC Energy:	-34.422454136520287	-936.6826	-21600.42	-90376.14
Dispersion Energy:	-0.431364817230082	-11.7380	-270.69	-1132.55
Total Bonding Energy:	-36.040236563716405	-980.7047	-22615.59	-94623.63