Supportina Material

Iridium Derivatives of Fluorinated Aromatics by C–H activation: Isolation of Classical and Non-classical Hydrides

Marcel Ahijado Salomon, Thomas Braun*,§ and Ingo Krossing‡

Coordinates are deposited in the PDB format and may be viewed e.g. with Jmol.

cis-trans-[Ir(4-C_5NF_4)$(H)_2$($PiPr_3$)$_2$] (2)

SCF-energy: -2143.166325084 H

Xyz-Coordinates (PDB-Format):

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HEADER
REMARK test basis
HETATM    1 ir         1      0.257  -0.723  -0.001
HETATM    2  p         1      2.614  -0.451   0.018
HETATM    3  p         1     -1.956  -1.557   0.000
HETATM    4  c         1      3.180  -0.958   1.766
HETATM    5  c         1      3.479   1.191  -0.360
HETATM    6  c         1      3.511  -1.722  -1.090
HETATM    7  c         1      2.261  -0.348   2.841
HETATM    8  c         1      4.659  -0.752   2.131
HETATM    9  c         1      3.083   2.304   0.627
HETATM   10  c         1      3.229   1.635  -1.813
HETATM   11  c         1      4.999  -1.442  -1.378
HETATM   12  c         1      2.761  -2.009  -2.403
HETATM   13  c         1     -2.593  -1.801   1.781
HETATM   14  c         1     -2.206  -3.222  -0.870
HETATM   15  c         1     -3.237  -0.347  -0.720
HETATM   16  c         1     -1.444  -2.136   2.749
HETATM   17  c         1     -3.767  -2.779   1.983
HETATM   18  c         1     -1.484  -4.377  -0.151
HETATM   19  c         1     -4.725  -0.693  -0.538
HETATM   20  c         1     -1.754  -3.181  -2.341
HETATM   21  c         1     -2.956   0.049  -2.182
HETATM   22  c         1     -0.375   1.315   0.006
HETATM   23  c         1     -0.434   2.190  -1.092
HETATM   24  c         1     -0.879   3.516  -0.963
HETATM   25  n         1     -1.289   4.034   0.183
HETATM   26  c         1     -1.268   3.246   1.246
HETATM   27  c         1     -0.824   1.917   1.196
HETATM   28  f         1     -0.846   1.186   2.354
HETATM   29  f         1     -1.699   3.766   2.410
HETATM   30  f         1     -0.053   1.774  -2.336
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HETATM   31  f         1     -0.902   4.316  -2.044
HETATM   32  h         1      0.729  -2.329   0.037
HETATM   33  h         1      0.270  -0.773  -1.550
HETATM   34  h         1      2.971  -2.053   1.742
HETATM   35  h         1      4.567   0.985  -0.238
HETATM   36  h         1      3.442  -2.642  -0.464
HETATM   37  h         1      2.422  -0.861   3.816
HETATM   38  h         1      1.184  -0.451   2.583
HETATM   39  h         1      2.452   0.735   2.995
HETATM   40  h         1      4.834  -1.094   3.177
HETATM   41  h         1      4.959   0.318   2.085
HETATM   42  h         1      5.348  -1.332   1.482
HETATM   43  h         1      3.562   3.262   0.318
HETATM   44  h         1      3.413   2.093   1.666
HETATM   45  h         1      1.984   2.465   0.638
HETATM   46  h         1      3.757   2.598  -2.003
HETATM   47  h         1      2.150   1.793  -2.015
HETATM   48  h         1      3.608   0.901  -2.555
HETATM   49  h         1      5.450  -2.329  -1.879
HETATM   50  h         1      5.598  -1.242  -0.466
HETATM   51  h         1      5.132  -0.580  -2.068
HETATM   52  h         1      3.288  -2.814  -2.965
HETATM   53  h         1      2.717  -1.115  -3.064
HETATM   54  h         1      1.722  -2.344  -2.208
HETATM   55  h         1     -2.943  -0.772   2.030
HETATM   56  h         1     -3.305  -3.407  -0.833
HETATM   57  h         1     -3.011   0.547  -0.094
HETATM   58  h         1     -1.821  -2.140   3.797
HETATM   59  h         1     -0.630  -1.383   2.693
HETATM   60  h         1     -0.999  -3.132   2.541
HETATM   61  h         1     -4.173  -2.657   3.014
HETATM   62  h         1     -3.443  -3.838   1.889
HETATM   63  h         1     -4.607  -2.621   1.278
HETATM   64  h         1     -1.659  -5.325  -0.708
HETATM   65  h         1     -1.833  -4.535   0.890
HETATM   66  h         1     -0.388  -4.191  -0.121
HETATM   67  h         1     -5.344   0.097  -1.023
HETATM   68  h         1     -5.033  -0.732   0.527
HETATM   69  h         1     -4.999  -1.658  -1.020
HETATM   70  h         1     -1.931  -4.175  -2.812
HETATM   71  h         1     -0.666  -2.962  -2.407
HETATM   72  h         1     -2.294  -2.424  -2.944
HETATM   73  h         1     -3.473   1.009  -2.407
HETATM   74  h         1     -3.354  -0.706  -2.896
HETATM   75  h         1     -1.877   0.198  -2.389
END

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)       km/mol        IR     RAMAN
    1                       0.00        0.00000       -      -
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2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	16.03	0.11513	YES	YES
8	a	24.48	0.27374	YES	YES
9	a	28.75	0.33544	YES	YES
10	a	37.17	0.28258	YES	YES
11	a	38.76	0.73554	YES	YES
12	a	41.98	0.52147	YES	YES
13	a	53.79	0.30266	YES	YES
14	a	62.56	0.57132	YES	YES
15	a	76.87	0.13334	YES	YES
16	a	79.14	0.48359	YES	YES
17	a	86.62	0.07508	YES	YES
18	a	92.34	0.15920	YES	YES
19	a	100.14	1.67775	YES	YES
20	a	108.99	0.05731	YES	YES
21	a	113.90	0.01332	YES	YES
22	a	118.48	0.63063	YES	YES
23	a	124.57	1.29207	YES	YES
24	a	127.63	0.57800	YES	YES
25	a	137.99	0.58919	YES	YES
26	a	143.68	0.29218	YES	YES
27	a	149.76	0.50728	YES	YES
28	a	158.99	0.18860	YES	YES
29	a	167.63	1.07721	YES	YES
30	a	171.04	0.30606	YES	YES
31	a	178.83	0.15486	YES	YES
32	a	182.42	0.29274	YES	YES
33	a	190.46	0.82562	YES	YES
34	a	193.02	0.07232	YES	YES
35	a	202.93	0.27161	YES	YES
36	a	209.34	0.75986	YES	YES
37	a	211.53	0.22346	YES	YES
38	a	214.92	0.95050	YES	YES
39	a	218.35	0.02279	YES	YES
40	a	224.73	0.57821	YES	YES
41	a	227.21	0.59982	YES	YES
42	a	236.52	0.58209	YES	YES
43	a	239.21	0.88868	YES	YES
44	a	247.03	0.19251	YES	YES
45	a	248.56	0.45439	YES	YES
46	a	251.69	1.62404	YES	YES
47	a	258.60	0.25521	YES	YES
48	a	260.56	0.51728	YES	YES
49	a	261.73	0.60026	YES	YES
50	a	274.42	0.18104	YES	YES
51	a	285.78	0.42764	YES	YES
52	a	290.36	0.27489	YES	YES

53	a	296.87	0.46945	YES	YES
54	a	302.05	0.33584	YES	YES
55	a	303.64	0.16747	YES	YES
56	a	325.87	1.35880	YES	YES
57	a	341.98	0.88383	YES	YES
58	a	347.67	0.98430	YES	YES
59	a	370.12	0.16734	YES	YES
60	a	373.08	0.29062	YES	YES
61	a	381.40	2.81110	YES	YES
62	a	390.80	2.05078	YES	YES
63	a	401.00	2.18115	YES	YES
64	a	425.32	5.53090	YES	YES
65	a	429.20	5.17101	YES	YES
66	a	447.61	0.95899	YES	YES
67	a	453.05	28.43124	YES	YES
68	a	458.06	9.04870	YES	YES
69	a	460.92	4.68829	YES	YES
70	a	461.08	0.48354	YES	YES
71	a	464.12	6.61847	YES	YES
72	a	469.50	8.48442	YES	YES
73	a	497.53	0.63167	YES	YES
74	a	549.55	10.06457	YES	YES
75	a	569.71	38.22407	YES	YES
76	a	580.99	66.67077	YES	YES
77	a	593.16	20.48554	YES	YES
78	a	596.52	16.68214	YES	YES
79	a	622.79	12.93763	YES	YES
80	a	638.19	13.53272	YES	YES
81	a	644.36	56.52327	YES	YES
82	a	646.32	12.17858	YES	YES
83	a	650.69	2.07760	YES	YES
84	a	664.97	10.03884	YES	YES
85	a	669.50	0.71125	YES	YES
86	a	704.38	2.45831	YES	YES
87	a	744.02	13.49354	YES	YES
88	a	790.85	40.01697	YES	YES
89	a	871.60	3.54726	YES	YES
90	a	875.16	6.98254	YES	YES
91	a	879.95	5.40662	YES	YES
92	a	881.24	4.44628	YES	YES
93	a	882.21	7.54999	YES	YES
94	a	883.56	7.95404	YES	YES
95	a	899.75	1.37849	YES	YES
96	a	900.27	9.71289	YES	YES
97	a	903.24	2.24438	YES	YES
98	a	907.65	5.31212	YES	YES
99	a	910.14	17.79253	YES	YES
100	a	913.41	58.67371	YES	YES
101	a	914.85	57.36784	YES	YES
102	a	942.10	1.62042	YES	YES
103	a	943.55	0.66978	YES	YES

104	a	945.33	1.69401	YES	YES
105	a	949.76	0.16421	YES	YES
106	a	951.52	2.02815	YES	YES
107	a	952.83	0.02655	YES	YES
108	a	1007.61	9.81200	YES	YES
109	a	1011.03	13.25191	YES	YES
110	a	1016.87	8.90839	YES	YES
111	a	1019.43	8.80868	YES	YES
112	a	1044.30	37.78748	YES	YES
113	a	1047.39	7.05423	YES	YES
114	a	1080.81	2.04274	YES	YES
115	a	1083.61	0.88060	YES	YES
116	a	1088.31	2.42246	YES	YES
117	a	1099.21	4.49772	YES	YES
118	a	1100.78	10.19609	YES	YES
119	a	1102.43	2.73517	YES	YES
120	a	1109.43	3.90577	YES	YES
121	a	1141.47	0.69951	YES	YES
122	a	1145.40	2.53826	YES	YES
123	a	1147.97	5.41431	YES	YES
124	a	1148.75	4.19267	YES	YES
125	a	1149.14	2.30454	YES	YES
126	a	1151.78	3.25825	YES	YES
127	a	1174.07	160.61478	YES	YES
128	a	1220.16	31.33268	YES	YES
129	a	1225.26	19.84246	YES	YES
130	a	1228.86	7.28290	YES	YES
131	a	1241.05	6.22607	YES	YES
132	a	1251.85	4.37553	YES	YES
133	a	1257.90	5.75605	YES	YES
134	a	1273.62	0.33512	YES	YES
135	a	1278.44	0.58591	YES	YES
136	a	1278.77	1.71365	YES	YES
137	a	1284.95	2.31748	YES	YES
138	a	1290.08	0.60670	YES	YES
139	a	1292.44	1.12986	YES	YES
140	a	1324.79	15.18487	YES	YES
141	a	1344.60	3.04827	YES	YES
142	a	1348.21	1.63356	YES	YES
143	a	1349.66	0.60448	YES	YES
144	a	1351.81	1.93852	YES	YES
145	a	1357.40	1.96259	YES	YES
146	a	1357.81	1.10828	YES	YES
147	a	1364.15	6.44520	YES	YES
148	a	1367.09	45.26913	YES	YES
149	a	1368.44	12.53180	YES	YES
150	a	1369.00	9.49674	YES	YES
151	a	1371.57	9.08997	YES	YES
152	a	1376.29	4.10120	YES	YES
153	a	1378.19	4.65087	YES	YES
154	a	1412.32	34.74122	YES	YES

155	a	1414.90	35.59753	YES	YES
156	a	1417.85	35.60123	YES	YES
157	a	1420.71	70.46093	YES	YES
158	a	1421.19	13.86525	YES	YES
159	a	1422.50	8.00754	YES	YES
160	a	1424.29	136.96286	YES	YES
161	a	1426.94	1.77868	YES	YES
162	a	1429.86	61.12355	YES	YES
163	a	1430.26	32.56044	YES	YES
164	a	1431.10	1.89125	YES	YES
165	a	1431.90	8.58777	YES	YES
166	a	1435.14	2.66218	YES	YES
167	a	1437.17	12.99561	YES	YES
168	a	1438.04	10.03159	YES	YES
169	a	1440.60	4.33529	YES	YES
170	a	1441.68	4.52767	YES	YES
171	a	1442.59	16.98349	YES	YES
172	a	1445.45	3.56558	YES	YES
173	a	1447.56	18.15982	YES	YES
174	a	1450.77	0.24828	YES	YES
175	a	1451.60	6.45756	YES	YES
176	a	1453.24	2.20277	YES	YES
177	a	1454.58	17.41708	YES	YES
178	a	1459.01	11.64847	YES	YES
179	a	1459.81	1.31575	YES	YES
180	a	1570.07	53.54660	YES	YES
181	a	1595.59	181.77618	YES	YES
182	a	1939.73	273.71321	YES	YES
183	a	2409.95	1.58377	YES	YES
184	a	2938.05	29.10476	YES	YES
185	a	2940.63	19.75930	YES	YES
186	a	2941.74	4.67639	YES	YES
187	a	2942.30	31.07481	YES	YES
188	a	2942.87	18.73462	YES	YES
189	a	2942.98	1.21571	YES	YES
190	a	2944.46	8.09747	YES	YES
191	a	2944.95	45.93063	YES	YES
192	a	2946.21	3.55842	YES	YES
193	a	2946.95	16.90254	YES	YES
194	a	2947.23	44.80992	YES	YES
195	a	2947.34	33.76815	YES	YES
196	a	2947.79	10.57036	YES	YES
197	a	2948.03	44.61191	YES	YES
198	a	2949.05	2.42751	YES	YES
199	a	2949.54	56.96600	YES	YES
200	a	2950.59	4.10982	YES	YES
201	a	2951.17	45.10095	YES	YES
202	a	3008.21	13.78554	YES	YES
203	a	3015.41	12.89620	YES	YES
204	a	3018.47	21.74726	YES	YES
205	a	3018.61	40.13303	YES	YES

206	a	3019.60	3.06253	YES	YES
207	a	3021.89	6.67628	YES	YES
208	a	3022.15	44.89679	YES	YES
209	a	3024.27	22.68552	YES	YES
210	a	3024.70	20.66340	YES	YES
211	a	3025.30	11.57524	YES	YES
212	a	3027.30	22.88318	YES	YES
213	a	3031.75	8.34470	YES	YES
214	a	3045.50	15.29617	YES	YES
215	a	3048.47	14.93758	YES	YES
216	a	3049.51	19.16125	YES	YES
217	a	3051.35	7.63738	YES	YES
218	a	3054.96	9.37539	YES	YES
219	a	3056.24	8.74134	YES	YES
220	a	3056.64	18.48916	YES	YES
221	a	3057.69	10.89964	YES	YES
222	a	3065.67	2.57702	YES	YES
223	a	3071.35	8.16059	YES	YES
224	a	3071.85	1.99649	YES	YES
225	a	3074.63	9.06605	YES	YES

cis-trans-[Ir(4-C_5NF_4)$(H)_2$$(H_2)$$(P$*i*$Pr_3)_2$] (3)

SCF-energy: -2144.358292760 H

HEADER
REMARK test basis

HETATM	1 ir	1	-0.630	-0.065	-0.124
HETATM	2 p	1	-1.182	2.235	0.075
HETATM	3 p	1	-0.548	-2.442	-0.053
HETATM	4 c	1	0.178	3.398	0.727
HETATM	5 c	1	-2.627	2.615	1.255
HETATM	6 c	1	-1.661	3.078	-1.565
HETATM	7 c	1	0.679	3.021	2.133
HETATM	8 c	1	-0.161	4.901	0.686
HETATM	9 c	1	-2.555	1.771	2.542
HETATM	10 c	1	-4.032	2.493	0.641
HETATM	11 c	1	-0.427	3.411	-2.427
HETATM	12 c	1	-2.660	2.264	-2.413
HETATM	13 c	1	-1.548	-3.301	-1.432
HETATM	14 c	1	-1.154	-3.203	1.567
HETATM	15 c	1	1.216	-3.138	-0.253
HETATM	16 c	1	-2.895	-2.633	-1.765
HETATM	17 c	1	-1.740	-4.818	-1.240
HETATM	18 c	1	-2.641	-2.921	1.840
HETATM	19 c	1	1.716	-2.965	-1.699
HETATM	20 c	1	-0.298	-2.758	2.767
HETATM	21 c	1	1.521	-4.555	0.269
HETATM	22 c	1	1.512	0.226	-0.043
HETATM	23 c	1	2.286	0.123	1.131
HETATM	24 c	1	3.672	0.359	1.140

HETATM 25 n 1 4.362 0.675 0.058
HETATM 26 c 1 3.689 0.767 -1.075
HETATM 27 c 1 2.304 0.553 -1.162
HETATM 28 f 1 1.746 0.660 -2.408
HETATM 29 f 1 4.385 1.083 -2.181
HETATM 30 f 1 1.717 -0.199 2.326
HETATM 31 f 1 4.351 0.261 2.297
HETATM 32 h 1 -0.258 0.005 -1.913
HETATM 33 h 1 -0.603 -0.089 1.473
HETATM 34 h 1 1.007 3.196 0.011
HETATM 35 h 1 -2.470 3.685 1.526
HETATM 36 h 1 -2.156 4.030 -1.259
HETATM 37 h 1 -0.029 3.362 2.920
HETATM 38 h 1 1.650 3.532 2.329
HETATM 39 h 1 0.840 1.933 2.257
HETATM 40 h 1 0.739 5.488 0.982
HETATM 41 h 1 -0.964 5.162 1.410
HETATM 42 h 1 -0.474 5.266 -0.315
HETATM 43 h 1 -2.798 0.710 2.324
HETATM 44 h 1 -3.298 2.155 3.278
HETATM 45 h 1 -1.557 1.790 3.024
HETATM 46 h 1 -4.791 2.723 1.423
HETATM 47 h 1 -4.229 1.458 0.283
HETATM 48 h 1 -4.203 3.200 -0.198
HETATM 49 h 1 0.243 4.167 -1.967
HETATM 50 h 1 -0.762 3.823 -3.406
HETATM 51 h 1 -3.502 1.840 -1.832
HETATM 52 h 1 -2.151 1.420 -2.923
HETATM 53 h 1 -3.086 2.918 -3.208
HETATM 54 h 1 -0.884 -3.146 -2.312
HETATM 55 h 1 -1.023 -4.300 1.428
HETATM 56 h 1 1.786 -2.420 0.377
HETATM 57 h 1 -3.635 -2.749 -0.945
HETATM 58 h 1 -3.326 -3.113 -2.674
HETATM 59 h 1 -2.791 -1.548 -1.962
HETATM 60 h 1 -2.224 -5.250 -2.146
HETATM 61 h 1 -2.405 -5.046 -0.378
HETATM 62 h 1 -0.785 -5.361 -1.088
HETATM 63 h 1 -2.835 -1.827 1.885
HETATM 64 h 1 -2.929 -3.363 2.821
HETATM 65 h 1 -3.310 -3.358 1.070
HETATM 66 h 1 1.492 -1.956 -2.106
HETATM 67 h 1 1.276 -3.726 -2.382
HETATM 68 h 1 2.821 -3.097 -1.733
HETATM 69 h 1 -0.594 -3.341 3.669
HETATM 70 h 1 -0.454 -1.681 2.986
HETATM 71 h 1 0.791 -2.904 2.612
HETATM 72 h 1 1.045 -5.348 -0.346
HETATM 73 h 1 1.216 -4.708 1.325
HETATM 74 h 1 2.620 -4.727 0.220
HETATM 75 h 1 0.181 2.504 -2.636

HETATM 76 h 1 -1.126 -0.116 -1.863
HETATM 77 h 1 -2.272 -0.276 0.041
END

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.62	0.26336	YES	YES
8	a	16.56	0.02491	YES	YES
9	a	28.59	0.19147	YES	YES
10	a	34.36	0.34110	YES	YES
11	a	41.97	0.21947	YES	YES
12	a	47.80	0.94113	YES	YES
13	a	56.25	0.44758	YES	YES
14	a	63.12	1.03129	YES	YES
15	a	86.84	0.08468	YES	YES
16	a	94.01	0.19383	YES	YES
17	a	102.24	0.30968	YES	YES
18	a	110.20	0.31770	YES	YES
19	a	113.84	0.44902	YES	YES
20	a	118.03	0.33944	YES	YES
21	a	122.02	0.45220	YES	YES
22	a	124.61	0.31434	YES	YES
23	a	126.95	1.02966	YES	YES
24	a	134.97	0.39687	YES	YES
25	a	140.57	0.73633	YES	YES
26	a	148.27	0.14950	YES	YES
27	a	152.89	0.68520	YES	YES
28	a	161.71	0.73338	YES	YES
29	a	170.20	0.52969	YES	YES
30	a	173.13	0.23680	YES	YES
31	a	179.44	0.14318	YES	YES
32	a	184.68	0.16728	YES	YES
33	a	188.09	0.99279	YES	YES
34	a	198.48	0.72081	YES	YES
35	a	203.91	1.24134	YES	YES
36	a	213.02	1.06715	YES	YES
37	a	215.63	0.95028	YES	YES
38	a	218.41	0.17519	YES	YES
39	a	224.20	0.17731	YES	YES
40	a	227.67	0.10876	YES	YES
41	a	238.65	0.37178	YES	YES
42	a	242.32	0.32935	YES	YES
43	a	247.99	0.43330	YES	YES
44	a	258.33	1.47855	YES	YES

45	a	262.63	0.26459	YES	YES
46	a	265.54	2.85611	YES	YES
47	a	275.96	0.03730	YES	YES
48	a	281.61	0.93330	YES	YES
49	a	284.37	0.05897	YES	YES
50	a	293.69	0.48399	YES	YES
51	a	294.61	0.70796	YES	YES
52	a	296.24	0.21363	YES	YES
53	a	302.65	1.04403	YES	YES
54	a	310.61	0.20696	YES	YES
55	a	315.59	0.56436	YES	YES
56	a	326.86	4.93767	YES	YES
57	a	334.12	0.07555	YES	YES
58	a	354.38	3.64207	YES	YES
59	a	361.17	1.54657	YES	YES
60	a	367.89	1.23587	YES	YES
61	a	378.34	1.02185	YES	YES
62	a	383.06	1.59587	YES	YES
63	a	389.28	4.17142	YES	YES
64	a	403.84	4.51073	YES	YES
65	a	416.28	0.50544	YES	YES
66	a	429.87	5.51378	YES	YES
67	a	431.55	1.88009	YES	YES
68	a	437.74	8.88284	YES	YES
69	a	452.96	7.83174	YES	YES
70	a	456.17	2.53003	YES	YES
71	a	458.84	1.18574	YES	YES
72	a	465.10	34.48972	YES	YES
73	a	468.30	10.39976	YES	YES
74	a	495.44	1.68646	YES	YES
75	a	497.36	8.97760	YES	YES
76	a	559.14	32.09888	YES	YES
77	a	571.15	53.80344	YES	YES
78	a	594.26	11.33066	YES	YES
79	a	609.86	31.87387	YES	YES
80	a	617.94	27.32640	YES	YES
81	a	628.90	55.25550	YES	YES
82	a	641.42	23.83839	YES	YES
83	a	652.86	0.08625	YES	YES
84	a	665.08	11.46516	YES	YES
85	a	669.25	0.58058	YES	YES
86	a	684.71	10.10373	YES	YES
87	a	729.41	57.56890	YES	YES
88	a	767.00	16.56191	YES	YES
89	a	786.62	21.93135	YES	YES
90	a	849.63	20.40812	YES	YES
91	a	864.17	141.48859	YES	YES
92	a	876.90	5.57394	YES	YES
93	a	878.16	6.75481	YES	YES
94	a	879.11	5.44556	YES	YES
95	a	881.83	3.84668	YES	YES

96	a	882.30	4.44599	YES	YES
97	a	886.49	5.34258	YES	YES
98	a	902.24	3.31692	YES	YES
99	a	903.28	1.87238	YES	YES
100	a	906.58	3.41014	YES	YES
101	a	907.62	6.48362	YES	YES
102	a	910.27	7.92049	YES	YES
103	a	911.94	3.81913	YES	YES
104	a	914.62	122.88230	YES	YES
105	a	943.23	0.20729	YES	YES
106	a	945.21	2.11624	YES	YES
107	a	945.58	0.82398	YES	YES
108	a	949.78	0.74031	YES	YES
109	a	951.02	0.07828	YES	YES
110	a	952.25	0.14011	YES	YES
111	a	973.22	17.87475	YES	YES
112	a	1010.75	8.86987	YES	YES
113	a	1013.23	9.78687	YES	YES
114	a	1025.70	32.89393	YES	YES
115	a	1028.75	0.72241	YES	YES
116	a	1040.34	7.96463	YES	YES
117	a	1042.29	20.83727	YES	YES
118	a	1069.49	4.76216	YES	YES
119	a	1082.15	3.62634	YES	YES
120	a	1088.74	7.05287	YES	YES
121	a	1092.36	10.06258	YES	YES
122	a	1098.63	0.75416	YES	YES
123	a	1104.10	2.22789	YES	YES
124	a	1109.20	4.60821	YES	YES
125	a	1144.19	5.49076	YES	YES
126	a	1145.37	2.75372	YES	YES
127	a	1147.31	5.12082	YES	YES
128	a	1149.44	3.27525	YES	YES
129	a	1150.54	3.20866	YES	YES
130	a	1153.33	3.87641	YES	YES
131	a	1176.40	150.37954	YES	YES
132	a	1226.54	6.85806	YES	YES
133	a	1236.01	38.71675	YES	YES
134	a	1241.11	28.74478	YES	YES
135	a	1244.61	4.75398	YES	YES
136	a	1249.39	4.12746	YES	YES
137	a	1251.07	8.23685	YES	YES
138	a	1279.82	0.75008	YES	YES
139	a	1285.11	0.94369	YES	YES
140	a	1287.89	2.94856	YES	YES
141	a	1289.58	3.99473	YES	YES
142	a	1295.67	1.31969	YES	YES
143	a	1296.15	2.60161	YES	YES
144	a	1326.17	14.89053	YES	YES
145	a	1344.62	1.41982	YES	YES
146	a	1347.90	0.54572	YES	YES

147	a	1348.99	0.89041	YES	YES
148	a	1353.46	9.89093	YES	YES
149	a	1354.15	1.06252	YES	YES
150	a	1357.21	3.54498	YES	YES
151	a	1358.44	20.31075	YES	YES
152	a	1363.98	7.17574	YES	YES
153	a	1367.84	7.95977	YES	YES
154	a	1370.58	15.14709	YES	YES
155	a	1371.41	11.08159	YES	YES
156	a	1374.76	2.24003	YES	YES
157	a	1375.70	2.87464	YES	YES
158	a	1416.08	180.52829	YES	YES
159	a	1418.13	107.92600	YES	YES
160	a	1420.94	1.30462	YES	YES
161	a	1420.98	30.54574	YES	YES
162	a	1423.27	58.02585	YES	YES
163	a	1424.13	3.78906	YES	YES
164	a	1425.97	31.30143	YES	YES
165	a	1427.91	1.38071	YES	YES
166	a	1428.15	11.70204	YES	YES
167	a	1430.18	6.29322	YES	YES
168	a	1430.36	19.78295	YES	YES
169	a	1432.54	13.16416	YES	YES
170	a	1433.34	6.78631	YES	YES
171	a	1435.37	7.25747	YES	YES
172	a	1438.30	7.58768	YES	YES
173	a	1442.29	6.21245	YES	YES
174	a	1443.95	8.12229	YES	YES
175	a	1444.79	7.34358	YES	YES
176	a	1445.06	1.11651	YES	YES
177	a	1447.60	7.46400	YES	YES
178	a	1448.34	12.16377	YES	YES
179	a	1449.67	8.71518	YES	YES
180	a	1453.24	4.50712	YES	YES
181	a	1454.51	10.46544	YES	YES
182	a	1457.29	8.61029	YES	YES
183	a	1460.86	6.90686	YES	YES
184	a	1572.04	59.30822	YES	YES
185	a	1592.66	26.19098	YES	YES
186	a	1595.47	165.40876	YES	YES
187	a	1990.74	233.61227	YES	YES
188	a	2275.53	24.95914	YES	YES
189	a	2870.06	63.84524	YES	YES
190	a	2938.04	3.60477	YES	YES
191	a	2939.02	25.03640	YES	YES
192	a	2939.55	19.68486	YES	YES
193	a	2940.19	34.74961	YES	YES
194	a	2942.58	14.06721	YES	YES
195	a	2943.51	12.68394	YES	YES
196	a	2945.11	51.37433	YES	YES
197	a	2946.40	30.77303	YES	YES

198	a	2946.91	20.71984	YES	YES
199	a	2947.27	55.32854	YES	YES
200	a	2947.41	41.63470	YES	YES
201	a	2947.95	38.81792	YES	YES
202	a	2951.32	21.23878	YES	YES
203	a	2953.05	34.06214	YES	YES
204	a	2955.37	18.36110	YES	YES
205	a	2955.51	3.81389	YES	YES
206	a	2964.44	4.37344	YES	YES
207	a	2969.13	2.85499	YES	YES
208	a	3010.45	6.29601	YES	YES
209	a	3013.18	16.35969	YES	YES
210	a	3013.29	5.90614	YES	YES
211	a	3016.77	31.62751	YES	YES
212	a	3016.90	16.69253	YES	YES
213	a	3020.09	22.69417	YES	YES
214	a	3023.60	21.13769	YES	YES
215	a	3026.12	9.07831	YES	YES
216	a	3028.63	15.67784	YES	YES
217	a	3031.60	20.48028	YES	YES
218	a	3032.03	4.16458	YES	YES
219	a	3032.45	37.27554	YES	YES
220	a	3044.93	7.43602	YES	YES
221	a	3045.23	14.82641	YES	YES
222	a	3045.89	17.98062	YES	YES
223	a	3048.61	12.73732	YES	YES
224	a	3053.22	11.19038	YES	YES
225	a	3053.57	10.70177	YES	YES
226	a	3057.55	10.91987	YES	YES
227	a	3059.21	11.15829	YES	YES
228	a	3068.74	10.25848	YES	YES
229	a	3070.01	5.91462	YES	YES
230	a	3076.64	5.39462	YES	YES
231	a	3085.82	0.51422	YES	YES

trans-[Ir(Cl)(H)$_2$(P*i*Pr$_3$)$_2$]

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*                                                          *
*  zero point VIBRATIONAL energy :     0.5704794  Hartree  *
*    SCF-energy                  : -1959.1313076          *
*    SCF + E(vib0)               : -1958.5608282          *
*                                                          *
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HEADER
REMARK test basis
HETATM    1 ir         1     -0.006   0.012   0.070
HETATM    2  p         1      2.363   0.010   0.243
HETATM    3  p         1     -2.357   0.057   0.054
HETATM    4  c         1      2.929   1.725   0.859
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HETATM    5  c         1      3.451  -0.419  -1.245
HETATM    6  c         1      2.987  -1.154   1.629
HETATM    7  c         1      2.296   2.876   0.052
HETATM    8  c         1      4.441   1.951   1.033
HETATM    9  c         1      3.309   0.593  -2.396
HETATM   10  c         1      3.155  -1.846  -1.749
HETATM   11  c         1      4.480  -1.537   1.586
HETATM   12  c         1      2.127  -2.425   1.765
HETATM   13  c         1     -3.072   1.322  -1.185
HETATM   14  c         1     -3.227   0.429   1.691
HETATM   15  c         1     -3.032  -1.596  -0.589
HETATM   16  c         1     -2.120   2.514  -1.396
HETATM   17  c         1     -4.507   1.809  -0.910
HETATM   18  c         1     -2.772   1.784   2.265
HETATM   19  c         1     -4.558  -1.781  -0.564
HETATM   20  c         1     -3.036  -0.685   2.735
HETATM   21  c         1     -2.300  -2.801   0.033
HETATM   22 cl         1     -0.136  -0.583  -2.313
HETATM   23  h         1      0.001   1.265   1.032
HETATM   24  h         1     -0.035  -0.440   1.593
HETATM   25  h         1      2.456   1.737   1.869
HETATM   26  h         1      4.498  -0.383  -0.866
HETATM   27  h         1      2.810  -0.533   2.538
HETATM   28  h         1      2.378   3.826   0.630
HETATM   29  h         1      1.221   2.688  -0.159
HETATM   30  h         1      2.811   3.035  -0.919
HETATM   31  h         1      4.624   2.997   1.371
HETATM   32  h         1      4.997   1.817   0.080
HETATM   33  h         1      4.893   1.283   1.795
HETATM   34  h         1      3.918   0.248  -3.264
HETATM   35  h         1      3.673   1.606  -2.123
HETATM   36  h         1      2.252   0.666  -2.730
HETATM   37  h         1      3.849  -2.092  -2.586
HETATM   38  h         1      2.113  -1.913  -2.130
HETATM   39  h         1      3.296  -2.620  -0.966
HETATM   40  h         1      4.750  -2.076   2.523
HETATM   41  h         1      5.161  -0.666   1.499
HETATM   42  h         1      4.701  -2.226   0.742
HETATM   43  h         1      2.423  -2.984   2.683
HETATM   44  h         1      2.265  -3.110   0.900
HETATM   45  h         1      1.045  -2.186   1.831
HETATM   46  h         1     -3.068   0.731  -2.129
HETATM   47  h         1     -4.311   0.496   1.445
HETATM   48  h         1     -2.688  -1.534  -1.648
HETATM   49  h         1     -2.515   3.171  -2.206
HETATM   50  h         1     -1.109   2.166  -1.692
HETATM   51  h         1     -2.017   3.136  -0.480
HETATM   52  h         1     -4.864   2.415  -1.774
HETATM   53  h         1     -4.556   2.467  -0.014
HETATM   54  h         1     -5.235   0.984  -0.764
HETATM   55  h         1     -3.359   2.021   3.182
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HETATM   56  h         1     -2.912   2.624   1.552
HETATM   57  h         1     -1.697   1.755   2.545
HETATM   58  h         1     -4.819  -2.776  -0.993
HETATM   59  h         1     -5.092  -1.018  -1.168
HETATM   60  h         1     -4.971  -1.754   0.469
HETATM   61  h         1     -3.485  -0.371   3.705
HETATM   62  h         1     -1.958  -0.893   2.913
HETATM   63  h         1     -3.525  -1.636   2.437
HETATM   64  h         1     -2.529  -3.717  -0.557
HETATM   65  h         1     -2.609  -2.993   1.082
HETATM   66  h         1     -1.199  -2.649   0.020
END
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