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Supporting information for paper:

Why Does $[HIrCl(PMe_3)_4]^+$ Adopt The Sterically And Electronically Unfavorable *cis* Geometry?

by Ofer Blum, Ra`anan Carmielli, Jan M.L. Martin* and David Milstein*

- B3LYP/LANL2DZ frequencies (cm-1) and infrared intensities (km/mol, given in parentheses) (ASCII text)
- B3LYP/LANL2DZ geometries for all molecules (XMol format). The fourth column contains partial charges computed according to the Atomic Polar Tensor method [J. Cioslowski, *J. Am. Chem. Soc.* **1989**, *111* , 8333.]
- View above structures using the CHIME plugin

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CIS H (ultrafine grid)
--- cis-h-tight.log ---
Total energy (Hartree)= -153.2520901
61.4(A",0.2300E-02);89.8(A",0.5500E-02);92.9(A',0.9500E-02);98.0(A",0.6100E-02);
98.8(A',0.1870E-01);110.3(A',0.1770E-01);114.6(A",0.3750E-01);
137.1(A",0.3900E-01);138.3(A',0.5020E-01);139.2(A",0.5470E-01);
142.2(A',0.5030E-01);233.2(A',0.2858);302.7(A",0.5128);306.8(A',0.7685);
312.2(A',0.5009);333.9(A',1.096);441.8(A',0.1338);445.5(A",0.1335);
519.5(A",0.1801);532.0(A",0.1861);547.7(A',0.2038);555.4(A",0.2114);
563.4(A',0.2211);567.5(A',0.2221);840.1(A',0.4290);899.4(A",0.4894);
980.7(A",0.6205);988.0(A',0.6230);1000.5(A',0.6367);1028.6(A',0.6791);
1120.7(A",0.7596);1122.7(A',0.7616);1124.8(A",0.7652);1126.9(A',0.7667);
1130.4(A',0.7722);1133.0(A",0.7758);1135.6(A',0.7792);1136.5(A",0.7805);
2192.3(A',2.866);2350.0(A',3.345);2362.3(A',3.373);2372.4(A",3.408);
2373.4(A',3.411);2386.6(A',3.495);2387.6(A',3.491);2394.6(A",3.525);
2400.0(A",3.541);2404.6(A",3.550);2405.1(A',3.551);2440.2(A",3.656);
2440.2(A',3.655);
--- Zero-point energy (kcal/mol): 75.14 ---
Total number of freqs. 51
TRANS H (ultrafine grid)
--- trans-h-tight.log ---
Total energy (Hartree)= -153.2530444
46.2(B1,0.1300E-02);62.0(E,0.2400E-02);62.0(E,0.2400E-02);65.5(A2,0.2600E-02);
69.6(B2,0.1360E-01);81.2(E,0.4220E-01);81.2(E,0.4220E-01);137.4(A1,0.5490E-01);
160.0(E,0.6890E-01);160.0(E,0.6890E-01);173.0(B1,0.7720E-01);
294.3(A1,1.844);299.2(E,0.5095);299.2(E,0.5095);305.5(B2,0.5126);
314.4(A1,0.4912);518.4(E,0.1770);518.4(E,0.1770);533.7(B1,0.1914);
536.1(A2,0.1869);561.4(B2,0.2150);567.6(A1,0.2282);573.3(E,0.2262);
573.3(E,0.2262);833.2(E,0.4199);833.2(E,0.4199);987.5(E,0.6279);
987.5(E,0.6279);993.3(B2,0.6233);1032.2(A1,0.6808);1123.0(E,0.7618);
1123.0(E,0.7618);1123.0(B2,0.7609);1123.6(A2,0.7637);1126.9(A1,0.7671);
1129.7(E,0.7714);1129.7(E,0.7714);1131.3(B1,0.7746);2204.7(A1,2.899);
2379.3(E,3.415);2379.3(E,3.415);2379.6(B2,3.415);2380.8(A1,3.421);
2410.4(B2,3.571);2410.6(E,3.574);2410.6(E,3.574);2411.7(A1,3.577);
2412.0(A2,3.579);2413.6(E,3.582);2413.6(E,3.582);2413.9(B1,3.584);
--- Zero-point energy (kcal/mol): 75.32 ---
Total number of freqs. 51
CIS Me (ultrafine grid)
--- cis-me-tight.log ---
Total energy (Hartree)= -625.1241285
17.7(a,0.6000E-03);41.2(a,0.2900E-02);55.5(a,0.5100E-02);71.0(a,0.9200E-02);
79.7(a,0.1350E-01);84.5(a,0.1440E-01);90.7(a,0.1690E-01);111.3(a,0.2880E-01);
118.4(a,0.2240E-01);122.8(a,0.1330E-01);127.8(a,0.4090E-01);136.9(a,0.2180E-01);
139.7(a,0.1860E-01);145.9(a,0.2250E-01);149.6(a,0.1940E-01);153.9(a,0.2100E-01);
156.3(a,0.2450E-01);157.5(a,0.2210E-01);166.4(a,0.2040E-01);170.6(a,0.5550E-01);
174.5(a,0.4150E-01);177.7(a,0.3430E-01);182.6(a,0.5560E-01);184.3(a,0.3430E-01);
188.4(a,0.3010E-01);190.7(a,0.3750E-01);192.4(a,0.4200E-01);197.3(a,0.3220E-01);
203.2(a,0.3680E-01);207.8(a,0.5010E-01);215.9(a,0.7180E-01);222.4(a,0.7530E-01);
232.7(a,0.8220E-01);236.1(a,0.3910E-01);249.2(a,0.9020E-01);253.9(a,0.9960E-01);
257.2(a,0.1021);261.4(a,0.9300E-01);262.4(a,0.1051);265.4(a,0.1087);
270.6(a,0.9190E-01);274.8(a,0.9750E-01);285.2(a,0.9770E-01);289.8(a,0.2508);
319.9(a,0.1837);335.6(a,0.2233);337.6(a,0.2211);362.3(a,0.2382);
634.0(a,1.151);639.7(a,1.185);641.6(a,1.200);646.6(a,1.212);691.1(a,1.458);
694.8(a,1.442);698.8(a,1.468);700.0(a,1.457);700.6(a,1.455);705.2(a,1.449);
707.8(a,1.481);710.3(a,1.493);850.1(a,0.4395);860.9(a,0.5049);
866.7(a,0.5121);873.5(a,0.5209);874.7(a,0.5220);891.9(a,0.5142);
916.8(a,0.6043);923.3(a,0.6077);925.8(a,0.6140);928.6(a,0.6233);
929.9(a,0.6259);931.6(a,0.6204);937.4(a,0.6404);942.6(a,0.6079);
1004.4(a,0.7973);1008.9(a,0.8063);1012.4(a,0.8061);1013.1(a,0.8103);
1015.4(a,0.8119);1016.5(a,0.8164);1019.4(a,0.8519);1022.1(a,0.8540);
1023.6(a,0.8310);1026.1(a,0.8396);1027.2(a,0.8529);1045.2(a,0.9108);
1364.3(a,1.283);1367.9(a,1.290);1368.5(a,1.287);1371.7(a,1.296);
1372.4(a,1.294);1372.8(a,1.295);1376.6(a,1.301);1377.6(a,1.303);
1394.8(a,1.333);1395.7(a,1.333);1397.5(a,1.337);1403.9(a,1.348);
1477.3(a,1.353);1477.9(a,1.354);1479.4(a,1.355);1480.9(a,1.360);
1481.9(a,1.362);1489.7(a,1.373);1491.2(a,1.376);1491.4(a,1.377);
1494.0(a,1.382);1494.5(a,1.382);1495.9(a,1.383);1497.8(a,1.386);
1498.4(a,1.391);1501.0(a,1.396);1502.5(a,1.397);1503.4(a,1.400);

1505.1(a,1.403);1508.6(a,1.408);1511.4(a,1.415);1513.1(a,1.414);
1514.0(a,1.419);1516.9(a,1.421);1522.6(a,1.429);1527.1(a,1.436);
2190.5(a,2.862);3060.6(a,5.700);3065.9(a,5.719);3066.4(a,5.722);
3067.2(a,5.726);3067.6(a,5.728);3069.5(a,5.737);3070.2(a,5.737);
3070.5(a,5.741);3073.3(a,5.755);3074.0(a,5.760);3074.7(a,5.765);
3077.2(a,5.772);3161.1(a,6.486);3165.8(a,6.502);3166.0(a,6.505);
3167.2(a,6.508);3169.0(a,6.517);3169.7(a,6.514);3172.6(a,6.534);
3172.9(a,6.534);3174.3(a,6.534);3174.8(a,6.541);3176.4(a,6.535);
3178.0(a,6.542);3180.7(a,6.559);3184.2(a,6.582);3189.5(a,6.595);
3192.2(a,6.616);3192.3(a,6.617);3192.8(a,6.609);3196.0(a,6.631);
3198.6(a,6.636);3200.6(a,6.650);3205.7(a,6.670);3209.2(a,6.680);
3219.5(a,6.705);
--- Zero-point energy (kcal/mol): 300.44 ---
Total number of freqs. 159
TRANS CH3 (ultrafine grid)
--- trans-me-tight.log ---
Total energy (Hartree)= -625.1252047
43.8(A2,0.2200E-02);60.7(A1,0.7400E-02);77.0(B1,0.1890E-01);80.5(A2,0.4700E-02);
83.0(B2,0.1000E-01);86.7(B2,0.5300E-02);95.1(A1,0.2170E-01);109.1(B1,0.2450E-01)
;
110.2(A2,0.1640E-01);115.1(B1,0.1180E-01);118.8(A2,0.9600E-02);
126.7(B2,0.3210E-01);132.8(B1,0.1780E-01);138.6(B2,0.6530E-01);
143.8(A2,0.2610E-01);146.5(B2,0.1350E-01);150.1(A2,0.1920E-01);
155.3(B1,0.1730E-01);158.7(B2,0.6000E-01);163.4(A1,0.5110E-01);
165.6(B1,0.4840E-01);167.0(A2,0.5030E-01);171.6(B1,0.4890E-01);
175.1(A1,0.4230E-01);175.6(B2,0.4790E-01);176.4(A2,0.1870E-01);
187.0(A1,0.4580E-01);189.5(A1,0.3010E-01);191.5(A2,0.5410E-01);
202.1(B1,0.3310E-01);205.3(A1,0.4090E-01);206.6(B2,0.5030E-01);
212.2(B2,0.4370E-01);215.3(B1,0.6470E-01);219.7(A1,0.6770E-01);
258.2(B1,0.1106);258.3(A2,0.9920E-01);258.5(B2,0.1133);264.5(A1,0.2291);
274.2(A1,0.2045);275.6(A2,0.1288);294.2(B2,0.1548);295.1(B1,0.1580);
305.5(A1,0.1619);333.3(A1,0.2121);344.3(B1,0.2045);345.5(B2,0.2014);
358.5(A1,0.2123);635.5(A1,1.166);637.3(B1,1.166);637.4(B2,1.180);
643.5(A1,1.201);688.9(A2,1.462);691.7(B2,0.8247);695.6(B1,1.464);
696.3(A2,1.455);697.6(B2,0.6940);704.9(B1,1.459);707.4(A1,1.517);
707.8(A1,1.467);717.5(B2,0.4966);865.4(A2,0.5100);869.4(B2,0.5129);
875.7(B1,0.5192);876.7(B1,0.4674);879.6(A2,0.5227);916.0(A2,0.6050);
924.1(B2,0.6179);926.1(A1,0.6257);928.1(B2,0.6234);929.6(B1,0.6180);
933.1(B1,0.6301);933.4(A1,0.6335);934.7(A2,0.6244);1011.0(A1,0.8137);
1011.8(B1,0.8035);1014.5(A2,0.7971);1016.2(B2,0.8124);1018.3(B2,0.8097);
1018.4(B1,0.8138);1018.4(A2,0.8218);1018.5(A1,0.8168);1024.0(B1,0.8644);
1025.9(A1,0.8480);1028.1(B2,0.8648);1048.1(A1,0.9185);1362.0(A2,1.278);
1366.5(B1,1.281);1370.0(B2,1.292);1374.8(A1,1.297);1375.0(B2,1.298);
1377.9(B1,1.302);1377.9(A1,1.303);1378.6(A2,1.299);1393.4(A1,1.330);
1397.5(B2,1.332);1401.4(B1,1.341);1406.9(A1,1.347);1477.2(A2,1.358);
1479.6(B2,1.360);1481.4(B1,1.364);1481.5(A2,1.361);1492.0(B1,1.377);
1492.2(B2,1.380);1494.0(A1,1.382);1494.7(A2,1.381);1495.6(B2,1.383);
1497.7(A2,1.393);1499.0(A1,1.392);1499.8(B1,1.394);1501.0(A1,1.394);
1503.5(A2,1.395);1506.0(B1,1.403);1506.0(B2,1.403);1507.5(A2,1.411);
1508.7(B2,1.411);1510.8(B1,1.418);1514.1(A1,1.416);1518.8(B1,1.420);
1519.4(A1,1.427);1523.6(B2,1.432);1527.1(A1,1.437);2201.8(A1,2.892);
3071.8(B2,5.747);3071.9(A1,5.747);3072.0(A2,5.749);3072.6(B1,5.751);
3072.6(B2,5.752);3073.7(A1,5.754);3074.8(A2,5.767);3075.3(B1,5.765);
3075.4(A1,5.765);3076.0(B2,5.769);3076.4(B1,5.772);3077.4(A1,5.775);
3169.3(A2,6.521);3169.4(B2,6.521);3172.7(A1,6.532);3172.7(B1,6.531);
3174.3(A2,6.539);3174.6(B1,6.540);3175.3(B2,6.539);3175.5(A1,6.539);
3177.8(B2,6.550);3177.9(A1,6.551);3183.3(B1,6.570);3183.3(A1,6.570);
3190.5(A2,6.603);3190.6(B1,6.603);3199.7(A2,6.643);3199.9(B2,6.643);
3201.8(A2,6.650);3202.1(B1,6.654);3202.4(B2,6.654);3202.8(A1,6.658);
3214.4(A2,6.678);3214.7(B2,6.680);3214.7(B1,6.681);3214.9(A1,6.682);
--- Zero-point energy (kcal/mol): 300.48 ---
Total number of freqs. 159
DMPE H CIS (ultrafine grid)
--- cis-h-dmpe.log ---
Total energy (Hartree)= -308.1202995
52.6(a,0.5600E-02);69.2(a,0.9900E-02);88.1(a,0.2100E-01);104.0(a,0.4330E-01);
117.5(a,0.5750E-01);138.3(a,0.4890E-01);140.6(a,0.4540E-01);185.6(a,0.1052);
192.2(a,0.4300E-01);200.6(a,0.4340E-01);228.7(a,0.2702);264.9(a,0.3118);

307.2(a,0.8149);321.3(a,0.6690);334.7(a,0.6271);354.3(a,0.5928);
376.4(a,0.1369);403.6(a,0.1914);422.8(a,0.1712);478.2(a,0.1827);
496.6(a,0.1937);522.0(a,0.2664);611.3(a,0.9157);614.4(a,0.9096);
632.9(a,0.5748);635.8(a,0.5790);728.2(a,0.3430);742.9(a,0.3519);
744.9(a,0.3558);756.5(a,0.3895);798.0(a,0.4314);804.1(a,0.4591);
813.6(a,0.4344);828.1(a,0.4862);851.8(a,0.4565);868.5(a,0.4640);
903.3(a,0.7271);905.4(a,0.7160);995.6(a,1.003);1001.6(a,1.005);
1043.6(a,1.404);1050.3(a,1.384);1093.5(a,0.7349);1096.0(a,0.7426);
1105.8(a,0.7511);1113.5(a,0.7635);1173.0(a,0.8501);1180.5(a,0.8610);
1211.1(a,1.054);1214.1(a,1.060);1324.0(a,1.324);1324.7(a,1.321);
1340.4(a,1.240);1346.2(a,1.251);1488.2(a,1.407);1489.2(a,1.405);
1492.5(a,1.428);1493.0(a,1.425);2187.6(a,2.854);2333.9(a,3.320);
2348.2(a,3.358);2359.0(a,3.393);2365.9(a,3.413);2375.4(a,3.464);
2386.1(a,3.493);2416.8(a,3.584);2419.2(a,3.590);3084.9(a,5.941);
3087.8(a,5.946);3092.6(a,5.980);3097.2(a,5.990);3153.5(a,6.471);
3153.8(a,6.473);3165.9(a,6.532);3171.2(a,6.553);
--- Zero-point energy (kcal/mol): 126.97 ---
Total number of freqs. 75
DMPE H TRANS (ultrafine grid)
--- trans-h-dmpe.log ---
Total energy (Hartree)= -308.1311939
46.3(A,0.4200E-02);60.1(B,0.1040E-01);81.4(A,0.1540E-01);93.5(B,0.3920E-01);
104.0(B,0.3140E-01);113.2(B,0.4120E-01);152.2(A,0.4610E-01);189.7(A,0.7370E-01);
197.9(B,0.4150E-01);205.3(A,0.5950E-01);239.9(B,0.3080);287.3(A,1.653);
303.7(B,0.5016);307.5(A,0.4630);331.6(B,0.4695);350.2(A,0.5515);
393.1(B,0.1546);394.4(A,0.2050);455.9(B,0.1521);486.5(A,0.1790);
496.9(B,0.2599);512.5(A,0.2549);619.0(B,0.9631);622.0(A,0.9864);
637.8(B,0.6097);641.3(A,0.6070);736.6(B,0.3369);751.7(B,0.3828);
755.9(A,0.3699);759.2(A,0.3713);803.0(B,0.4278);810.6(B,0.4422);
817.7(B,0.4175);819.0(A,0.4376);832.4(B,0.4311);834.0(A,0.4966);
906.6(B,0.7456);907.3(A,0.7327);997.7(B,1.028);1003.5(A,1.015);
1050.6(B,1.346);1050.8(A,1.340);1091.6(B,0.7382);1093.0(A,0.7331);
1094.5(B,0.7370);1100.2(A,0.7496);1178.0(B,0.8571);1179.0(A,0.8593);
1211.9(B,1.069);1213.8(A,1.071);1324.4(A,1.322);1324.8(B,1.323);
1345.7(B,1.250);1346.0(A,1.252);1488.5(B,1.406);1488.8(A,1.406);
1492.2(B,1.426);1492.5(A,1.427);2207.4(A,2.906);2367.4(A,3.409);
2367.6(B,3.411);2370.6(B,3.415);2371.7(A,3.421);2397.1(B,3.536);
2397.5(A,3.536);2399.4(B,3.539);2399.8(A,3.540);3090.0(B,5.955);
3090.0(A,5.955);3097.2(B,5.992);3097.2(A,5.992);3157.6(A,6.494);
3157.6(B,6.494);3172.0(A,6.560);3172.0(B,6.560);
--- Zero-point energy (kcal/mol): 127.14 ---
Total number of freqs. 75
DMPE ME CIS (ultrafine grid)
--- cis-me-dmpe.log ---
Total energy (Hartree)= -622.7156041
24.4(a,0.1000E-02);41.1(a,0.3000E-02);55.1(a,0.6400E-02);81.4(a,0.1370E-01);
98.1(a,0.2420E-01);107.0(a,0.2070E-01);115.5(a,0.2550E-01);117.8(a,0.2380E-01);
123.8(a,0.1440E-01);127.1(a,0.3220E-01);134.9(a,0.2930E-01);138.1(a,0.1340E-01);
146.5(a,0.1890E-01);147.5(a,0.1480E-01);152.3(a,0.2150E-01);156.5(a,0.1870E-01);
161.4(a,0.2920E-01);166.5(a,0.2800E-01);169.1(a,0.2420E-01);172.2(a,0.3440E-01);
181.3(a,0.3180E-01);186.7(a,0.3400E-01);189.8(a,0.5090E-01);198.4(a,0.5670E-01);
200.9(a,0.6780E-01);205.7(a,0.7200E-01);214.2(a,0.7730E-01);234.4(a,0.9830E-01);
237.2(a,0.9190E-01);243.2(a,0.9480E-01);250.6(a,0.1089);253.6(a,0.1023);
256.5(a,0.1132);290.3(a,0.2196);295.7(a,0.1715);298.4(a,0.1391);
308.1(a,0.2032);332.2(a,0.3250);332.9(a,0.2900);350.2(a,0.3300);
435.9(a,0.4087);442.2(a,0.4394);609.9(a,0.9588);616.6(a,1.007);
623.0(a,0.6955);626.1(a,0.6287);675.1(a,1.364);685.0(a,1.370);
689.0(a,1.367);692.9(a,1.423);703.3(a,1.466);711.0(a,1.469);719.5(a,1.512);
722.1(a,1.524);821.2(a,0.4948);832.4(a,0.6381);846.5(a,0.5394);
852.9(a,0.4462);879.0(a,0.5631);881.5(a,0.5693);912.3(a,0.6131);
917.2(a,0.6258);922.2(a,0.6235);926.2(a,0.6281);933.5(a,0.6254);
934.8(a,0.6197);965.2(a,0.7992);970.8(a,0.8211);989.6(a,0.8214);
992.1(a,0.8338);997.3(a,0.8454);1004.9(a,0.8443);1014.2(a,0.8217);
1017.5(a,0.8231);1023.8(a,0.8494);1027.7(a,0.8942);1037.5(a,1.639);
1040.3(a,1.607);1147.8(a,0.8246);1154.2(a,0.8314);1195.4(a,1.046);
1197.7(a,1.050);1312.9(a,1.332);1314.1(a,1.325);1328.1(a,1.237);
1334.2(a,1.250);1367.9(a,1.287);1370.3(a,1.294);1370.9(a,1.294);
1373.7(a,1.298);1386.2(a,1.318);1388.3(a,1.322);1391.5(a,1.328);

1392.2(a,1.327);1475.8(a,1.352);1477.5(a,1.363);1478.2(a,1.365);
1480.1(a,1.367);1488.1(a,1.382);1489.2(a,1.385);1489.4(a,1.390);
1490.5(a,1.398);1492.6(a,1.390);1493.3(a,1.396);1494.1(a,1.402);
1494.8(a,1.387);1498.6(a,1.392);1499.1(a,1.394);1501.1(a,1.398);
1504.4(a,1.402);1507.2(a,1.404);1508.3(a,1.405);1510.7(a,1.409);
1511.7(a,1.412);2173.7(a,2.818);3061.2(a,5.819);3062.6(a,5.724);
3063.4(a,5.710);3063.8(a,5.720);3066.1(a,5.789);3066.3(a,5.783);
3066.4(a,5.724);3067.4(a,5.727);3068.5(a,5.731);3072.9(a,5.756);
3074.8(a,5.903);3076.3(a,5.912);3125.8(a,6.353);3128.2(a,6.365);
3142.5(a,6.429);3148.3(a,6.449);3162.6(a,6.492);3166.0(a,6.505);
3167.0(a,6.512);3168.8(a,6.517);3171.4(a,6.528);3171.6(a,6.530);
3174.0(a,6.536);3175.6(a,6.543);3176.9(a,6.544);3177.9(a,6.559);
3181.9(a,6.572);3185.6(a,6.586);3190.6(a,6.607);3194.2(a,6.625);
3194.4(a,6.623);3196.8(a,6.628);
--- Zero-point energy (kcal/mol): 275.17 ---
Total number of freqs. 147
DMPE ME TRANS (ultrafine grid)
--- trans-me-dmpe.log ---
Total energy (Hartree)= -622.7306938
31.2(B,0.1900E-02);40.0(A,0.2800E-02);51.6(A,0.5600E-02);87.7(B,0.2330E-01);
88.5(A,0.1900E-01);98.3(B,0.4520E-01);112.8(B,0.1810E-01);122.1(B,0.2440E-01);
122.2(A,0.2220E-01);132.9(A,0.1140E-01);138.4(B,0.1490E-01);139.6(A,0.1310E-01);
142.5(B,0.1550E-01);148.1(A,0.3430E-01);154.8(B,0.4330E-01);162.1(B,0.3750E-01);
164.0(A,0.2300E-01);167.6(B,0.2070E-01);172.4(A,0.3090E-01);175.3(B,0.3640E-01);
181.3(A,0.4340E-01);188.7(A,0.2920E-01);189.3(B,0.2630E-01);192.3(A,0.5020E-01);
196.9(B,0.6390E-01);207.2(B,0.9170E-01);207.9(A,0.7770E-01);234.4(B,0.8310E-01);
239.4(A,0.1060);242.5(A,0.1000);249.7(A,0.1164);252.3(B,0.1100);
253.6(B,0.1280);274.5(A,0.6686);303.2(A,0.1241);305.4(B,0.1380);
319.7(A,0.2840);326.3(B,0.2761);334.2(B,0.3000);342.5(A,0.2870);
439.8(A,0.4280);449.5(B,0.4409);617.2(B,1.083);623.2(A,1.056);
627.7(A,0.6693);628.6(B,0.6547);685.7(A,1.334);688.1(B,1.421);
690.2(B,1.355);691.2(A,1.453);713.7(B,1.464);714.9(A,1.539);718.1(B,1.407);
724.4(A,1.493);804.1(B,0.3935);818.1(B,0.4126);838.1(A,0.6431);
843.5(B,0.6508);885.5(A,0.5702);885.9(B,0.5715);918.7(B,0.6241);
921.4(A,0.6352);927.7(A,0.6316);927.9(B,0.6274);933.0(B,0.6182);
937.8(A,0.6252);968.6(B,0.7950);969.4(A,0.8209);986.6(A,0.8153);
992.2(B,0.8278);999.2(B,0.8785);1007.3(A,0.8618);1021.8(A,0.8284);
1023.6(B,0.8500);1024.3(B,0.8387);1031.1(A,0.9137);1043.4(B,1.600);
1044.9(A,1.514);1150.2(B,0.8266);1151.3(A,0.8303);1195.3(B,1.062);
1198.1(A,1.069);1313.7(A,1.331);1314.1(B,1.332);1333.0(B,1.253);
1333.0(A,1.254);1372.2(A,1.294);1372.9(B,1.295);1376.7(B,1.300);
1378.3(A,1.303);1386.6(B,1.321);1388.2(A,1.324);1394.5(B,1.331);
1395.9(A,1.332);1474.3(B,1.352);1475.2(A,1.352);1480.9(A,1.371);
1481.7(B,1.373);1489.1(B,1.387);1489.7(A,1.383);1489.8(A,1.383);
1491.6(B,1.380);1492.9(B,1.403);1494.0(A,1.393);1494.8(B,1.399);
1495.3(A,1.413);1498.0(B,1.386);1499.3(A,1.388);1499.6(B,1.395);
1501.3(A,1.398);1504.2(A,1.397);1505.0(B,1.403);1513.8(B,1.416);
1514.3(A,1.417);2212.6(A,2.920);3063.2(B,5.707);3063.3(A,5.707);
3063.8(B,5.713);3063.8(A,5.712);3066.3(B,5.723);3066.3(A,5.726);
3068.9(B,5.865);3068.9(A,5.863);3071.1(B,5.743);3071.1(A,5.743);
3076.2(B,5.912);3076.3(A,5.912);3131.9(A,6.384);3131.9(B,6.384);
3146.2(B,6.445);3146.2(A,6.445);3165.9(A,6.505);3166.0(B,6.505);
3166.2(A,6.506);3166.3(B,6.506);3172.0(B,6.533);3172.0(A,6.533);
3178.3(A,6.553);3178.3(B,6.553);3179.4(A,6.559);3179.5(B,6.559);
3180.6(B,6.567);3180.7(A,6.567);3185.7(A,6.595);3185.7(B,6.595);
3194.8(B,6.624);3194.8(A,6.624);
--- Zero-point energy (kcal/mol): 275.38 ---
Total number of freqs. 147

19
Cis no methyls --- Cs symmetry. 4th column are computed APT partial charges

Cl	2.32098665	-0.63727814	0.00000000	-0.3839
Ir	0.00010051	0.21837639	0.00000000	-0.4776
P	-0.62591806	-2.22701936	0.00000000	0.6317
P	0.33004755	0.34601123	2.37668680	0.7717
P	0.33004755	0.34601123	-2.37668680	0.7717
P	-2.18488177	1.15870520	0.00000000	0.8202
H	0.55511456	1.71797078	0.00000000	0.0109
H	-1.98052315	-2.69269686	0.00000000	-0.1191
H	-3.31306233	0.28154640	0.00000000	-0.1194
H	1.52517399	1.03679094	2.71113154	-0.0503
H	1.52517399	1.03679094	-2.71113154	-0.0503
H	-0.63644148	1.00583062	3.19496234	-0.1274
H	-0.63644148	1.00583062	-3.19496234	-0.1274
H	0.49787519	-0.88468310	3.07562119	-0.1001
H	0.49787519	-0.88468310	-3.07562119	-0.1001
H	-0.10677116	-2.99024290	1.08942478	-0.0776
H	-0.10677116	-2.99024290	-1.08942478	-0.0776
H	-2.51257164	2.01045520	1.09716099	-0.0978
H	-2.51257164	2.01045520	-1.09716099	-0.0978

19
Trans no methyls --- C4v symmetry

Ir	0.00000000	0.00000000	0.28865395	-0.5334
H	0.00000000	0.00000000	1.88520895	-0.0305
P	2.40477700	0.00000000	0.20756495	0.7815
Cl	0.00000000	0.00000000	-2.25874705	-0.4564
P	0.00000000	-2.40477700	0.20756495	0.7815
P	-2.40477700	0.00000000	0.20756495	0.7815
P	0.00000000	2.40477700	0.20756495	0.7815
H	3.14016600	0.00000000	1.42876795	-0.1062
H	2.99229900	-1.09791800	-0.48522905	-0.0851
H	2.99229900	1.09791800	-0.48522905	-0.0851
H	0.00000000	-3.14016600	1.42876795	-0.1062
H	-1.09791800	-2.99229900	-0.48522905	-0.0851
H	1.09791800	-2.99229900	-0.48522905	-0.0851
H	-3.14016600	0.00000000	1.42876795	-0.1062
H	-2.99229900	1.09791800	-0.48522905	-0.0851
H	-2.99229900	-1.09791800	-0.48522905	-0.0851
H	0.00000000	3.14016600	1.42876795	-0.1062
H	1.09791800	2.99229900	-0.48522905	-0.0851
H	-1.09791800	2.99229900	-0.48522905	-0.0851

55
CIS FORM WITh METHYLs --- C1 symmetry

Cl	0.20231342	-2.36814845	-1.21283974	-0.4866
Ir	0.01203936	-0.02257984	-0.33368866	-0.4852
P	0.12088571	-0.90622876	2.05258594	0.7758
P	-2.37271199	-0.45889813	-0.73780745	0.8868
P	2.43825050	-0.08570640	-0.75902019	0.8892
P	-0.26305620	2.28521200	0.23988706	0.9849
H	-0.02665254	0.47679767	-1.85494456	-0.0393
C	-3.03063228	-2.11120238	-0.11869528	-0.2386
C	-2.65199526	-0.57575528	-2.59292587	-0.2107
C	-3.76056296	0.70153150	-0.19084341	-0.2513
C	-1.41073555	-0.77246959	3.15855136	-0.2004
C	1.41003443	-0.09891054	3.17989292	-0.1935
C	0.52477701	-2.73830132	2.24055643	-0.1938
C	-0.94887944	3.31047342	-1.18294558	-0.2063
C	1.22483007	3.32555240	0.74957978	-0.2231
C	-1.41974627	2.70165648	1.67274908	-0.2337
C	2.71721599	-0.31405160	-2.60430439	-0.2133
C	3.34585121	-1.55977086	-0.01535491	-0.2425
C	3.65091680	1.30851662	-0.36706734	-0.2465
H	-2.20051105	-1.42839979	2.78256416	0.0321
H	-1.78353057	0.25446247	3.18482473	0.0304
H	-1.16004808	-1.08528152	4.17838948	0.0032
H	-1.95047235	-1.30894237	-2.99808772	0.0772
H	-2.45899203	0.39427202	-3.06004106	0.0398

H	-3.68069092	-0.88797654	-2.80486938	0.0085
H	3.62485931	1.57241201	0.69296514	0.0371
H	3.42596513	2.19322375	-0.96795882	0.0319
H	4.66044808	0.96656609	-0.62078959	0.0024
H	-3.58438189	1.72564426	-0.52992636	0.0310
H	-3.86098372	0.69056514	0.89860875	0.0330
H	-4.70201901	0.34962883	-0.62695714	0.0051
H	3.45642523	-1.43933854	1.06660677	0.0226
H	4.34279677	-1.63192296	-0.46409135	0.0067
H	2.78111653	-2.46791950	-0.23333198	0.0861
H	-2.34820862	-2.90279224	-0.43266285	0.0904
H	-4.02345319	-2.28658435	-0.54779754	0.0084
H	-3.11377895	-2.10828861	0.97126269	0.0257
H	3.78353854	-0.45889098	-2.81094356	0.0090
H	2.35599363	0.56772127	-3.14155736	0.0401
H	2.15116414	-1.18755665	-2.93485932	0.0820
H	1.16699880	0.95794494	3.33366510	0.0199
H	2.40460823	-0.16865264	2.72982822	0.0259
H	1.42990923	-0.59813811	4.15513368	0.0065
H	-0.18826079	-3.32991502	1.66174309	0.0581
H	0.47888584	-3.02400048	3.29751329	0.0030
H	1.52323030	-2.94559427	1.85017843	0.0428
H	-1.05065158	4.35940212	-0.88333365	0.0109
H	-1.92501808	2.92979943	-1.49366184	0.0331
H	-0.26627204	3.23906767	-2.03443713	0.0502
H	-0.94568979	2.41980780	2.61798521	0.0288
H	-2.37097081	2.17864341	1.57961878	0.0479
H	-1.60484704	3.78146335	1.68535933	0.0103
H	1.77305704	2.84117754	1.56146451	0.0387
H	0.86808209	4.30288697	1.09295501	0.0100
H	1.89503237	3.47658578	-0.09794956	0.0398

55

TRANS FORM WITH METHYLs --- C2v symmetry

P	2.43724467	0.00000000	-0.18229486	0.9027
Ir	0.00000000	0.00000000	0.15433303	-0.5196
P	-2.43724467	0.00000000	-0.18229486	0.9027
P	0.00000000	2.41985796	0.50604999	0.9049
Cl	0.00000000	0.00000000	-2.42585131	-0.5084
P	0.00000000	-2.41985796	0.50604999	0.9049
H	0.00000000	0.00000000	1.75234319	-0.0286
C	0.00000000	3.57712445	-0.97883791	-0.2535
C	1.41565350	3.06223782	1.57920198	-0.2154
C	-1.41565350	3.06223782	1.57920198	-0.2154
C	-3.59296526	0.00000000	1.30706069	-0.2431
C	-3.07398155	-1.42160909	-1.24722810	-0.2263
C	-3.07398155	1.42160909	-1.24722810	-0.2263
C	0.00000000	-3.57712445	-0.97883791	-0.2535
C	-1.41565350	-3.06223782	1.57920198	-0.2154
C	1.41565350	-3.06223782	1.57920198	-0.2154
C	3.59296526	0.00000000	1.30706069	-0.2431
C	3.07398155	1.42160909	-1.24722810	-0.2263
C	3.07398155	-1.42160909	-1.24722810	-0.2263
H	-3.41303078	0.88613176	1.92083934	0.0408
H	-3.41303078	-0.88613176	1.92083934	0.0408
H	-4.63684110	0.00000000	0.97433827	0.0011
H	-0.88183887	3.38790069	-1.59428583	0.0531
H	0.88183887	3.38790069	-1.59428583	0.0531
H	0.00000000	4.62058368	-0.64464158	0.0028
H	3.41303078	0.88613176	1.92083934	0.0408
H	4.63684110	0.00000000	0.97433827	0.0011
H	3.41303078	-0.88613176	1.92083934	0.0408
H	0.00000000	-4.62058368	-0.64464158	0.0028
H	0.88183887	-3.38790069	-1.59428583	0.0531
H	-0.88183887	-3.38790069	-1.59428583	0.0531
H	-2.98405845	2.38837921	-0.75024358	0.0220
H	-4.13008534	1.24686784	-1.47972655	0.0110
H	-2.49172504	1.42725249	-2.17241199	0.0833
H	-4.13008534	-1.24686784	-1.47972655	0.0110

H	-2.98405845	-2.38837921	-0.75024358	0.0220
H	-2.49172504	-1.42725249	-2.17241199	0.0833
H	-2.38676032	2.94310500	1.09812860	0.0305
H	-1.25803412	4.12706932	1.78246830	0.0120
H	-1.41502610	2.51492494	2.52657961	0.0459
H	2.38676032	2.94310500	1.09812860	0.0305
H	1.41502610	2.51492494	2.52657961	0.0459
H	1.25803412	4.12706932	1.78246830	0.0120
H	4.13008534	-1.24686784	-1.47972655	0.0110
H	2.49172504	-1.42725249	-2.17241199	0.0833
H	2.98405845	-2.38837921	-0.75024358	0.0220
H	2.98405845	2.38837921	-0.75024358	0.0220
H	2.49172504	1.42725249	-2.17241199	0.0833
H	4.13008534	1.24686784	-1.47972655	0.0110
H	1.25803412	-4.12706932	1.78246830	0.0120
H	1.41502610	-2.51492494	2.52657961	0.0459
H	2.38676032	-2.94310500	1.09812860	0.0305
H	-1.25803412	-4.12706932	1.78246830	0.0120
H	-2.38676032	-2.94310500	1.09812860	0.0305
H	-1.41502610	-2.51492494	2.52657961	0.0459

27
CIS NOMETHYL DMPE --- C1 symmetry

P	2.03876123	1.15400435	0.70393285	0.8206
Ir	0.09597652	0.16376598	-0.26202489	-0.5695
P	-1.89595529	-0.49909862	-1.41541293	0.7917
P	-1.19557008	-0.49060253	1.78320654	0.6468
H	0.68751742	0.69466571	-1.65277953	0.0099
P	1.45746066	-1.74844505	-0.56570885	0.8176
Cl	-1.08701718	2.32855488	-0.02932745	-0.3972
C	-3.32021309	-0.51753121	-0.15110026	-0.0814
H	-1.97309956	-1.76769844	-2.07039699	-0.1664
H	-2.32484012	0.38461834	-2.44377314	-0.0961
C	-2.88324315	-1.16803787	1.17746600	-0.0459
H	-1.55595494	0.59989936	2.63102287	-0.1006
H	-0.83003065	-1.46734806	2.76720057	-0.1546
H	1.81466363	-2.07510141	-1.90903085	-0.1316
H	1.05810259	-3.03517316	-0.08474878	-0.1541
C	3.13002562	-1.44602868	0.31406594	-0.0632
H	2.37754851	2.45073288	0.22734400	-0.0979
C	3.52638594	0.04530784	0.26798647	-0.0917
H	2.12092151	1.34165012	2.11768812	-0.1540
H	3.90102190	-2.06543867	-0.15513261	0.0260
H	3.00928960	-1.78824163	1.34831399	0.0205
H	4.35474052	0.23934182	0.95674038	0.0289
H	3.85119866	0.33416685	-0.73758572	0.0308
H	-4.17876930	-1.04962307	-0.57384406	0.0234
H	-3.59909033	0.53005536	-0.00266930	0.0533
H	-3.63976778	-0.98870378	1.94780151	0.0214
H	-2.77253156	-2.25334837	1.06755932	0.0132

27
TRANS DMPE NOMETHYL --- C2 symmetry

P	1.23010611	2.05310940	0.24230142	0.8010
Ir	0.00000000	0.00000000	0.30977769	-0.6274
P	-1.23010611	-2.05310940	0.24230142	0.8010
Cl	0.00000000	0.00000000	-2.24436019	-0.4703
H	0.00000000	0.00000000	1.90676895	-0.0175
P	-1.92094181	1.42386343	0.20209129	0.8028
P	1.92094181	-1.42386343	0.20209129	0.8028
H	-0.45332410	-4.37351346	-0.23122553	0.0283
C	-1.32419460	3.12390312	-0.41347075	-0.0846
H	-2.65814368	1.70124942	1.39326447	-0.1508
H	-2.17341634	-2.37787836	1.26262922	-0.1447
H	-2.09462479	3.87737585	-0.22156980	0.0294
H	-2.00068873	-2.24408368	-0.94211164	-0.1173
H	-0.15828824	3.78081424	1.32211583	0.0212
H	0.45332410	4.37351346	-0.23122553	0.0283
H	2.09462479	-3.87737585	-0.22156980	0.0294
H	-2.96154414	1.06554288	-0.70330017	-0.1184

H	-1.19554972	3.02353959	-1.49588109	0.0497
H	0.15828824	-3.78081424	1.32211583	0.0212
H	2.17341634	2.37787836	1.26262922	-0.1447
C	0.00031030	3.51326387	0.27137476	-0.0590
H	2.96154414	-1.06554288	-0.70330017	-0.1184
C	1.32419460	-3.12390312	-0.41347075	-0.0846
H	2.00068873	2.24408368	-0.94211164	-0.1173
H	2.65814368	-1.70124942	1.39326447	-0.1508
C	-0.00031030	-3.51326387	0.27137476	-0.0590
H	1.19554972	-3.02353959	-1.49588109	0.0497

51

CIS METHYL DMPE --- C1 symmetry

P	-2.34744044	-0.64747254	-0.51546583	0.9422
Ir	-0.06391430	0.08447872	-0.38382004	-0.6200
P	2.23781245	0.75560133	-0.67747036	0.9130
P	0.88262219	-1.48916837	1.35491075	0.7609
H	-0.44599855	1.01851771	-1.63305538	-0.0239
P	-0.89446521	1.86612127	0.94096197	0.9590
Cl	0.48481432	-1.69957270	-2.05397543	-0.4694
C	3.29561655	-0.66141101	0.01958270	-0.1548
C	2.92450254	2.28844609	0.17671288	-0.2520
C	2.79393709	0.96037223	-2.45533738	-0.2198
C	2.76480498	-1.13695292	1.38666516	-0.1065
C	0.79541551	-3.33501884	0.98314990	-0.2088
C	0.46147738	-1.46256662	3.19870903	-0.2118
C	-1.04915166	3.50675739	0.03373477	-0.2152
C	-0.14263164	2.37606421	2.58961623	-0.2406
C	-2.69136994	1.42777881	1.41092062	-0.1309
C	-2.99993075	-0.86552451	-2.25766458	-0.2258
C	-3.42467164	0.72489511	0.25186195	-0.1555
C	-2.86974377	-2.22904284	0.35599557	-0.2603
H	-3.21453555	2.34552645	1.70603003	-0.0023
H	-2.63961135	0.77757177	2.29349616	0.0102
H	-4.37303219	0.29730961	0.59745655	0.0026
H	-3.65813078	1.43546822	-0.55045262	0.0142
H	4.33702783	-0.32690052	0.10383964	-0.0061
H	3.25454533	-1.46841024	-0.71989119	0.0422
H	3.28739778	-2.04830797	1.70110767	-0.0066
H	2.94079955	-0.37716833	2.15986670	0.0008
H	2.37502543	3.17741592	-0.14826033	0.0379
H	3.98040779	2.41720219	-0.08520682	0.0139
H	2.84147977	2.19131926	1.26342802	0.0318
H	2.36249897	1.87745852	-2.86793057	0.0380
H	2.42870485	0.10711768	-3.03121584	0.0906
H	3.88680751	1.01495733	-2.51121307	0.0127
H	-0.75659353	3.15969774	3.04734932	0.0143
H	0.86744170	2.76651891	2.43879441	0.0397
H	-0.10019506	1.51941834	3.26624845	0.0402
H	-1.53921139	4.25336752	0.66842898	0.0108
H	-1.62777594	3.36370730	-0.88259551	0.0540
H	-0.05518521	3.86957190	-0.24399056	0.0398
H	-3.93934632	-2.41081351	0.20406381	0.0128
H	-2.66494394	-2.15945782	1.42876497	0.0313
H	-2.30403678	-3.06461048	-0.06587500	0.0587
H	-4.05821599	-1.14844196	-2.24368508	0.0148
H	-2.41004019	-1.64051061	-2.75379014	0.0814
H	-2.87050335	0.06859686	-2.81118442	0.0515
H	-0.22227761	-3.69856080	1.15541619	0.0316
H	1.48291956	-3.88236957	1.63752392	0.0047
H	1.05247681	-3.50237180	-0.06482257	0.0887
H	-0.59840091	-1.69468041	3.34632823	0.0313
H	0.67387827	-0.47875723	3.62695474	0.0261
H	1.05871784	-2.21051570	3.73206787	0.0086

51

TRANS METHYL DMPE --- C2 symmetry

P	-1.94833440	-1.42962563	0.18736242	0.9190
Ir	0.00000000	0.00000000	0.16183549	-0.6763
P	1.94833440	1.42962563	0.18736242	0.9190

Cl	0.00000000	0.00000000	-2.41007059	-0.4994
H	0.00000000	0.00000000	1.75940679	-0.0239
P	1.24071443	-2.06723047	0.13651421	0.9240
P	-1.24071443	2.06723047	0.13651421	0.9240
H	2.10376527	3.90610640	0.04499937	0.0000
C	0.00214798	-3.44148152	-0.30034612	-0.1474
C	1.99696101	-2.63400330	1.76244077	-0.2318
C	3.20307078	1.22288416	1.57223141	-0.2307
H	0.43569520	-4.41318754	-0.03519339	-0.0015
C	2.99402174	1.51222753	-1.37137519	-0.2482
H	-1.23795776	-3.39399348	1.50174580	0.0098
H	-2.10376527	-3.90610640	0.04499937	0.0000
H	-0.43569520	4.41318754	-0.03519339	-0.0015
C	2.60977385	-2.29724007	-1.12758680	-0.2431
H	-0.12776293	-3.41354423	-1.38851029	0.0308
H	1.23795776	3.39399348	1.50174580	0.0098
C	-3.20307078	-1.22288416	1.57223141	-0.2307
C	-1.33729279	-3.21943622	0.42296863	-0.1346
C	-2.60977385	2.29724007	-1.12758680	-0.2431
C	-0.00214798	3.44148152	-0.30034612	-0.1474
C	-2.99402174	-1.51222753	-1.37137519	-0.2482
C	-1.99696101	2.63400330	1.76244077	-0.2318
C	1.33729279	3.21943622	0.42296863	-0.1346
H	0.12776293	3.41354423	-1.38851029	0.0308
H	2.26945352	-1.88865331	-2.08281118	0.0872
H	2.84491055	-3.36149387	-1.23853671	0.0168
H	3.51518864	-1.77226840	-0.80722610	0.0252
H	1.21792201	-2.69875040	2.52767138	0.0445
H	2.74381796	-1.90843967	2.09743814	0.0389
H	2.47592026	-3.61222271	1.64446278	0.0092
H	2.68228346	1.16996452	2.53251440	0.0506
H	3.90148220	2.06696899	1.58197565	0.0159
H	3.77563891	0.30134255	1.42774661	0.0296
H	2.34013976	1.67238519	-2.23156057	0.0853
H	3.51676849	0.56387426	-1.52078909	0.0408
H	3.72900902	2.32032485	-1.28684226	0.0097
H	-2.84491055	3.36149387	-1.23853671	0.0168
H	-3.51518864	1.77226840	-0.80722610	0.0252
H	-2.26945352	1.88865331	-2.08281118	0.0872
H	-2.47592026	3.61222271	1.64446278	0.0092
H	-1.21792201	2.69875040	2.52767138	0.0445
H	-2.74381796	1.90843967	2.09743814	0.0389
H	-3.51676849	-0.56387426	-1.52078909	0.0408
H	-3.72900902	-2.32032485	-1.28684226	0.0097
H	-2.34013976	-1.67238519	-2.23156057	0.0853
H	-3.77563891	-0.30134255	1.42774661	0.0296
H	-2.68228346	-1.16996452	2.53251440	0.0506
H	-3.90148220	-2.06696899	1.58197565	0.0159