Supporting Information

Buchwald-Hartwig Cross-Coupling of Amides (Transamidation) by Selective N–C(O) Cleavage Mediated by Air- and Moisture-Stable [Pd(NHC)(allyl)Cl] Precatalysts: Catalyst Evaluation and Mechanism

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List of Known Compounds/General Methods

All starting materials reported in the manuscript have been previously described in literature or prepared by the method reported previously. Amides were prepared by standard methods.[1–3] Unless stated otherwise, all products reported in the manuscript have been previously well described in literature. All experiments were performed using standard Schlenk techniques under argon or nitrogen atmosphere unless stated otherwise. All solvents were purchased at the highest commercial grade and used as received or after purification by passing through activated alumina columns or distillation from sodium/benzophenone under nitrogen. All other chemicals were purchased at the highest commercial grade and used as received. Reaction glassware was oven-dried at 140 °C for at least 24 h or flame-dried prior to use, allowed to cool under vacuum and purged with argon or nitrogen (three cycles). All products were identified using ^{1}H NMR analysis and comparison with authentic samples. GC and/or GC/MS analysis was used for volatile products. All yields refer to yields determined by ^{1}H NMR and/or GC or GC/MS using an internal standard (optimization) and isolated yields (preparative runs) unless stated otherwise. ^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ on Bruker spectrometers at 500 (^{1}H NMR) and 125 MHz (^{13}C NMR). All shifts are reported in parts per million (ppm) relative to residual $CHCl_3$ peak (7.27 and 77.2 ppm, ^{1}H NMR and ^{13}C NMR, respectively). All coupling constants (J) are reported in hertz (Hz). Abbreviations are: s, singlet; d, doublet; t, triplet; q, quartet; brs, broad singlet. GC-MS chromatography was performed using Agilent HP6890 GC System and Agilent 5973A inert XL EI/CI MSD using helium as the carrier gas at a flow rate of 1 mL/min and an initial oven temperature of 50 °C. The injector temperature was 280 °C. The detector temperature was 280 °C. For runs with the initial oven temperature of 50 °C, temperature was increased with a 10 °C/min ramp after 50 °C hold for 3 min to a final temperature of 280 °C, then hold at 280 °C for 10 min (splitless mode of injection, total run time of 33.00 min). All flash chromatography was performed using silica gel, 60 Å, 300 mesh. TLC analysis was carried out on glass plates coated with silica gel 60 F254, 0.2 mm thickness. The plates were visualized using a 254 nm ultraviolet lamp or aqueous potassium permanganate solutions. ^{1}H NMR and ^{13}C NMR data are given for all compounds in the Supporting Experimental for characterization purposes. ^{1}H NMR, ^{13}C NMR and HRMS data are reported for all new compounds.

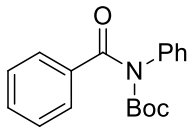
Experimental Procedures and Characterization Data

General Procedure for Transamidation. An oven-dried vial equipped with a stir bar was charged with an amide substrate (neat, 1.0 equiv), amine (2.0 equiv), K_2CO_3 (typically, 3.0 equiv) and Pd(II)–NHC pre-catalyst (typically, 3 mol%), placed under a positive pressure of argon, and subjected to three evacuation/backfilling cycles. DME (typically, 0.25 M) was added with vigorous stirring at room temperature, the reaction mixture was placed in a preheated oil bath at 110 °C, and stirred for the indicated time at 110 °C. After the indicated time, the reaction mixture was diluted with ethyl acetate, filtered, and concentrated. The sample was analyzed by ^{1}H NMR ($CDCl_3$, 500 MHz) and GC-MS to obtain conversion, yield and selectivity using internal standard and comparison with authentic samples. Purification of an analytical sample by chromatography (hexanes/ethyl acetate) afforded the title product.

Note: all Pd(II)–NHC catalysts used in this study are commercially-available, bench-, air- and moisture-stable solids. Pd(II)–NHC catalysts can be prepared on large scale using established methods. For lead references, see: Marion, N.; Navarro, O.; Mei, J.; Stevens, E. D.; Scott, N. M.; Nolan, S. P. *J. Am. Chem. Soc.* **2006**, *128*, 4101; Navarro, O.; Marion, N.; Mei, J.; Nolan, S. P. *Chem. Eur. J.* **2006**, *12*, 5142; Marion, N.; Nolan, S. P. *Acc. Chem. Res.* **2008**, *41*, 1440; Rivas-Nass, A.; Winde, R.; Briel, O.; Le Ret, C.; Karch, R. *Chim. Oggi* **2007**, *25*, 15. All Pd(II)–NHC catalysts are available from commercial suppliers; for example, Strem, Sigma-Aldrich, Umicore.

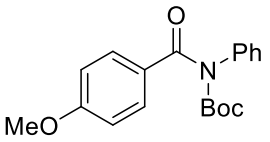
Characterization Data for Amides Starting Materials

Amides used in this study were prepared by procedures reported in the literature. **8a**,[1] **8b**,[1] **8c**[1] are known compounds. Spectroscopic data matched those reported in the literature.

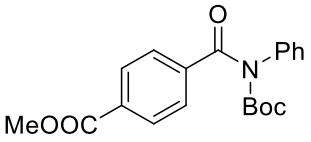


***tert*-Butyl benzoyl(phenyl)carbamate (8a).** White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 (d, J = 7.1 Hz, 2 H), 7.55 (t, J = 7.4 Hz, 1 H), 7.49-7.43 (m, 4 H), 7.37 (t, J = 7.4 Hz, 1 H), 7.30 (d, J = 7.4 Hz, 2 H), 1.26 (s, 9 H). ^{13}C NMR

(125 MHz, $CDCl_3$) δ 172.78, 153.30, 139.10, 136.98, 131.72, 129.21, 128.28, 128.14, 127.96, 127.80, 83.50, 27.49.



***tert*-Butyl (4-methoxybenzoyl)(phenyl)carbamate (8b).** Oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.6 Hz, 2 H), 7.43 (t, *J* = 7.2 Hz, 2 H), 7.33 (t, *J* = 7.3 Hz, 1 H), 7.28 (d, *J* = 7.9 Hz, 2 H), 6.95 (d, *J* = 7.7 Hz, 2 H), 3.88 (s, 3 H), 1.32 (s, 9 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.07, 162.78, 153.53, 139.48, 130.86, 129.12, 128.72, 127.75, 127.48, 113.56, 83.10, 55.49, 27.65.

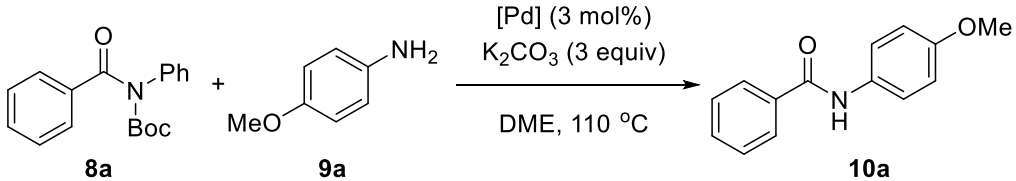


***tert*-Butyl phenyl((4-(methoxycarbonyl)benzoyl)carbamate (8c).** White solid. ^{1}H NMR (500 MHz, CDCl3) δ 8.14 (d, *J* = 8.1 Hz, 2 H), 7.78 (d, *J* = 8.1 Hz, 2 H), 7.46 (t, *J* = 7.6 Hz, 2 H), 7.38 (t, *J* = 7.3 Hz, 1 H), 7.28 (d, *J* = 7.8 Hz, 2 H), 3.97 (s, 3 H), 1.26 (s, 9 H). ^{13}C NMR (125 MHz, CDCl3) δ 171.83, 166.21, 152.93, 141.01, 138.62, 132.53, 129.52, 129.27, 128.07, 127.99, 127.78, 84.01, 52.42, 27.51.

Characterization Data of Transamidation Products

All products reported in the manuscript are known compounds. **10a**,[2] **10b**,[3] **10c**,[2] **10d**,[2] **10e**,[2] **10f**,[4] **10g**,[5] **10h**,[6] **10i**,[7] **10j**[8] have been previously reported. Spectroscopic data matched those reported in the literature.

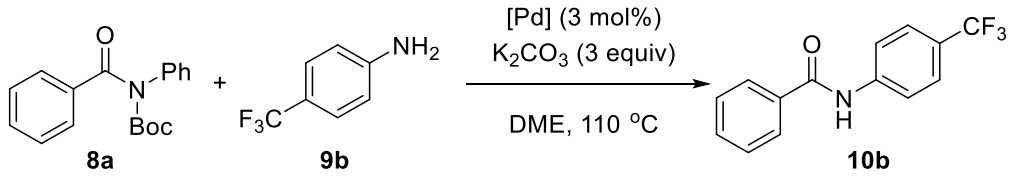
N-(4-Methoxyphenyl)benzamide (3a, Table 1)



According to the general procedure, the reaction of *tert*-butyl benzoyl(phenyl)carbamate (0.10 mmol, 1.0 equiv), 4-methoxyaniline (2.0 equiv), K_2CO_3 (3.0 equiv), Pd(II)–NHC (3.0 mol%) in DME (0.25 M) for 16 h at 110 °C, afforded after the standard work-up as described above and

chromatography the title compound. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, J = 7.6 Hz, 2H), 7.81 (s, 1H), 7.55 (dd, J = 7.6, 5.7 Hz, 3H), 7.48 (t, J = 7.6 Hz, 2H), 6.91 (d, J = 8.9 Hz, 2H), 3.82 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.47, 157.48, 135.89, 132.54, 131.85, 129.59, 127.83, 122.96, 115.09, 56.36.

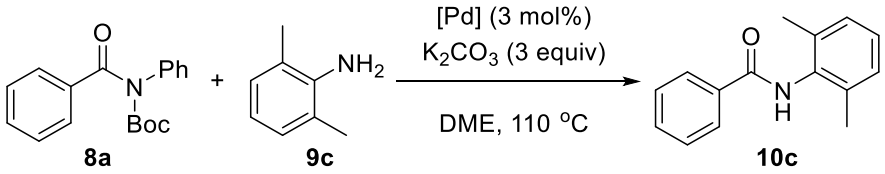
_N_-(4-(Trifluoromethyl)phenyl)benzamide (10b, Table 1)



8a **9b** **10b**

According to the general procedure, the reaction of *tert*-butyl benzoyl(phenyl)carbamate (0.10 mmol, 1.0 equiv), 4-(trifluoromethyl)aniline (2.0 equiv), K_2CO_3 (3.0 equiv), Pd(II)–NHC (3.0 mol%) in DME (0.25 M) for 16 h at 110 °C, afforded after the standard work-up as described above and chromatography the title compound. White solid. ^{1}H NMR (500 MHz, DMSO-d^6) δ 10.60 (s, 1H), 8.03 (d, J = 8.4 Hz, 2H), 7.98 (d, J = 7.4 Hz, 2H), 7.73 (d, J = 8.5 Hz, 2H), 7.63 (t, J = 7.3 Hz, 1H), 7.56 (t, J = 7.5 Hz, 2H). ^{13}C NMR (125 MHz, DMSO-d^6) δ 167.42, 144.25, 135.88, 133.27, 129.82, 129.15, 127.26 (q, J^F = 3.8 Hz), 126.83 (J^F = 224.5 Hz), 124.77 (d, J^F = 15.0), 121.46. ^{19}F NMR (471 MHz, DMSO) δ -60.33.

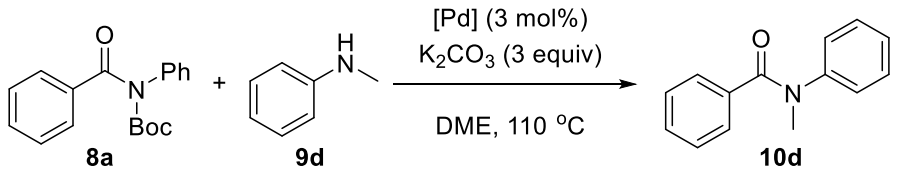
_N_-(2,6-Dimethylphenyl)benzamide (10c, Table 1)



8a **9c** **10c**

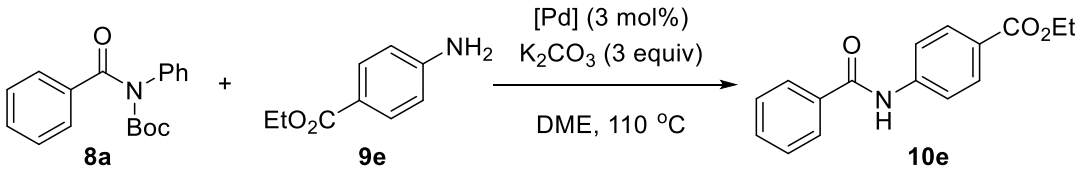
According to the general procedure, the reaction of *tert*-butyl benzoyl(phenyl)carbamate (0.10 mmol, 1.0 equiv), 2,6-dimethylaniline (2.0 equiv), K_2CO_3 (3.0 equiv), Pd(II)–NHC (3.0 mol%) in DME (0.25 M) for 16 h at 110 °C, afforded after the standard work-up as described above and chromatography the title compound. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, J = 8.3 Hz, 2H), 7.60 (t, J = 7.4 Hz, 1H), 7.53 (t, J = 7.4 Hz, 2H), 7.39 (s, 1H), 7.20 – 7.09 (m, 3H), 2.32 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.87, 135.57, 134.56, 133.85, 131.84, 128.81, 128.33, 127.48, 127.2, 18.53.

_N_-Methyl-_N_-phenylbenzamide (10d, Table 1)



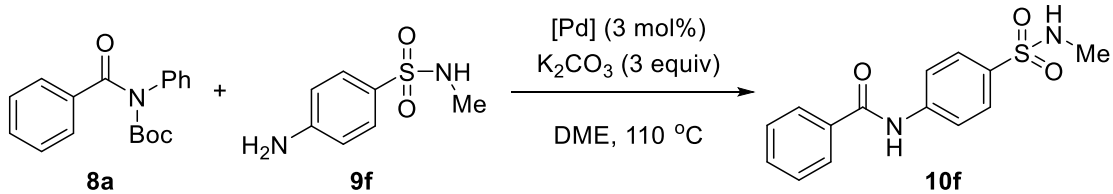
According to the general procedure, the reaction of *tert*-butyl benzoyl(phenyl)carbamate (0.10 mmol, 1.0 equiv), *N*-methylaniline (2.0 equiv), K_2CO_3 (3.0 equiv), Pd(II)–NHC (3.0 mol%) in DME (0.25 M) for 16 h at 110 °C, afforded after the standard work-up as described above and chromatography the title compound. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 (d, J = 7.3 Hz, 2H), 7.16 – 7.10 (m, 3H), 7.10 – 7.04 (m, 3H), 6.96 (d, J = 7.7 Hz, 2H), 3.42 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.69, 144.94, 135.95, 129.59, 129.15, 128.73, 127.73, 126.93, 126.49, 38.41.

Ethyl 4-benzamidobenzoate (10e, Table 1)



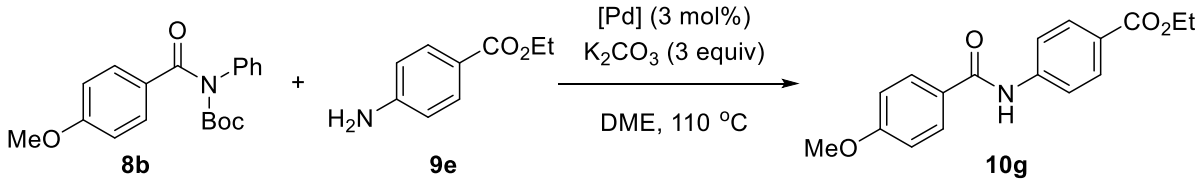
According to the general procedure, the reaction of *tert*-butyl benzoyl(phenyl)carbamate (0.10 mmol, 1.0 equiv), ethyl 4-aminobenzoate (2.0 equiv), K_2CO_3 (3.0 equiv), Pd(II)–NHC (3.0 mol%) in DME (0.25 M) for 16 h at 110 °C, afforded after the standard work-up as described above and chromatography the title compound. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 – 8.02 (m, 2H), 7.91 – 7.83 (m, 2H), 7.74 (d, J = 8.6 Hz, 2H), 7.58 – 7.53 (m, 1H), 7.52 – 7.41 (m, 2H), 4.42 – 4.30 (m, 2H), 1.39 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.16, 142.10, 134.57, 132.21, 130.85, 128.88, 127.12, 126.18, 119.20, 60.94, 14.37.

_N_-(4-(_N_-Methylsulfamoyl)phenyl)benzamide (10f, Table 1)



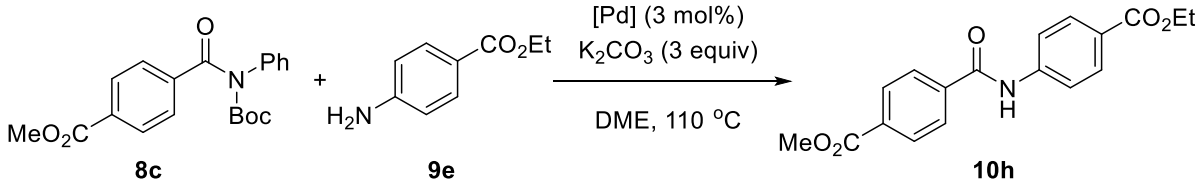
According to the general procedure, the reaction of *tert*-butyl benzoyl(phenyl)carbamate (0.10 mmol, 1.0 equiv), 4-amino-*N*-methylbenzenesulfonamide (2.0 equiv), K_2CO_3 (3.0 equiv), Pd(II)–NHC (3.0 mol%) in DME (0.25 M) for 16 h at 110 °C, afforded after the standard work-up as described above and chromatography the title compound. White solid. ^{1}H NMR (500 MHz, DMSO-d^6) δ 10.56 (s, 1H), 8.00 – 7.92 (m, 4H), 7.74 (d, J = 8.7 Hz, 2H), 7.60 (t, J = 7.3 Hz, 1H), 7.53 (t, J = 7.5 Hz, 2H), 7.30 (q, J = 5.0 Hz, 1H), 2.38 (d, J = 5.0 Hz, 3H). ^{13}C NMR (125 MHz, DMSO-d^6) δ 166.53, 143.22, 134.97, 134.02, 132.43, 128.95, 128.28, 128.15, 120.45, 29.14.

Ethyl 4-(4-methoxybenzamido)benzoate (10g, Table 2)



According to the general procedure, the reaction of *tert*-butyl (4-methoxybenzoyl) (phenyl)carbamate (0.10 mmol, 1.0 equiv), ethyl 4-aminobenzoate (2.0 equiv), K_2CO_3 (3.0 equiv), Pd(II)–NHC (3.0 mol%) in DME (0.25 M) for 16 h at 110 °C, afforded after the standard work-up as described above and chromatography the title compound. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, J = 8.3 Hz, 2H), 7.99 (s, 1H), 7.85 (d, J = 8.2 Hz, 2H), 7.73 (d, J = 8.0 Hz, 2H), 6.97 (d, J = 8.5 Hz, 2H), 4.36 (q, J = 6.4 Hz, 2H), 3.87 (s, 3H), 1.39 (t, J = 6.8 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.18, 165.27, 162.79, 142.28, 130.85, 129.03, 126.66, 125.97, 119.07, 114.10, 60.89, 55.52, 14.37.

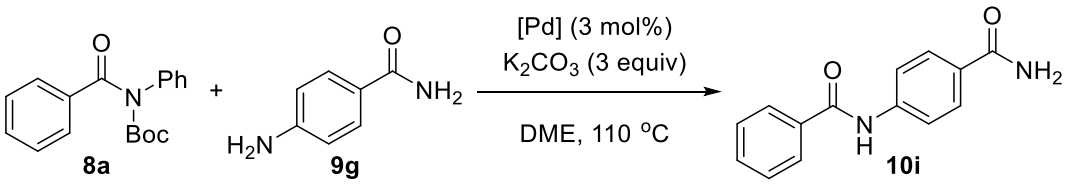
Ethyl 4-(4-(methoxycarbonyl)benzamido)benzoate (10h, Table 2)



According to the general procedure, the reaction of methyl 4-((*tert*-butoxycarbonyl) (phenyl)carbamoyl)benzoate (0.10 mmol, 1.0 equiv), ethyl 4-aminobenzoate (2.0 equiv), K_2CO_3 (3.0 equiv), Pd(II)–NHC (3.0 mol%) in DME (0.25 M) for 16 h at 110 °C, afforded after the

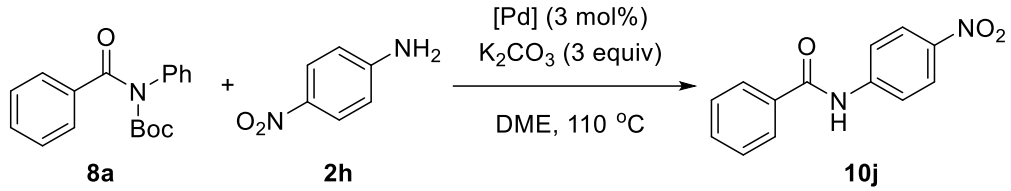
standard work-up as described above and chromatography the title compound. White solid. ^{1}H NMR (500 MHz, DMSO-d^6) δ 10.74 (s, 1H), 8.13 – 8.06 (m, 4H), 7.97 (q, J = 9.0 Hz, 4H), 4.31 (dd, J = 14.1, 7.0 Hz, 2H), 3.91 (s, 3H), 1.33 (t, J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, DMSO-d^6) δ 166.12, 165.79, 165.62, 143.78, 139.10, 132.75, 130.57, 129.68, 128.71, 125.34, 120.16, 60.97, 52.91, 14.68.

N-(4-Carbamoylphenyl)benzamide (10i, Table 2)



According to the general procedure, the reaction of *tert*-butyl benzoyl(phenyl)carbamate (0.10 mmol, 1.0 equiv), 4-aminobenzamide (2.0 equiv), K_2CO_3 (3.0 equiv), Pd(II)–NHC (3.0 mol%) in DME (0.25 M) for 16 h at 110 °C, afforded after the standard work-up as described above and chromatography the title compound. White solid. ^{1}H NMR (500 MHz, DMSO-d^6) δ 10.46 (s, 1H), 7.98 (d, J = 7.3 Hz, 2H), 7.93 – 7.80 (m, 5H), 7.61 (t, J = 7.2 Hz, 1H), 7.54 (t, J = 7.4 Hz, 2H), 7.26 (s, 1H). ^{13}C NMR (125 MHz, DMSO-d^6) δ 167.90, 166.34, 142.40, 135.05, 132.08, 129.41, 128.86, 128.67, 128.23, 119.90.

N-(4-Nitrophenyl)benzamide (10j, Table 2)



According to the general procedure, the reaction of *tert*-butyl benzoyl(phenyl)carbamate (0.10 mmol, 1.0 equiv), 4-nitroaniline (2.0 equiv), K_2CO_3 (3.0 equiv), Pd(II)–NHC (3.0 mol%) in DME (0.25 M) for 16 h at 110 °C, afforded after the standard work-up as described above and chromatography the title compound. White solid. ^{1}H NMR (500 MHz, DMSO-d^6) δ 10.82 (s, 1H), 8.28 (d, J = 9.1 Hz, 2H), 8.08 (d, J = 8.7 Hz, 2H), 7.99 (d, J = 7.6 Hz, 2H), 7.65 (t, J = 7.3 Hz, 1H), 7.57 (t, J = 7.5 Hz, 2H). ^{13}C NMR (125 MHz, DMSO-d^6) δ 166.84, 146.90, 142.92, 134.74, 132.63, 129.01, 128.38, 125.29, 120.30.

General Procedure for Determination of Kinetic Profiles.

An oven-dried vial equipped with a stir bar was charged with an amide substrate (neat, 1.0 equiv), amine (2.0 equiv), K_2CO_3 (3.0 equiv) and Pd(II)–NHC pre-catalyst (3 mol%), placed under a positive pressure of argon, and subjected to three evacuation/backfilling cycles. DME (0.25 M) was added with vigorous stirring at room temperature, the reaction mixture was placed in a preheated oil bath at 110 °C, and stirred for the indicated time at 110 °C. After the indicated time, the reaction mixture was diluted with ethyl acetate, filtered, and concentrated. The sample was analyzed by ^{1}H NMR ($CDCl_3$, 500 MHz) and GC-MS to obtain conversion, yield and selectivity using internal standard and comparison with authentic samples.

General Procedure for Determination of Turnover Number.

An oven-dried vial equipped with a stir bar was charged with an amide substrate (neat, 1.0 equiv), amine (2.0 equiv), K_2CO_3 (3.0 equiv) and Pd(II)–NHC pre-catalyst (0.25 mol%), placed under a positive pressure of argon, and subjected to three evacuation/backfilling cycles. DME (0.25 M) was added with vigorous stirring at room temperature, the reaction mixture was placed in a preheated oil bath at 110 °C, and stirred for the indicated time at 110 °C. After the indicated time, the reaction mixture was diluted with ethyl acetate, filtered, and concentrated. The sample was analyzed by ^{1}H NMR ($CDCl_3$, 500 MHz) and/or GC-MS to obtain conversion, selectivity and yield using internal standard and comparison with authentic samples.

References

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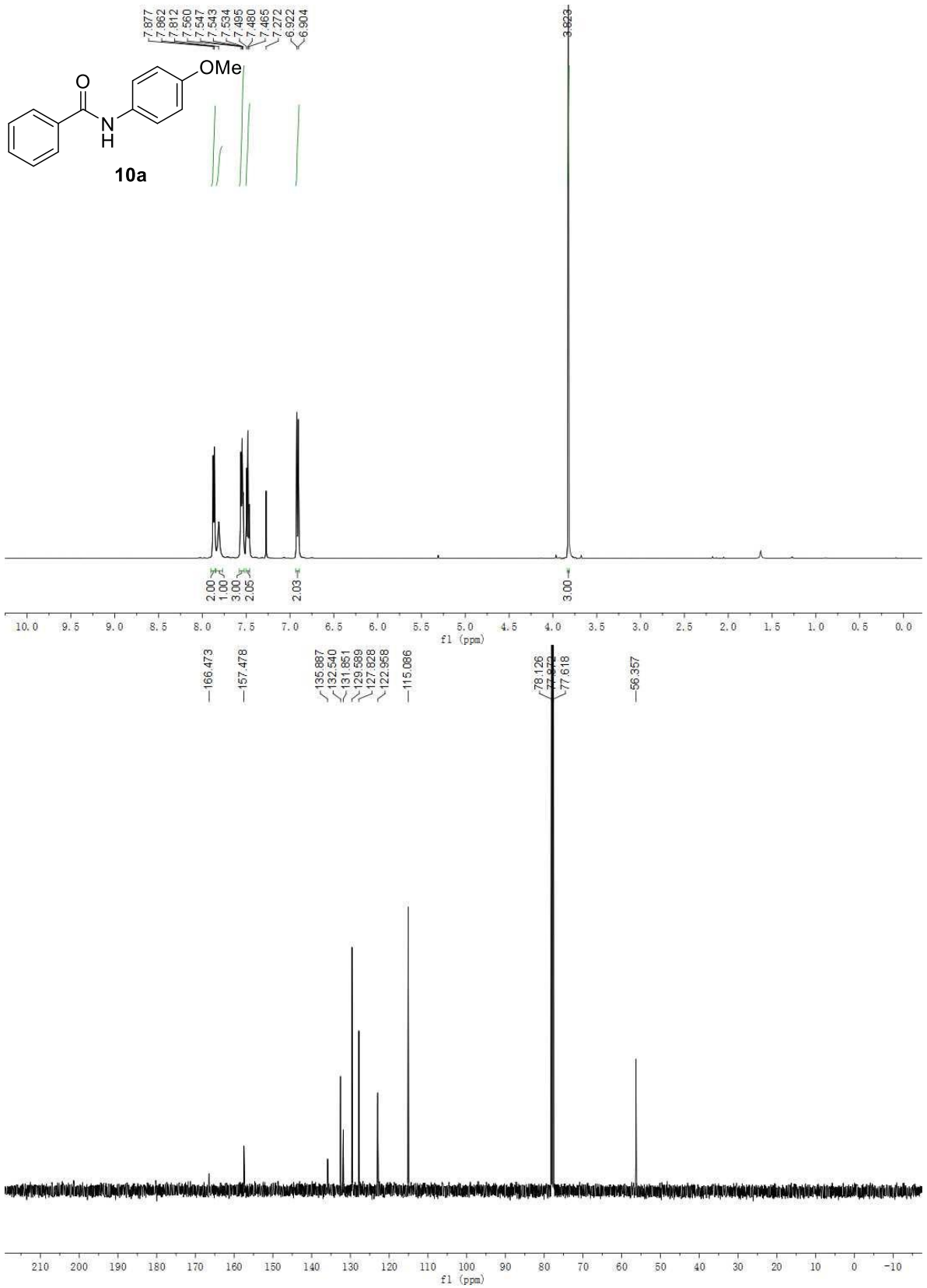
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1.00
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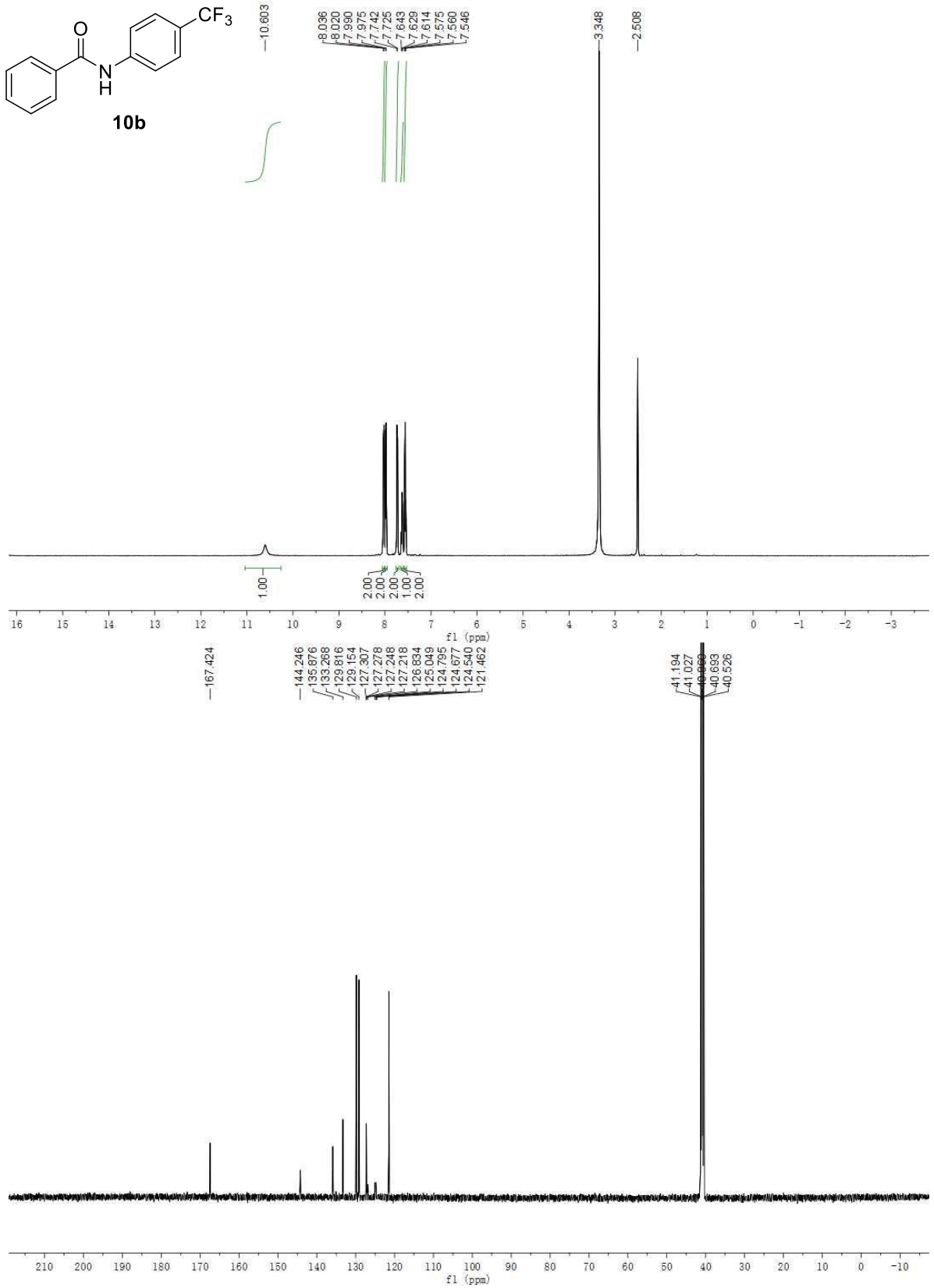
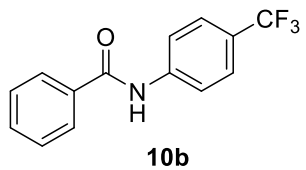
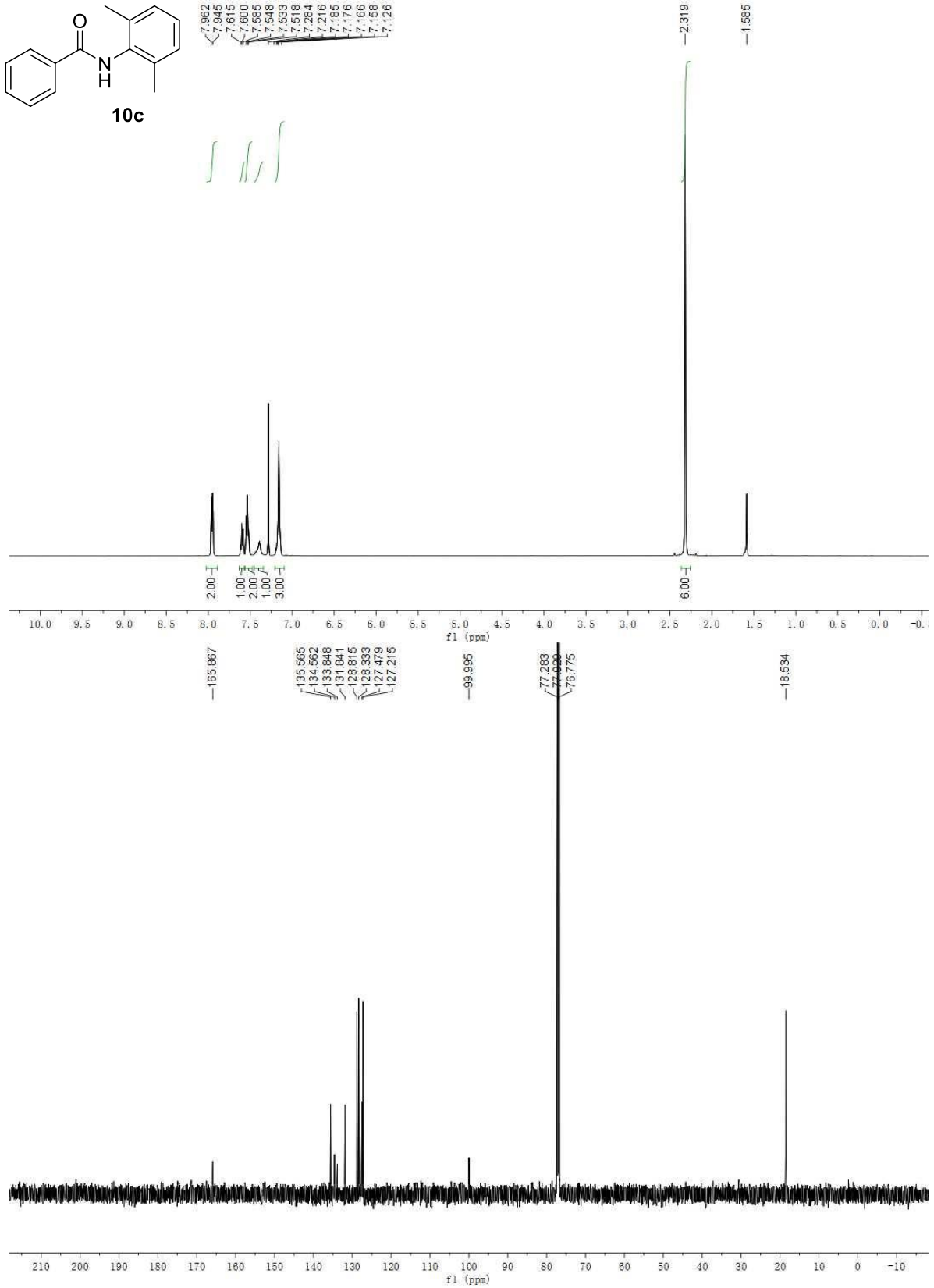
f1 (ppm)

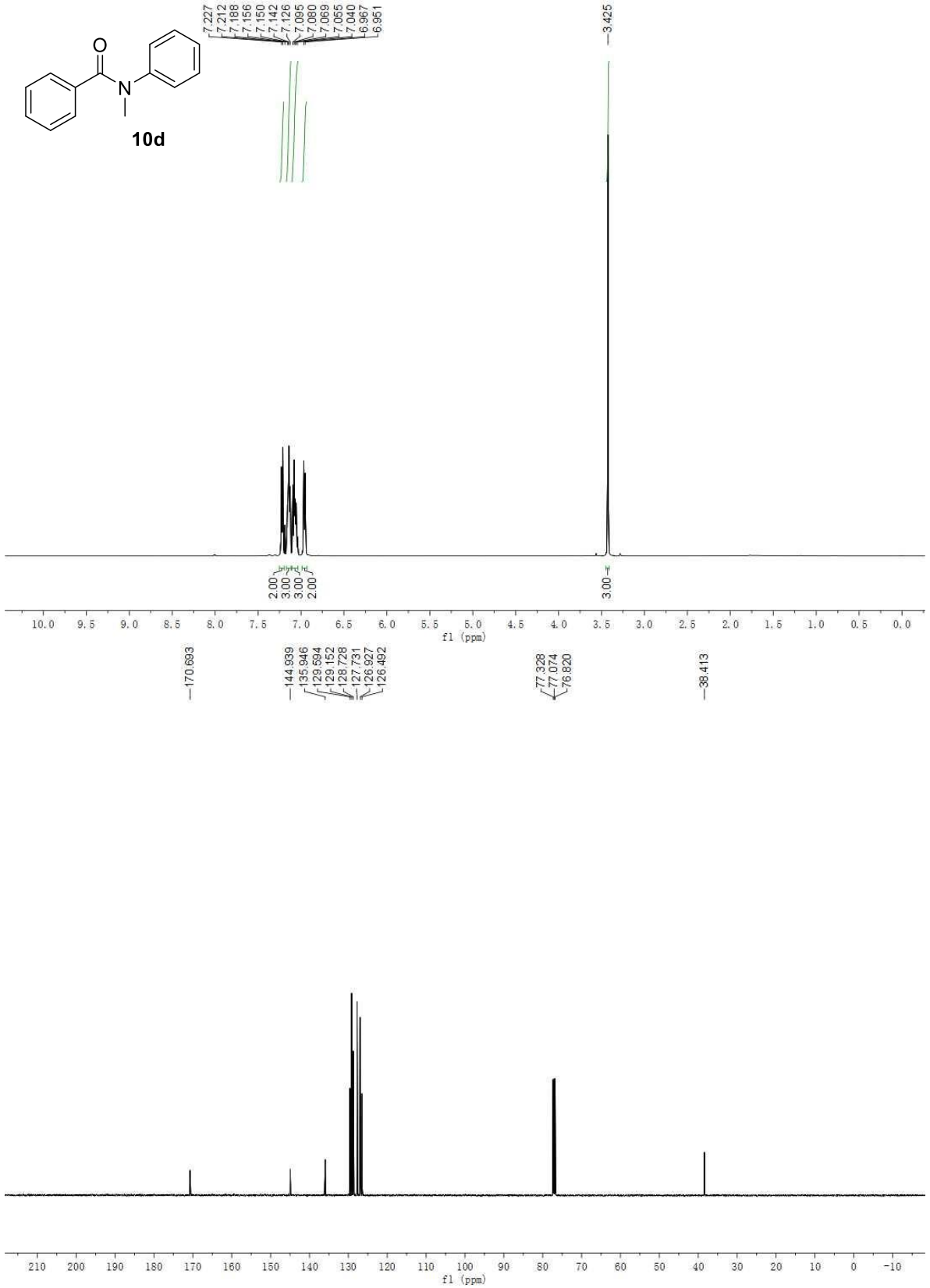

CF3
O
N
H
10b
10.603
8.036
8.020
7.990
7.975
7.742
7.725
7.643
7.629
7.614
7.575
7.560
7.546
3.348
2.508
1.00
2.00
2.00
2.00
1.00
2.00
f1 (ppm)
167.424
144.246
135.876
133.268
129.816
129.154
127.307
127.278
127.248
127.218
126.834
125.049
124.795
124.677
124.540
121.462
41.194
41.027
40.860
40.693
40.526
f1 (ppm)

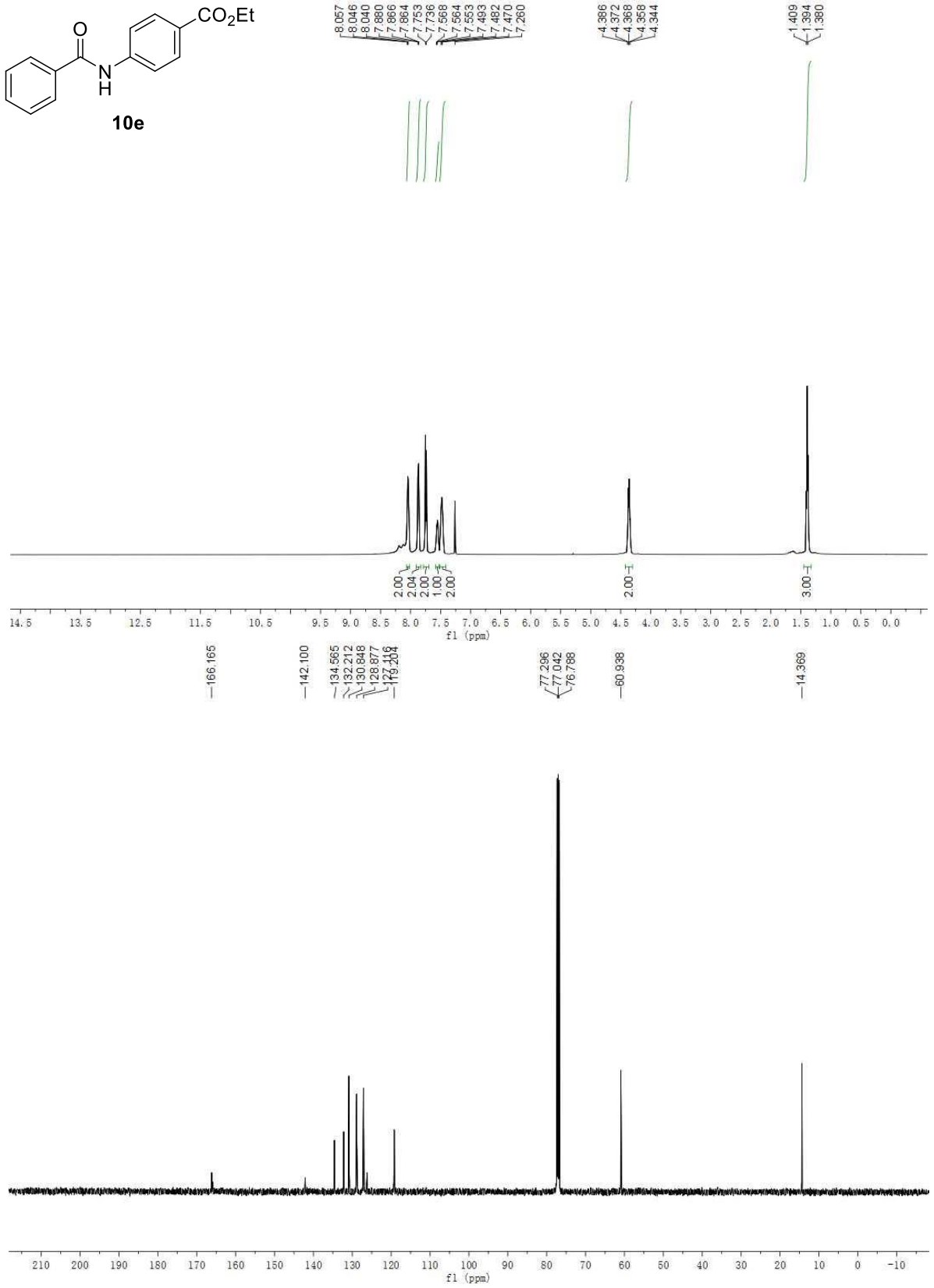

O
N
H
CF3

10b

-60.412
20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -110 -120
f1 (ppm)


10c
7.962
7.945
7.615
7.600
7.585
7.548
7.533
7.518
7.284
7.216
7.185
7.176
7.166
7.158
7.126
2.319
1.585
2.00
1.00
2.00
1.00
3.00
6.00
f1 (ppm)
165.867
135.565
134.562
133.848
131.841
128.815
128.333
127.479
127.215
99.995
77.283
77.000
76.775
18.534
f1 (ppm)


10d
7.227
7.212
7.188
7.156
7.150
7.142
7.126
7.095
7.080
7.069
7.055
7.040
6.967
6.951
3.425
2.00
3.00
3.00
2.00
3.00
f1 (ppm)
170.693
144.939
135.946
129.594
129.152
128.728
127.731
126.927
126.492
77.328
77.074
76.820
38.413
f1 (ppm)


CO2Et
O
N
H
10e
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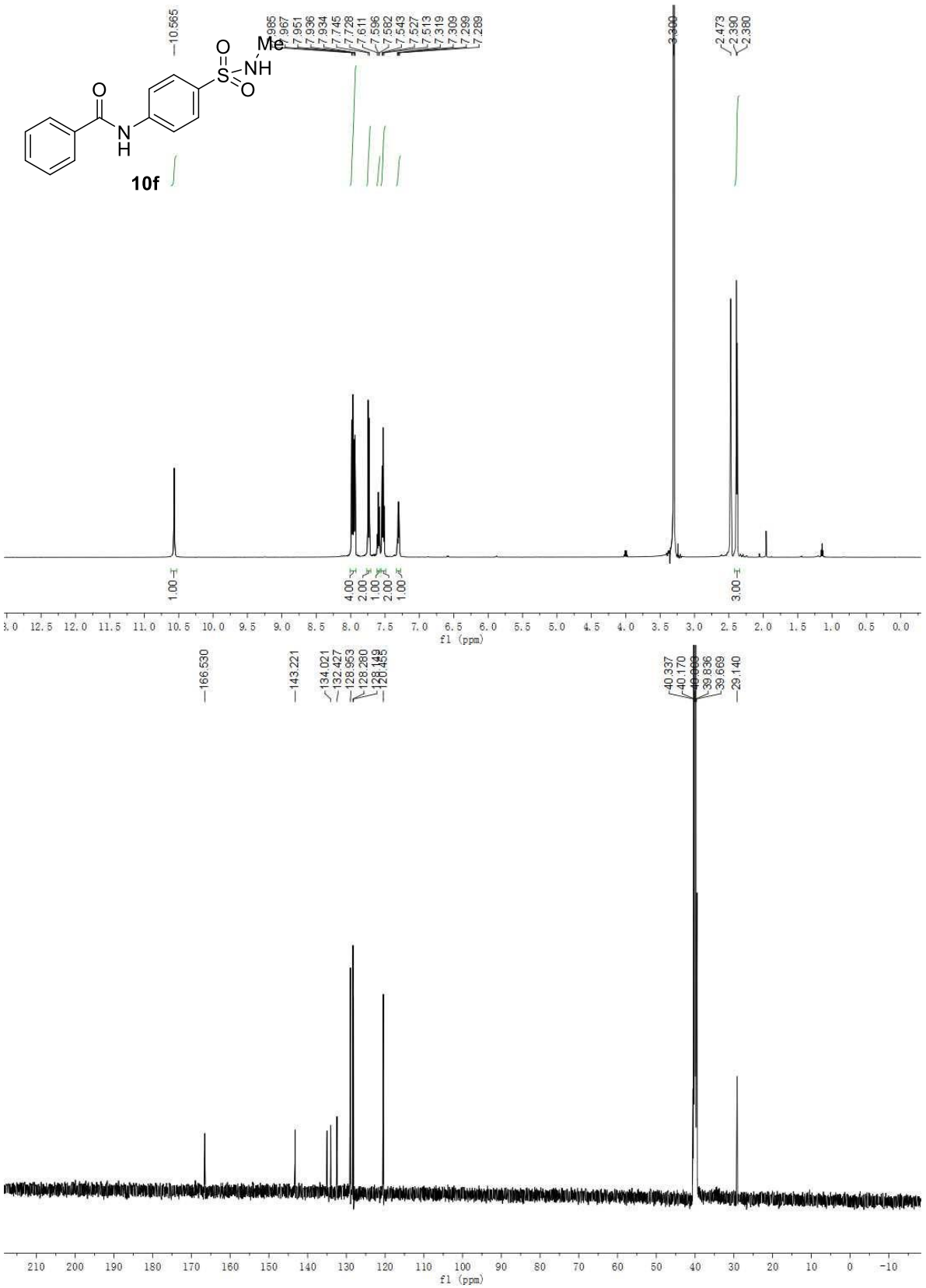
8.046
8.040
7.880
7.866
7.864
7.753
7.736
7.568
7.564
7.553
7.493
7.482
7.470
7.260
4.386
4.372
4.368
4.358
4.344
1.409
1.394
1.380
2.00
2.04
2.00
1.00
2.00
2.00
3.00
f1 (ppm)
166.165
142.100
134.565
132.212
130.848
128.877
127.116
119.204
77.296
77.042
76.788
60.938
14.369
f1 (ppm)


10f
10.565
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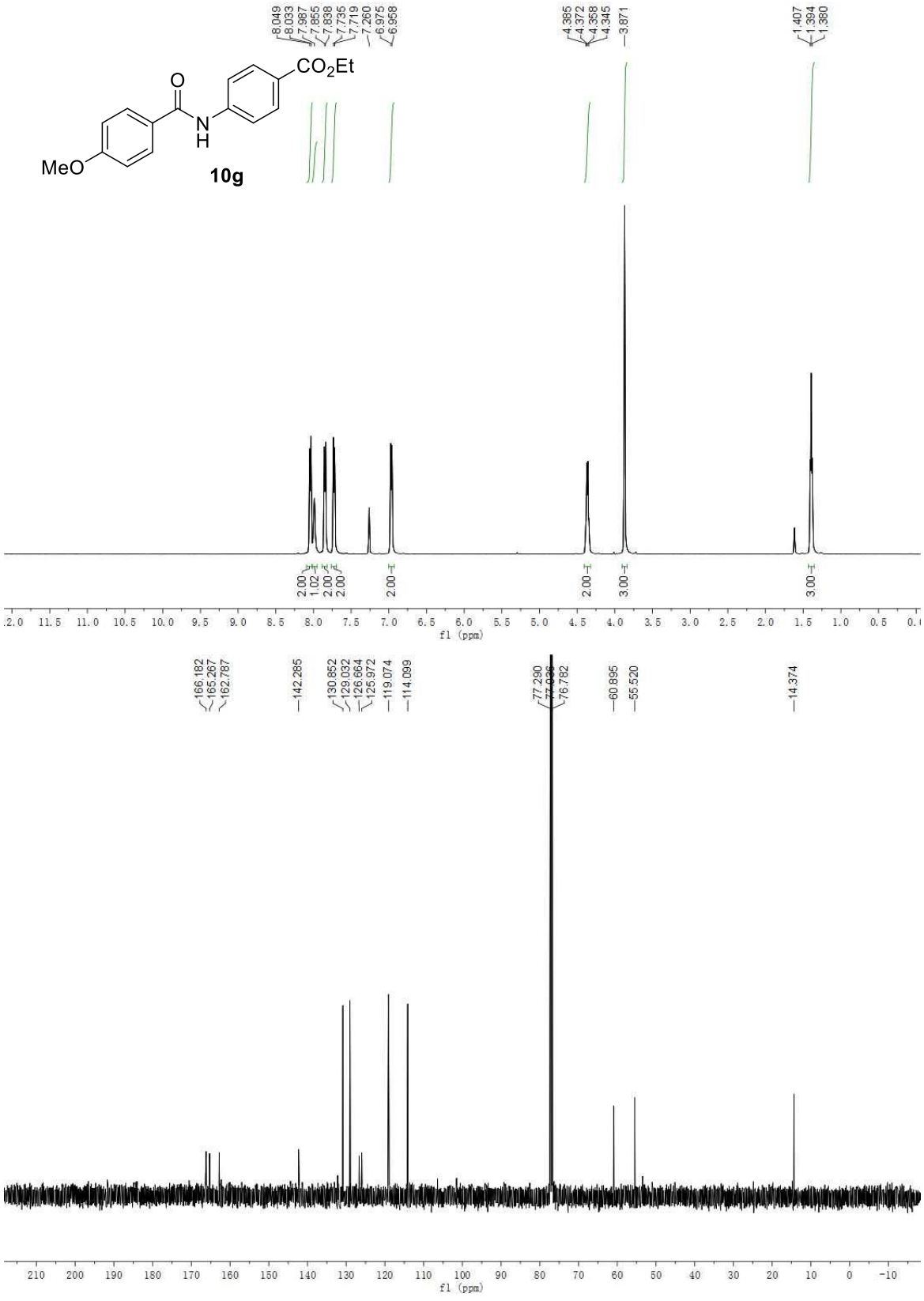
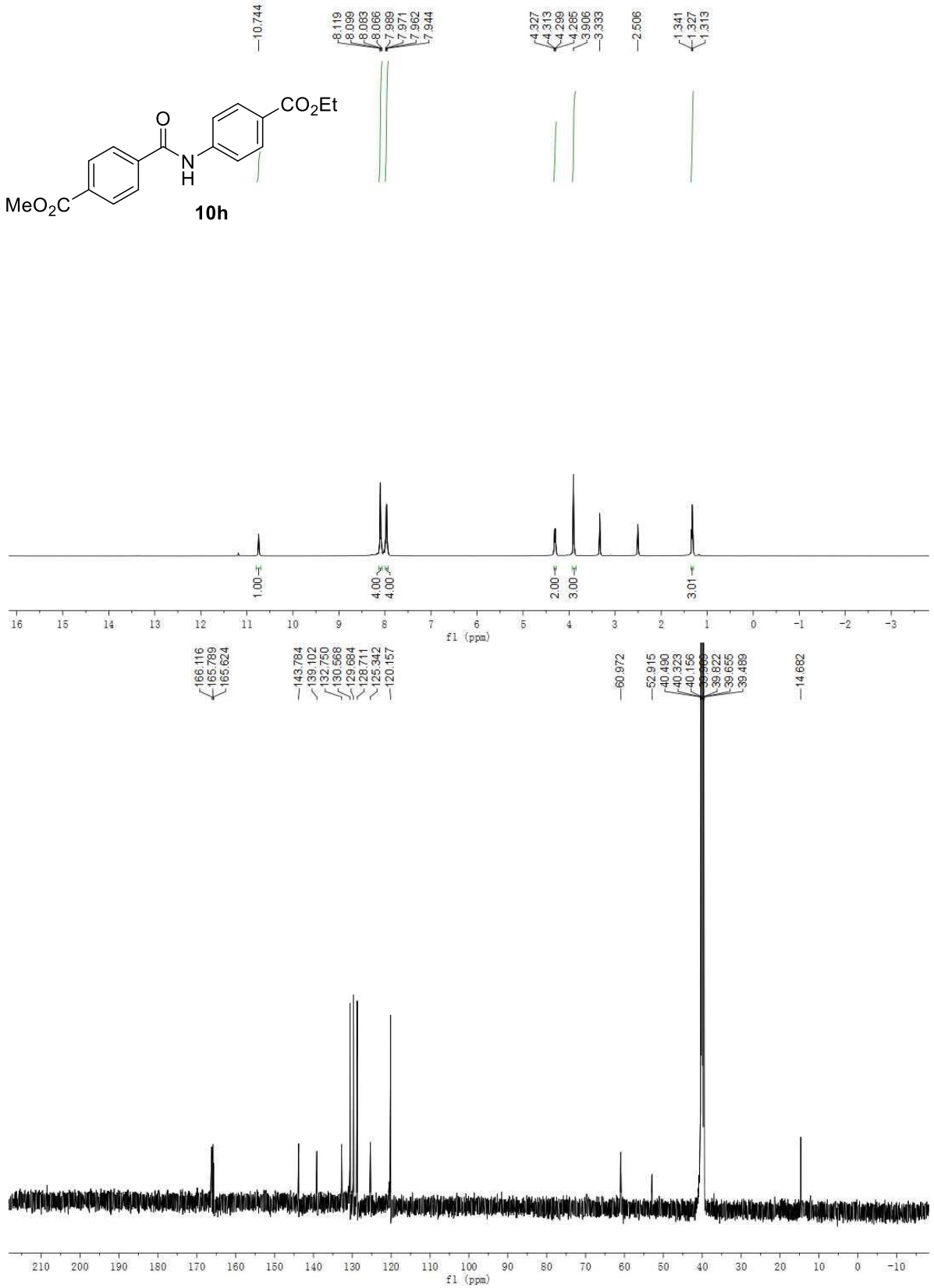
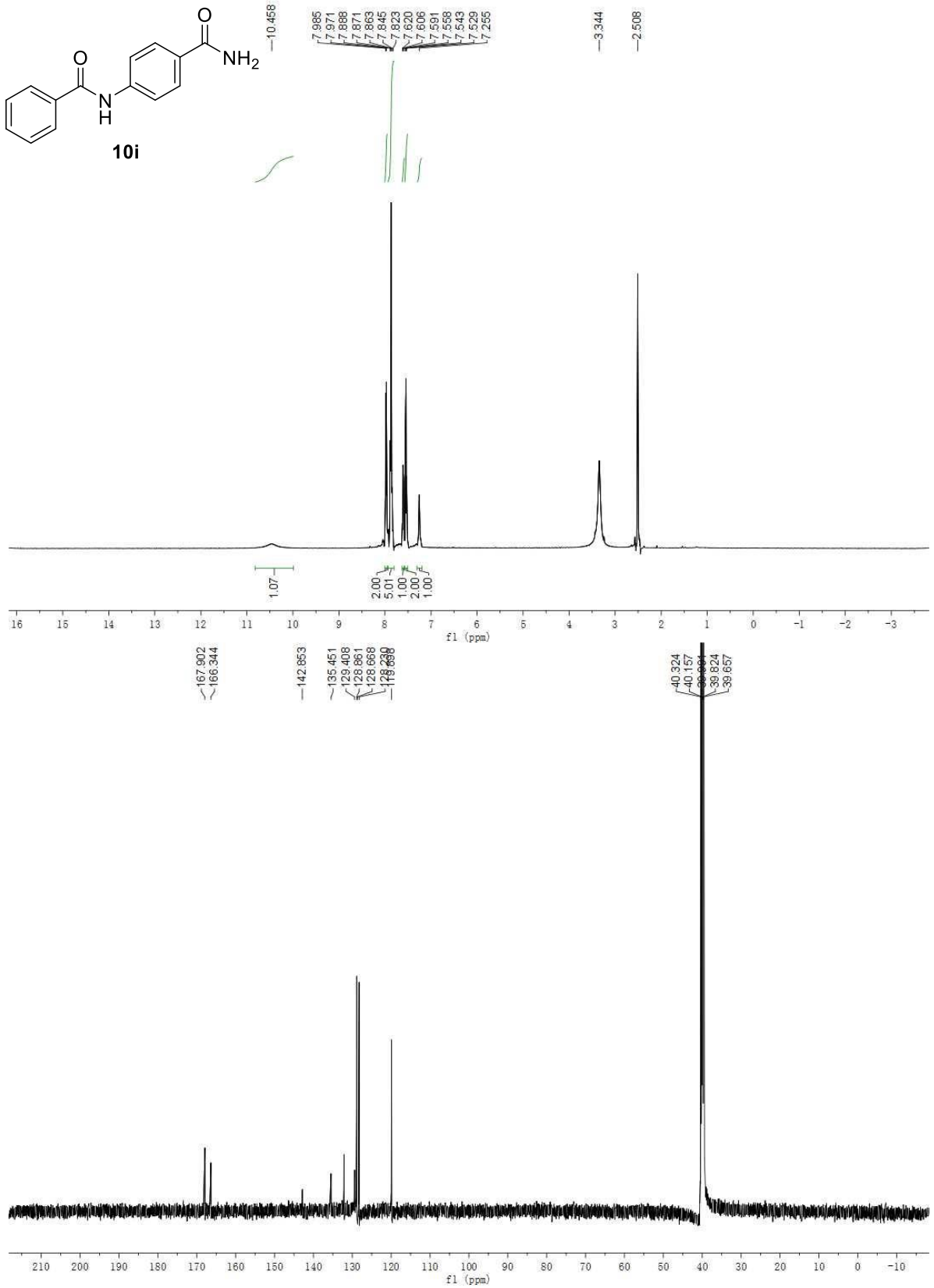
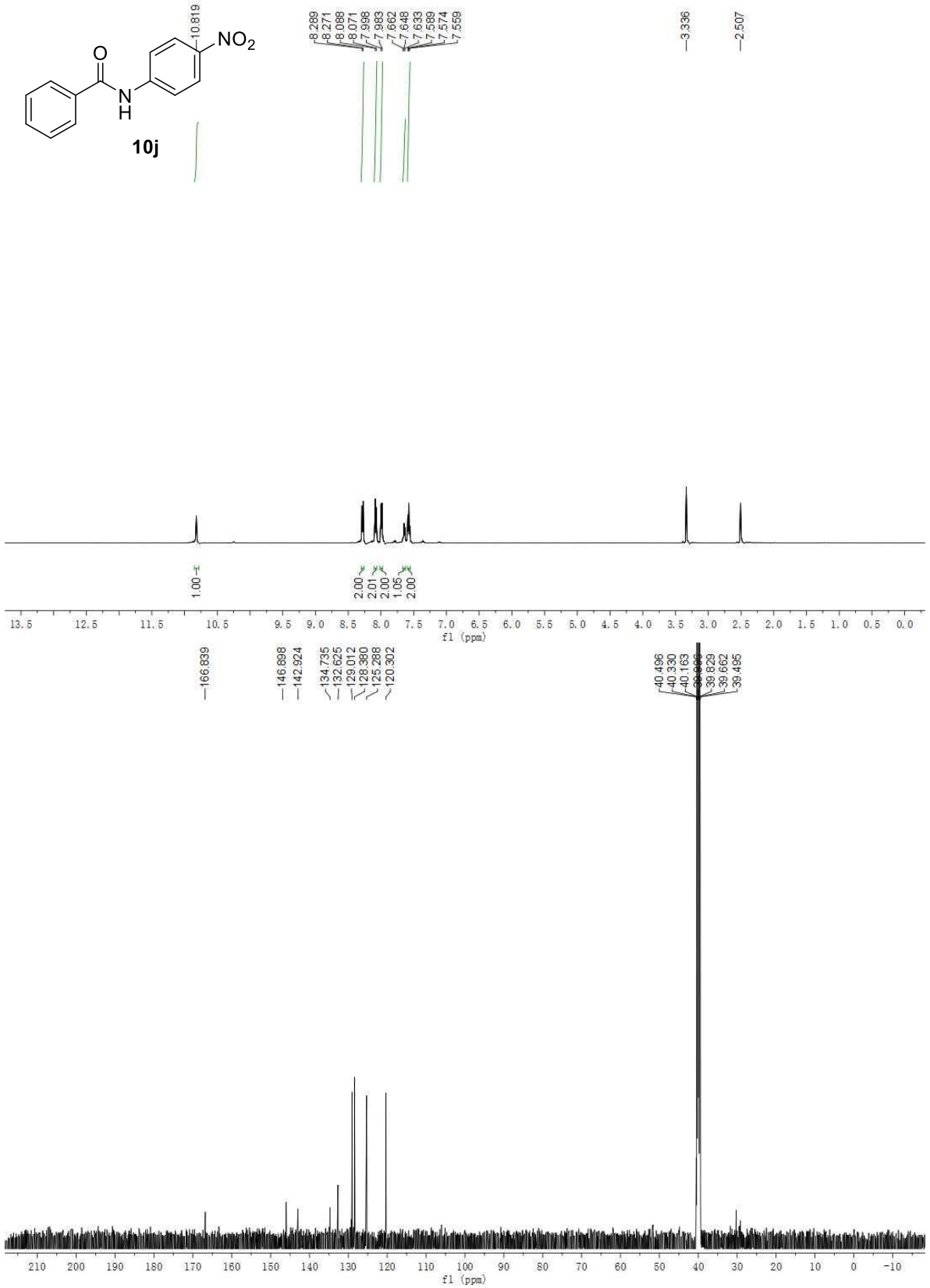
7.967
7.951
7.936
7.934
7.745
7.728
7.611
7.596
7.582
7.543
7.527
7.513
7.319
7.309
7.299
7.289
3.300
2.473
2.390
2.380
1.00
4.00
2.00
1.00
2.00
1.00
3.00
f1 (ppm)
166.530
143.221
134.021
132.427
128.953
128.280
128.149
120.453
40.337
40.170
40.003
39.836
39.669
29.140
f1 (ppm)


8.049
8.033
7.987
7.865
7.838
7.735
7.719
7.260
6.975
6.958
4.385
4.372
4.358
4.345
3.871
1.407
1.394
1.380
CO2Et
O
N
H
MeO
10g
2.00
1.02
2.00
2.00
2.00
2.00
3.00
3.00
f1 (ppm)
166.182
165.267
162.787
142.285
130.852
129.032
126.664
125.972
119.074
114.099
77.290
77.038
76.782
60.895
55.520
14.374
f1 (ppm)


10.744
8.119
8.099
8.083
8.066
7.989
7.971
7.962
7.944
4.327
4.313
4.299
4.285
3.906
3.333
2.506
1.341
1.327
1.313
CO2Et
O
N
H
MeO2C
10h
1.00
4.00
4.00
2.00
3.00
3.01
f1 (ppm)
166.116
165.789
165.624
143.784
139.102
132.750
130.568
129.684
128.711
125.342
120.157
60.972
52.915
40.490
40.323
40.156
39.822
39.655
39.489
14.682
f1 (ppm)


10i
10.458
7.985
7.971
7.888
7.871
7.863
7.845
7.823
7.620
7.606
7.591
7.558
7.543
7.529
7.255
3.344
2.508
1.07
2.00
5.01
1.00
2.00
1.00
f1 (ppm)
167.902
166.344
142.853
135.451
129.408
128.861
128.668
128.230
119.898
40.324
40.157
39.824
39.657
f1 (ppm)


10.819
8.289
8.271
8.088
8.071
7.998
7.983
7.662
7.648
7.633
7.589
7.574
7.559
3.336
2.507
NO2
O
N
H
10j
1.00
2.00
2.01
2.00
1.05
2.00
f1 (ppm)
166.839
146.898
142.924
134.735
132.625
129.012
128.380
125.268
120.302
40.496
40.330
40.163
39.829
39.662
39.495
f1 (ppm)

Computational Details

Computational Details: All DFT static calculations were performed at the GGA level with the Gaussian09 set of programs,[1] using the BP86 functional of Becke and Perdew.[2] The electronic configuration of the molecular systems was described with the standard split-valence basis set with a polarization function of Ahlrichs and co-workers for H, C, B, N, O and Cl (SVP keyword in Gaussian)[3] and Def2-QZVPP for K.[4] For Pd we used the quasi-relativistic Stuttgart/Dresden effective core potential,[5] with an associated valence basis set (standard SDD keywords in Gaussian09). Geometry optimizations were carried out without symmetry constraints, and the characterization of the stationary points was performed by analytical frequency calculations. These frequencies were used to calculate unscaled zero-point energies (ZPEs) as well as thermal corrections and entropy effects at 298 K and 1 atm by using the standard statistical mechanics relationships for an ideal gas. Moreover, we also included the D3 Grimme pairwise scheme to account for dispersion corrections in the BP86 geometry optimizations.[6] Energies were obtained via single-point calculations on the BP86-D3 optimized geometries using the M06 functional,[7] including solvent effects of DME solution estimated with the polarizable continuous solvation model (PCM) as implemented in Gaussian09.[9] In these single-point energy calculations, H, C, B, N, O and Cl were described by using the Def2-TZVP basis set that includes polarization functions,[8] Def2-QZVPP for K, whereas for the metal (Pd), the SDD basis set has been employed. On top of the M06/Def2-TZVP~sdd (PCM-DME)//BP86-D3/SVP~sdd energies, we added the ZPEs thermal and entropy corrections obtained at the BP86-D3/SVP~sdd level.

[1] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; et al. Gaussian 09; Gaussian Inc.: Wallingford, CT, USA, 2009.

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[3] Schäfer, A.; Huber, C.; Ahlrichs, R. *J. Chem. Phys.* **1994**, *100*, 5829.

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[5] (a) Kuechle,W.; Dolg, M.; Stoll, H.; Preuss, H. *J. Chem. Phys.* **1994**, *100*, 7535–7542. (b) Leininger, T.; Nicklass, A.; Stoll, H.; Dolg, M.; Schwerdtfeger, P. *J. Chem. Phys.* **1996**, *105*, 1052-1059.

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[8] Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.

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Table S1. Coordinate date sets, absolute energies (a.u.) for DFT optimized complexes.

[Pd(IPr)(allyl)Cl]			**[Pd(IPr)(allyl)Cl]-I**		
75			81		
I-PREallyl SCF Done: -1864.75392019 A.U.			I-PREallyl+K2CO3 SCF Done: -3328.52921378 A.U.		
Cl	-0.709969	-2.505458	1.379674	Cl	0.131379	-2.381145	0.909979
N	0.997658	-0.120581	-1.277778	N	-2.571071	-0.031694	0.433976
C	2.381771	-0.129609	-0.870968	C	-3.080284	-1.148411	-0.325736
N	-1.153026	0.112167	-1.157016	N	-1.288812	1.593684	1.075435
C	3.045737	1.119184	-0.749659	C	-3.225579	-0.978278	-1.729790
C	4.386455	1.096346	-0.317517	C	-3.737253	-2.067712	-2.460837
H	4.939042	2.041768	-0.209941	H	-3.863269	-1.979701	-3.550028
C	5.023157	-0.116345	-0.009433	C	-4.093924	-3.264851	-1.820784
H	6.070502	-0.111904	0.332467	H	-4.493388	-4.104033	-2.412401
C	4.332148	-1.331418	-0.123238	C	-3.939090	-3.399497	-0.434998
H	4.840049	-2.272641	0.135160	H	-4.213437	-4.347164	0.052481
C	2.989677	-1.367871	-0.553436	C	-3.420110	-2.346805	0.346831
C	2.339116	2.432025	-1.086088	C	-2.894349	0.350798	-2.411319
H	1.253669	2.271999	-0.912709	H	-2.038833	0.794612	-1.862662
C	2.773918	3.612380	-0.197755	C	-2.438174	0.197420	-3.870742
H	2.751041	3.352885	0.878684	H	-1.619351	-0.546318	-3.959089
H	2.096430	4.476740	-0.358690	H	-2.065190	1.169857	-4.254292
H	3.801035	3.956964	-0.442069	H	-3.264730	-0.120435	-4.541523
C	2.527559	2.794803	-2.575971	C	-4.077758	1.336135	-2.297063
H	3.602576	2.959956	-2.801616	H	-4.973438	0.943702	-2.824131
H	1.975186	3.725293	-2.825676	H	-3.812922	2.316189	-2.747325
H	2.160627	1.993783	-3.246852	H	-4.355618	1.516414	-1.238731

C	2.231561	-2.681398	-0.706105
H	1.149084	-2.460731	-0.602084
C	2.559666	-3.700662	0.396659
H	3.599346	-4.086746	0.322929
H	1.873109	-4.567480	0.318864
H	2.409783	-3.253503	1.399513
C	2.469842	-3.268237	-2.114531
H	2.162351	-2.557672	-2.910086
H	1.887293	-4.203472	-2.250765
H	3.544309	-3.505099	-2.271756
C	-0.033425	-0.025790	-0.379212
C	0.530657	-0.074724	-2.592494
H	1.202173	-0.163243	-3.450939
C	-0.828557	0.081419	-2.515795
H	-1.591400	0.178701	-3.293027
C	-2.467182	0.400157	-0.633632
C	-2.704664	1.707205	-0.127202
C	-4.004132	1.992837	0.333020
H	-4.232882	2.993278	0.729255
C	-5.015354	1.019450	0.293417
H	-6.026277	1.265566	0.655607
C	-4.740963	-0.266351	-0.189435
H	-5.536365	-1.026970	-0.194339
C	-3.455047	-0.612552	-0.655415
C	-1.602350	2.766838	-0.113978
H	-0.645932	2.229977	0.049879
C	-1.501473	3.485393	-1.476019
H	-1.323723	2.766090	-2.301136
H	-0.659125	4.209923	-1.474022
H	-2.435850	4.042191	-1.701407
C	-1.729687	3.770101	1.043184
H	-2.606789	4.441935	0.928985
H	-0.829584	4.418667	1.083333
H	-1.822130	3.246842	2.017248
C	-3.162367	-2.019222	-1.170091
H	-2.060457	-2.152943	-1.149576
C	-3.748198	-3.109680	-0.253871
H	-3.408064	-2.961098	0.789553
H	-3.395827	-4.108420	-0.585085
H	-4.858962	-3.126307	-0.280364
C	-3.663626	-2.188865	-2.620445
H	-4.766429	-2.062715	-2.674756
H	-3.417717	-3.201754	-3.003124
H	-3.211437	-1.447163	-3.310240
C	1.106135	1.500306	2.252296
H	0.805210	2.481857	1.851388
H	2.174014	1.247711	2.114288
C	0.363913	0.953169	3.351118
H	-0.551388	1.472415	3.691021
C	0.598377	-0.376361	3.768829
H	1.600040	-0.832106	3.680797
Pd	0.102719	-0.281037	1.607829
H	-0.100541	-0.868336	4.462872

Zero-point correction=	0.624857 (Hartree/Particle)
Thermal correction to Energy=	0.663061
Thermal correction to Enthalpy=	0.664005
Thermal correction to Gibbs Free Energy=	0.554582
Sum of electronic and zero-point Energies=	-1864.129063

C	-3.269756	-2.497592	1.858623
H	-2.526701	-1.740773	2.187825
C	-2.722608	-3.877406	2.270208
H	-3.462953	-4.686694	2.091965
H	-2.490178	-3.882595	3.355585
H	-1.792798	-4.111278	1.716528
C	-4.613931	-2.222101	2.569326
H	-5.016194	-1.215643	2.336910
H	-4.497216	-2.294872	3.671214
H	-5.380091	-2.963940	2.257443
C	-1.278062	0.427298	0.353760
C	-3.365551	0.831475	1.193725
H	-4.429119	0.641030	1.359597
C	-2.553753	1.854504	1.604379
H	-2.756576	2.741474	2.210613
C	-0.174034	2.510256	1.065364
C	-0.224796	3.583174	0.139458
C	0.911922	4.412301	0.053557
H	0.914802	5.258406	-0.650987
C	2.049623	4.150611	0.830404
H	2.943268	4.785423	0.723917
C	2.068224	3.076487	1.734070
H	2.981708	2.874371	2.309167
C	0.948158	2.235554	1.887825
C	-1.464165	3.853785	-0.716499
H	-2.092582	2.938812	-0.705201
C	-2.297787	4.999264	-0.101142
H	-2.570707	4.786057	0.952301
H	-3.235396	5.161579	-0.673959
H	-1.722261	5.949388	-0.107451
C	-1.147324	4.149125	-2.194651
H	-0.565182	5.086333	-2.318379
H	-2.090222	4.273467	-2.767575
H	-0.572453	3.325700	-2.661435
C	0.921474	1.086502	2.896827
H	0.518639	0.195407	2.363900
C	2.311091	0.708236	3.430845
H	3.030446	0.507023	2.607708
H	2.224060	-0.198596	4.068624
H	2.730053	1.506322	4.081785
C	-0.032426	1.410582	4.070126
H	0.322058	2.306487	4.623582
H	-0.064445	0.559659	4.782765
H	-1.071493	1.603511	3.737218
C	0.841477	0.983900	-2.021265
H	0.869500	2.045257	-1.729223
H	0.203692	0.748730	-2.893784
C	1.997804	0.181616	-1.734415
H	2.855669	0.605492	-1.175775
C	1.913914	-1.219521	-1.883286
H	1.236142	-1.682479	-2.624692
Pd	0.306797	-0.452335	-0.540029
H	2.724648	-1.844128	-1.466666
O	4.732887	-1.950695	-0.318713
C	4.695978	-0.632570	-0.046298
O	4.182745	-0.243029	1.066561
O	5.132430	0.197425	-0.941158
K	3.124223	-2.420503	1.610784
K	5.724036	-1.511308	-2.532496

Zero-point correction=	0.642142 (Hartree/Particle)
Thermal correction to Energy=	0.688977
Thermal correction to Enthalpy=	0.689922
Thermal correction to Gibbs Free Energy=	0.556232
Sum of electronic and zero-point Energies=	-3327.887072

Sum of electronic and thermal Energies= -1864.090859 Sum of electronic and thermal Enthalpies= -1864.089915 Sum of electronic and thermal Free Energies= -1864.199339 SCF Done (in solvent): -1865.0159802	Sum of electronic and thermal Energies= -3327.840236 Sum of electronic and thermal Enthalpies= -3327.839292 Sum of electronic and thermal Free Energies= -3327.972982 SCF Done (in solvent): -3328.8407743

[Pd(IPr)(allyl)Cl]-I-II				**[Pd(IPr)(allyl)Cl]-II**			
81				81			
I-PREallyl--K2CO3 SCF Done: -3328.50414434 A.U.				I-PREallyl--K2CO3post SCF Done: -3328.56875991 A.U.			
Cl	1.233600	0.211450	-2.120580	Cl	1.427802	-0.996054	-1.872134
N	-1.100784	1.899909	0.501090	N	-0.114665	2.144044	-0.443588
C	0.210980	2.488925	0.625581	C	1.227536	2.421663	-0.018700
N	-2.736782	0.539755	0.094872	N	-2.029347	1.189620	-0.732004
C	1.029566	2.141644	1.737696	C	1.525805	2.368944	1.373153
C	2.263741	2.812636	1.870978	C	2.829706	2.737022	1.772835
H	2.921138	2.569993	2.718301	H	3.086957	2.717501	2.843029
C	2.667350	3.785515	0.938294	C	3.795640	3.139409	0.834038
H	3.622985	4.317418	1.079597	H	4.799481	3.443219	1.172872
C	1.860206	4.073604	-0.172891	C	3.482592	3.151286	-0.535597
H	2.194218	4.818813	-0.911997	H	4.249252	3.453670	-1.266736
C	0.621552	3.421328	-0.362505	C	2.198577	2.778649	-0.994530
C	0.586359	1.091087	2.752897	C	0.482916	1.985364	2.422388
H	0.110651	0.283098	2.153643	H	-0.347118	1.472599	1.896445
C	1.746153	0.445655	3.528592	C	1.025629	0.967976	3.442875
H	2.557069	0.074403	2.864726	H	1.433352	0.067504	2.936326
H	1.364256	-0.419751	4.109149	H	0.203707	0.637856	4.111710
H	2.200168	1.147354	4.262060	H	1.820456	1.397296	4.089880
C	-0.480864	1.662654	3.711448	C	-0.089525	3.250478	3.093729
H	-0.066151	2.504053	4.307281	H	0.698248	3.815528	3.637270
H	-0.820675	0.877327	4.417930	H	-0.878224	2.974099	3.824545
H	-1.373596	2.032938	3.167101	H	-0.541413	3.932877	2.343218
C	-0.229144	3.744143	-1.590545	C	1.891436	2.774698	-2.491831
H	-1.028459	2.976977	-1.652817	H	0.918889	2.258230	-2.628094
C	0.575494	3.653809	-2.902316	C	2.933320	1.976211	-3.300633
H	1.371807	4.427300	-2.955021	H	3.948392	2.422901	-3.232112
H	-0.097030	3.819614	-3.770103	H	2.652099	1.966033	-4.374348
H	1.032472	2.648841	-3.002225	H	2.966630	0.922586	-2.957656
C	-0.893844	5.131177	-1.450069	C	1.767321	4.216114	-3.031879
H	-1.505695	5.212481	-0.528777	H	1.008081	4.805798	-2.478921
H	-1.554491	5.339103	-2.317850	H	1.480371	4.209961	-4.104220
H	-0.125697	5.933141	-1.409507	H	2.734124	4.756473	-2.942527
C	-1.359958	0.587180	0.152205	C	-0.746448	0.920969	-0.293963
C	-2.283524	2.633598	0.656873	C	-0.979220	3.125144	-0.949481
H	-2.276347	3.688590	0.943997	H	-0.655166	4.155888	-1.118161
C	-3.315895	1.777001	0.387912	C	-2.189025	2.515206	-1.139617
H	-4.398969	1.932153	0.373125	H	-3.146043	2.900502	-1.504267
C	-3.465233	-0.660674	-0.221525	C	-3.110908	0.259569	-0.542069
C	-4.167816	-1.321328	0.821654	C	-3.937613	0.438425	0.595368
C	-4.853243	-2.506337	0.488094	C	-4.985219	-0.485362	0.789227
H	-5.404111	-3.054876	1.266122	H	-5.645598	-0.378256	1.664490
C	-4.837038	-3.007086	-0.823366	C	-5.183651	-1.547818	-0.104211
H	-5.380305	-3.935885	-1.060683	H	-6.006174	-2.260967	0.065245
C	-4.134879	-2.331283	-1.829928	C	-4.327780	-1.715356	-1.204140
H	-4.133454	-2.731638	-2.855480	H	-4.483218	-2.563944	-1.888174
C	-3.428349	-1.142052	-1.553775	C	-3.265103	-0.821497	-1.443632
C	-4.118827	-0.805590	2.262038	C	-3.698576	1.561186	1.604767
H	-4.131871	0.305034	2.223024	H	-2.801993	2.128471	1.282025
C	-5.322643	-1.236364	3.116547	C	-4.881746	2.549649	1.631939
H	-6.288538	-0.994084	2.626395	H	-5.078263	2.971093	0.624105
H	-5.295285	-0.720142	4.098456	H	-4.675005	3.392833	2.324381
H	-5.310216	-2.326798	3.327255	H	-5.815000	2.054272	1.975064
C	-2.789588	-1.213126	2.934043	C	-3.380872	1.009519	3.008652
H	-2.711118	-2.318512	3.001045	H	-4.228148	0.424853	3.425215

H	-2.726250	-0.796796	3.961060
H	-1.918451	-0.853182	2.353460
C	-2.699882	-0.397933	-2.670781
H	-2.007428	0.330869	-2.204141
C	-1.820006	-1.332302	-3.519949
H	-1.123002	-1.898640	-2.868989
H	-1.200719	-0.736139	-4.219878
H	-2.422468	-2.049629	-4.118067
C	-3.709032	0.390425	-3.531704
H	-4.432992	-0.291427	-4.028114
H	-3.182754	0.964880	-4.323173
H	-4.291392	1.107337	-2.915313
C	-0.084262	-2.488432	1.162875
H	-0.980726	-3.132145	1.113476
H	0.152316	-2.130454	2.181846
C	0.994989	-2.731037	0.236611
H	0.877626	-3.487451	-0.561977
C	2.193861	-1.941288	0.283465
H	2.214760	-1.113804	1.008422
Pd	-0.018158	-0.868021	-0.201690
H	2.640459	-1.712589	-0.701201
O	5.280938	-1.591291	-0.391185
C	4.577918	-1.541090	0.698789
O	3.781418	-2.632839	0.956293
O	4.473620	-0.514534	1.428433
K	4.562526	-3.880177	-1.061402
K	3.824979	0.903938	-0.642179

Zero-point correction= 0.641920 (Hartree/Particle)
Thermal correction to Energy= 0.687759
Thermal correction to Enthalpy= 0.688703
Thermal correction to Gibbs Free Energy= 0.561125
Sum of electronic and zero-point Energies= -3327.862225
Sum of electronic and thermal Energies= -3327.816386
Sum of electronic and thermal Enthalpies= -3327.815442
Sum of electronic and thermal Free Energies= -3327.943019

SCF Done (in solvent): -3328.8053792

H	-3.171198	1.843191	3.711439
H	-2.492441	0.349655	2.977788
C	-2.327086	-1.014695	-2.631406
H	-1.413156	-0.416915	-2.441341
C	-1.854589	-2.474462	-2.762543
H	-1.459044	-2.822584	-1.785027
H	-1.038278	-2.539246	-3.511216
H	-2.669404	-3.159019	-3.081937
C	-2.977757	-0.498571	-3.930537
H	-3.904941	-1.063511	-4.168732
H	-2.280362	-0.605088	-4.788373
H	-3.251279	0.573733	-3.842484
C	-1.215300	-1.736952	1.805709
H	-2.291344	-1.745996	1.548010
H	-0.997272	-1.264496	2.784278
C	-0.352285	-2.799528	1.355941
H	-0.835986	-3.591302	0.740897
C	0.736450	-3.325125	2.270530
H	0.404817	-4.232829	2.823593
Pd	-0.123307	-0.946666	0.243535
H	1.045824	-2.554274	3.005717
O	3.661901	-3.050517	0.338108
C	2.940179	-2.810528	1.358011
O	1.906684	-3.755283	1.523980
O	3.020638	-1.844925	2.153947
K	1.633812	-3.844740	-1.130263
K	3.647386	-0.366103	0.136839

Zero-point correction= 0.643394 (Hartree/Particle)
Thermal correction to Energy= 0.689486
Thermal correction to Enthalpy= 0.690430
Thermal correction to Gibbs Free Energy= 0.562521
Sum of electronic and zero-point Energies= -3327.925366
Sum of electronic and thermal Energies= -3327.879274
Sum of electronic and thermal Enthalpies= -3327.878330
Sum of electronic and thermal Free Energies= -3328.006239

SCF Done (in solvent): -3328.8632747

[Pd(IPr)(allyl)Cl]-III

79

I-PREallyl+KCO3menysKClISOMERopen SCF Done: -2268.31153883 A.U.

N	-0.714797	1.170248	1.254371
C	-2.061300	1.338168	0.778871
N	1.371323	0.621422	1.352457
C	-2.286242	2.231127	-0.309595
C	-3.612052	2.360800	-0.774136
H	-3.830244	3.043645	-1.608755
C	-4.663698	1.638738	-0.178867
H	-5.692869	1.762223	-0.553207
C	-4.409423	0.766767	0.890314
H	-5.237742	0.201088	1.343218
C	-3.099987	0.589077	1.393310
C	-1.138465	3.036355	-0.920750
H	-0.243388	2.376752	-0.914115
C	-1.364806	3.426223	-2.388328
H	-1.599030	2.534628	-3.007388
H	-0.441602	3.883261	-2.799806
H	-2.182534	4.167696	-2.514573
C	-0.809621	4.267794	-0.049732
H	-1.666140	4.974852	-0.019427
H	0.069913	4.806763	-0.460202
H	-0.568921	3.975358	0.992554
C	-2.840947	-0.349364	2.570958

[Pd(IPr)(allyl)Cl]-I'

79

I-PREallyl+KCO3menysKCl SCF Done: -2268.30105435 A.U.

N	-0.014677	1.530818	1.086377
C	-0.878140	2.490465	0.439644
N	1.371373	-0.117229	1.331095
C	-0.326182	3.258720	-0.620284
C	-1.174810	4.189342	-1.249856
H	-0.786763	4.804842	-2.075074
C	-2.508319	4.342123	-0.839047
H	-3.156871	5.073861	-1.347024
C	-3.021650	3.563035	0.206128
H	-4.073265	3.681085	0.507636
C	-2.221364	2.608112	0.865543
C	1.144322	3.128743	-1.021275
H	1.450753	2.082570	-0.817961
C	1.396358	3.355662	-2.520134
H	0.732038	2.713301	-3.134189
H	2.448338	3.103314	-2.769432
H	1.233405	4.411678	-2.824510
C	2.023634	4.049958	-0.149245
H	1.758866	5.117365	-0.307315
H	3.098457	3.920397	-0.397635
H	1.894605	3.824360	0.929578
C	-2.776155	1.778687	2.019335

H	-1.750120	-0.555106	2.598699
C	-3.553289	-1.708758	2.436494
H	-4.658769	-1.599554	2.481829
H	-3.259898	-2.362592	3.283715
H	-3.278589	-2.231201	1.494759
C	-3.236084	0.348150	3.893522
H	-2.721642	1.321368	4.032973
H	-2.988586	-0.298411	4.760876
H	-4.329101	0.546245	3.918471
C	0.273507	0.533087	0.531158
C	-0.234173	1.650994	2.476620
H	-0.872909	2.188580	3.182466
C	1.087453	1.297616	2.538746
H	1.849474	1.471944	3.304155
C	2.696497	0.226271	0.939176
C	3.523564	1.226999	0.372098
C	4.834131	0.854876	0.009514
H	5.506718	1.602144	-0.439884
C	5.282195	-0.460042	0.197849
H	6.311890	-0.733380	-0.083456
C	4.419553	-1.438933	0.717311
H	4.780819	-2.471698	0.825104
C	3.096156	-1.126660	1.090944
C	2.987341	2.621623	0.047580
H	2.034661	2.763522	0.599461
C	3.935652	3.752342	0.485813
H	4.182656	3.680058	1.565311
H	3.466974	4.742197	0.303843
H	4.890281	3.734801	-0.081161
C	2.648021	2.707285	-1.456984
H	3.563340	2.601569	-2.077426
H	2.174957	3.682697	-1.700357
H	1.943956	1.891480	-1.743505
C	2.117221	-2.190830	1.582680
H	1.145476	-2.002341	1.073149
C	2.522633	-3.622514	1.199659
H	2.784508	-3.697985	0.123924
H	1.661681	-4.295823	1.375907
H	3.389971	-3.989143	1.791226
C	1.869491	-2.099831	3.104407
H	2.809824	-2.272888	3.671259
H	1.131565	-2.869740	3.410073
H	1.464404	-1.113458	3.406511
C	0.458786	-0.994462	-3.382587
H	1.078554	-0.285546	-3.959363
H	-0.529135	-1.221368	-3.825690
C	1.060076	-1.909212	-2.499803
H	2.161853	-1.877056	-2.380750
C	0.437217	-3.213303	-2.036704
H	0.635274	-3.993534	-2.813308
Pd	0.350113	-0.222043	-1.353130
H	0.913071	-3.548631	-1.091471
O	-2.688511	-3.036072	-0.396954
C	-1.448313	-3.269718	-0.436398
O	-0.620699	-3.543826	0.435069
O	-0.968331	-3.131002	-1.834333
K	-2.711984	-1.058840	-1.896765

H	-2.110195	0.897962	2.135881
C	-4.191659	1.239151	1.751016
H	-4.936547	2.060823	1.673612
H	-4.510493	0.597734	2.600427
H	-4.216839	0.615882	0.833143
C	-2.741793	2.603423	3.326943
H	-1.726194	2.982439	3.565213
H	-3.088587	1.992053	4.186963
H	-3.410882	3.487096	3.246535
C	0.445279	0.400517	0.458798
C	0.607743	1.712734	2.323083
H	0.374625	2.565418	2.966493
C	1.479608	0.668285	2.482908
H	2.170082	0.415294	3.292639
C	2.288074	-1.166279	0.963584
C	3.590169	-0.776478	0.561956
C	4.484193	-1.797129	0.175885
H	5.506501	-1.532608	-0.137596
C	4.078959	-3.137798	0.163347
H	4.786195	-3.922099	-0.150723
C	2.770811	-3.487939	0.536525
H	2.469457	-4.544636	0.502707
C	1.839640	-2.513475	0.948333
C	4.029794	0.687935	0.513283
H	3.150165	1.321673	0.744897
C	5.098146	0.979757	1.586864
H	4.731773	0.720355	2.601756
H	5.374651	2.055137	1.584894
H	6.022841	0.391457	1.405149
C	4.510469	1.104633	-0.890626
H	5.407029	0.533322	-1.210969
H	4.781998	2.181036	-0.899276
H	3.715855	0.947332	-1.645568
C	0.411920	-2.872755	1.355445
H	-0.267052	-2.153162	0.844672
C	-0.036145	-4.258654	0.873287
H	0.065789	-4.351712	-0.226360
H	-1.110835	-4.389930	1.109899
H	0.523770	-5.084628	1.364613
C	0.217552	-2.737399	2.881530
H	0.861205	-3.459173	3.429749
H	-0.839242	-2.941483	3.154414
H	0.460252	-1.719122	3.245552
C	1.582706	-0.640879	-2.427357
H	2.490373	-1.036343	-1.943234
H	1.717157	0.311769	-2.973031
C	0.578918	-1.573514	-2.859360
H	0.679045	-2.635610	-2.568528
C	-0.669881	-1.109142	-3.323274
H	-0.759775	-0.140263	-3.845359
Pd	-0.208027	-0.376636	-1.269045
H	-1.511457	-1.810606	-3.424723
O	-4.047971	-1.357130	-0.197489
C	-2.793080	-1.365108	-0.495736
O	-2.165106	-0.204552	-0.565056
O	-2.144980	-2.472940	-0.717750
K	-4.205164	-3.775236	-0.429224

Zero-point correction=	0.641222 (Hartree/Particle)
Thermal correction to Energy=	0.683424
Thermal correction to Enthalpy=	0.684368
Thermal correction to Gibbs Free Energy=	0.566014
Sum of electronic and zero-point Energies=	-2267.670317
Sum of electronic and thermal Energies=	-2267.628115
Sum of electronic and thermal Enthalpies=	-2267.627170
Sum of electronic and thermal Free Energies=	-2267.745524

Zero-point correction=	0.640014 (Hartree/Particle)
Thermal correction to Energy=	0.682561
Thermal correction to Enthalpy=	0.683506
Thermal correction to Gibbs Free Energy=	0.563819
Sum of electronic and zero-point Energies=	-2267.661040
Sum of electronic and thermal Energies=	-2267.618493
Sum of electronic and thermal Enthalpies=	-2267.617549
Sum of electronic and thermal Free Energies=	-2267.737236

SCF Done (in solvent): -2268.5920949	SCF Done (in solvent): -2268.5827314

[Pd(IPr)(allyl)Cl]-I'-III				**[Pd(IPr)(allyl)Cl]-IV**			
79				66			
I-PREallyl+KCO3--C-O SCF Done: -2268.27120149 A.U.				IPr-Pd SCF Done: -1287.32550879 A.U.			
N	0.112606	1.252983	-1.439039	N	1.083488	0.011775	0.980144
C	1.430301	1.760953	-1.147199	C	2.454394	0.019288	0.542433
N	-1.781605	0.215598	-1.257141	N	-1.083488	-0.011591	0.980163
C	1.530938	3.001077	-0.473314	C	3.116703	-1.222713	0.378546
C	2.823498	3.490863	-0.196499	C	4.457045	-1.189010	-0.054636
H	2.936982	4.446378	0.339044	H	5.001787	-2.134189	-0.203840
C	3.960364	2.760595	-0.561963	C	5.102522	0.030594	-0.310780
H	4.963220	3.148226	-0.323013	H	6.150444	0.034894	-0.651006
C	3.830275	1.519681	-1.204651	C	4.418573	1.243899	-0.141619
H	4.737834	0.950117	-1.448786	H	4.932621	2.193488	-0.358504
C	2.563660	0.988328	-1.514233	C	3.077297	1.266108	0.290480
C	0.297954	3.734049	0.047109	C	2.382708	-2.547203	0.574846
H	-0.598677	3.267129	-0.411476	H	1.461285	-2.337495	1.158797
C	0.191374	3.515775	1.571208	C	1.934197	-3.100851	-0.794712
H	0.202042	2.428749	1.794720	H	1.303127	-2.349647	-1.322967
H	-0.747686	3.952216	1.971805	H	1.342678	-4.032445	-0.669684
H	1.048095	3.983307	2.101034	H	2.813765	-3.329151	-1.433977
C	0.279740	5.227128	-0.327297	C	3.205080	-3.579264	1.368283
H	1.117066	5.782179	0.146355	H	4.101657	-3.914786	0.805061
H	-0.663241	5.700028	0.019068	H	2.594233	-4.483523	1.571964
H	0.356839	5.372516	-1.425042	H	3.550098	-3.168463	2.339997
C	2.404501	-0.372048	-2.193639	C	2.311304	2.581340	0.408425
H	1.556027	-0.872086	-1.677049	H	1.357805	2.367860	0.936225
C	3.638907	-1.273433	-2.017153	C	1.941495	3.101268	-0.996542
H	4.501206	-0.919633	-2.621835	H	2.852916	3.325700	-1.590889
H	3.406816	-2.296923	-2.390785	H	1.333883	4.028134	-0.927513
H	3.956251	-1.316775	-0.952912	H	1.346967	2.329567	-1.538662
C	2.064026	-0.231808	-3.693614	C	3.070668	3.638234	1.232481
H	1.122196	0.326086	-3.858380	H	3.341411	3.254358	2.238149
H	1.944230	-1.232623	-4.161870	H	2.445760	4.546183	1.365248
H	2.877764	0.300602	-4.230983	H	4.007848	3.958127	0.729538
C	-0.578666	0.405368	-0.593346	C	-0.000004	0.000013	0.118410
C	-0.638253	1.591464	-2.567707	C	0.684858	0.007931	2.318510
H	-0.256807	2.274770	-3.332448	H	1.411130	0.015191	3.136826
C	-1.830514	0.925614	-2.460314	C	-0.684837	-0.007623	2.318521
H	-2.695495	0.879872	-3.129085	H	-1.411098	-0.014740	3.136850
C	-2.844008	-0.581235	-0.709149	C	-2.454395	-0.019211	0.542452
C	-3.965037	0.077052	-0.135316	C	-3.077211	-1.266073	0.290505
C	-4.942554	-0.730359	0.478903	C	-4.418483	-1.243953	-0.141610
H	-5.820742	-0.260809	0.945664	H	-4.932468	-2.193580	-0.358480
C	-4.812518	-2.128021	0.515294	C	-5.102508	-0.030695	-0.310796
H	-5.585346	-2.736657	1.011301	H	-6.150422	-0.035069	-0.651045
C	-3.712127	-2.750468	-0.088196	C	-4.457116	1.188955	-0.054657
H	-3.631059	-3.849031	-0.071093	H	-5.001916	2.134094	-0.203894
C	-2.706806	-1.990830	-0.721084	C	-3.116786	1.222747	0.378549
C	-4.079015	1.603626	-0.145452	C	-2.311163	-2.581273	0.408491
H	-3.652932	1.959354	-1.108167	H	-1.357602	-2.367719	0.936150
C	-5.529715	2.111742	-0.083711	C	-3.070410	-3.638084	1.232758
H	-6.168895	1.640287	-0.859116	H	-3.340962	-3.254119	2.238444
H	-5.553970	3.210322	-0.238137	H	-2.445504	-4.546039	1.365483
H	-5.993389	1.916735	0.906625	H	-4.007693	-3.957981	0.730009
C	-3.224775	2.230344	0.976622	C	-1.941515	-3.101338	-0.996467
H	-3.609884	1.928912	1.973180	H	-2.853000	-3.325760	-1.590719
H	-3.250461	3.338591	0.914241	H	-1.333957	-4.028238	-0.927420
H	-2.170840	1.898419	0.915109	H	-1.346972	-2.329714	-1.538686
C	-1.539707	-2.688494	-1.417518	C	-2.382840	2.547270	0.574834

H -0.884539 -1.902367 -1.845323 C -0.679316 -3.486429 -0.418805 H -0.262297 -2.795883 0.349060 H 0.158796 -3.983376 -0.958022 H -1.266116 -4.280901 0.089510 C -2.038398 -3.568065 -2.582444 H -2.674267 -4.403463 -2.219959 H -1.181157 -4.013598 -3.131106 H -2.639312 -2.978126 -3.305088 C -1.228014 0.073594 2.695916 H -2.234850 -0.381149 2.642715 H -1.254267 1.150712 2.948620 C -0.150402 -0.733189 3.258538 H -0.324001 -1.812145 3.427594 C 1.096840 -0.193288 3.678531 H 1.187866 0.898307 3.786324 Pd 0.051659 -0.353325 1.124380 H 1.733886 -0.781647 4.354090 O 4.050523 -1.600797 1.394734 C 2.905566 -1.054835 1.586371 O 2.722301 -0.159376 2.507898 O 1.891068 -1.446365 0.812247 K 3.063155 -3.564208 0.271634	H -1.461531 2.337624 1.158986 C -1.934049 3.100745 -0.794707 H -1.303021 2.349410 -1.322827 H -1.342410 4.032262 -0.669669 H -2.813493 3.329119 -1.434114 C -3.205355 3.579425 1.367989 H -4.101781 3.914954 0.804528 H -2.594517 4.483672 1.571746 H -3.550625 3.168715 2.339652 Pd -0.000032 -0.000112 -1.812866
Zero-point correction= 0.640145 (Hartree/Particle) Thermal correction to Energy= 0.681531 Thermal correction to Enthalpy= 0.682476 Thermal correction to Gibbs Free Energy= 0.565583 Sum of electronic and zero-point Energies= -2267.631056 Sum of electronic and thermal Energies= -2267.589670 Sum of electronic and thermal Enthalpies= -2267.588726 Sum of electronic and thermal Free Energies= -2267.705618 SCF Done (in solvent): -2268.5435554	Zero-point correction= 0.552882 (Hartree/Particle) Thermal correction to Energy= 0.585580 Thermal correction to Enthalpy= 0.586525 Thermal correction to Gibbs Free Energy= 0.487302 Sum of electronic and zero-point Energies= -1286.772627 Sum of electronic and thermal Energies= -1286.739928 Sum of electronic and thermal Enthalpies= -1286.738984 Sum of electronic and thermal Free Energies= -1286.838207 SCF Done (in solvent): -1287.489106

[Pd(IPr)(allyl)Cl]-V	**[Pd(IPr)(allyl)Cl]-V-VI**
107 I5 SCF Done: -2264.54452787 A.U. C -1.316556 1.567453 -1.822137 O -0.949184 1.402134 -2.974938 Pd 0.145211 0.177040 -0.192076 N -0.445798 2.205838 -0.788667 C -5.499902 0.981991 -0.866211 C -5.086897 1.419379 -2.137157 H -4.847456 0.331018 1.108499 C -4.537682 0.700599 0.120739 C -3.721176 1.596365 -2.407882 C -2.753468 1.342558 -1.410727 C -3.172770 0.866236 -0.149995 H -3.378540 1.934302 -3.397680 H -2.416909 0.588956 0.602722 H -6.571478 0.847974 -0.647365 H -5.832065 1.627764 -2.921467 C 0.907324 2.623496 -1.166360 O 1.400811 2.511631 -2.266675 O 1.469234 3.186261 -0.076002 C 2.926878 3.439995 -0.038418 C 3.273176 4.586473 -0.997205 H 3.068605 4.294653 -2.044284 H 2.677924 5.489640 -0.751773 H 4.348933 4.840294 -0.900402 C 3.142346 3.846838 1.423877 H 4.208759 4.094730 1.598145 H 2.524719 4.732024 1.676712 H 2.854286 3.016497 2.099019	107 I5-I6 SCF Done: -2264.54164124 A.U. C 0.323032 -1.326781 -1.466876 O 0.034787 -0.996669 -2.609283 Pd -0.227553 0.015703 0.120799 N -0.973796 -1.900335 -0.424341 C 3.929303 -3.597415 -0.689887 C 3.314373 -3.618641 -1.955354 H 3.866736 -2.769653 1.326122 C 3.379175 -2.813708 0.340033 C 2.146471 -2.873816 -2.182690 C 1.584563 -2.098156 -1.145684 C 2.220038 -2.061153 0.109449 H 1.645432 -2.883862 -3.163056 H 1.797286 -1.408352 0.888667 H 4.843406 -4.185837 -0.509970 H 3.744503 -4.224999 -2.768742 C -2.296445 -1.658133 -0.873043 O -2.617165 -0.749519 -1.622020 O -3.146087 -2.554646 -0.309900 C -4.604077 -2.317007 -0.339234 C -5.125746 -2.397067 -1.781213 H -4.725556 -1.565334 -2.389202 H -4.818984 -3.357168 -2.243985 H -6.234430 -2.348888 -1.781023 C -5.143142 -3.476602 0.507235 H -6.248444 -3.419698 0.575089 H -4.864879 -4.449293 0.053977 H -4.720123 -3.439295 1.531181

C	3.677814	2.143518	-0.365224
H	3.587581	1.871636	-1.432324
H	4.751935	2.258481	-0.117866
H	3.272479	1.304389	0.233544
N	-0.415973	-2.712452	0.466580
N	1.689636	-2.402954	0.083258
C	0.491902	-1.724024	0.148814
C	0.198295	-3.963890	0.581323
C	1.531654	-3.767280	0.339755
C	-1.818474	-2.501645	0.722720
C	-2.749990	-2.900700	-0.268071
C	-4.117188	-2.842865	0.070197
C	-4.527816	-2.397480	1.334062
C	-3.585320	-1.932711	2.264628
C	-2.206753	-1.958280	1.975899
C	-2.279238	-3.270210	-1.673713
H	-5.600601	-2.374278	1.583445
C	-1.165217	-1.396991	2.943054
C	2.970209	-1.767641	-0.088772
C	3.666700	-1.358771	1.076968
C	4.957585	-0.821907	0.904988
C	5.511555	-0.679317	-0.376489
C	4.777234	-1.048277	-1.513148
C	3.488103	-1.608169	-1.396598
C	2.993820	-1.389137	2.448195
H	6.520986	-0.253467	-0.491972
C	2.651802	-1.950702	-2.625882
H	-0.371653	-4.866152	0.823146
H	2.379329	-4.458805	0.331080
H	-4.873083	-3.143833	-0.669454
H	-3.929731	-1.534231	3.230459
H	-1.306268	-3.799712	-1.574698
H	-0.384938	-0.930590	2.300424
H	5.529466	-0.491582	1.785713
H	5.211582	-0.898213	-2.513122
H	2.147330	-2.105074	2.395926
H	1.868264	-2.669731	-2.302406
C	1.927775	-0.683575	-3.130074
H	2.651293	0.101958	-3.430590
H	1.278576	-0.914044	-3.999483
H	1.281459	-0.250404	-2.331764
C	3.467273	-2.625461	-3.743906
H	2.792380	-2.961201	-4.558298
H	4.197467	-1.924860	-4.201817
H	4.028691	-3.508411	-3.372374
C	3.922497	-1.861037	3.580346
H	4.744490	-1.138733	3.769989
H	3.352233	-1.959253	4.527687
H	4.380855	-2.844902	3.349346
C	2.388699	0.000193	2.750041
H	1.812921	-0.015542	3.699829
H	3.188561	0.765425	2.841185
H	1.700237	0.311585	1.928665
C	-0.492793	-2.503542	3.781184
H	0.311850	-2.075999	4.416469
H	-1.229360	-3.000501	4.448585
H	-0.033944	-3.282946	3.139773
C	-1.711598	-0.272244	3.836830
H	-2.428357	-0.643749	4.600450
H	-0.875459	0.211612	4.384185
H	-2.219964	0.510781	3.236761
C	-3.237630	-4.210494	-2.423281
H	-4.190961	-3.703056	-2.682970
C	-4.910417	-0.962569	0.320507
H	-4.498060	-0.122400	-0.269136
H	-6.008057	-0.830208	0.411727
H	-4.468649	-0.923285	1.337422
N	-0.177808	2.941735	0.537501
C	-1.221360	3.301114	-2.142920
H	-0.173948	3.341764	-1.780442
C	-2.128868	3.099676	-0.932449
C	-1.610870	2.921737	0.374321
C	0.574422	1.805178	0.345202
C	-2.423978	2.636835	1.498501
C	-1.813334	2.300590	2.856873
H	-0.747854	2.613758	2.831808
C	-3.527247	3.018228	-1.086075
H	-3.965512	3.135369	-2.089265
C	-4.361791	2.761243	0.011120
H	-5.451555	2.692006	-0.133624
C	-3.814930	2.564795	1.288637
H	-4.479752	2.331189	2.134770
C	0.624666	4.064449	0.733643
C	-1.830558	0.771691	3.066333
H	-1.322672	0.488022	4.011881
H	-2.869688	0.381432	3.090563
H	-1.300202	0.258356	2.223629
C	-2.491228	3.042261	4.023535
H	-1.964332	2.828795	4.977013
H	-2.487788	4.140399	3.864080
H	-3.546769	2.723451	4.155658
C	-1.315550	2.101217	-3.107659
H	-2.320372	2.039333	-3.576996
H	-0.567997	2.208203	-3.921977
H	-1.132943	1.137953	-2.591173
C	-1.504949	4.639826	-2.852794
H	-1.400103	5.500789	-2.159583
H	-0.796959	4.786111	-3.695494
H	-2.532339	4.668428	-3.274201
C	1.923434	3.627143	0.661529
H	2.874089	4.161762	0.750398
H	0.202134	5.060866	0.893187
N	1.870351	2.250651	0.419232
C	3.014159	1.400576	0.198156
C	3.333865	1.028835	-1.135218
C	3.751382	0.965379	1.327134
C	4.475785	0.222125	-1.311791
C	4.889714	0.170581	1.087829
C	5.250658	-0.188926	-0.218359
H	4.755725	-0.106932	-2.322026
H	5.490731	-0.190619	1.935518
H	6.133817	-0.825041	-0.385841
C	2.466511	1.470866	-2.316464
H	1.410409	1.334927	-1.996337
C	3.262672	1.265677	2.745197
H	2.758377	2.256147	2.726025
C	2.673022	2.963793	-2.657011
H	1.989750	3.263947	-3.479160
H	2.467404	3.629946	-1.796350
H	3.715748	3.150280	-2.992515
C	2.654169	0.612792	-3.575988
H	1.882336	0.882978	-4.324221
H	3.649025	0.773821	-4.045360
H	2.530273	-0.464085	-3.354606
C	4.393856	1.351851	3.783870
H	3.992567	1.696647	4.759292

H	-2.778855	-4.537556	-3.379023
H	-3.482095	-5.116340	-1.829608
C	-2.018013	-1.976336	-2.480161
H	-1.639187	-2.214118	-3.495872
H	-2.950554	-1.383369	-2.583185
H	-1.270253	-1.325917	-1.977869
C	-1.095131	3.014805	0.240583
C	-0.957407	2.690992	1.601518
C	-1.877616	4.112350	-0.155528
C	-1.624222	3.457073	2.567975
H	-0.341600	1.815876	1.868773
C	-2.548505	4.873885	0.816320
H	-1.975659	4.349763	-1.225992
C	-2.426341	4.546732	2.177920
H	-1.523350	3.194805	3.632927
H	-3.174714	5.724492	0.504650
H	-2.957465	5.141396	2.937775

Zero-point correction= 0.878942 (Hartree/Particle)
Thermal correction to Energy= 0.933277
Thermal correction to Enthalpy= 0.934221
Thermal correction to Gibbs Free Energy= 0.790578
Sum of electronic and zero-point Energies= -2263.665586
Sum of electronic and thermal Energies= -2263.611251
Sum of electronic and thermal Enthalpies= -2263.610307
Sum of electronic and thermal Free Energies= -2263.753950

SCF Done (in solvent): -2265.0133024

H	4.866534	0.362725	3.962286
H	5.190308	2.057417	3.468556
C	2.198510	0.225642	3.167410
H	1.350072	0.197646	2.449083
H	2.642439	-0.792124	3.203033
H	1.794887	0.460682	4.175011
C	-0.702603	-3.077121	0.357327
C	-0.588886	-4.325806	-0.285689
C	-0.482536	-2.984276	1.744341
C	-0.246403	-5.468017	0.452325
H	-0.752309	-4.380393	-1.372636
C	-0.140957	-4.129386	2.481345
H	-0.561586	-1.997464	2.226196
C	-0.017811	-5.373687	1.837922
H	-0.146297	-6.438427	-0.059327
H	0.037655	-4.046700	3.565349
H	0.259865	-6.270118	2.414606

Zero-point correction= 0.878158 (Hartree/Particle)
Thermal correction to Energy= 0.932026
Thermal correction to Enthalpy= 0.932970
Thermal correction to Gibbs Free Energy= 0.790423
Sum of electronic and zero-point Energies= -2263.663483
Sum of electronic and thermal Energies= -2263.609616
Sum of electronic and thermal Enthalpies= -2263.608671
Sum of electronic and thermal Free Energies= -2263.751218

SCF Done (in solvent): -2264.9988566

[Pd(IPr)(allyl)Cl]-VI

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I6 SCF Done: -2264.56837771 A.U.

Pd	-0.225174	0.209134	0.140420
N	1.529440	2.579904	-0.109743
C	-0.049642	3.124061	-2.480238
H	0.596317	2.237196	-2.316189
C	-0.441881	3.661614	-1.108075
C	0.340589	3.385697	0.038638
C	1.483581	1.213821	-0.015992
C	-0.024180	3.784646	1.348371
C	0.746274	3.303472	2.577218
H	1.710963	2.873137	2.234484
C	-1.601593	4.437415	-0.917243
H	-2.241973	4.667874	-1.781253
C	-1.968154	4.889014	0.359278
H	-2.884332	5.487545	0.484876
C	-1.195926	4.555303	1.482199
H	-1.519525	4.881597	2.482996
C	2.837797	3.042064	-0.225128
C	-0.034604	2.166598	3.272305
H	0.550359	1.740400	4.114321
H	-1.005223	2.530014	3.670237
H	-0.260633	1.340019	2.561537
C	1.083909	4.439401	3.560263
H	1.702118	4.054602	4.398304
H	1.647887	5.252983	3.059227
H	0.169816	4.885883	4.005044
C	-1.261085	2.621006	-3.283771
H	-1.913628	3.455725	-3.620424
H	-0.910194	2.087383	-4.190569
H	-1.864352	1.919511	-2.673171
C	0.771782	4.174585	-3.257284
H	1.683107	4.476969	-2.699064
H	1.090815	3.772098	-4.241811
H	0.170286	5.090904	-3.440261

[Pd(IPr)(allyl)Cl]-VII

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I6+K2CO3 SCF Done: -3728.40801581 A.U.

Pd	-0.128619	-0.046806	-0.188848
N	-2.984725	-1.067650	-0.286102
C	-2.234578	-1.837061	-3.014918
H	-2.343346	-0.817650	-2.595109
C	-2.382404	-2.845064	-1.881831
C	-2.654934	-2.447300	-0.550481
C	-2.106219	-0.038642	-0.044163
C	-2.674072	-3.356564	0.543335
C	-2.832113	-2.873590	1.983149
H	-2.484998	-1.821296	1.996018
C	-2.214853	-4.229220	-2.123241
H	-2.020384	-4.574445	-3.151196
C	-2.302903	-5.162273	-1.076956
H	-2.195259	-6.238844	-1.288879
C	-2.511042	-4.726063	0.244973
H	-2.537659	-5.461494	1.063529
C	-4.310793	-0.643376	-0.161323
C	-1.931317	-3.641044	2.968047
H	-1.940610	-3.132538	3.953915
H	-2.281460	-4.683169	3.133365
H	-0.881748	-3.662097	2.616533
C	-4.303801	-2.922075	2.446809
H	-4.391812	-2.536379	3.484028
H	-4.965730	-2.307017	1.806011
H	-4.688823	-3.964640	2.435456
C	-0.812667	-1.890932	-3.610148
H	-0.601681	-2.871493	-4.091269
H	-0.696679	-1.098725	-4.376747
H	-0.044055	-1.699464	-2.832355
C	-3.322372	-2.028979	-4.089749
H	-4.340573	-1.962580	-3.651920
H	-3.232407	-1.244761	-4.869895
H	-3.235290	-3.016189	-4.593407

C	3.643711	1.931555	-0.198705	C	-4.267759	0.673688	0.201847
H	4.731166	1.826722	-0.244275	H	-5.060813	1.387613	0.437470
H	3.070992	4.107954	-0.303705	H	-5.149716	-1.319889	-0.345928
N	2.799113	0.824723	-0.073353	N	-2.917289	1.023185	0.274080
C	3.234729	-0.542815	0.070913	C	-2.457290	2.312164	0.732208
C	3.635870	-1.253769	-1.086559	C	-2.637195	3.429255	-0.121490
C	3.205608	-1.125088	1.367946	C	-1.873809	2.407448	2.030052
C	4.074194	-2.582741	-0.908980	C	-2.249668	4.693069	0.371334
C	3.659363	-2.452765	1.484678	C	-1.501030	3.697355	2.459907
C	4.096537	-3.171332	0.360905	C	-1.695370	4.827313	1.648721
H	4.386358	-3.169293	-1.785691	H	-2.367550	5.579835	-0.269359
H	3.651887	-2.944496	2.468246	H	-1.044489	3.823208	3.451431
H	4.435572	-4.212823	0.476266	H	-1.392676	5.821363	2.014632
C	3.608532	-0.615456	-2.473828	C	-3.228386	3.299150	-1.524834
H	2.897914	0.236851	-2.431761	H	-3.180188	2.227843	-1.810477
C	2.668683	-0.353453	2.573843	C	-1.640405	1.178731	2.914462
H	1.817851	0.255354	2.201596	H	-1.144190	0.405805	2.283237
C	5.003622	-0.068063	-2.848675	C	-4.706494	3.747955	-1.541101
H	5.372415	0.675484	-2.113887	H	-5.328730	3.179558	-0.820409
H	5.747164	-0.892470	-2.890850	H	-4.792615	4.823313	-1.274654
H	4.978027	0.421549	-3.844753	H	-5.146120	3.611804	-2.551640
C	3.096487	-1.576743	-3.563021	C	-2.422394	4.079175	-2.582160
H	2.939162	-1.022685	-4.510792	H	-2.806589	3.843721	-3.595922
H	3.824917	-2.388679	-3.772229	H	-2.511480	5.177473	-2.441320
H	2.132297	-2.037284	-3.275399	H	-1.350070	3.809509	-2.555867
C	3.721324	0.620211	3.144808	C	-2.963989	0.580996	3.442778
H	3.287514	1.216513	3.975209	H	-2.750567	-0.318141	4.057195
H	4.599100	0.066156	3.540468	H	-3.500035	1.314799	4.082816
H	4.083619	1.330647	2.374552	H	-3.652574	0.269582	2.633271
C	2.094739	-1.260995	3.673298	C	-0.684951	1.429793	4.090558
H	1.362010	-1.984672	3.260856	H	0.253474	1.917105	3.759407
H	2.885669	-1.830724	4.206278	H	-1.147074	2.062114	4.880450
H	1.570225	-0.644964	4.432661	H	-0.394492	0.455723	4.528473
C	0.156807	-0.815142	-1.507032	C	-0.255026	1.279435	-1.662353
O	0.261334	-0.279153	-2.593069	O	-0.958895	1.103982	-2.658864
N	-2.069779	-0.634605	0.517507	N	2.010052	0.026078	-0.225733
C	0.144650	-5.090041	-0.979928	C	2.209032	4.834314	-1.608531
C	-0.272228	-4.520154	-2.198665	C	2.133004	4.038058	-2.767508
H	0.891883	-4.703017	1.032488	H	1.557894	5.071829	0.459616
C	0.578366	-4.265918	0.072920	C	1.500743	4.459803	-0.453508
C	-0.250496	-3.128114	-2.368039	C	1.332524	2.884871	-2.775846
C	0.173859	-2.298510	-1.304424	C	0.634176	2.497641	-1.610978
C	0.578989	-2.874433	-0.084117	C	0.735156	3.284618	-0.447557
H	-0.569259	-2.661548	-3.312843	H	1.232054	2.267940	-3.682514
H	0.891322	-2.209310	0.733014	H	0.198128	2.975081	0.458651
H	0.120543	-6.183623	-0.848821	H	2.829308	5.745075	-1.604756
H	-0.618739	-5.166986	-3.020432	H	2.692223	4.326251	-3.672590
C	-3.126139	-0.065094	-0.148977	C	2.674333	-0.985302	-0.809151
O	-3.020478	0.905497	-0.908297	O	2.196227	-1.826785	-1.597070
O	-4.324011	-0.655016	0.166489	O	3.996999	-1.099590	-0.360241
C	-5.575846	-0.232023	-0.466652	C	5.015813	-1.800918	-1.143212
C	-5.492616	-0.428295	-1.989451	C	5.047458	-1.256672	-2.579658
H	-4.739515	0.251392	-2.429335	H	4.087346	-1.453766	-3.093211
H	-5.208550	-1.475332	-2.223086	H	5.231453	-0.162996	-2.575024
H	-6.480319	-0.224663	-2.452398	H	5.864125	-1.742123	-3.152317
C	-6.601754	-1.194158	0.148830	C	6.314906	-1.443862	-0.404481
H	-7.616789	-0.982258	-0.244886	H	7.194549	-1.857885	-0.937372
H	-6.337985	-2.244423	-0.090168	H	6.423280	-0.342680	-0.333175
H	-6.617547	-1.087225	1.252219	H	6.314488	-1.864706	0.623545
C	-5.896470	1.223875	-0.090247	C	4.775411	-3.320582	-1.113527
H	-5.138003	1.907434	-0.514526	H	3.891465	-3.582460	-1.723696
H	-6.899144	1.503209	-0.475658	H	5.660290	-3.856111	-1.516100
H	-5.902275	1.338257	1.013254	H	4.604572	-3.661565	-0.071211

C	-2.132295	-1.892735	1.147190
C	-1.456511	-2.073480	2.380871
C	-2.738483	-3.026122	0.547287
C	-1.375973	-3.337016	2.985739
H	-0.981845	-1.195024	2.846391
C	-2.659422	-4.284849	1.157692
H	-3.245548	-2.905901	-0.420115
C	-1.977233	-4.454233	2.377923
H	-0.842346	-3.447419	3.944211
H	-3.120282	-5.154278	0.661354
H	-1.914274	-5.447998	2.848576

Zero-point correction= 0.878591 (Hartree/Particle)
Thermal correction to Energy= 0.933575
Thermal correction to Enthalpy= 0.934519
Thermal correction to Gibbs Free Energy= 0.786900
Sum of electronic and zero-point Energies= -2263.689787
Sum of electronic and thermal Energies= -2263.634803
Sum of electronic and thermal Enthalpies= -2263.633859
Sum of electronic and thermal Free Energies= -2263.781477

SCF Done (in solvent): -2265.0220783

K	0.874158	-3.676153	-0.368917
K	3.581489	-1.123832	2.519167
C	0.940327	-1.868927	2.022757
O	1.781012	-2.862755	1.889365
O	1.065418	-0.995242	2.944755
O	-0.039546	-1.781345	1.125024
C	2.688929	1.092846	0.403750
C	2.236508	1.559436	1.663718
C	3.769245	1.770498	-0.216576
C	2.862471	2.649036	2.291952
H	1.397270	1.024629	2.138132
C	4.386252	2.858144	0.415144
H	4.090190	1.454855	-1.219198
C	3.943859	3.304706	1.676420
H	2.486985	2.993996	3.269636
H	5.207276	3.385328	-0.097244
H	4.425422	4.168763	2.160882

Zero-point correction= 0.897804 (Hartree/Particle)
Thermal correction to Energy= 0.959840
Thermal correction to Enthalpy= 0.960784
Thermal correction to Gibbs Free Energy= 0.802704
Sum of electronic and zero-point Energies= -3727.510212
Sum of electronic and thermal Energies= -3727.448176
Sum of electronic and thermal Enthalpies= -3727.447232
Sum of electronic and thermal Free Energies= -3727.605311

SCF Done (in solvent): -3728.878878

[Pd(IPr)(allyl)Cl]-VII-VIII

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I6+K2CO3--KN SCF Done: -3728.37682165 A.U.

Pd	0.182472	-0.496537	-0.376835
N	3.024185	-1.194218	-0.150542
C	2.996822	-1.005797	2.738376
H	2.524304	-0.194552	2.141900
C	2.690170	-2.314876	2.007639
C	2.690276	-2.387604	0.587046
C	2.128558	-0.173925	-0.379977
C	2.357627	-3.560405	-0.135927
C	2.301712	-3.564036	-1.660982
H	2.143024	-2.515647	-1.989294
C	2.385998	-3.500799	2.706550
H	2.367055	-3.491176	3.805809
C	2.098863	-4.694034	2.021548
H	1.882225	-5.612260	2.591794
C	2.077903	-4.722616	0.616795
H	1.836170	-5.660104	0.092225
C	4.296538	-0.876658	-0.628556
C	1.108532	-4.366219	-2.211188
H	1.014598	-4.200553	-3.302907
H	1.220264	-5.459690	-2.045206
H	0.156898	-4.025501	-1.756350
C	3.633082	-4.072664	-2.254774
H	3.602257	-4.034778	-3.363641
H	4.495876	-3.462341	-1.918254
H	3.826196	-5.124585	-1.952060
C	2.393256	-0.922624	4.149532
H	2.901165	-1.608616	4.861232
H	2.515362	0.107718	4.542490
H	1.310480	-1.153242	4.131303
C	4.515894	-0.726032	2.792905
H	4.974157	-0.681600	1.786065
H	4.707513	0.249581	3.286979
H	5.038039	-1.514353	3.375792

[Pd(IPr)(allyl)Cl]-VIII

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I6+K2CO3menysKNisomer1 SCF Done: -2495.86298673 A.U.

Pd	-0.040404	0.844449	-0.075083
N	2.245965	-1.059759	-0.527276
C	2.344047	0.374846	-3.083769
H	1.590024	-0.360079	-2.736927
C	3.267512	0.703846	-1.915934
C	3.190523	0.020315	-0.679608
C	0.937390	-0.861591	-0.174339
C	3.971889	0.365527	0.451867
C	3.794719	-0.317672	1.807072
H	2.976029	-1.060249	1.713614
C	4.225606	1.732882	-2.020331
H	4.321312	2.284843	-2.968678
C	5.045203	2.072818	-0.933963
H	5.784779	2.882886	-1.037459
C	4.911141	1.403536	0.291534
H	5.536197	1.703091	1.147517
C	2.583768	-2.413390	-0.485463
C	3.355362	0.689080	2.889612
H	3.158338	0.156193	3.844692
H	4.149164	1.440074	3.090212
H	2.433759	1.229038	2.587765
C	5.061880	-1.095639	2.214914
H	4.899105	-1.628647	3.175442
H	5.344017	-1.846384	1.446964
H	5.928226	-0.414026	2.352463
C	1.548980	1.616925	-3.531911
H	2.208573	2.400526	-3.962743
H	0.802247	1.330492	-4.300002
H	0.998399	2.053218	-2.672770
C	3.124722	-0.261998	-4.250941
H	3.656078	-1.181772	-3.927758
H	2.435211	-0.534610	-5.077419

C	4.211091	0.387621	-1.146043
H	4.965608	1.036442	-1.599079
H	5.137066	-1.571420	-0.547741
N	2.889969	0.808354	-0.972791
C	2.466656	2.182398	-1.106216
C	2.773665	3.056788	-0.031537
C	1.758035	2.585294	-2.265614
C	2.333947	4.390690	-0.142535
C	1.324284	3.925752	-2.310160
C	1.605625	4.816334	-1.262144
H	2.544361	5.098576	0.673765
H	0.760832	4.280096	-3.185622
H	1.249418	5.857224	-1.319977
C	3.592774	2.598733	1.176518
H	3.614321	1.490554	1.171083
C	1.549120	1.622568	-3.429178
H	1.383624	0.608669	-3.011535
C	5.051937	3.086096	1.040222
H	5.507760	2.752275	0.085895
H	5.100891	4.195716	1.064367
H	5.674597	2.697070	1.873457
C	3.000545	3.014650	2.535171
H	3.631498	2.613130	3.356070
H	2.965789	4.117217	2.658361
H	1.974310	2.625504	2.669973
C	2.818174	1.579443	-4.310555
H	2.686396	0.850759	-5.137554
H	3.028138	2.575984	-4.756247
H	3.713591	1.272035	-3.733021
C	0.312349	1.928953	-4.286525
H	-0.598673	2.021003	-3.664338
H	0.423982	2.862191	-4.880714
H	0.139170	1.094311	-4.994974
C	-0.094561	-0.136766	1.557082
O	-0.199612	-1.085568	2.351268
N	-2.530903	0.190666	0.196480
C	-0.713638	3.887757	3.006494
C	-0.756579	2.795062	3.896964
H	-0.407397	4.514072	0.937736
C	-0.433818	3.674410	1.646939
C	-0.542830	1.493779	3.421425
C	-0.258318	1.271294	2.052969
C	-0.190640	2.374785	1.177537
H	-0.600224	0.622761	4.092016
H	0.042423	2.202398	0.118344
H	-0.902554	4.907910	3.378072
H	-0.970654	2.962984	4.964998
C	-3.476172	-0.643167	0.612296
O	-3.321839	-1.742552	1.194626
O	-4.781463	-0.279422	0.171080
C	-5.983566	-0.735511	0.869322
C	-5.840430	-0.516397	2.383993
H	-5.035641	-1.152346	2.798359
H	-5.597875	0.545149	2.594697
H	-6.793588	-0.761571	2.895882
C	-7.079765	0.173981	0.295896
H	-8.064629	-0.064126	0.747363
H	-6.837012	1.236884	0.496715
H	-7.158965	0.043563	-0.803631
C	-6.264331	-2.212061	0.538261
H	-5.427947	-2.843801	0.891315
H	-7.207118	-2.548003	1.018188
H	-6.383458	-2.348462	-0.558771
H	3.884725	0.437652	-4.661003
C	1.458126	-3.086222	-0.086834
H	1.274957	-4.148763	0.094247
H	3.592411	-2.761692	-0.725783
N	0.461768	-2.122890	0.094461
C	-0.842030	-2.365391	0.658631
C	-1.846154	-2.944721	-0.154930
C	-1.063667	-1.981713	2.011042
C	-3.099268	-3.195965	0.443376
C	-2.337290	-2.249050	2.551593
C	-3.340735	-2.860335	1.781818
H	-3.902503	-3.646503	-0.159000
H	-2.546672	-1.969396	3.594531
H	-4.327445	-3.062432	2.228386
C	-1.594370	-3.288969	-1.620648
H	-0.705530	-2.709664	-1.946166
C	0.033980	-1.331466	2.853386
H	0.674935	-0.742675	2.166962
C	-1.284072	-4.792917	-1.783733
H	-0.410353	-5.106048	-1.176733
H	-2.150471	-5.410640	-1.463483
H	-1.065464	-5.035010	-2.845003
C	-2.761929	-2.871432	-2.535307
H	-2.474831	-3.007992	-3.597907
H	-3.669772	-3.486202	-2.355518
H	-3.024288	-1.805166	-2.394236
C	0.921580	-2.409272	3.510566
H	1.757239	-1.934379	4.065940
H	0.337247	-3.027696	4.225443
H	1.363146	-3.089023	2.752496
C	-0.496797	-0.317440	3.877576
H	-1.128742	0.446464	3.381510
H	-1.076881	-0.797841	4.695065
H	0.353506	0.223285	4.338179
C	-1.195845	0.274311	-1.566356
O	-0.911026	-0.220623	-2.652139
C	-5.276570	1.503088	-0.694617
C	-4.664970	1.864583	-1.912448
H	-5.047244	0.394182	1.175717
C	-4.567561	0.711144	0.235000
C	-3.359487	1.426490	-2.204901
C	-2.635769	0.667002	-1.261260
C	-3.246199	0.317085	-0.036413
H	-2.879783	1.679189	-3.163624
H	-2.675156	-0.267039	0.701129
H	-6.310913	1.818547	-0.479945
H	-5.217823	2.472972	-2.647033
K	-2.988100	3.882626	0.998676
C	-0.339829	2.867184	1.462305
O	-0.958848	2.686303	0.266124
O	-0.752933	3.768340	2.238592
O	0.608968	2.010033	1.696184

K -1.176252 -3.139732 1.036783 K -3.659547 -1.282892 -2.268942 C -0.892444 -1.752305 -2.481420 O -1.347634 -2.086160 -1.274078 O -1.541045 -2.037580 -3.525912 O 0.213645 -1.045211 -2.479044 C -2.781968 1.511108 -0.168463 C -2.134742 2.045186 -1.315822 C -3.558606 2.401287 0.623565 C -2.252121 3.403072 -1.651228 H -1.484962 1.374593 -1.905203 C -3.671756 3.755273 0.284346 H -4.037362 2.012939 1.534464 C -3.020380 4.271301 -0.854738 H -1.719151 3.787987 -2.535181 H -4.262245 4.426258 0.929817 H -3.103199 5.339398 -1.110211	
Zero-point correction= 0.896153 (Hartree/Particle) Thermal correction to Energy= 0.958095 Thermal correction to Enthalpy= 0.959039 Thermal correction to Gibbs Free Energy= 0.799436 Sum of electronic and zero-point Energies= -3727.480668 Sum of electronic and thermal Energies= -3727.418726 Sum of electronic and thermal Enthalpies= -3727.417782 Sum of electronic and thermal Free Energies= -3727.577385 SCF Done (in solvent): -3728.8549761	Zero-point correction= 0.669780 (Hartree/Particle) Thermal correction to Energy= 0.715433 Thermal correction to Enthalpy= 0.716377 Thermal correction to Gibbs Free Energy= 0.589859 Sum of electronic and zero-point Energies= -2495.193207 Sum of electronic and thermal Energies= -2495.147554 Sum of electronic and thermal Enthalpies= -2495.146609 Sum of electronic and thermal Free Energies= -2495.273127 SCF Done (in solvent): -2496.2126867

[Pd(IPr)(allyl)Cl]-IX	**[Pd(IPr)(allyl)Cl]-IX-X**
102 I6+KCO3+NH2 SCF Done: -2897.74689089 A.U. Pd -0.151304 -0.498248 -0.303152 C 1.300665 0.679139 -0.979164 O 1.326933 1.257568 -2.063840 C 4.720938 1.085802 1.659739 C 4.877021 1.210522 0.265891 H 3.319421 0.717817 3.289844 C 3.452913 0.807929 2.200023 C 3.765323 1.082472 -0.578919 C 2.490781 0.795232 -0.042692 C 2.349016 0.641481 1.350886 H 3.862030 1.187176 -1.670337 H 1.354566 0.402913 1.760088 H 5.593817 1.196046 2.323250 H 5.874466 1.399433 -0.161749 K -0.737011 -4.283512 3.796077 C 2.456303 -2.289466 -0.608124 C 3.288101 -2.317467 0.533828 C 3.048935 -2.126791 -1.872498 C 4.670606 -2.167295 0.410234 H 2.823238 -2.414290 1.526604 C 4.441680 -1.983185 -2.007490 H 2.408734 -2.068927 -2.766886 C 5.261054 -1.986815 -0.860092 H 5.323171 -2.148049 1.295395 H 4.866119 -1.840362 -3.011005 C -1.386149 -2.611743 1.592596 O -2.306159 -3.062880 2.369313 O -0.127648 -2.991907 1.789018 O -1.683091 -1.786371 0.630907 N -2.534797 1.049209 -1.202412 N -1.401846 2.270023 0.185678 C -1.417078 1.032696 -0.406802 C -3.190038 2.277922 -1.125770	102 I6+KCO3+NH2--HKCO3 SCF Done: -2897.75014994 A.U. Pd 0.261221 -0.174317 0.665124 C -0.473710 1.423285 1.584079 O 0.151985 2.168901 2.335785 C -4.736415 2.010117 1.071147 C -4.121048 2.298613 2.304454 H -4.437680 1.305554 -0.971834 C -3.964520 1.537887 -0.005286 C -2.736088 2.123984 2.456215 C -1.960174 1.630846 1.383621 C -2.586776 1.334221 0.156002 H -2.229847 2.367441 3.403810 H -1.975028 0.950218 -0.673626 H -5.823080 2.150119 0.951251 H -4.724995 2.667552 3.149421 K -1.496126 -5.116701 -0.425073 C -2.431516 -1.576968 1.128297 C -2.584954 -1.845910 -0.262180 C -3.609292 -1.413351 1.890269 C -3.850717 -1.942249 -0.849921 H -1.680539 -1.895931 -0.890692 C -4.884998 -1.494108 1.304609 H -3.526614 -1.167098 2.961136 C -5.019022 -1.757913 -0.074533 H -3.960251 -2.106100 -1.933811 H -5.766650 -1.317842 1.936460 C 0.540527 -3.148288 -0.359573 O 0.565903 -4.014061 -1.292073 O 0.003886 -3.516365 0.827065 O 0.951005 -1.936658 -0.512686 N 3.019476 0.799317 -0.024624 N 1.537948 2.003936 -1.053511 C 1.666591 0.936837 -0.201181 C 3.719825 1.780272 -0.726901

C	-2.483817	3.046105	-0.239137	C	2.786729	2.534277	-1.388097
C	-3.059888	-0.124664	-1.862164	C	3.625786	-0.341339	0.624692
C	-4.108876	-0.826542	-1.213544	C	4.103890	-1.391839	-0.202468
C	-4.606738	-1.973336	-1.861297	C	4.685456	-2.500322	0.442126
C	-4.073098	-2.404337	-3.084804	C	4.771648	-2.562552	1.841035
C	-3.023056	-1.697467	-3.688079	C	4.265034	-1.519191	2.627901
C	-2.485113	-0.541226	-3.086248	C	3.669008	-0.385688	2.037604
C	-4.718537	-0.346611	0.102670	C	4.032314	-1.324790	-1.727411
H	-4.476143	-3.307780	-3.570338	H	5.226954	-3.442547	2.323128
C	-1.346508	0.225137	-3.753119	C	3.101287	0.733053	2.904955
C	-0.489693	2.634855	1.238933	C	0.286858	2.374959	-1.666970
C	0.523077	3.587921	0.971534	C	-0.350783	3.571449	-1.259124
C	1.383544	3.930430	2.034465	C	-1.563026	3.907180	-1.897290
C	1.239146	3.342123	3.297141	C	-2.113127	3.077766	-2.882890
C	0.236806	2.386073	3.525439	C	-1.471371	1.882347	-3.245129
C	-0.649182	1.999155	2.501067	C	-0.258462	1.493814	-2.642916
C	0.661459	4.251307	-0.397168	C	0.251824	4.473620	-0.184832
H	1.927886	3.618681	4.111177	H	-3.064968	3.355257	-3.363069
C	-1.736969	0.952456	2.740720	C	0.436642	0.187108	-3.024251
H	-4.095860	2.483715	-1.701964	H	4.810657	1.842988	-0.694514
H	-2.649942	4.059668	0.134652	H	2.891805	3.383643	-2.068108
H	-5.418102	-2.546805	-1.388091	H	5.063810	-3.337019	-0.164688
H	-2.607679	-2.048686	-4.645749	H	4.322894	-1.585354	3.725567
H	-3.990988	0.345232	0.575240	H	3.269801	-0.564123	-1.991885
H	-0.946842	0.963903	-3.030133	H	2.501348	1.407725	2.262408
H	2.189888	4.659073	1.862411	H	-2.091883	4.824642	-1.599074
H	0.147964	1.919976	4.517970	H	-1.927820	1.230612	-4.004856
H	0.128048	3.611325	-1.131077	H	0.965888	3.856151	0.399625
H	-1.904910	0.411142	1.787911	H	0.932926	-0.211882	-2.117159
C	-1.329257	-0.139856	3.742889	C	-0.531065	-0.924938	-3.461745
H	-1.243298	0.241572	4.784039	H	-0.913786	-0.778172	-4.495327
H	-2.089145	-0.947224	3.720033	H	-0.010566	-1.903091	-3.411728
H	-0.362005	-0.595756	3.442545	H	-1.402900	-0.980891	-2.778389
C	-3.070644	1.621870	3.132356	C	1.531739	0.430806	-4.084252
H	-3.402163	2.345126	2.358421	H	2.289200	1.158852	-3.727620
H	-3.866507	0.855580	3.240731	H	2.058518	-0.518459	-4.315259
H	-2.977584	2.169728	4.095027	H	1.094430	0.824850	-5.027007
C	2.121562	4.357908	-0.873232	C	-0.795853	5.009490	0.808333
H	2.150632	4.739147	-1.914673	H	-0.289285	5.545982	1.636701
H	2.711830	5.060769	-0.247389	H	-1.493376	5.727953	0.327103
H	2.621324	3.371808	-0.857597	H	-1.389516	4.187561	1.250425
C	-0.004770	5.645468	-0.386045	C	1.029278	5.641456	-0.831910
H	0.512770	6.318800	0.330481	H	0.343122	6.290530	-1.417363
H	0.044543	6.113343	-1.391878	H	1.513694	6.269101	-0.054591
H	-1.070234	5.598620	-0.082787	H	1.819877	5.287127	-1.523957
C	-4.971646	-1.476598	1.115192	C	3.586174	-2.644765	-2.381669
H	-5.362912	-1.041893	2.060495	H	3.475953	-2.495874	-3.477309
H	-5.742211	-2.191111	0.752325	H	4.340776	-3.449114	-2.245034
H	-4.039678	-2.029963	1.350343	H	2.613601	-2.993011	-1.983225
C	-6.020264	0.440420	-0.173715	C	5.388870	-0.865447	-2.307584
H	-6.787533	-0.224915	-0.624681	H	6.178961	-1.614769	-2.086612
H	-6.437819	0.851320	0.769901	H	5.325147	-0.751283	-3.410510
H	-5.864272	1.285684	-0.874813	H	5.723261	0.102645	-1.882387
C	-0.163666	-0.694279	-4.108017	C	2.125601	0.191160	3.966385
H	-0.427259	-1.437591	-4.890441	H	2.638285	-0.428296	4.733230
H	0.691584	-0.090886	-4.472586	H	1.618913	1.032789	4.479819
H	0.177458	-1.235885	-3.202260	H	1.343308	-0.428205	3.480776
C	-1.859712	0.999795	-4.984465	C	4.234493	1.566186	3.536996
H	-1.040668	1.593759	-5.442298	H	3.816845	2.404132	4.134188
H	-2.256609	0.309475	-5.759879	H	4.864185	0.946153	4.211304
H	-2.677819	1.697615	-4.707844	H	4.899786	1.995861	2.758848
N	1.041935	-2.320894	-0.450380	N	-1.137329	-1.475637	1.673753
H	0.576592	-2.814866	-1.223302	H	-1.177206	-1.287292	2.683458

H	0.674331	-2.714212	0.501064
O	6.619846	-1.800197	-0.867783
C	7.245945	-1.515497	-2.105331
H	6.841027	-0.587488	-2.574358
H	8.321663	-1.366999	-1.888458
H	7.141113	-2.352934	-2.835083

Zero-point correction= 0.817317 (Hartree/Particle)
Thermal correction to Energy= 0.872120
Thermal correction to Enthalpy= 0.873065
Thermal correction to Gibbs Free Energy= 0.726918
Sum of electronic and zero-point Energies= -2896.929574
Sum of electronic and thermal Energies= -2896.874770
Sum of electronic and thermal Enthalpies= -2896.873826
Sum of electronic and thermal Free Energies= -2897.019973

SCF Done (in solvent): -2898.2195406

H	-0.474883	-2.537915	1.360717
O	-6.212477	-1.827579	-0.750603
C	-7.397331	-1.520353	-0.038097
H	-7.370593	-0.490962	0.391452
H	-8.229580	-1.584003	-0.765708
H	-7.591729	-2.241824	0.790905

Zero-point correction= 0.813743 (Hartree/Particle)
Thermal correction to Energy= 0.868025
Thermal correction to Enthalpy= 0.868969
Thermal correction to Gibbs Free Energy= 0.724668
Sum of electronic and zero-point Energies= -2896.936407
Sum of electronic and thermal Energies= -2896.882125
Sum of electronic and thermal Enthalpies= -2896.881181
Sum of electronic and thermal Free Energies= -2897.025482

SCF Done (in solvent): -2898.2172034

[Pd(IPr)(allyl)Cl]-X (adduct)

102

TS5NH2PhOMePOST SCF Done: -2897.71451373 A.U.

Pd	0.069587	0.472686	0.467441
C	-1.321506	0.442089	-0.933477
O	-1.359224	1.225925	-1.876716
C	-4.559468	-2.334135	-0.190175
C	-4.808954	-1.082118	-0.781817
H	-3.033023	-3.712004	0.536705
C	-3.238820	-2.717974	0.106944
C	-3.741744	-0.221096	-1.077050
C	-2.422197	-0.574226	-0.723206
C	-2.177641	-1.834023	-0.141181
H	-3.916792	0.762670	-1.534877
H	-1.141161	-2.123463	0.089681
H	-5.397894	-3.010749	0.041370
H	-5.842037	-0.764512	-0.992967
K	0.492916	-3.070250	4.714337
C	-2.639247	1.192931	1.812801
C	-3.619078	0.411043	2.497315
C	-3.139232	2.199039	0.941832
C	-4.988914	0.602201	2.300157
H	-3.277087	-0.394677	3.169953
C	-4.514191	2.398625	0.736985
H	-2.414540	2.822188	0.399994
C	-5.456275	1.588670	1.403885
H	-5.732135	-0.029417	2.811713
H	-4.834043	3.185095	0.037816
C	1.410454	-0.915174	2.890771
O	2.068458	-1.360896	3.866904
O	0.217791	-1.660356	2.627701
O	1.651241	0.060721	2.139596
N	2.510168	1.070391	-1.192619
N	1.575781	-0.716370	-1.978907
C	1.478546	0.197227	-0.954255
C	3.204797	0.741138	-2.354878
C	2.620733	-0.393931	-2.849798
C	2.883094	2.140198	-0.296768
C	3.904769	1.884067	0.654412
C	4.281011	2.951763	1.491334
C	3.655091	4.204170	1.392197
C	2.625644	4.411489	0.463844
C	2.208068	3.378102	-0.399692
C	4.579391	0.517302	0.757516
H	3.963319	5.023850	2.060874
C	1.070410	3.597361	-1.390897
C	0.804358	-1.932031	-2.061728

[Pd(IPr)(allyl)Cl]-X

96

I6+NH SCF Done: -2033.39828600 A.U.

Pd	-0.087873	0.315628	-0.647700
C	0.805647	1.626598	0.551303
O	0.548317	1.721261	1.740772
C	3.702683	4.277599	-1.267844
C	3.178426	4.557622	0.009459
H	3.677799	2.913180	-2.967550
C	3.268177	3.139625	-1.970601
C	2.234810	3.696058	0.585807
C	1.801238	2.545181	-0.113844
C	2.314996	2.283225	-1.399581
H	1.808342	3.901297	1.579766
H	1.964619	1.383846	-1.929101
H	4.447627	4.953527	-1.717743
H	3.507591	5.456092	0.555760
C	-2.413023	1.962630	-1.398998
C	-2.926299	3.293450	-1.350348
C	-3.316200	0.918196	-1.052499
C	-4.238855	3.558228	-0.951015
H	-2.259806	4.132222	-1.613079
C	-4.628192	1.178545	-0.631574
H	-2.965951	-0.126202	-1.107286
C	-5.103967	2.506355	-0.573183
H	-4.622542	4.589368	-0.905600
H	-5.268825	0.328264	-0.359779
N	-0.175600	-2.233060	0.896567
N	1.900539	-1.646296	0.695087
C	0.626400	-1.262330	0.343471
C	0.575214	-3.202181	1.561831
C	1.889940	-2.835890	1.426323
C	-1.608649	-2.253487	0.730220
C	-2.144411	-3.043255	-0.319656
C	-3.546324	-3.072739	-0.456583
C	-4.369478	-2.346136	0.417537
C	-3.806375	-1.542792	1.418363
C	-2.409180	-1.460303	1.587955
C	-1.233683	-3.734751	-1.332303
H	-5.463950	-2.387791	0.298450
C	-1.803111	-0.531339	2.634488
C	3.066148	-0.900827	0.294630
C	3.691823	-0.049129	1.242992
C	4.780383	0.724999	0.794908
C	5.224193	0.649565	-0.532678
C	4.594732	-0.211578	-1.441535
C	3.496328	-1.004239	-1.051871

C	-0.186186	-2.050057	-3.067880
C	-0.909958	-3.259741	-3.127551
C	-0.653169	-4.300248	-2.229159
C	0.337311	-4.157098	-1.243982
C	1.090311	-2.972327	-1.130582
C	-0.446406	-0.944370	-4.088617
H	-1.235649	-5.233235	-2.288787
C	2.167307	-2.811704	-0.054204
H	4.040677	1.344723	-2.719048
H	2.857631	-1.008590	-3.721932
H	5.067409	2.795525	2.244882
H	2.125267	5.390819	0.412069
H	3.863881	-0.226227	0.349617
H	0.767498	2.612611	-1.800017
H	-1.697281	-3.378277	-3.886639
H	0.521181	-4.987340	-0.547083
H	-0.045148	0.000076	-3.667001
H	2.036444	-1.796919	0.379027
C	2.035258	-3.812557	1.106650
H	2.307425	-4.845364	0.799214
H	2.719204	-3.510559	1.926714
H	1.001497	-3.819521	1.506763
C	3.593461	-2.885820	-0.645377
H	3.772820	-2.104991	-1.409623
H	4.347540	-2.740732	0.156385
H	3.773237	-3.876359	-1.115493
C	-1.944810	-0.715583	-4.360870
H	-2.077624	0.192126	-4.984282
H	-2.399555	-1.565320	-4.913786
H	-2.506701	-0.564701	-3.420901
C	0.292817	-1.252476	-5.410640
H	-0.092606	-2.191444	-5.862805
H	0.140141	-0.432499	-6.143443
H	1.384665	-1.379959	-5.266309
C	4.884928	0.095347	2.205494
H	5.246684	-0.954831	2.220110
H	5.687422	0.717800	2.656688
H	3.978586	0.152544	2.837484
C	5.862718	0.468013	-0.100741
H	6.611309	1.197744	0.275649
H	6.320701	-0.543285	-0.061341
H	5.666216	0.708175	-1.164478
C	-0.179337	4.167831	-0.696453
H	-0.029385	5.213672	-0.353009
H	-1.040190	4.155221	-1.395311
H	-0.444597	3.546763	0.183373
C	1.531568	4.476273	-2.571169
H	0.710619	4.602898	-3.308109
H	1.838559	5.486828	-2.224778
H	2.399102	4.024016	-3.096760
N	-1.274424	0.990619	1.957868
H	-1.104079	0.401209	2.783279
H	-0.210238	-1.241333	1.817541
O	-6.825186	1.671408	1.248745
C	-7.325448	2.624867	0.335433
H	-6.953056	2.452178	-0.703793
H	-8.428804	2.522375	0.338876
H	-7.063891	3.671145	0.625329

Zero-point correction=	0.815977 (Hartree/Particle)
Thermal correction to Energy=	0.871193
Thermal correction to Enthalpy=	0.872137
Thermal correction to Gibbs Free Energy=	0.724325
Sum of electronic and zero-point Energies=	-2896.898536
Sum of electronic and thermal Energies=	-2896.843321
Sum of electronic and thermal Enthalpies=	-2896.842377

C	3.238965	-0.007277	2.701440
H	6.064505	1.278807	-0.864864
C	2.830965	-1.942455	-2.058349
H	0.106713	-4.057628	2.057649
H	2.811017	-3.313474	1.770479
H	-4.001366	-3.666175	-1.263779
H	-4.461471	-0.941018	2.065995
H	-0.250661	-3.908210	-0.844079
H	-0.726465	-0.407191	2.400593
H	5.279708	1.412426	1.493218
H	4.952802	-0.258786	-2.482111
H	2.169796	-0.308762	2.724046
H	1.980037	-2.442353	-1.550539
C	2.246677	-1.176194	-3.260830
H	3.030137	-0.612512	-3.809998
H	1.772597	-1.877878	-3.977790
H	1.467514	-0.457415	-2.928115
C	3.811099	-3.046615	-2.507096
H	4.213823	-3.606500	-1.637672
H	3.302928	-3.769750	-3.179265
H	4.674226	-2.622582	-3.062797
C	3.327030	1.391506	3.334830
H	2.861098	1.377677	4.341445
H	4.378767	1.723690	3.465479
H	2.789160	2.139619	2.724835
C	4.053023	-1.020156	3.539053
H	5.128218	-0.740759	3.544899
H	3.696808	-1.036113	4.590510
H	3.982102	-2.051092	3.139339
C	-0.989297	-2.791058	-2.530952
H	-0.290912	-3.249118	-3.262249
H	-1.942008	-2.561002	-3.052095
H	-0.549609	-1.823943	-2.201676
C	-1.760063	-5.104010	-1.797971
H	-2.683115	-5.006186	-2.407364
H	-1.005137	-5.608677	-2.435917
H	-1.987933	-5.768680	-0.939135
C	-2.413353	0.881003	2.564176
H	-3.478463	0.895549	2.878611
H	-1.849525	1.565580	3.228572
H	-2.353231	1.282878	1.532864
C	-1.917027	-1.146392	4.044230
H	-1.444755	-0.482648	4.798641
H	-2.980577	-1.288772	4.333865
H	-1.417905	-2.137107	4.096443
N	-1.102468	1.666795	-1.751856
H	-0.602851	2.507114	-2.072023
O	-6.369506	2.871750	-0.177118
C	-7.247696	1.852183	0.254033
H	-6.844249	1.290868	1.131334
H	-8.190716	2.350157	0.553592
H	-7.473843	1.116470	-0.554824

Zero-point correction=	0.787537 (Hartree/Particle)
Thermal correction to Energy=	0.836448
Thermal correction to Enthalpy=	0.837392
Thermal correction to Gibbs Free Energy=	0.703607
Sum of electronic and zero-point Energies=	-2032.610749
Sum of electronic and thermal Energies=	-2032.561838
Sum of electronic and thermal Enthalpies=	-2032.560894

Sum of electronic and thermal Free Energies= -2896.990188 SCF Done (in solvent): -2898.1990086	Sum of electronic and thermal Free Energies= -2032.694679 SCF Done (in solvent): -2033.7672359

[Pd(IPr)(allyl)Cl]-X-XI				**[Pd(IPr)(allyl)Cl]-XI**			
96				96			
I6--PROD SCF Done: -2033.39010873 A.U.				TS5NH2PhOMe--CNmin SCF Done: -2033.40623542 A.U.			
Pd	-0.047953	0.061315	-0.832033	Pd	0.096784	0.371324	-0.401801
C	-0.014013	1.902583	0.105474	C	0.319294	3.020623	0.010863
O	-0.673456	2.061882	1.121245	O	-0.273612	3.478034	0.985991
C	3.266334	4.500717	-0.982586	C	4.607889	3.519450	-0.351741
C	2.285779	4.921992	-0.063319	C	3.857387	4.259814	0.578849
H	3.951506	2.874294	-2.263259	H	4.537982	1.992522	-1.909676
C	3.177763	3.221311	-1.560827	C	3.958173	2.603209	-1.201319
C	1.225229	4.069432	0.278154	C	2.466239	4.087733	0.660259
C	1.134110	2.782092	-0.301470	C	1.806549	3.172455	-0.188658
C	2.118808	2.366552	-1.221916	C	2.570186	2.426678	-1.119423
H	0.450333	4.378069	0.996840	H	1.861434	4.645181	1.391140
H	2.053143	1.345209	-1.633281	H	2.091900	1.632469	-1.719549
H	4.101715	5.170022	-1.243770	H	5.701169	3.644474	-0.406723
H	2.349973	5.924034	0.390800	H	4.360135	4.972043	1.252372
C	-2.433389	1.916103	-1.316157	C	-1.813985	2.280572	-1.173577
C	-3.111002	3.093589	-1.733148	C	-2.404219	2.288973	-2.455118
C	-3.168050	0.966812	-0.565388	C	-2.624359	2.054966	-0.041379
C	-4.460930	3.292534	-1.430468	C	-3.773056	2.042415	-2.610123
H	-2.562446	3.859856	-2.305969	H	-1.778041	2.456036	-3.347093
C	-4.518299	1.167124	-0.242587	C	-3.996570	1.815564	-0.195204
H	-2.652089	0.050400	-0.234401	H	-2.176547	2.040084	0.958757
C	-5.179987	2.335908	-0.676898	C	-4.580676	1.789813	-1.480718
H	-4.990304	4.199687	-1.760096	H	-4.239555	2.025513	-3.606140
H	-5.035884	0.395837	0.345410	H	-4.589068	1.610825	0.705579
N	0.175613	-2.485536	0.657431	N	-0.446735	-2.152531	1.094037
N	2.130805	-1.555140	0.655893	N	1.589341	-2.153952	0.360572
C	0.842708	-1.362378	0.217553	C	0.450044	-1.378015	0.387756
C	1.028338	-3.366312	1.321470	C	0.115732	-3.367225	1.491373
C	2.268293	-2.779911	1.317016	C	1.406607	-3.369173	1.025237
C	-1.255825	-2.610145	0.527200	C	-1.785055	-1.710440	1.396222
C	-1.782364	-3.255267	-0.617116	C	-2.818664	-1.973946	0.462902
C	-3.185419	-3.331294	-0.730651	C	-4.123063	-1.567267	0.806654
C	-4.017236	-2.780715	0.254989	C	-4.379305	-0.909872	2.018568
C	-3.464983	-2.119514	1.362908	C	-3.327233	-0.612080	2.897101
C	-2.069744	-2.003785	1.519686	C	-2.004625	-1.003440	2.604753
C	-0.867707	-3.725761	-1.744769	C	-2.528291	-2.565078	-0.913304
H	-5.111380	-2.846262	0.146244	H	-5.407710	-0.604261	2.271449
C	-1.457097	-1.237666	2.689618	C	-0.847962	-0.574351	3.502937
C	3.169765	-0.562189	0.533673	C	2.799405	-1.721080	-0.289132
C	3.211770	0.494205	1.484341	C	3.772626	-1.034069	0.478608
C	4.252146	1.433852	1.344471	C	4.933802	-0.597054	-0.189134
C	5.191402	1.328918	0.308397	C	5.113663	-0.838071	-1.559333
C	5.106027	0.290407	-0.628909	C	4.127145	-1.510521	-2.296036
C	4.086029	-0.678502	-0.539248	C	2.945850	-1.967302	-1.676744
C	2.160229	0.615209	2.590149	C	3.533596	-0.689305	1.946262
H	5.987505	2.084423	0.217542	H	6.030408	-0.488993	-2.061431
C	3.914307	-1.758681	-1.606218	C	1.835997	-2.624268	-2.493819
H	0.678328	-4.319442	1.728766	H	-0.448570	-4.109109	2.064450
H	3.229475	-3.113188	1.719732	H	2.204848	-4.113431	1.103716
H	-3.633320	-3.812786	-1.613353	H	-4.947785	-1.752377	0.100796
H	-4.129965	-1.660307	2.109203	H	-3.532755	-0.057096	3.825584
H	0.157173	-3.825404	-1.327335	H	-1.496787	-2.976889	-0.894170
H	-0.473109	-0.858049	2.344609	H	0.049453	-1.154497	3.200110
H	4.318199	2.280433	2.042001	H	5.701797	-0.042513	0.370821
H	5.836090	0.240050	-1.450776	H	4.272892	-1.679542	-3.374452
H	1.180659	0.388816	2.115609				

H	3.391649	-2.617730	-1.132781
C	2.998594	-1.236101	-2.735881
H	3.463634	-0.362938	-3.241560
H	2.819746	-2.023006	-3.498731
H	2.013637	-0.910242	-2.333448
C	5.246964	-2.286612	-2.165840
H	5.935104	-2.607856	-1.356561
H	5.066180	-3.156039	-2.831359
H	5.771754	-1.520080	-2.774204
C	2.045458	2.028635	3.181248
H	1.147592	2.088861	3.828506
H	2.927219	2.286848	3.806881
H	1.938899	2.796115	2.391570
C	2.387135	-0.406914	3.726556
H	3.366573	-0.231824	4.220715
H	1.592392	-0.303251	4.494882
H	2.363262	-1.454143	3.368952
C	-0.810898	-2.641363	-2.842525
H	-0.090445	-2.914185	-3.641549
H	-1.809553	-2.485021	-3.300923
H	-0.488865	-1.657728	-2.417787
C	-1.266801	-5.094566	-2.325247
H	-2.248280	-5.053387	-2.842923
H	-0.519270	-5.428476	-3.074599
H	-1.333338	-5.869234	-1.533550
C	-2.278502	-0.003358	3.097397
H	-3.246406	-0.281617	3.567057
H	-1.711111	0.591064	3.842577
H	-2.468275	0.653801	2.226279
C	-1.207506	-2.175614	3.890187
H	-0.723268	-1.622162	4.722012
H	-2.164628	-2.595081	4.267784
H	-0.547324	-3.024969	3.619332
N	-1.080945	1.697369	-1.575061
H	-0.652543	2.391168	-2.198396
O	-6.497322	2.632533	-0.425683
C	-7.249407	1.714642	0.343956
H	-6.822045	1.571316	1.365032
H	-8.267088	2.140931	0.440342
H	-7.325239	0.714687	-0.146492

H	2.742676	-1.370441	2.327536
H	1.125994	-3.092989	-1.779574
C	1.050686	-1.544302	-3.267695
H	1.708307	-1.021889	-3.995229
H	0.200021	-1.992445	-3.822624
H	0.643742	-0.788046	-2.550780
C	2.354631	-3.735581	-3.425057
H	2.937819	-4.497364	-2.866911
H	1.505214	-4.246827	-3.924490
H	3.007067	-3.330977	-4.227724
C	2.988338	0.750514	2.054078
H	2.774026	1.013985	3.110800
H	3.717431	1.484893	1.651578
H	2.050639	0.852016	1.467074
C	4.781038	-0.894685	2.825081
H	5.583328	-0.167474	2.578156
H	4.525525	-0.740792	3.894166
H	5.201427	-1.915989	2.713062
C	-2.547216	-1.431916	-1.962295
H	-2.303005	-1.823079	-2.972181
H	-3.539795	-0.936541	-2.006518
H	-1.792244	-0.654062	-1.694372
C	-3.480724	-3.714839	-1.290175
H	-4.526156	-3.360734	-1.413585
H	-3.175410	-4.165969	-2.257359
H	-3.482001	-4.514435	-0.520306
C	-0.534835	0.914710	3.242808
H	-1.401510	1.558151	3.504080
H	0.336407	1.250062	3.842324
H	-0.296178	1.077180	2.168900
C	-1.103159	-0.860087	4.994153
H	-0.203857	-0.607142	5.593631
H	-1.941192	-0.250490	5.393920
H	-1.347324	-1.928499	5.170780
N	-0.380118	2.376944	-1.076073
H	0.075612	2.515400	-1.987439
O	-5.898082	1.515296	-1.730072
C	-6.748084	1.256660	-0.624659
H	-6.812035	2.128726	0.067152
H	-7.753620	1.056024	-1.041949
H	-6.414801	0.367447	-0.040795

Zero-point correction=	0.787136 (Hartree/Particle)
Thermal correction to Energy=	0.835168
Thermal correction to Enthalpy=	0.836112
Thermal correction to Gibbs Free Energy=	0.705221
Sum of electronic and zero-point Energies=	-2032.602973
Sum of electronic and thermal Energies=	-2032.554941
Sum of electronic and thermal Enthalpies=	-2032.553997
Sum of electronic and thermal Free Energies=	-2032.684888

SCF Done (in solvent): -2033.7591989

Zero-point correction=	0.788436 (Hartree/Particle)
Thermal correction to Energy=	0.836994
Thermal correction to Enthalpy=	0.837938
Thermal correction to Gibbs Free Energy=	0.705333
Sum of electronic and zero-point Energies=	-2032.617799
Sum of electronic and thermal Energies=	-2032.569241
Sum of electronic and thermal Enthalpies=	-2032.568297
Sum of electronic and thermal Free Energies=	-2032.700903

SCF Done (in solvent): -2033.7938724

[Pd(IPr*)(allyl)Cl]			
131			
StI-PREallyl SCF Done: -3397.66039395 A.U.			
Cl	-2.734788	-0.377916	-2.125012
C	1.606899	-1.334780	-2.765030
H	2.300440	-1.714657	-2.003149
H	1.974427	-0.453761	-3.317119

[Pd(IPr*)(allyl)Cl]-I			
137			
StI-PREallyl+K2CO3 SCF Done: -4861.44043390 A.U.			
Cl	2.645320	-0.896178	-1.077177
C	-0.761522	1.966342	-1.930247
H	-1.398791	2.504941	-1.209925
H	-1.306608	1.334996	-2.652973

C	0.676395	-2.229363	-3.386477
H	0.582984	-3.266839	-3.014448
C	-0.330885	-1.695095	-4.223527
H	-0.150333	-0.780730	-4.815486
Pd	-0.377586	-0.791213	-2.192965
H	-1.174450	-2.323645	-4.549138
N	0.074570	-0.912958	0.770560
C	-2.079339	-2.856324	0.447344
H	-2.116308	-1.928962	-0.166617
C	-0.615659	-3.275548	0.569461
C	0.416703	-2.314712	0.695704
C	-0.128474	-0.096022	-0.318066
C	1.783290	-2.686352	0.801096
C	2.871491	-1.617454	0.913234
H	2.551238	-0.781398	0.249030
C	-0.253809	-4.637919	0.596947
H	-1.043169	-5.396917	0.492996
C	1.082235	-5.027790	0.758890
H	1.341155	-6.097465	0.801368
C	2.092127	-4.059972	0.856695
H	3.142289	-4.369119	0.966446
C	-0.021504	-0.198103	1.969529
C	-0.265986	1.100982	1.629253
H	-0.423665	1.988381	2.247439
H	0.104136	-0.678321	2.942727
N	-0.333153	1.148320	0.228102
C	-0.379781	2.381892	-0.525731
C	-1.619778	3.034442	-0.754329
C	0.849170	2.950456	-0.938505
C	-1.600758	4.253147	-1.458536
C	0.821926	4.189753	-1.612251
C	-0.393298	4.826248	-1.888138
H	-2.555801	4.763211	-1.653392
H	1.775567	4.660661	-1.897592
H	-0.402463	5.789771	-2.421657
C	-2.916310	2.479150	-0.161183
H	-2.918054	1.389051	-0.391019
C	2.190502	2.308308	-0.597026
H	1.978038	1.447214	0.069697
C	2.968621	1.734303	-1.781949
C	4.062391	0.884682	-1.501867
C	2.673662	2.021098	-3.129130
C	4.838389	0.330457	-2.529904
H	4.325270	0.659572	-0.456685
C	3.459572	1.480279	-4.165382
H	1.810279	2.654792	-3.378510
C	4.541341	0.632497	-3.871873
H	5.668334	-0.345523	-2.272722
H	3.209771	1.714235	-5.212516
H	5.145657	0.201315	-4.685393
C	3.021718	3.293661	0.240869
C	2.594358	3.595249	1.553318
C	4.173232	3.933871	-0.257604
C	3.304749	4.504162	2.351544
H	1.693452	3.101405	1.950539
C	4.884552	4.850227	0.539297
H	4.521314	3.705787	-1.276795
C	4.456570	5.136460	1.846133
H	2.956283	4.722611	3.373881
H	5.783276	5.341313	0.133118
H	5.016651	5.850373	2.470531
C	-4.168278	3.064406	-0.821105
C	-4.478943	2.684412	-2.147333
C	0.516013	2.509430	-2.283972
H	0.914790	3.397356	-1.759619
C	1.398823	1.723946	-3.056332
H	1.017654	0.987145	-3.787428
Pd	0.737392	0.632380	-1.222659
H	2.446384	2.055270	-3.163685
O	4.178210	3.497113	-2.461140
C	3.368802	3.868457	-1.456493
O	3.266807	3.123940	-0.417259
O	2.672032	4.959711	-1.604324
K	4.753715	1.266137	-1.359039
K	3.330636	5.306290	-3.905821
N	-0.117909	-0.548471	1.514432
C	2.707143	-0.939875	2.390074
H	2.385405	-1.096041	1.334244
C	1.756556	0.083862	3.005730
C	0.502374	0.389416	2.426841
C	-0.290544	-0.425030	0.153020
C	-0.232741	1.534640	2.819292
C	-1.500564	1.990098	2.092711
H	-1.628096	1.333852	1.205425
C	2.189755	0.862587	4.098319
H	3.163804	0.630503	4.555608
C	1.439754	1.954645	4.552356
H	1.800251	2.559433	5.398891
C	0.264997	2.313409	3.881385
H	-0.275748	3.226731	4.169033
C	-0.874918	-1.608194	2.027651
C	-1.549047	-2.159556	0.976299
H	-2.178229	-3.051151	0.903534
H	-0.847836	-1.867482	3.089380
N	-1.197485	-1.416322	-0.156583
C	-1.767948	-1.684421	-1.460121
C	-1.089291	-2.576866	-2.330012
C	-3.044972	-1.159380	-1.779823
C	-1.702450	-2.915692	-3.550137
C	-3.654810	-1.589352	-2.978848
C	-2.985199	-2.440814	-3.865625
H	-1.173030	-3.593444	-4.236719
H	-4.678847	-1.252538	-3.201138
H	-3.472089	-2.752352	-4.803234
C	0.212087	-3.238560	-1.879978
H	0.843004	-2.448164	-1.421170
C	-3.778915	-0.179242	-0.868091
H	-3.160062	-0.062122	0.042501
C	-3.948946	1.236665	-1.435021
C	-4.214435	2.277188	-0.516895
C	-3.888595	1.555627	-2.806226
C	-4.410804	3.594503	-0.956604
H	-4.264003	2.047847	0.559806
C	-4.079143	2.877217	-3.248521
H	-3.659811	0.774457	-3.544803
C	-4.341070	3.902530	-2.326452
H	-4.600936	4.390571	-0.222446
H	-4.012115	3.103444	-4.324738
H	-4.482416	4.939320	-2.669891
C	-5.122189	-0.770074	-0.411822
C	-5.145680	-1.752404	0.601205
C	-6.343666	-0.377335	-0.995844
C	-6.355128	-2.326924	1.023128
H	-4.200340	-2.064956	1.070480
C	-7.556453	-0.956460	-0.581595
H	-6.344176	0.403365	-1.772553

C	-5.009397	3.988368	-0.168099
C	-5.598174	3.221988	-2.801078
H	-3.832311	1.951911	-2.656177
C	-6.131545	4.527823	-0.824715
H	-4.789917	4.288833	0.867856
C	-6.429397	4.148698	-2.143761
H	-5.826477	2.909753	-3.832959
H	-6.777435	5.247758	-0.296453
H	-7.308779	4.569085	-2.657692
C	-2.900942	2.636197	1.357619
C	-3.369964	1.587373	2.172401
C	-2.379165	3.792975	1.976892
C	-3.293073	1.671784	3.571505
H	-3.756503	0.671229	1.701769
C	-2.305371	3.885106	3.378292
H	-1.999622	4.616741	1.351497
C	-2.754291	2.819551	4.180639
H	-3.635075	0.820860	4.180762
H	-1.886975	4.791269	3.845448
H	-2.681695	2.883487	5.278156
C	4.251696	-2.039948	0.377677
C	5.442523	-1.609762	1.000401
C	4.365851	-2.784296	-0.819694
C	6.700566	-1.897674	0.440137
H	5.389021	-1.032823	1.935198
C	5.618924	-3.081436	-1.377023
H	3.459044	-3.147149	-1.324866
C	6.796587	-2.634106	-0.751863
H	7.612409	-1.543965	0.947085
H	5.672824	-3.661167	-2.312110
H	7.781366	-2.862186	-1.189263
C	2.930492	-1.041630	2.331697
C	3.204420	0.327774	2.526208
C	2.710000	-1.850839	3.464793
C	3.235938	0.884977	3.813705
H	3.387885	0.978569	1.658404
C	2.736301	-1.297171	4.757267
H	2.492263	-2.922123	3.331938
C	2.993519	0.073894	4.936630
H	3.441856	1.960777	3.928993
H	2.550336	-1.942707	5.630524
H	3.006200	0.508137	5.948849
C	-2.885555	-3.897241	-0.334286
C	-2.786362	-3.920417	-1.742124
C	-3.676758	-4.871976	0.307932
C	-3.459909	-4.899092	-2.489575
H	-2.190618	-3.143808	-2.246049
C	-4.350277	-5.854637	-0.440220
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C	-4.242754	-5.872557	-1.841511
H	-3.382055	-4.895029	-3.588732
H	-4.965592	-6.608532	0.076835
H	-4.774312	-6.638439	-2.428708
C	-2.717721	-2.505894	1.790506
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C	-4.667236	-1.631300	2.986763
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C	-2.755448	-2.457289	4.238035
H	-1.098463	-3.220735	3.052951
C	-4.042678	-1.896114	4.221312
H	-5.671847	-1.179982	2.961517
H	-2.256444	-2.667561	5.197697
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H	-6.350289	-3.086770	1.821082
H	-8.500809	-0.635248	-1.049545
H	-8.519183	-2.379605	0.759219
C	1.031550	-3.781890	-3.047008
C	1.714660	-2.857635	-3.870486
C	1.117780	-5.154400	-3.351574
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H	1.671531	-1.786695	-3.615854
C	1.861438	-5.597095	-4.461865
H	0.603213	-5.886234	-2.709753
C	2.529692	-4.671378	-5.280243
H	2.984543	-2.564693	-5.607661
H	1.919846	-6.674791	-4.684448
H	3.113302	-5.017940	-6.148213
C	-0.089294	-4.250160	-0.775798
C	0.718591	-4.277447	0.377997
C	-1.209927	-5.106642	-0.840699
C	0.404026	-5.120833	1.455770
H	1.575004	-3.588401	0.446682
C	-1.522620	-5.960588	0.231504
H	-1.861712	-5.080885	-1.728761
C	-0.719927	-5.963197	1.387119
H	1.029969	-5.098466	2.359783
H	-2.404418	-6.618539	0.167623
H	-0.973511	-6.617494	2.236600
C	-1.289662	3.402766	1.523917
C	-2.308907	4.375377	1.498685
C	-0.044906	3.716352	0.928077
C	-2.087793	5.630433	0.901653
H	-3.292345	4.151132	1.938228
C	0.180317	4.962962	0.321926
H	0.775609	2.980013	0.911426
C	-0.847345	5.925513	0.312255
H	-2.899035	6.377258	0.895152
H	1.157748	5.145712	-0.168220
H	-0.677511	6.908345	-0.157521
C	-2.731949	1.771666	2.972926
C	-3.533861	0.630098	2.764041
C	-3.086786	2.642996	4.027494
C	-4.668186	0.371865	3.550914
H	-3.259287	-0.076193	1.967458
C	-4.213995	2.386679	4.825922
H	-2.485880	3.545856	4.213218
C	-5.014204	1.253933	4.587906
H	-5.284157	-0.515910	3.336815
H	-4.474815	3.085058	5.637298
H	-5.905121	1.063555	5.207170
C	4.096198	-0.275478	2.293698
C	4.169468	1.004165	1.694411
C	5.274262	-0.832740	2.828140
C	5.380900	1.712438	1.650156
H	3.272536	1.481239	1.265906
C	6.496991	-0.134559	2.761075
H	5.243523	-1.818256	3.316514
C	6.556732	1.142194	2.178299
H	5.375786	2.719208	1.199490
H	7.404851	-0.591529	3.187429
H	7.508310	1.697386	2.149185
C	2.723422	-2.309324	3.055119
C	3.395159	-3.369720	2.401613
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H -4.560611 -1.664495 5.165675	H 3.851553 -3.183367 1.415817 C 2.221488 -3.836100 4.903291 H 1.599959 -1.751120 4.829548 C 2.915245 -4.872954 4.257812 H 4.029146 -5.445158 2.472474 H 1.752121 -4.013225 5.884394 H 2.992770 -5.866602 4.726732
Zero-point correction= 1.039105 (Hartree/Particle) Thermal correction to Energy= 1.102793 Thermal correction to Enthalpy= 1.103737 Thermal correction to Gibbs Free Energy= 0.936609 Sum of electronic and zero-point Energies= -3396.621289 Sum of electronic and thermal Energies= -3396.557601 Sum of electronic and thermal Enthalpies= -3396.556657 Sum of electronic and thermal Free Energies= -3396.723785 SCF Done (in solvent): -3398.2257711	Zero-point correction= 1.056635 (Hartree/Particle) Thermal correction to Energy= 1.128706 Thermal correction to Enthalpy= 1.129650 Thermal correction to Gibbs Free Energy= 0.942412 Sum of electronic and zero-point Energies= -4860.383799 Sum of electronic and thermal Energies= -4860.311728 Sum of electronic and thermal Enthalpies= -4860.310784 Sum of electronic and thermal Free Energies= -4860.498021 SCF Done (in solvent): -4862.0479335

[Pd(IPr*)(allyl)Cl]-I-II	**[Pd(IPr*)(allyl)Cl]-II**
137 StI-PREallyl--K2CO3 SCF Done: -4861.42331053 A.U.	137 StI-PREallyl--K2CO3post SCF Done: -4861.49290802 A.U.
Cl 2.811492 -1.450316 0.374922 C 0.113537 -0.746424 -3.092063 H 0.053519 0.237612 -3.582820 H -0.797778 -1.363451 -3.176056 C 1.393577 -1.380668 -2.967577 H 2.293821 -0.782452 -3.206199 C 1.514720 -2.662678 -2.359472 H 0.635090 -3.316057 -2.273043 Pd 0.778723 -0.701483 -1.034604 H 2.311878 -2.826113 -1.628164 O 4.119392 -4.631328 -1.773955 C 2.938982 -4.823447 -2.311868 O 2.632024 -4.101094 -3.399057 O 2.057961 -5.544218 -1.738311 K 4.540353 -2.454861 -2.899904 K 2.856347 -4.627204 0.548236 N -0.420155 0.572669 1.545233 C -1.658033 -2.004677 1.832432 H -1.590804 -1.426057 0.885623 C -0.434116 -1.601777 2.659350 C 0.201229 -0.357505 2.450099 C -0.280353 0.552306 0.174225 C 1.416497 0.003690 3.087914 C 2.199118 1.240095 2.615810 H 2.321975 1.053318 1.526137 C 0.127467 -2.471943 3.616059 H -0.349373 -3.448440 3.793691 C 1.283899 -2.105425 4.319130 H 1.704705 -2.787767 5.075186 C 1.934391 -0.890590 4.041498 H 2.879334 -0.641968 4.546788 C -1.311767 1.561109 1.968402 C -1.714879 2.230652 0.848213 H -2.406155 3.065562 0.710995 H -1.560912 1.705081 3.020234 N -1.081956 1.603120 -0.226504 C -1.437676 1.813417 -1.598960 C -2.619561 1.189593 -2.065277 C -0.582149 2.566823 -2.430145 C -2.924924 1.314279 -3.432861 C -0.971948 2.738628 -3.774402 C -2.120002 2.102473 -4.273695 H -3.799840 0.780940 -3.836885	Cl 2.943845 0.336615 -0.104995 C -0.377667 3.394424 -0.815827 H -0.866439 3.628766 0.149373 H -1.066788 3.423672 -1.681003 C 1.000446 3.710082 -1.036475 H 1.553532 4.161134 -0.189535 C 1.487089 4.200568 -2.381239 H 1.494620 5.313267 -2.422973 Pd 0.694700 1.609859 -0.581044 H 0.852038 3.821161 -3.206442 O 4.188029 2.074127 -3.100435 C 3.059759 2.606338 -3.331983 O 2.862339 3.807891 -2.618132 O 2.127845 2.175929 -4.054266 K 4.370897 2.875673 -0.571607 K 2.623465 -0.186038 -3.216327 N -0.217428 -1.406490 0.019398 C -2.035553 -0.830777 -2.192191 H -1.836855 -0.149909 -1.334752 C -0.795592 -1.712982 -2.345890 C 0.075461 -1.994908 -1.259243 C -0.200169 -0.038173 0.267489 C 1.181454 -2.882250 -1.411494 C 2.112720 -3.207556 -0.238061 H 2.236804 -2.257173 0.326841 C -0.543007 -2.324753 -3.592067 H -1.215464 -2.099261 -4.433907 C 0.532217 -3.207960 -3.757375 H 0.708457 -3.689676 -4.732401 C 1.384744 -3.482035 -2.673759 H 2.235278 -4.168085 -2.803422 C -0.760718 -2.126158 1.098097 C -1.066278 -1.211571 2.064154 H -1.512650 -1.328584 3.055133 H -0.887527 -3.210329 1.075035 N -0.724598 0.039253 1.544300 C -1.106541 1.288941 2.145088 C -2.450892 1.699520 1.989980 C -0.145218 2.071490 2.829399 C -2.833251 2.937674 2.543088 C -0.592330 3.258157 3.442776 C -1.919482 3.694691 3.290577

H	-0.363533	3.369716	-4.438796	H	-3.855191	3.308731	2.368003
H	-2.387104	2.215247	-5.336083	H	0.120150	3.869691	4.016922
C	-3.522087	0.440902	-1.082862	H	-2.236940	4.646105	3.745638
H	-2.905957	0.204396	-0.194372	C	-3.442801	0.818490	1.233059
C	0.715879	3.125699	-1.855482	H	-2.846969	0.099502	0.637504
H	0.687831	2.876017	-0.776016	C	1.300914	1.583798	2.892559
C	1.970101	2.427572	-2.387731	H	1.483487	1.038555	1.938687
C	2.791037	1.712620	-1.490212	C	2.388180	2.658886	2.876936
C	2.365616	2.497735	-3.740501	C	3.686751	2.343634	3.340205
C	3.997101	1.125411	-1.910840	C	2.190963	3.923247	2.277174
H	2.493480	1.619855	-0.436531	C	4.745998	3.260584	3.221227
C	3.554746	1.889482	-4.177338	H	3.868014	1.358027	3.795662
H	1.751851	3.056224	-4.462284	C	3.244302	4.850893	2.166684
C	4.384744	1.215159	-3.259204	H	1.199828	4.186906	1.882936
H	4.609681	0.591834	-1.167297	C	4.530754	4.525858	2.638848
H	3.847805	1.962787	-5.236634	H	5.745672	2.988301	3.596887
H	5.343932	0.788217	-3.599424	H	3.052904	5.834330	1.706892
C	0.797243	4.655569	-1.868916	H	5.353452	5.255788	2.567296
C	-0.377578	5.433981	-1.781909	C	1.454245	0.564647	4.019651
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C	-0.307185	6.828681	-1.627736	C	1.261638	0.943895	5.365206
H	-1.359619	4.937497	-1.826510	C	1.872708	-1.725358	4.761401
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H	2.972069	4.718871	-1.866796	C	1.374984	0.001638	6.399117
C	0.941666	7.471415	-1.557463	H	1.015817	1.992118	5.599262
H	-1.236340	7.416954	-1.559963	C	1.679058	-1.339420	6.098519
H	3.102060	7.197633	-1.595877	H	2.102688	-2.773852	4.520783
H	0.998183	8.564607	-1.435265	H	1.221391	0.312696	7.444895
C	-3.965297	-0.932416	-1.591165	H	1.762795	-2.082854	6.907186
C	-2.987255	-1.952034	-1.635801	C	-4.224288	1.598998	0.174308
C	-5.292716	-1.248030	-1.934913	C	-3.483644	2.108816	-0.914812
C	-3.325490	-3.260448	-2.008494	C	-5.624264	1.733461	0.169322
H	-1.949859	-1.707538	-1.348202	C	-4.124160	2.714300	-2.004189
C	-5.633646	-2.559783	-2.319208	H	-2.389786	1.978908	-0.919543
H	-6.071390	-0.471899	-1.876218	C	-6.270908	2.355067	-0.917302
C	-4.655555	-3.568204	-2.354088	H	-6.216185	1.319128	0.999858
H	-2.551335	-4.043620	-2.003578	C	-5.527412	2.837549	-2.008769
H	-6.677884	-2.795433	-2.580615	H	-3.525707	3.054134	-2.864748
H	-4.928266	-4.596193	-2.640535	H	-7.369155	2.446310	-0.916061
C	-4.653340	1.329033	-0.560679	H	-6.040000	3.300385	-2.866923
C	-4.906488	1.366567	0.827221	C	-4.297191	-0.048046	2.156956
C	-5.468275	2.103383	-1.413682	C	-4.443002	-1.418076	1.853135
C	-5.957191	2.137942	1.349103	C	-4.964926	0.465436	3.288753
H	-4.266122	0.784190	1.505949	C	-5.245412	-2.252597	2.647148
C	-6.520988	2.877507	-0.894517	H	-3.913131	-1.833167	0.982666
H	-5.276043	2.109265	-2.497402	C	-5.768513	-0.367624	4.086939
C	-6.771782	2.895458	0.489162	H	-4.852276	1.526941	3.556206
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H	-7.147607	3.473429	-1.577349	H	-5.346144	-3.317086	2.381855
H	-7.596198	3.503054	0.895252	H	-6.282505	0.051274	4.966989
C	3.616536	1.313958	3.194322	H	-6.542420	-2.381726	4.395728
C	3.903189	2.002754	4.391624	C	3.507278	-3.642788	-0.710988
C	4.669858	0.650440	2.527189	C	3.831186	-5.002705	-0.907365
C	5.208569	2.024837	4.913645	C	4.482130	-2.666434	-1.013680
H	3.100228	2.539441	4.919426	C	5.086204	-5.376399	-1.420446
C	5.975309	0.676232	3.045875	H	3.092695	-5.779412	-0.653936
H	4.441085	0.086648	1.607953	C	5.737151	-3.039753	-1.525009
C	6.250956	1.362491	4.242400	H	4.249785	-1.605192	-0.821163
H	5.412213	2.570740	5.848915	C	6.042615	-4.396423	-1.738258
H	6.784664	0.153661	2.510283	H	5.318593	-6.443339	-1.567909
H	7.274986	1.384724	4.648337	H	6.485688	-2.262077	-1.748623
C	1.455941	2.565531	2.760894	H	7.026466	-4.689521	-2.137996
C	1.527542	3.523028	1.727782	C	1.504263	-4.239827	0.711794

C	0.695734	2.872344	3.908439	C	1.918395	-4.257045	2.059593
C	0.817041	4.731871	1.804995	C	0.555210	-5.191373	0.283782
H	2.150050	3.317280	0.843185	C	1.377465	-5.181452	2.966104
C	0.001377	4.091545	4.004938	H	2.672858	-3.526726	2.393630
H	0.621933	2.128220	4.718898	C	0.010527	-6.119777	1.190071
C	0.046171	5.017192	2.947070	H	0.223459	-5.191409	-0.766656
H	0.865917	5.445730	0.966881	C	0.414107	-6.113188	2.536157
H	-0.592197	4.312937	4.906670	H	1.703686	-5.174063	4.018564
H	-0.514946	5.962740	3.013202	H	-0.737215	-6.849800	0.841119
C	-1.561634	-3.468595	1.402224	H	-0.017411	-6.833665	3.248704
C	-0.713135	-3.788739	0.321670	C	-2.159219	0.095246	-3.406087
C	-2.259300	-4.507349	2.049505	C	-1.166995	1.089284	-3.562438
C	-0.575067	-5.112579	-0.130511	C	-3.148132	-0.035241	-4.400218
H	-0.160728	-2.961199	-0.166855	C	-1.163749	1.939931	-4.676962
C	-2.116451	-5.838557	1.613949	H	-0.388865	1.205230	-2.778673
H	-2.931996	-4.270904	2.889128	C	-3.160999	0.831556	-5.510200
C	-1.280840	-6.142774	0.524712	H	-3.919506	-0.815570	-4.310541
H	0.102010	-5.340571	-0.976074	C	-2.172746	1.820742	-5.652723
H	-2.670803	-6.641171	2.127037	H	-0.348879	2.672981	-4.781662
H	-1.177866	-7.183039	0.176390	H	-3.948229	0.723322	-6.273797
C	-3.006628	-1.624576	2.442735	H	-2.179683	2.489118	-6.528695
C	-4.189857	-1.967042	1.745277	C	-3.279039	-1.643895	-1.814882
C	-3.119789	-0.906745	3.649720	C	-4.545217	-1.015342	-1.753050
C	-5.448513	-1.608519	2.248583	C	-3.197807	-3.004673	-1.444470
H	-4.115719	-2.516399	0.794079	C	-5.684761	-1.722089	-1.340510
C	-4.383345	-0.538541	4.151639	H	-4.639901	0.043674	-2.028605
H	-2.207139	-0.640318	4.206050	C	-4.340407	-3.715466	-1.032359
C	-5.551511	-0.892059	3.456013	H	-2.227231	-3.522900	-1.476652
H	-6.353958	-1.872781	1.680666	C	-5.590877	-3.078126	-0.980120
H	-4.451710	0.022681	5.097470	H	-6.650960	-1.196545	-1.289004
H	-6.539948	-0.603822	3.847079	H	-4.246375	-4.775771	-0.747834
				H	-6.484866	-3.630049	-0.650074
Zero-point correction= 1.055581 (Hartree/Particle) Thermal correction to Energy= 1.127234 Thermal correction to Enthalpy= 1.128179 Thermal correction to Gibbs Free Energy= 0.942847 Sum of electronic and zero-point Energies= -4860.367730 Sum of electronic and thermal Energies= -4860.296076 Sum of electronic and thermal Enthalpies= -4860.295132 Sum of electronic and thermal Free Energies= -4860.480463 SCF Done (in solvent): -4862.0190172				Zero-point correction= 1.057772 (Hartree/Particle) Thermal correction to Energy= 1.129236 Thermal correction to Enthalpy= 1.130180 Thermal correction to Gibbs Free Energy= 0.946291 Sum of electronic and zero-point Energies= -4860.435136 Sum of electronic and thermal Energies= -4860.363672 Sum of electronic and thermal Enthalpies= -4860.362728 Sum of electronic and thermal Free Energies= -4860.546617 SCF Done (in solvent): -4862.0788396				

[Pd(IPr*)(allyl)Cl]-III				**[Pd(IPr*)(allyl)Cl]-I'**			
135 StI-PREallyl+KCO3menysKClISOMERopen SCF Done: -3801.23095887 A.U.				135 StI-PREallyl+KCO3menysKCl SCF Done: -3801.22675111 A.U.			
N	0.159123	1.116426	0.485241	N	-0.129192	-1.128587	0.230810
C	0.101074	2.212139	-0.439819	C	-0.040156	-2.208177	-0.715387
N	0.078783	-0.879929	1.302929	N	-0.320364	0.842710	1.093294
C	1.156894	2.395823	-1.373400	C	-1.127019	-2.412550	-1.598325
C	1.041553	3.461236	-2.292264	C	-1.027159	-3.458471	-2.534256
H	1.849523	3.625687	-3.021414	H	-1.857176	-3.622735	-3.238531
C	-0.087884	4.299836	-2.292122	C	0.108526	-4.280129	-2.568632
H	-0.162171	5.119149	-3.025110	H	0.179451	-5.087253	-3.314482
C	-1.112805	4.105501	-1.352413	C	1.151097	-4.087125	-1.650179
H	-2.001740	4.755590	-1.347300	H	2.039735	-4.735663	-1.685102
C	-1.024898	3.072954	-0.393998	C	1.096583	-3.050094	-0.698112
C	2.404662	1.508638	-1.346076	C	-2.418363	-1.602731	-1.468722
H	2.063024	0.485155	-1.068542	H	-2.137241	-0.615915	-1.039933
C	-2.067234	2.945790	0.716098	C	2.161241	-2.889917	0.386748
H	-2.100568	1.878873	1.025208	H	2.123373	-1.830076	0.719518
C	0.006156	-0.203943	0.107006	C	-0.087664	0.206578	-0.106851
C	0.330326	1.244972	1.869471	C	-0.396916	-1.310051	1.591203

H	0.471174	2.215631	2.350532	H	-0.499969	-2.304151	2.030529
C	0.267379	-0.019480	2.384714	C	-0.495183	-0.063680	2.140349
H	0.362663	-0.387310	3.408941	H	-0.704417	0.265633	3.160612
C	0.307635	-2.302346	1.362259	C	-0.668893	2.233695	1.185276
C	1.658525	-2.719816	1.421228	C	-2.049855	2.540574	1.241305
C	1.923857	-4.102172	1.466367	C	-2.422933	3.899256	1.230316
H	2.968782	-4.449293	1.445183	H	-3.492718	4.160951	1.223417
C	0.866769	-5.021632	1.511058	C	-1.442747	4.901169	1.174713
H	1.078978	-6.100253	1.580321	H	-1.744069	5.960378	1.154666
C	-0.465389	-4.581129	1.429266	C	-0.077817	4.568059	1.111865
H	-1.282533	-5.316598	1.425854	H	0.675524	5.365029	1.031734
C	-0.776536	-3.212812	1.303081	C	0.342256	3.223253	1.111156
C	2.786774	-1.690694	1.392538	C	-3.090574	1.420363	1.272506
H	2.353016	-0.737713	1.031133	H	-2.600612	0.509713	0.874404
C	-2.185820	-2.699896	0.982183	C	1.792981	2.794621	0.892822
H	-2.073685	-2.179655	-0.003383	H	1.802324	2.258592	-0.088448
C	0.033327	-2.213836	-3.631060	C	-0.879547	2.824084	-2.113974
H	1.040100	-2.664876	-3.668503	H	-1.204357	3.421305	-1.248656
H	-0.230404	-1.557021	-4.479303	H	-1.696168	2.478266	-2.772339
C	-0.978188	-2.798960	-2.860318	C	0.405113	3.075240	-2.691971
H	-0.725310	-3.706239	-2.276165	H	1.109831	3.748336	-2.170284
C	-2.461317	-2.590372	-3.076833	C	0.882587	2.232626	-3.718711
H	-2.822284	-3.369995	-3.793596	H	0.188428	1.753809	-4.430810
Pd	-0.081377	-1.161136	-1.687140	Pd	0.429128	1.090709	-1.864938
H	-3.022007	-2.730802	-2.127699	H	1.942593	2.269057	-4.012881
O	-3.813183	0.659498	-3.336776	O	4.035718	-0.344003	-3.012860
C	-3.658574	-0.464132	-2.788908	C	3.098322	0.234623	-2.364930
O	-4.067657	-0.924726	-1.713876	O	1.903459	-0.339900	-2.303880
O	-2.772121	-1.307430	-3.603690	O	3.308410	1.339594	-1.697893
K	-1.406075	1.150188	-3.701885	K	5.646588	0.564787	-1.311213
C	3.415301	1.921714	-0.272000	C	2.792259	3.942897	0.747887
C	4.618407	1.185834	-0.164319	C	3.101660	4.803837	1.824154
C	3.191311	2.983093	0.628717	C	3.449635	4.135461	-0.486779
C	5.570966	1.506894	0.812943	C	4.029865	5.846569	1.666903
H	4.806041	0.352061	-0.857719	H	2.610004	4.656036	2.798633
C	4.148481	3.306316	1.610091	C	4.381704	5.178515	-0.642649
H	2.262241	3.570869	0.563790	H	3.252256	3.422504	-1.305055
C	5.342793	2.572835	1.703229	C	4.672849	6.039755	0.429933
H	6.489807	0.904866	0.887056	H	4.254841	6.511658	2.516275
H	3.952998	4.138537	2.304923	H	4.883459	5.317835	-1.614519
H	6.088298	2.820423	2.474932	H	5.399882	6.858467	0.305901
C	3.011215	1.358775	-2.740322	C	2.309556	1.781234	1.914452
C	4.073679	2.162135	-3.200870	C	2.074128	1.911057	3.297782
C	2.448038	0.411081	-3.619590	C	3.095587	0.702597	1.453761
C	4.554413	2.023350	-4.516142	C	2.656829	1.011065	4.209005
H	4.534604	2.894394	-2.519053	H	1.419285	2.719035	3.663905
C	2.924561	0.267773	-4.932000	C	3.686057	-0.191232	2.361736
H	1.629538	-0.233113	-3.236991	H	3.203711	0.592608	0.358990
C	3.981943	1.079152	-5.387007	C	3.478930	-0.031830	3.746361
H	5.387338	2.656502	-4.861431	H	2.469168	1.127485	5.288660
H	2.478974	-0.490834	-5.596288	H	4.284656	-1.039124	1.987262
H	4.365038	0.968601	-6.413933	H	3.937759	-0.735045	4.459579
C	3.838924	-2.013342	0.327424	C	1.814136	-3.751597	1.611243
C	5.212434	-2.123461	0.610894	C	1.843622	-3.191010	2.906260
C	3.409956	-2.077967	-1.018670	C	1.491475	-5.119266	1.482914
C	6.145090	-2.270443	-0.434261	C	1.559418	-3.970855	4.040684
H	5.558218	-2.060206	1.654100	H	2.080186	-2.123217	3.022218
C	4.338668	-2.206785	-2.060699	C	1.206391	-5.902328	2.614232
H	2.327122	-1.985030	-1.246568	H	1.455518	-5.578952	0.483913
C	5.714732	-2.299477	-1.771716	C	1.238847	-5.332049	3.899569
H	7.218838	-2.346774	-0.198786	H	1.585403	-3.506935	5.039883
H	3.987252	-2.211776	-3.104583	H	0.954200	-6.967589	2.489153
H	6.447605	-2.391824	-2.588817	H	1.012269	-5.945881	4.785844

C	3.349333	-1.367310	2.775443
C	3.563933	-0.015167	3.116875
C	3.687063	-2.361207	3.717857
C	4.114854	0.338322	4.358562
H	3.288463	0.769123	2.396120
C	4.237271	-2.010933	4.963648
H	3.513016	-3.421771	3.482042
C	4.455847	-0.660064	5.288195
H	4.275841	1.402111	4.595464
H	4.493782	-2.801037	5.687477
H	4.885015	-0.387306	6.265518
C	-2.700900	-1.644673	1.955178
C	-2.440812	-1.723685	3.338277
C	-3.534131	-0.615186	1.466505
C	-3.015886	-0.797860	4.227064
H	-1.789183	-2.527397	3.719590
C	-4.109381	0.308918	2.354718
H	-3.753895	-0.567465	0.385401
C	-3.859894	0.215243	3.737812
H	-2.813159	-0.875275	5.307571
H	-4.753909	1.109160	1.956095
H	-4.325143	0.931299	4.434588
C	-3.213557	-3.815390	0.754138
C	-4.332668	-3.990674	1.592427
C	-3.058045	-4.696727	-0.340730
C	-5.268765	-5.011000	1.343305
H	-4.483190	-3.311559	2.444531
C	-3.988900	-5.715216	-0.593338
H	-2.178460	-4.589755	-0.992834
C	-5.103894	-5.875902	0.249684
H	-6.139242	-5.122805	2.009434
H	-3.845681	-6.384021	-1.457153
H	-5.841138	-6.669860	0.050711
C	-3.473221	3.273595	0.213198
C	-4.086849	2.351148	-0.659503
C	-4.153644	4.461453	0.546582
C	-5.350676	2.611503	-1.207673
H	-3.586321	1.406538	-0.920598
C	-5.428075	4.720185	0.006521
H	-3.687314	5.183032	1.235959
C	-6.026636	3.800157	-0.873202
H	-5.776479	1.873719	-1.904268
H	-5.954878	5.649824	0.276460
H	-7.022013	4.009729	-1.296913
C	-1.644681	3.750028	1.951596
C	-0.862558	4.920913	1.867060
C	-2.048036	3.302628	3.228557
C	-0.492867	5.626199	3.027842
H	-0.527099	5.286625	0.884472
C	-1.679611	4.002875	4.387293
H	-2.638000	2.378012	3.307844
C	-0.898646	5.170059	4.292909
H	0.120391	6.537238	2.938675
H	-1.999108	3.628998	5.373295
H	-0.604661	5.718001	5.202184

Zero-point correction= 1.055286 (Hartree/Particle)
Thermal correction to Energy= 1.123094
Thermal correction to Enthalpy= 1.124038
Thermal correction to Gibbs Free Energy= 0.947096
Sum of electronic and zero-point Energies= -3800.175673
Sum of electronic and thermal Energies= -3800.107865
Sum of electronic and thermal Enthalpies= -3800.106920
Sum of electronic and thermal Free Energies= -3800.283863

SCF Done (in solvent): -3801.8132666

C	3.609149	-3.107443	-0.078148
C	3.996194	-2.784433	-1.395253
C	4.603200	-3.538261	0.832014
C	5.339975	-2.906861	-1.796802
H	3.260234	-2.395198	-2.114718
C	5.948174	-3.642870	0.436856
H	4.320475	-3.798817	1.863621
C	6.323326	-3.334034	-0.885281
H	5.599901	-2.644143	-2.834505
H	6.704092	-3.983202	1.163053
H	7.373542	-3.439726	-1.203999
C	-3.396361	-2.211601	-0.453261
C	-3.042569	-3.305150	0.366544
C	-4.668524	-1.621297	-0.261225
C	-3.927153	-3.790577	1.348296
H	-2.062018	-3.788644	0.238268
C	-5.553650	-2.108194	0.712329
H	-4.968698	-0.764617	-0.880034
C	-5.188007	-3.196795	1.524657
H	-3.623125	-4.643383	1.976292
H	-6.529384	-1.615234	0.844673
H	-5.879096	-3.573770	2.295017
C	-3.005615	-1.263909	-2.839966
C	-4.184104	-1.834798	-3.356292
C	-2.305904	-0.325333	-3.629246
C	-4.675096	-1.440970	-4.615972
H	-4.733653	-2.582977	-2.764817
C	-2.792748	0.072332	-4.881723
H	-1.359873	0.093446	-3.231258
C	-3.990460	-0.479403	-5.377828
H	-5.604058	-1.890814	-5.001674
H	-2.235556	0.815891	-5.474268
H	-4.381874	-0.167486	-6.359231
C	-3.531009	1.045621	2.686349
C	-3.805771	2.007381	3.679846
C	-3.692811	-0.320607	3.002844
C	-4.244259	1.612220	4.956891
H	-3.669145	3.076878	3.457343
C	-4.132206	-0.717586	4.274889
H	-3.462109	-1.078618	2.239280
C	-4.411393	0.249056	5.258366
H	-4.453728	2.376679	5.722288
H	-4.252633	-1.790346	4.494729
H	-4.752820	-0.059043	6.259530
C	-4.245375	1.647443	0.293340
C	-5.592251	1.751908	0.684617
C	-3.936627	1.620597	-1.084260
C	-6.609426	1.815363	-0.288263
H	-5.850911	1.749720	1.754798
C	-4.944874	1.668552	-2.056112
H	-2.885502	1.508163	-1.387147
C	-6.292172	1.765506	-1.657009
H	-7.661842	1.887070	0.030434
H	-4.676004	1.586730	-3.121537
H	-7.093078	1.789945	-2.412760

Zero-point correction= 1.056103 (Hartree/Particle)
Thermal correction to Energy= 1.123273
Thermal correction to Enthalpy= 1.124217
Thermal correction to Gibbs Free Energy= 0.952258
Sum of electronic and zero-point Energies= -3800.170648
Sum of electronic and thermal Energies= -3800.103478
Sum of electronic and thermal Enthalpies= -3800.102534
Sum of electronic and thermal Free Energies= -3800.274493

SCF Done (in solvent): -3801.7968399

[Pd(IPr*)(allyl)Cl]-I'-III				[Pd(IPr*)(allyl)Cl]-IV			
135				122			
StI-PREallyl+KCO3--C-O SCF Done: -3801.19521560 A.U.				StIPr-Pd SCF Done: -2820.24979116 A.U.			
N	-0.395512	-1.173145	0.787325	Pd	0.923630	0.061581	-2.001375
C	-0.142636	-2.425517	0.134362	N	-0.189700	-1.038731	0.671601
N	-0.580372	0.955897	1.144017	C	-2.849486	-2.065756	0.208261
C	-1.216769	-3.055974	-0.533496	H	-2.489107	-1.048067	0.468736
C	-0.980304	-4.308608	-1.132072	C	-1.605594	-2.940580	0.053717
H	-1.793947	-4.802086	-1.685867	C	-0.314556	-2.398955	0.227162
C	0.288300	-4.903332	-1.057480	C	0.075798	0.009576	-0.184032
H	0.461351	-5.885140	-1.525424	C	0.862943	-3.149107	-0.026712
C	1.346168	-4.244793	-0.411961	C	2.225071	-2.472664	0.123956
H	2.346087	-4.703911	-0.392854	H	2.131427	-1.499042	-0.429323
C	1.156710	-2.980960	0.181112	C	-1.711868	-4.295409	-0.324466
C	-2.582060	-2.372129	-0.578617	H	-2.711285	-4.736060	-0.460206
H	-2.385011	-1.280098	-0.502398	C	-0.563167	-5.067298	-0.538321
C	2.276320	-2.240065	0.915078	H	-0.659741	-6.125124	-0.829654
H	2.048567	-1.153722	0.837091	C	0.715043	-4.494369	-0.405823
C	-0.156109	0.051509	0.180850	H	1.615945	-5.093672	-0.606556
C	-0.931329	-1.036498	2.069686	C	-0.347724	-0.614624	1.996470
H	-1.156203	-1.903280	2.696040	C	-0.188234	0.743485	1.988949
C	-1.038995	0.304801	2.302358	H	-0.266714	1.484547	2.789050
H	-1.368256	0.865678	3.180965	H	-0.552819	-1.315087	2.809942
C	-0.698888	2.376703	0.981878	N	0.076142	1.105597	0.663163
C	-1.999071	2.943821	0.945373	C	0.205790	2.463692	0.199825
C	-2.109326	4.345893	1.044174	C	-0.979967	3.154446	-0.148384
H	-3.111161	4.801445	1.081628	C	1.483678	3.059452	0.074849
C	-0.963759	5.156003	1.074351	C	-0.876467	4.498344	-0.551808
H	-1.066889	6.250102	1.146764	C	1.545712	4.411272	-0.317308
C	0.312424	4.577465	0.979311	C	0.377079	5.129286	-0.612790
H	1.210693	5.213131	0.945597	H	-1.791096	5.042942	-0.832838
C	0.467765	3.179314	0.942245	H	2.531380	4.894068	-0.403520
C	-3.221930	2.064393	0.668150	H	0.444894	6.185348	-0.918244
H	-2.918324	1.022721	0.886161	C	-2.316229	2.416749	-0.097108
C	1.838265	2.520555	0.833199	H	-2.090101	1.371259	-0.398241
H	1.670220	1.620894	0.178113	C	2.750546	2.220342	0.235407
C	-0.959130	0.889231	-2.789854	H	2.455815	1.354554	0.868773
H	-1.461832	1.817314	-2.473801	C	3.188146	1.581762	-1.093802
H	-1.658356	0.041308	-2.899158	C	4.314999	0.749978	-1.143596
C	0.148348	1.012103	-3.710573	C	2.333737	1.661536	-2.251226
H	0.577713	2.015459	-3.884326	C	4.573725	-0.080385	-2.265795
C	0.667262	-0.058482	-4.484056	H	4.999093	0.716254	-0.280101
H	0.121843	-1.014762	-4.488835	C	2.588600	0.815477	-3.388448
Pd	0.646917	0.368072	-1.581820	H	1.652533	2.523955	-2.346658
H	1.232719	0.162246	-5.400040	C	3.706870	-0.073227	-3.360186
O	4.416581	-0.173475	-3.507344	H	5.441554	-0.757105	-2.253540
C	3.186275	-0.259544	-3.177619	H	2.068886	1.006451	-4.343099
O	2.342192	-0.973757	-3.875340	H	3.897191	-0.733414	-4.221220
O	2.776312	0.349125	-2.067877	C	3.840888	2.959096	1.002408
K	5.167172	0.850925	-1.362259	C	3.777084	2.999593	2.412350
C	2.215572	-2.611073	2.398550	C	4.888538	3.643350	0.352913
C	2.487960	-3.930098	2.824776	C	4.736858	3.703593	3.157265
C	1.848976	-1.653080	3.362072	H	2.958986	2.467185	2.925682
C	2.392655	-4.280783	4.180071	C	5.849733	4.352172	1.095787
H	2.780267	-4.688648	2.081600	H	4.954957	3.602501	-0.745925
C	1.747839	-2.001364	4.720901	C	5.778251	4.384143	2.499350
H	1.640583	-0.621052	3.045859	H	4.674312	3.719657	4.257274
C	2.016871	-3.315884	5.135097	H	6.663557	4.879717	0.572859
H	2.609807	-5.314135	4.494723	H	6.534624	4.934751	3.080923
H	1.463749	-1.230651	5.454751	C	-3.297265	2.928153	-1.149342
H	1.938104	-3.591321	6.198974	C	-2.998081	2.685690	-2.509256

C	3.663730	-2.396136	0.286324	C	-4.472950	3.629895	-0.824319
C	4.826945	-2.326560	1.085990	C	-3.858100	3.134258	-3.521845
C	3.814331	-2.504683	-1.114679	H	-2.072812	2.139487	-2.762790
C	6.107729	-2.385892	0.503876	C	-5.336474	4.082271	-1.840223
H	4.724530	-2.235320	2.178246	H	-4.717163	3.815024	0.233556
C	5.091692	-2.583903	-1.699040	C	-5.033398	3.835497	-3.189472
H	2.929161	-2.500439	-1.769152	H	-3.614015	2.933153	-4.577369
C	6.245054	-2.527065	-0.891322	H	-6.254846	4.628822	-1.572017
H	7.001748	-2.341881	1.147578	H	-5.712085	4.186282	-3.983121
H	5.172457	-2.641747	-2.794421	C	-2.883832	2.322731	1.317591
H	7.245649	-2.594445	-1.348840	C	-3.717389	1.233837	1.649441
C	-3.438011	-2.750679	0.632632	C	-2.574458	3.266120	2.317136
C	-3.649014	-4.098837	0.992163	C	-4.196822	1.062879	2.956313
C	-4.056919	-1.749595	1.409165	H	-3.982870	0.503810	0.868621
C	-4.458540	-4.431956	2.091195	C	-3.063812	3.107188	3.627115
H	-3.167266	-4.897683	0.407486	H	-1.924303	4.120699	2.071605
C	-4.870703	-2.074619	2.507266	C	-3.865830	1.999840	3.953196
H	-3.893151	-0.692018	1.157811	H	-4.816462	0.184265	3.194802
C	-5.074331	-3.421504	2.852990	H	-2.806929	3.850273	4.399219
H	-4.607683	-5.490815	2.356630	H	-4.233446	1.865214	4.982912
H	-5.342484	-1.265706	3.087835	C	3.349850	-3.220261	-0.583305
H	-5.708950	-3.685029	3.714002	C	4.368186	-3.903878	0.108510
C	-3.296468	-2.540262	-1.923691	C	3.369403	-3.219264	-1.996118
C	-4.684092	-2.766108	-2.015652	C	5.386918	-4.572924	-0.596032
C	-2.559390	-2.362853	-3.117359	H	4.368102	-3.904108	1.209775
C	-5.321661	-2.810631	-3.270506	C	4.381619	-3.887101	-2.700213
H	-5.274890	-2.901621	-1.096877	H	2.582061	-2.668910	-2.537090
C	-3.194032	-2.399504	-4.367656	C	5.397632	-4.566884	-2.001157
H	-1.472306	-2.195618	-3.055675	H	6.178974	-5.099794	-0.039924
C	-4.581287	-2.624247	-4.450053	H	4.384893	-3.868857	-3.802025
H	-6.407755	-2.988236	-3.321938	H	6.197055	-5.087620	-2.552162
H	-2.600224	-2.247898	-5.282965	C	2.527180	-2.122435	1.577695
H	-5.081731	-2.655089	-5.430795	C	3.315876	-0.989932	1.864500
C	-3.614917	2.073679	-0.817798	C	2.039457	-2.893529	2.652595
C	-4.181381	0.905845	-1.374047	C	3.593462	-0.617409	3.188941
C	-3.448366	3.196268	-1.655161	H	3.717856	-0.403196	1.025809
C	-4.540386	0.844353	-2.728709	C	2.316553	-2.526923	3.982166
H	-4.339543	0.017524	-0.744988	H	1.424803	-3.783776	2.443027
C	-3.829726	3.147968	-3.008663	C	3.087161	-1.383062	4.255636
H	-2.983214	4.111049	-1.259482	H	4.205836	0.277532	3.383240
C	-4.366354	1.969585	-3.553236	H	1.924473	-3.138912	4.810600
H	-4.939358	-0.096412	-3.138602	H	3.297367	-1.091926	5.297156
H	-3.679859	4.033816	-3.646112	C	-3.538715	-1.928838	-1.151436
H	-4.636509	1.922204	-4.619731	C	-3.100980	-0.920759	-2.036992
C	-4.403416	2.361029	1.594405	C	-4.550196	-2.814126	-1.581136
C	-5.415398	3.280388	1.249362	C	-3.674416	-0.784567	-3.311476
C	-4.487492	1.701352	2.840148	H	-2.277044	-0.252064	-1.734454
C	-6.473661	3.548108	2.135886	C	-5.121296	-2.683137	-2.858667
H	-5.382929	3.774527	0.265351	H	-4.907500	-3.604118	-0.901395
C	-5.546848	1.961437	3.724843	C	-4.688768	-1.664627	-3.726878
H	-3.716354	0.962072	3.110605	H	-3.328913	0.021424	-3.977089
C	-6.543394	2.891389	3.376820	H	-5.914008	-3.379681	-3.175684
H	-7.256067	4.268683	1.848645	H	-5.143329	-1.556828	-4.724508
H	-5.596910	1.431159	4.689546	C	-3.749181	-2.463870	1.379933
H	-7.376928	3.095958	4.067216	C	-5.090358	-2.023595	1.443410
C	2.397639	1.982795	2.143526	C	-3.227193	-3.170959	2.484430
C	1.801536	2.197047	3.401103	C	-5.883770	-2.283777	2.573244
C	3.586431	1.219487	2.089826	H	-5.518598	-1.466305	0.596071
C	2.393647	1.676660	4.569193	C	-4.016643	-3.427219	3.619020
H	0.872362	2.784931	3.466503	H	-2.185783	-3.528293	2.452214
C	4.184320	0.703097	3.244481	C	-5.349779	-2.985418	3.669009
H	4.042993	1.114196	1.096130	H	-6.927247	-1.930988	2.597328
C	3.584427	0.934633	4.497629	H	-3.585690	-3.980398	4.468881

H	1.916546	1.856118	5.545988
H	5.109182	0.110729	3.169274
H	4.036685	0.520960	5.411864
C	2.830355	3.367511	0.034649
C	3.919663	4.043112	0.625643
C	2.664572	3.443171	-1.368603
C	4.840073	4.754697	-0.169330
H	4.059036	3.996204	1.717295
C	3.579865	4.152978	-2.162342
H	1.830166	2.892254	-1.833794
C	4.677448	4.806668	-1.566222
H	5.686650	5.274042	0.308314
H	3.445422	4.178735	-3.255353
H	5.399408	5.359039	-2.188891

Zero-point correction= 1.053891 (Hartree/Particle)
Thermal correction to Energy= 1.121113
Thermal correction to Enthalpy= 1.122058
Thermal correction to Gibbs Free Energy= 0.947646
Sum of electronic and zero-point Energies= -3800.141325
Sum of electronic and thermal Energies= -3800.074102
Sum of electronic and thermal Enthalpies= -3800.073158
Sum of electronic and thermal Free Energies= -3800.247569

SCF Done (in solvent): -3801.7548012

H	-5.971083	-3.189626	4.555307

Zero-point correction= 0.966219 (Hartree/Particle)
Thermal correction to Energy= 1.024263
Thermal correction to Enthalpy= 1.025207
Thermal correction to Gibbs Free Energy= 0.868123
Sum of electronic and zero-point Energies= -2819.283572
Sum of electronic and thermal Energies= -2819.225529
Sum of electronic and thermal Enthalpies= -2819.224584
Sum of electronic and thermal Free Energies= -2819.381668

SCF Done (in solvent): -2820.7127502

[Pd(IPr*)(allyl)Cl]-V			
163			
StI5 SCF Done: -3797.46552441 A.U.			
C	-1.563973	-2.774541	-1.179092
O	-2.760614	-2.589740	-0.938874
Pd	-0.180189	-1.135426	0.052725
N	-0.651020	-3.258595	-0.110739
C	-0.270807	-2.907292	-5.310158
C	-1.621411	-3.061581	-4.956305
H	1.746190	-2.537934	-4.581151
C	0.689855	-2.683520	-4.305832
C	-2.002660	-3.018016	-3.606336
C	-1.041924	-2.803547	-2.593146
C	0.309048	-2.616132	-2.960099
H	-3.053094	-3.153256	-3.314201
H	1.051878	-2.378121	-2.185966
H	0.034399	-2.946209	-6.368071
H	-2.386121	-3.219426	-5.732999
C	-1.307772	-3.683475	1.149461
O	-2.357639	-4.282564	1.195414
O	-0.492517	-3.360256	2.157416
C	-0.820928	-3.739384	3.563215
C	-0.945598	-5.264962	3.664847
H	-1.832559	-5.635471	3.118595
H	-0.038132	-5.752792	3.253454
H	-1.040150	-5.551832	4.732087
C	0.401189	-3.232157	4.331086
H	0.268455	-3.422476	5.415088
H	1.322716	-3.744289	3.992232
H	0.533876	-2.144390	4.177126
C	-2.094345	-3.001989	3.987942
H	-2.979834	-3.371027	3.439772
H	-2.261264	-3.149456	5.074300
H	-1.994074	-1.915793	3.791605
C	0.363643	-4.263940	-0.436666
C	1.719666	-4.028585	-0.161891
C	-0.060463	-5.495229	-0.971622
C	2.658238	-5.040908	-0.417170
H	2.027195	-3.043941	0.219087

[Pd(IPr*)(allyl)Cl]-V-VI			
163			
StI5-I6 SCF Done: -3797.45973947 A.U.			
C	-0.883327	-2.767907	0.186245
O	0.012826	-3.551738	-0.095095
Pd	-0.704358	-0.767240	-0.505913
N	-2.022114	-2.332889	-1.140856
C	-3.174733	-3.130303	3.839036
C	-2.408880	-4.206308	3.353824
H	-3.734117	-1.039392	3.537613
C	-3.160163	-1.899190	3.159471
C	-1.662634	-4.064211	2.173767
C	-1.664117	-2.836697	1.476214
C	-2.392751	-1.749164	1.997911
H	-1.077096	-4.903327	1.770401
H	-2.333198	-0.774474	1.488063
H	-3.773710	-3.248738	4.756315
H	-2.401326	-5.167703	3.891656
C	-1.603280	-2.620424	-2.461400
O	-0.458450	-2.884164	-2.793165
O	-2.656873	-2.500437	-3.316046
C	-2.446614	-2.595485	-4.779042
C	-1.910005	-3.986399	-5.148079
H	-0.886232	-4.133545	-4.758992
H	-2.569852	-4.773139	-4.728331
H	-1.896476	-4.098205	-6.251861
C	-3.862257	-2.395050	-5.333812
H	-3.852679	-2.483319	-6.438986
H	-4.552379	-3.158232	-4.921543
H	-4.249347	-1.391291	-5.068079
C	-1.513353	-1.462501	-5.233320
H	-0.498390	-1.583264	-4.810605
H	-1.442061	-1.460239	-6.340511
H	-1.915409	-0.481218	-4.909200
C	-3.417290	-2.459279	-0.827270
C	-4.007233	-3.740282	-0.813028
C	-4.183840	-1.339137	-0.468372
C	-5.353220	-3.888338	-0.447688
H	-3.392770	-4.614261	-1.079272

C	0.886644	-6.496522	-1.238548	C	-5.527527	-1.487959	-0.094772
H	-1.130715	-5.654115	-1.173133	H	-3.699302	-0.355798	-0.469579
C	2.246825	-6.273545	-0.955414	C	-6.118412	-2.763119	-0.084788
H	3.720425	-4.852870	-0.201020	H	-5.806434	-4.892350	-0.432214
H	0.558916	-7.457059	-1.666041	H	-6.106783	-0.599295	0.201502
H	2.988626	-7.061835	-1.159134	H	-7.171451	-2.884552	0.214495
N	-0.048645	1.671225	1.132845	N	0.984429	0.841728	1.499300
C	-2.655805	1.385537	2.365683	C	-1.201639	2.274279	2.671018
H	-2.366953	1.438962	1.294344	H	-0.734084	2.354165	1.667481
C	-1.366389	1.092128	3.129404	C	-0.691331	0.967983	3.274829
C	-0.111479	1.203741	2.489705	C	0.371397	0.259338	2.667422
C	-0.019123	0.817958	0.042393	C	0.660324	0.481857	0.212397
C	1.100126	0.860017	3.135419	C	0.842257	-0.982266	3.169228
C	2.428547	0.957403	2.385028	C	1.963795	-1.737319	2.449352
H	2.195208	0.840571	1.305594	H	1.594894	-1.922795	1.416185
C	-1.383198	0.684986	4.478543	C	-1.254555	0.440397	4.452327
H	-2.348553	0.591572	4.996995	H	-2.078558	0.978887	4.942589
C	-0.192609	0.369266	5.148226	C	-0.796779	-0.774302	4.974915
H	-0.225964	0.037967	6.197877	H	-1.261595	-1.192641	5.880693
C	1.038151	0.435029	4.475289	C	0.226323	-1.485640	4.329492
H	1.966374	0.125038	4.980320	H	0.550647	-2.457956	4.725540
C	0.104200	3.007726	0.758181	C	1.846135	1.943548	1.523820
C	0.224960	3.015536	-0.603928	C	2.083728	2.286339	0.219352
H	0.284304	3.841639	-1.317232	H	2.681945	3.085809	-0.225532
H	0.096193	3.822383	1.486690	H	2.203700	2.376176	2.460737
N	0.147218	1.680971	-1.019671	N	1.369608	1.378033	-0.562209
C	0.307757	1.238747	-2.380017	C	1.311216	1.341972	-2.001364
C	-0.848869	0.998987	-3.167289	C	0.169015	1.882049	-2.646213
C	1.617656	1.104586	-2.893243	C	2.343651	0.689562	-2.711298
C	-0.660238	0.599592	-4.500834	C	0.065768	1.732450	-4.040316
C	1.758569	0.775062	-4.257804	C	2.187262	0.543405	-4.104568
C	0.631914	0.510101	-5.046281	C	1.062535	1.056636	-4.762470
H	-1.537615	0.364270	-5.120135	H	-0.827066	2.119220	-4.555042
H	2.768053	0.717521	-4.693515	H	2.949532	-0.010100	-4.671411
H	0.757176	0.218293	-6.100519	H	0.951806	0.918103	-5.849162
C	-2.230647	1.239505	-2.549284	C	-0.891061	2.630022	-1.838290
H	-2.240628	0.666211	-1.596263	H	-0.886241	2.183494	-0.820775
C	2.834042	1.286915	-1.986879	C	3.574762	0.137916	-1.990223
H	2.449381	1.687351	-1.029333	H	3.413851	0.302066	-0.904841
C	3.557611	-0.012987	-1.617193	C	3.698544	-1.383328	-2.120990
C	4.422386	-0.001067	-0.500525	C	4.949724	-2.034609	-2.161247
C	3.427899	-1.208836	-2.346800	C	2.528865	-2.168558	-2.024436
C	5.124256	-1.152279	-0.117375	C	5.025752	-3.438131	-2.098849
H	4.550902	0.924205	0.081929	H	5.876075	-1.443110	-2.226475
C	4.133143	-2.365942	-1.970845	C	2.602281	-3.568262	-1.962003
H	2.760602	-1.235816	-3.217322	H	1.534421	-1.696428	-1.973914
C	4.983163	-2.341464	-0.853500	C	3.854213	-4.208433	-1.994749
H	5.765592	-1.124354	0.776436	H	6.011670	-3.929878	-2.124592
H	3.998441	-3.294048	-2.548251	H	1.662058	-4.130012	-1.869896
H	5.534253	-3.245598	-0.549634	H	3.918067	-5.306935	-1.937113
C	3.791731	2.349405	-2.533954	C	4.820172	0.948342	-2.348575
C	3.542314	3.712116	-2.262227	C	5.333281	1.877724	-1.419114
C	4.912375	2.010462	-3.319129	C	5.470994	0.821954	-3.595902
C	4.388699	4.713649	-2.765064	C	6.451502	2.671574	-1.728389
H	2.674540	3.985811	-1.640194	H	4.856906	1.961568	-0.429491
C	5.757180	3.011362	-3.830463	C	6.588738	1.612361	-3.909119
H	5.132864	0.948606	-3.513233	H	5.112918	0.077847	-4.323661
C	5.499634	4.365746	-3.555057	C	7.081148	2.545165	-2.978093
H	4.180990	5.771553	-2.537038	H	6.834905	3.388758	-0.984861
H	6.629410	2.729254	-4.441713	H	7.083041	1.495156	-4.886823
H	6.166365	5.148737	-3.949725	H	7.958103	3.164759	-3.224268
C	-3.400978	0.725945	-3.386557	C	-2.316736	2.400473	-2.343113
C	-4.042577	-0.472916	-3.017523	C	-2.735582	1.077610	-2.611087

C	-3.861225	1.420383	-4.527299	C	-3.264064	3.437745	-2.446179
C	-5.109524	-0.976750	-3.782663	C	-4.061035	0.793778	-2.971739
H	-3.692976	-1.029776	-2.133015	H	-2.011762	0.248630	-2.511436
C	-4.922885	0.914222	-5.295290	C	-4.593976	3.158784	-2.814748
H	-3.387594	2.371821	-4.815239	H	-2.962123	4.472930	-2.225652
C	-5.550856	-0.289726	-4.926214	C	-4.998188	1.838460	-3.078149
H	-5.598247	-1.915755	-3.475823	H	-4.352414	-0.253477	-3.142342
H	-5.267249	1.467833	-6.183707	H	-5.320621	3.983626	-2.888223
H	-6.387642	-0.684362	-5.524746	H	-6.040788	1.621086	-3.359461
C	-2.401656	2.718536	-2.187571	C	-0.490069	4.090861	-1.649615
C	-3.054756	3.084657	-0.993823	C	-0.342918	4.613795	-0.349775
C	-1.882788	3.738897	-3.013712	C	-0.250897	4.940304	-2.750786
C	-3.149689	4.431545	-0.607803	C	0.028220	5.953402	-0.144317
H	-3.472750	2.298151	-0.344640	H	-0.511870	3.956905	0.516386
C	-1.996280	5.090561	-2.644148	C	0.116128	6.281391	-2.552173
H	-1.347811	3.466103	-3.937590	H	-0.351248	4.542684	-3.772997
C	-2.618564	5.439578	-1.432211	C	0.257332	6.792639	-1.247990
H	-3.629576	4.689950	0.347865	H	0.137777	6.330697	0.884897
H	-1.581678	5.873225	-3.299974	H	0.298683	6.932247	-3.422188
H	-2.688973	6.495888	-1.127510	H	0.550519	7.843402	-1.094602
C	3.330898	-0.234424	2.714187	C	2.278617	-3.104837	3.064076
C	4.610779	-0.117080	3.286146	C	3.009834	-3.213378	4.267729
C	2.841034	-1.520675	2.391709	C	1.838198	-4.282301	2.428091
C	5.386837	-1.266295	3.538616	C	3.272344	-4.470198	4.836239
H	5.010838	0.879271	3.528969	H	3.380939	-2.301958	4.762757
C	3.617200	-2.662470	2.630415	C	2.105729	-5.541612	2.994525
H	1.836917	-1.609033	1.933979	H	1.283139	-4.201497	1.480915
C	4.894429	-2.540532	3.211450	C	2.817685	-5.641322	4.201731
H	6.386978	-1.159048	3.988397	H	3.842677	-4.536756	5.776796
H	3.225103	-3.654108	2.353802	H	1.756209	-6.452199	2.481422
H	5.504844	-3.437360	3.402989	H	3.027936	-6.628243	4.644403
C	3.059691	2.338996	2.552086	C	3.252558	-0.922595	2.322636
C	3.424086	3.088829	1.414949	C	4.100365	-1.161829	1.222855
C	3.287068	2.907192	3.824676	C	3.651549	0.015636	3.296674
C	4.014281	4.357701	1.533080	C	5.306285	-0.458175	1.082489
H	3.227042	2.680147	0.414102	H	3.807588	-1.907413	0.466566
C	3.876703	4.176648	3.951121	C	4.862388	0.718637	3.161523
H	2.992466	2.351502	4.728328	H	2.993917	0.210056	4.159995
C	4.244953	4.906937	2.805953	C	5.690037	0.490521	2.048300
H	4.289959	4.910988	0.621043	H	5.939712	-0.643256	0.201383
H	4.046462	4.600948	4.953721	H	5.157515	1.452751	3.928818
H	4.705950	5.902239	2.907559	H	6.632707	1.048303	1.931226
C	-3.634938	0.217157	2.480472	C	-2.705709	2.244297	2.398120
C	-3.591114	-0.809457	1.515959	C	-3.161467	1.881823	1.114316
C	-4.558279	0.112929	3.544018	C	-3.658775	2.591882	3.379317
C	-4.458537	-1.911443	1.596203	C	-4.530778	1.885661	0.802114
H	-2.848970	-0.761797	0.699182	H	-2.428695	1.587000	0.346275
C	-5.418894	-0.994478	3.634934	C	-5.032213	2.564867	3.082350
H	-4.622703	0.920978	4.290709	H	-3.318655	2.921304	4.374254
C	-5.374544	-2.006067	2.657804	C	-5.472336	2.218812	1.790835
H	-4.379024	-2.697145	0.832054	H	-4.851986	1.644426	-0.223580
H	-6.135863	-1.061059	4.469277	H	-5.763882	2.836699	3.860008
H	-6.053050	-2.871466	2.727186	H	-6.547887	2.222967	1.552750
C	-3.259301	2.756293	2.685179	C	-0.731482	3.523454	3.425194
C	-4.585801	3.050830	2.295599	C	-1.250537	4.788165	3.064729
C	-2.494582	3.781378	3.279712	C	0.274392	3.468431	4.412153
C	-5.129445	4.330041	2.495358	C	-0.768977	5.962294	3.664721
H	-5.197357	2.264390	1.826853	H	-2.043608	4.848684	2.302979
C	-3.033295	5.066344	3.472420	C	0.757032	4.644199	5.016214
H	-1.463269	3.568966	3.602794	H	0.682392	2.491516	4.715534
C	-4.353749	5.346874	3.082669	C	0.240753	5.896036	4.643042
H	-6.164822	4.535966	2.180544	H	-1.188726	6.936811	3.367616
H	-2.415518	5.851453	3.937202	H	1.541541	4.577470	5.786989

H -4.778496 6.351212 3.237824	H 0.617484 6.816546 5.116256
Zero-point correction= 1.295043 (Hartree/Particle) Thermal correction to Energy= 1.374487 Thermal correction to Enthalpy= 1.375432 Thermal correction to Gibbs Free Energy= 1.178664 Sum of electronic and zero-point Energies= -3796.170482 Sum of electronic and thermal Energies= -3796.091037 Sum of electronic and thermal Enthalpies= -3796.090093 Sum of electronic and thermal Free Energies= -3796.286861	Zero-point correction= 1.292687 (Hartree/Particle) Thermal correction to Energy= 1.372199 Thermal correction to Enthalpy= 1.373143 Thermal correction to Gibbs Free Energy= 1.172644 Sum of electronic and zero-point Energies= -3796.167052 Sum of electronic and thermal Energies= -3796.087541 Sum of electronic and thermal Enthalpies= -3796.086597 Sum of electronic and thermal Free Energies= -3796.287096
SCF Done (in solvent): -3798.236662	SCF Done (in solvent): -3798.217535

[Pd(IPr*)(allyl)Cl]-VI			**[Pd(IPr*)(allyl)Cl]-VII**		
163			169		
StI6 SCF Done: -3797.49819375 A.U.			StI6+K2CO3 SCF Done: -5261.32535883 A.U.		
Pd	-0.593587	-1.011103 -0.408445	Pd	-1.115283	-0.039834 0.042096
C	0.996188	-2.149929 -0.179739	C	-0.908038	-1.990569 0.238372
O	1.910641	-2.049087 -0.985741	O	-0.357336	-2.678657 -0.631911
N	-1.983898	-2.483482 -0.981410	N	-3.158344	-0.253178 0.656577
C	1.119798	-5.316805 2.759690	C	-2.854907	-4.081693 3.474691
C	2.233314	-5.049389 1.939769	C	-3.026097	-4.514190 2.144423
H	-0.927717	-4.748004 3.260018	H	-1.945199	-2.590745 4.782388
C	-0.047221	-4.543469 2.632609	C	-2.071464	-2.947672 3.748776
C	2.176298	-4.014567 0.996917	C	-2.389502	-3.831359 1.096692
C	1.005572	-3.230745 0.869174	C	-1.608249	-2.686890 1.371476
C	-0.103195	-3.502961 1.694004	C	-1.472333	-2.237630 2.697729
H	3.037418	-3.786784 0.350755	H	-2.489004	-4.167840 0.052718
H	-1.017755	-2.906999 1.579301	H	-0.895136	-1.325518 2.896454
H	1.162115	-6.135098 3.496764	H	-3.343388	-4.627320 4.297965
H	3.150857	-5.651528 2.038152	H	-3.648499	-5.397340 1.926905
C	-2.961122	-1.644557 -1.351957	C	-4.057033	-0.609330 -0.277373
O	-2.796683	-0.395209 -1.169247	O	-3.778360	-1.029493 -1.419226
O	-4.077570	-2.155745 -1.922473	O	-5.380036	-0.390782 0.094740
C	-4.751452	-1.427722 -3.021011	C	-6.482073	-1.065160 -0.599861
C	-3.704161	-0.967435 -4.046057	C	-6.245851	-2.584084 -0.603839
H	-3.067266	-0.165790 -3.625513	H	-5.343654	-2.836928 -1.192042
H	-3.060932	-1.816693 -4.354485	H	-6.104306	-2.958466 0.430767
H	-4.211345	-0.567722 -4.947456	H	-7.120254	-3.103459 -1.046664
C	-5.673072	-2.500689 -3.611845	C	-7.698780	-0.711783 0.268987
H	-6.256433	-2.083412 -4.457364	H	-8.610448	-1.209362 -0.118640
H	-5.079844	-3.363428 -3.975456	H	-7.535410	-1.035348 1.316742
H	-6.380946	-2.866826 -2.840978	H	-7.884330	0.383270 0.263760
C	-5.551139	-0.245023 -2.464397	C	-6.652564	-0.502740 -2.021496
H	-4.873216	0.522654 -2.049572	H	-5.819852	-0.830593 -2.669829
H	-6.166598	0.210759 -3.267648	H	-7.611290	-0.853177 -2.457168
H	-6.229953	-0.581314 -1.655285	H	-6.662280	0.606474 -1.994613
C	-2.023008	-3.885341 -1.003758	K	-2.838730	0.899641 -2.925588
C	-3.152797	-4.613490 -0.554855	K	-5.179149	2.348898 1.025774
C	-0.868786	-4.601974 -1.402335	C	-2.764498	2.529796 -0.391806
C	-3.121834	-6.015582 -0.512117	O	-3.808121	2.380111 -1.157399
H	-4.049702	-4.063339 -0.236240	O	-2.825249	3.212196 0.688033
C	-0.843508	-6.002723 -1.348702	O	-1.619268	1.943981 -0.752194
H	0.012340	-4.039938 -1.744202	C	-3.454253	-0.092104 2.026038
C	-1.968608	-6.720819 -0.903573	C	-2.642087	0.796417 2.778291
H	-4.009262	-6.565065 -0.157319	C	-4.441430	-0.839117 2.725217
H	0.070079	-6.538014 -1.653661	C	-2.808069	0.947585 4.161322
H	-1.946139	-7.821030 -0.857943	H	-1.878526	1.380940 2.248589
N	1.323579	0.934793 1.046515	C	-4.607500	-0.678396 4.109731
C	-0.261138	0.185022 3.339992	H	-5.041260	-1.582551 2.185276
H	-0.468699	0.883334 2.503788	C	-3.798190	0.212631 4.841542
C	1.087221	-0.478052 3.029072	H	-2.152284	1.653288 4.696940
C	1.869125	-0.067495 1.923437	H	-5.363213	-1.288881 4.630786
C	0.364609	0.669889 0.094380	H	-3.930851	0.321887 5.929542
C	3.153050	-0.611575 1.642689	N	1.892823	-0.236017 0.538085

C	3.941571	-0.151808	0.408291
H	3.231189	-0.216212	-0.443708
C	1.622419	-1.473326	3.871477
H	1.044119	-1.816153	4.739678
C	2.880485	-2.027820	3.616613
H	3.272054	-2.819219	4.273443
C	3.639580	-1.599072	2.515503
H	4.616558	-2.059320	2.309666
C	1.589558	2.305033	1.138366
C	0.806373	2.918252	0.204069
H	0.686072	3.972190	-0.054878
H	2.315220	2.711877	1.845545
N	0.057957	1.912033	-0.413371
C	-0.801245	2.129870	-1.550873
C	-2.160225	2.485433	-1.348519
C	-0.240022	1.964560	-2.834971
C	-2.950261	2.704900	-2.488767
C	-1.065136	2.209229	-3.951808
C	-2.405085	2.577635	-3.778488
H	-4.013580	2.956407	-2.362566
H	-0.643262	2.095285	-4.962062
H	-3.042915	2.753263	-4.658867
C	-2.723938	2.526051	0.073625
H	-2.426463	1.552945	0.513720
C	1.201032	1.485629	-3.010624
H	1.684105	1.522837	-2.011825
C	1.300119	0.020043	-3.447962
C	2.577169	-0.541534	-3.666959
C	0.170347	-0.815140	-3.553409
C	2.720660	-1.896618	-3.997829
H	3.471864	0.096059	-3.575068
C	0.312188	-2.176708	-3.876611
H	-0.834070	-0.408472	-3.371792
C	1.585228	-2.721921	-4.100596
H	3.727402	-2.314505	-4.157184
H	-0.584125	-2.814346	-3.925148
H	1.695105	-3.790912	-4.342614
C	1.982896	2.470218	-3.882049
C	2.487536	3.647272	-3.288174
C	2.177502	2.272199	-5.263987
C	3.170775	4.605347	-4.054067
H	2.343513	3.803655	-2.206206
C	2.859255	3.231240	-6.034288
H	1.805674	1.347519	-5.733017
C	3.358643	4.399985	-5.433400
H	3.560486	5.516539	-3.571844
H	3.005791	3.060447	-7.112879
H	3.896906	5.147724	-6.037175
C	-4.248086	2.582916	0.164474
C	-4.974665	1.410905	0.454911
C	-4.956921	3.791312	-0.011623
C	-6.374305	1.443247	0.574109
H	-4.429894	0.462382	0.560395
C	-6.357423	3.823389	0.090490
H	-4.404503	4.721212	-0.218326
C	-7.072034	2.648650	0.388903
H	-6.921844	0.516059	0.807209
H	-6.893977	4.775006	-0.052807
H	-8.169639	2.675378	0.479521
C	-2.087293	3.607473	0.944918
C	-1.820990	3.332839	2.301456
C	-1.746867	4.874850	0.429576
C	-1.179980	4.277589	3.117660
C	1.680179	1.767777	2.613410
H	1.534225	1.912615	1.521698
C	1.459075	0.279820	2.900179
C	1.712635	-0.689274	1.896612
C	0.855963	0.111459	-0.306777
C	1.867476	-2.068436	2.203278
C	2.404605	-3.051121	1.154839
H	1.888260	-2.825329	0.198856
C	1.207610	-0.177853	4.208855
H	0.965652	0.550868	4.994852
C	1.277275	-1.542691	4.517195
H	1.065504	-1.885349	5.541947
C	1.633653	-2.473648	3.530438
H	1.715925	-3.540904	3.781006
C	3.137357	-0.033331	-0.067582
C	2.887962	0.416537	-1.329322
H	3.566273	0.713025	-2.131161
H	4.078284	-0.204049	0.457870
N	1.497114	0.512628	-1.455971
C	0.864849	0.990796	-2.661214
C	0.685054	2.389455	-2.834556
C	0.499359	0.047320	-3.653073
C	0.154256	2.837051	-4.060074
C	0.006832	0.545078	-4.881865
C	-0.157733	1.925479	-5.084267
H	-0.007239	3.915509	-4.206338
H	-0.269006	-0.166524	-5.674729
H	-0.543936	2.295416	-6.047973
C	1.128138	3.358306	-1.735238
H	0.762308	2.916550	-0.784920
C	0.606826	-1.455110	-3.381921
H	0.411634	-1.608507	-2.296651
C	-0.506313	-2.220459	-4.101599
C	-0.332010	-2.759636	-5.394078
C	-1.768819	-2.336420	-3.481994
C	-1.404681	-3.375960	-6.063349
H	0.657482	-2.699580	-5.875611
C	-2.843913	-2.945431	-4.152269
H	-1.921157	-1.954674	-2.460521
C	-2.667348	-3.464667	-5.448613
H	-1.251896	-3.791547	-7.072547
H	-3.817746	-3.017248	-3.641813
H	-3.506261	-3.948370	-5.974424
C	1.989208	-2.046559	-3.649383
C	2.206587	-3.404436	-3.320280
C	3.050173	-1.310510	-4.211546
C	3.448295	-4.011618	-3.561770
H	1.383201	-3.982132	-2.870696
C	4.302417	-1.912752	-4.438170
H	2.895043	-0.252727	-4.477720
C	4.504977	-3.265635	-4.119819
H	3.599083	-5.070004	-3.296426
H	5.121834	-1.318838	-4.873988
H	5.481557	-3.740471	-4.304888
C	0.503170	4.751661	-1.833053
C	-0.644001	5.053114	-1.069218
C	1.041941	5.749167	-2.675350
C	-1.247123	6.319259	-1.160843
H	-1.077054	4.294808	-0.399598
C	0.434111	7.012938	-2.771058
H	1.955304	5.539894	-3.254413
C	-0.716254	7.302053	-2.014882
H	-2.141975	6.528744	-0.553385

H	-2.110199	2.356537	2.721799
C	-1.121914	5.833720	1.247406
H	-1.938044	5.093883	-0.633805
C	-0.822949	5.531638	2.588433
H	-0.954579	4.025557	4.165665
H	-0.854700	6.817959	0.829944
H	-0.315138	6.274619	3.223698
C	5.126101	-1.062480	0.058883
C	6.380519	-0.915931	0.690680
C	4.972992	-2.078928	-0.908901
C	7.448766	-1.774460	0.379670
H	6.528549	-0.113864	1.430272
C	6.043551	-2.933695	-1.224495
H	3.999218	-2.199781	-1.404323
C	7.284220	-2.789357	-0.579678
H	8.418855	-1.643467	0.885610
H	5.903066	-3.719244	-1.984629
H	8.122716	-3.459488	-0.828146
C	4.391831	1.304937	0.511447
C	4.429427	2.105053	-0.648649
C	4.786873	1.874049	1.740552
C	4.829584	3.448939	-0.581586
H	4.124415	1.672050	-1.615481
C	5.188761	3.219712	1.812188
H	4.747511	1.260293	2.655336
C	5.205857	4.013586	0.651264
H	4.840521	4.056928	-1.499858
H	5.486026	3.651732	2.781303
H	5.514291	5.069603	0.706572
C	-1.432574	-0.797670	3.336549
C	-2.339957	-0.783128	2.256840
C	-1.634137	-1.750156	4.358853
C	-3.371501	-1.731957	2.154311
H	-2.217568	-0.037003	1.457807
C	-2.667015	-2.697965	4.267082
H	-0.983355	-1.745529	5.246601
C	-3.526911	-2.706736	3.152436
H	-4.034388	-1.721173	1.275409
H	-2.797417	-3.440606	5.070269
H	-4.318551	-3.467401	3.067384
C	-0.187225	1.091329	4.576175
C	-1.345941	1.392080	5.324309
C	1.016539	1.749177	4.911377
C	-1.303595	2.325603	6.374485
H	-2.295415	0.894273	5.074431
C	1.060906	2.683709	5.959360
H	1.931638	1.526720	4.340291
C	-0.099981	2.977133	6.696907
H	-2.221638	2.547486	6.941500
H	2.011063	3.186158	6.201542
H	-0.066605	3.708668	7.519607

H	0.868834	7.779270	-3.433152
H	-1.190219	8.294474	-2.085298
C	2.656873	3.419534	-1.674260
C	3.299461	3.542833	-0.427458
C	3.451853	3.317597	-2.836240
C	4.698569	3.511303	-0.329871
H	2.691009	3.634739	0.485014
C	4.855319	3.301964	-2.746865
H	2.965040	3.210714	-3.818987
C	5.482435	3.382726	-1.490929
H	5.171171	3.567419	0.662187
H	5.460643	3.212212	-3.663393
H	6.580837	3.345683	-1.415457
C	2.109406	-4.516520	1.491790
C	2.992098	-5.295808	2.270837
C	0.901814	-5.099757	1.052892
C	2.663956	-6.616949	2.623139
H	3.950249	-4.867746	2.603945
C	0.571819	-6.417639	1.408123
H	0.221323	-4.507417	0.423586
C	1.448628	-7.181782	2.198166
H	3.366070	-7.208753	3.232459
H	-0.382809	-6.846373	1.063292
H	1.190024	-8.215994	2.476893
C	3.899085	-2.799380	0.925794
C	4.427245	-2.920708	-0.375054
C	4.761860	-2.403514	1.970346
C	5.773537	-2.626515	-0.637780
H	3.762074	-3.204548	-1.203107
C	6.113557	-2.109908	1.711830
H	4.366237	-2.298593	2.993247
C	6.622745	-2.210481	0.404674
H	6.148091	-2.704309	-1.670868
H	6.770482	-1.794578	2.538505
H	7.676622	-1.963696	0.199844
C	0.684162	2.699357	3.295452
C	-0.381383	3.236255	2.549439
C	0.810679	3.059637	4.657920
C	-1.308865	4.108090	3.147551
H	-0.530414	2.958481	1.491561
C	-0.118065	3.924068	5.259623
H	1.669002	2.689446	5.241287
C	-1.181502	4.452791	4.502945
H	-2.131840	4.484547	2.523458
H	-0.003971	4.195201	6.321678
H	-1.906509	5.136744	4.973368
C	3.148337	2.156601	2.896394
C	3.499418	3.518812	3.041337
C	4.182298	1.198379	2.955269
C	4.834938	3.905905	3.239601
H	2.712186	4.287356	3.003232
C	5.521828	1.583291	3.139238
H	3.946236	0.128747	2.860832
C	5.856403	2.939125	3.287743
H	5.078752	4.974594	3.349361
H	6.304784	0.808848	3.168360
H	6.904216	3.242832	3.439522

Zero-point correction=	1.294520 (Hartree/Particle)
Thermal correction to Energy=	1.374004
Thermal correction to Enthalpy=	1.374949
Thermal correction to Gibbs Free Energy=	1.176853
Sum of electronic and zero-point Energies=	-3796.203674
Sum of electronic and thermal Energies=	-3796.124189
Sum of electronic and thermal Enthalpies=	-3796.123245
Sum of electronic and thermal Free Energies=	-3796.321341

Zero-point correction=	1.312669 (Hartree/Particle)
Thermal correction to Energy=	1.400259
Thermal correction to Enthalpy=	1.401203
Thermal correction to Gibbs Free Energy=	1.184855
Sum of electronic and zero-point Energies=	-5260.012690
Sum of electronic and thermal Energies=	-5259.925100
Sum of electronic and thermal Enthalpies=	-5259.924155
Sum of electronic and thermal Free Energies=	-5260.140504

SCF Done (in solvent): -3798.2439604	SCF Done (in solvent): -5262.0951013

[Pd(IPr*)(allyl)Cl]-VII-VIII				**[Pd(IPr*)(allyl)Cl]-VIII**			
169				140			
StI6+K2CO3--KN SCF Done: -5261.29358531 A.U.				StI6+K2CO3menysKNisomer1 SCF Done: -4028.77978114 A.U.			
Pd	-1.125185	0.114746	-0.359257	Pd	-0.137570	-0.892128	-1.276421
C	-0.726397	-1.369874	-1.607124	C	1.747414	-1.380053	-1.095250
O	-0.623514	-1.091939	-2.814650	O	2.718093	-0.627970	-1.110777
N	-3.360129	-1.764765	-0.385798	C	2.103030	-5.676678	-1.496584
C	-0.467375	-5.505193	-0.397748	C	2.682977	-4.821126	-2.456722
C	-0.500160	-5.160985	-1.762787	H	1.003703	-5.786990	0.389341
H	-0.513872	-4.757743	1.650235	C	1.440974	-5.126776	-0.377359
C	-0.526946	-4.497947	0.581504	C	2.608229	-3.424824	-2.299497
C	-0.574590	-3.814770	-2.143230	C	1.918394	-2.878463	-1.196121
C	-0.621504	-2.796694	-1.162338	C	1.334717	-3.732997	-0.237688
C	-0.611692	-3.151792	0.201678	H	3.051860	-2.739266	-3.038523
H	-0.615116	-3.525212	-3.203932	H	0.794124	-3.289593	0.610381
H	-0.696469	-2.361308	0.961171	H	2.184464	-6.770298	-1.609898
H	-0.395132	-6.562444	-0.097072	H	3.208012	-5.247096	-3.327527
H	-0.460290	-5.949515	-2.531317	K	-1.140459	-4.656067	-2.955447
C	-4.187661	-1.695965	-1.415213	C	-1.868031	-1.886222	-2.889271
O	-3.888648	-1.516125	-2.618855	O	-0.577297	-2.275573	-2.777166
O	-5.573606	-1.698053	-1.048143	O	-2.685241	-2.602345	-3.521964
C	-6.614064	-2.113068	-1.984904	O	-2.140115	-0.791526	-2.235455
C	-6.244060	-3.460053	-2.626039	N	-0.419224	1.773493	-0.006429
H	-5.329552	-3.356863	-3.240093	C	1.427983	2.469750	-2.152236
H	-6.058754	-4.221044	-1.840515	H	1.627757	1.956870	-1.187158
H	-7.072722	-3.819901	-3.270022	C	-0.076011	2.727663	-2.242845
C	-7.851012	-2.269365	-1.086037	C	-0.964660	2.317276	-1.226805
H	-8.721773	-2.627278	-1.672347	C	0.002325	0.474204	0.128444
H	-7.644902	-2.992751	-0.271210	C	-2.373105	2.410344	-1.364789
H	-8.131622	-1.297728	-0.625477	C	-3.283807	1.825037	-0.283426
C	-6.848346	-1.025307	-3.047883	H	-2.830897	0.839257	-0.038448
H	-5.948854	-0.919700	-3.681524	C	-0.625751	3.342143	-3.386779
H	-7.719821	-1.284487	-3.684842	H	0.052511	3.676475	-4.186575
H	-7.056376	-0.048490	-2.561538	C	-2.010680	3.500426	-3.519707
K	-2.594813	0.598240	-3.257830	H	-2.424124	3.980045	-4.420798
K	-5.421734	0.379043	0.703807	C	-2.879444	3.018810	-2.524975
C	-3.015286	1.881339	0.275187	H	-3.969633	3.092639	-2.653741
O	-3.200419	1.089947	-0.777820	C	-0.193136	2.508482	1.160464
O	-3.968281	2.517306	0.802053	C	0.371452	1.649132	2.059354
O	-1.788628	1.885157	0.750948	H	0.702311	1.804446	3.088748
C	-3.731930	-2.168373	0.886346	H	-0.485119	3.557504	1.253080
C	-3.295786	-1.416296	2.017414	N	0.502176	0.411887	1.410934
C	-4.517365	-3.332087	1.144471	C	0.912007	-0.795077	2.086020
C	-3.692563	-1.758866	3.321791	C	2.290839	-1.023680	2.351068
H	-2.636314	-0.546377	1.849825	C	-0.096179	-1.680259	2.548011
C	-4.888144	-3.680577	2.449569	C	2.633852	-2.161206	3.107515
H	-4.833224	-3.948991	0.290499	C	0.296401	-2.764519	3.362017
C	-4.496790	-2.889419	3.550603	C	1.647855	-3.012063	3.628784
H	-3.376387	-1.119345	4.160953	H	3.697133	-2.364802	3.301074
H	-5.496499	-4.585848	2.613867	H	-0.482058	-3.400655	3.809712
H	-4.804512	-3.159434	4.572937	H	1.938643	-3.870053	4.255001
N	1.447760	0.274581	1.258970	C	3.372930	-0.061219	1.843634
C	-0.404468	0.947664	3.389497	H	3.109400	0.166500	0.790226
H	-0.744944	1.345592	2.411760	C	-1.575380	-1.476441	2.224617
C	0.068163	-0.493254	3.173366	H	-1.671655	-0.491303	1.723373
C	1.090016	-0.748330	2.218946	C	-2.162064	-2.498112	1.241355
C	0.769380	0.457438	0.074030	C	-3.155132	-2.062612	0.336708
C	1.781457	-1.983965	2.173156	C	-1.837084	-3.871167	1.255361
C	3.035156	-2.162795	1.316130				

H	2.985206	-1.391490	0.517430
C	-0.357451	-1.570598	3.969876
H	-1.176615	-1.417515	4.683141
C	0.256627	-2.829163	3.879096
H	-0.106173	-3.659673	4.504478
C	1.345526	-3.019388	3.022923
H	1.851351	-3.993900	2.982077
C	2.602675	1.067178	1.300733
C	2.667300	1.737935	0.113029
H	3.403500	2.449643	-0.265277
H	3.261958	1.089612	2.172369
N	1.549126	1.347541	-0.635481
C	1.320856	1.626533	-2.039813
C	0.482754	2.700741	-2.435084
C	1.963007	0.791144	-2.992286
C	0.262363	2.883081	-3.818542
C	1.713021	1.010249	-4.359343
C	0.857074	2.039935	-4.770379
H	-0.380035	3.713321	-4.147432
H	2.200409	0.359089	-5.099886
H	0.669556	2.205762	-5.843477
C	-0.112795	3.668284	-1.409887
H	-0.598024	3.055859	-0.612948
C	2.992778	-0.242558	-2.539672
H	2.575539	-0.718151	-1.622919
C	3.228801	-1.391538	-3.528511
C	4.514171	-1.729835	-3.995435
C	2.129928	-2.179936	-3.939946
C	4.701740	-2.837562	-4.843558
H	5.382575	-1.128747	-3.686609
C	2.317446	-3.283796	-4.785118
H	1.117710	-1.915608	-3.596214
C	3.606464	-3.622166	-5.238627
H	5.716054	-3.087712	-5.193528
H	1.446627	-3.888937	-5.085515
H	3.754805	-4.492855	-5.897078
C	4.283277	0.457681	-2.102028
C	5.074155	-0.124951	-1.091505
C	4.688139	1.693256	-2.646401
C	6.208048	0.529666	-0.590314
H	4.778566	-1.100383	-0.678945
C	5.830143	2.351845	-2.154328
H	4.087771	2.159045	-3.443198
C	6.585165	1.779996	-1.115115
H	6.779045	0.066942	0.229833
H	6.124391	3.323999	-2.581388
H	7.466694	2.305968	-0.715605
C	-1.203626	4.551455	-2.028950
C	-2.534153	4.087868	-2.100085
C	-0.899953	5.809791	-2.592919
C	-3.532610	4.853454	-2.727241
H	-2.797725	3.119114	-1.649659
C	-1.895260	6.575106	-3.225715
H	0.130802	6.193241	-2.533205
C	-3.216716	6.099241	-3.298562
H	-4.568582	4.478035	-2.749099
H	-1.636363	7.554437	-3.659472
H	-3.998724	6.703548	-3.785478
C	0.947378	4.534355	-0.725737
C	0.571277	5.260380	0.425792
C	2.249760	4.704917	-1.235605
C	1.473568	6.136148	1.047931
H	-0.452703	5.145450	0.816716
C	-3.813623	-2.958399	-0.518057
H	-3.422661	-0.997455	0.291137
C	-2.505456	-4.781516	0.415602
H	-1.060684	-4.249722	1.934221
C	-3.503769	-4.329878	-0.469008
H	-4.553315	-2.574252	-1.234663
H	-2.252431	-5.853862	0.471561
H	-4.046725	-5.040362	-1.115074
C	-2.389879	-1.362417	3.524087
C	-1.996577	-0.396871	4.478587
C	-3.519341	-2.158122	3.796027
C	-2.710161	-0.233509	5.674570
H	-1.120024	0.237365	4.269732
C	-4.237607	-1.995117	4.996229
H	-3.844766	-2.908628	3.059948
C	-3.836999	-1.035348	5.939427
H	-2.386541	0.525074	6.405384
H	-5.119717	-2.625849	5.190607
H	-4.400052	-0.908901	6.877595
C	4.761318	-0.714288	1.815820
C	5.094462	-1.578938	0.748662
C	5.703867	-0.520526	2.847368
C	6.332790	-2.239946	0.723638
H	4.376073	-1.711461	-0.074495
C	6.944367	-1.183734	2.822146
H	5.469965	0.160837	3.679822
C	7.262764	-2.049089	1.761945
H	6.573978	-2.906386	-0.120153
H	7.667695	-1.016960	3.636619
H	8.235257	-2.566628	1.740628
C	3.365727	1.267276	2.593081
C	3.611370	2.458890	1.880624
C	3.114041	1.344230	3.979199
C	3.586106	3.702468	2.531116
H	3.803319	2.409569	0.796361
C	3.088094	2.588677	4.634584
H	2.909675	0.419072	4.542233
C	3.318186	3.772794	3.910730
H	3.769383	4.620881	1.951488
H	2.881744	2.634022	5.716057
H	3.289997	4.748416	4.421406
C	-4.705647	1.531531	-0.777818
C	-5.818860	2.288060	-0.359355
C	-4.900995	0.470118	-1.692551
C	-7.107662	1.989348	-0.840347
H	-5.682504	3.114433	0.355313
C	-6.188783	0.173473	-2.166360
H	-4.022894	-0.108088	-2.037093
C	-7.298220	0.929714	-1.742849
H	-7.967725	2.589236	-0.501204
H	-6.321287	-0.656740	-2.879253
H	-8.308155	0.694397	-2.115895
C	-3.263082	2.648738	1.001140
C	-3.366898	2.002993	2.249906
C	-3.145618	4.053927	0.973214
C	-3.318490	2.736626	3.445437
H	-3.478963	0.907725	2.291476
C	-3.101327	4.793847	2.168465
H	-3.064002	4.566773	0.001400
C	-3.178129	4.136058	3.409368
H	-3.384056	2.203168	4.406360
H	-3.001507	5.890574	2.129419
H	-3.133788	4.713482	4.346576

C	3.164798	5.564852	-0.599736
H	2.558418	4.152025	-2.137157
C	2.779348	6.286633	0.541691
H	1.156753	6.701388	1.938977
H	4.183005	5.673254	-1.006616
H	3.491162	6.966539	1.036071
C	3.104347	-3.506932	0.595321
C	3.597202	-4.670846	1.226144
C	2.679773	-3.598959	-0.744094
C	3.652555	-5.892291	0.534298
H	3.972850	-4.610710	2.260210
C	2.754258	-4.811104	-1.446828
H	2.275426	-2.711295	-1.250751
C	3.236580	-5.964851	-0.807410
H	4.038986	-6.790175	1.042921
H	2.431724	-4.839544	-2.497932
H	3.293775	-6.919221	-1.354585
C	4.312973	-1.838263	2.114681
C	5.578414	-2.209084	1.604749
C	4.273776	-1.108758	3.321623
C	6.761848	-1.843155	2.266360
H	5.637006	-2.801056	0.678205
C	5.457021	-0.733297	3.981825
H	3.305230	-0.817749	3.753797
C	6.708164	-1.096005	3.457351
H	7.734493	-2.146112	1.846268
H	5.392579	-0.151784	4.915044
H	7.635983	-0.806142	3.975389
C	-1.588896	1.121209	4.341465
C	-2.802931	1.640293	3.842236
C	-1.509652	0.800188	5.716078
C	-3.918681	1.790273	4.684674
H	-2.873118	1.946081	2.787659
C	-2.628520	0.937452	6.554955
H	-0.559879	0.440652	6.141478
C	-3.843859	1.424745	6.039429
H	-4.851377	2.207800	4.271024
H	-2.547507	0.670403	7.621015
H	-4.720446	1.535153	6.697906
C	0.805448	1.787359	3.818103
C	1.031928	3.046238	3.227190
C	1.750194	1.295286	4.745583
C	2.185711	3.784842	3.537106
H	0.316765	3.421332	2.478220
C	2.899943	2.036812	5.066067
H	1.601428	0.299796	5.194374
C	3.125613	3.283188	4.454599
H	2.364666	4.743938	3.029051
H	3.628417	1.632856	5.787494
H	4.035982	3.858583	4.686539

Zero-point correction= 1.310179 (Hartree/Particle)
Thermal correction to Energy= 1.397583
Thermal correction to Enthalpy= 1.398527
Thermal correction to Gibbs Free Energy= 1.181347
Sum of electronic and zero-point Energies= -5259.983406
Sum of electronic and thermal Energies= -5259.896003
Sum of electronic and thermal Enthalpies= -5259.895058
Sum of electronic and thermal Free Energies= -5260.112239

SCF Done (in solvent): -5262.0669864

C	1.919189	1.464738	-3.200342
C	3.305208	1.273503	-3.385439
C	1.026729	0.588766	-3.853071
C	3.787939	0.243357	-4.206393
H	4.016354	1.925098	-2.854173
C	1.507727	-0.452476	-4.668000
H	-0.058642	0.697377	-3.712726
C	2.888536	-0.626621	-4.851597
H	4.874535	0.109138	-4.329987
H	0.786124	-1.142749	-5.130152
H	3.266486	-1.440716	-5.491507
C	2.172851	3.803637	-2.099532
C	2.680171	4.432999	-3.255108
C	2.295516	4.468486	-0.859677
C	3.296563	5.693983	-3.173296
H	2.605561	3.917363	-4.225580
C	2.908076	5.729531	-0.775696
H	1.901129	3.986105	0.050322
C	3.413175	6.347763	-1.934013
H	3.691043	6.168421	-4.086226
H	2.989771	6.235109	0.200337
H	3.897309	7.335203	-1.870427

Zero-point correction= 1.083592 (Hartree/Particle)
Thermal correction to Energy= 1.154750
Thermal correction to Enthalpy= 1.155695
Thermal correction to Gibbs Free Energy= 0.971527
Sum of electronic and zero-point Energies= -4027.696189
Sum of electronic and thermal Energies= -4027.625031
Sum of electronic and thermal Enthalpies= -4027.624087
Sum of electronic and thermal Free Energies= -4027.808254

SCF Done (in solvent): -4029.4220193

[Pd(IPr*)(allyl)Cl]-IX	**[Pd(IPr*)(allyl)Cl]-IX-X**
158 StI6+KCO3+NH2 SCF Done: -4430.67550625 A.U.	158

Pd	0.710258	-0.799160	-0.787751
C	2.238729	0.446635	-0.475188
O	2.342527	1.553339	-1.014438
C	5.520869	-0.741570	2.095017
C	5.766040	-0.053701	0.891701
H	3.991161	-1.596016	3.398077
C	4.202656	-1.068748	2.454558
C	4.700127	0.319775	0.062689
C	3.373439	-0.020921	0.410331
C	3.140485	-0.726800	1.604677
H	4.874951	0.873380	-0.871776
H	2.110037	-0.975454	1.882374
H	6.361632	-1.026419	2.747136
H	6.799653	0.190158	0.598706
K	-0.601070	-6.124196	0.061162
C	3.312446	-2.415826	-1.671075
C	3.741417	-3.209227	-0.584170
C	4.280245	-1.783211	-2.470578
C	5.099603	-3.339739	-0.290371
H	2.982869	-3.699765	0.041873
C	5.651657	-1.922390	-2.192041
H	3.956080	-1.143153	-3.305177
C	6.069201	-2.685584	-1.083387
H	5.443263	-3.921512	0.577786
H	6.377310	-1.396258	-2.827685
C	-0.900043	-3.465091	-0.919479
O	-1.917196	-4.134652	-0.509908
O	0.232605	-4.085326	-1.177431
O	-0.998989	-2.165783	-1.060665
N	1.921062	-2.218980	-1.896867
H	1.748816	-1.914225	-2.866236
H	1.289338	-3.086203	-1.661507
O	7.370946	-2.831107	-0.677455
C	8.370105	-2.110269	-1.374060
H	8.190487	-1.009246	-1.339354
H	9.330310	-2.332279	-0.869187
H	8.448497	-2.419536	-2.443160
N	-0.667173	1.073047	1.225044
C	-0.995810	-1.671034	2.270226
H	-0.904672	-1.543490	1.168544
C	-0.109491	-0.611117	2.938108
C	0.112876	0.670693	2.366185
C	-0.587549	0.531384	-0.035540
C	1.061447	1.584320	2.899696
C	1.342886	2.925580	2.206954
H	1.264485	2.737931	1.114551
C	0.573750	-0.915309	4.134344
H	0.410860	-1.897139	4.603011
C	1.477411	-0.010195	4.705246
H	2.008695	-0.275315	5.632738
C	1.742036	1.212808	4.074999
H	2.506912	1.886428	4.486346
C	-1.682615	2.034039	1.305070
C	-2.239882	2.111472	0.064307
H	-3.046663	2.736354	-0.322837
H	-1.913341	2.564944	2.230172
N	-1.592502	1.163917	-0.735415
C	-2.092572	0.847534	-2.055896
C	-3.393607	0.284878	-2.149881
C	-1.337363	1.173367	-3.204340
C	-3.939916	0.090141	-3.432394
C	-1.940293	0.992278	-4.466413
C	-3.228905	0.458368	-4.583873

StI6+KCO3+NH2--HFIIall SCF Done: -4430.66914439 A.U.

Pd	-0.977007	-0.143770	0.961282
C	-1.710353	1.660723	0.634340
O	-1.135012	2.702177	0.963763
C	-5.734861	1.888510	-0.922526
C	-5.363198	2.651552	0.201357
H	-5.084287	0.422052	-2.401476
C	-4.799054	1.034015	-1.531619
C	-4.050809	2.583281	0.695739
C	-3.111106	1.723897	0.085898
C	-3.499442	0.934375	-1.014029
H	-3.734411	3.185939	1.561896
H	-2.769686	0.243280	-1.457991
H	-6.762222	1.952124	-1.315504
H	-6.099582	3.311543	0.687900
K	-3.246263	-4.699172	1.840106
C	-3.832414	-1.257185	1.022273
C	-3.464214	-2.130411	-0.043675
C	-5.215773	-1.029258	1.215733
C	-4.421452	-2.735789	-0.866864
H	-2.393706	-2.281404	-0.256751
C	-6.185978	-1.627616	0.391341
H	-5.536302	-0.334178	2.008383
C	-5.799516	-2.491015	-0.658217
H	-4.108989	-3.377553	-1.706203
H	-7.245229	-1.392646	0.568380
C	-0.902909	-3.113674	2.108279
O	-0.724631	-4.350343	1.895233
O	-1.933056	-2.760411	2.917796
O	-0.206810	-2.179314	1.552063
N	1.935426	0.683740	0.797398
N	0.952157	1.010447	-1.109215
C	0.742995	0.483032	0.148179
C	2.853908	1.347523	-0.020609
C	2.244890	1.532110	-1.230014
C	2.306938	0.030388	2.028945
C	3.142509	-1.111866	1.926550
C	3.501017	-1.769932	3.117005
C	3.077079	-1.280859	4.362803
C	2.263066	-0.142879	4.434547
C	1.832941	0.518019	3.264964
C	3.655336	-1.601643	0.570796
H	3.378738	-1.798787	5.286768
C	0.900111	1.723235	3.347914
C	-0.028910	0.899764	-2.161196
C	-0.686177	2.064655	-2.635606
C	-1.689796	1.902797	-3.610674
C	-2.020119	0.632231	-4.097436
C	-1.329756	-0.501528	-3.645056
C	-0.305758	-0.395239	-2.683883
C	-0.263020	3.457682	-2.155628
H	-2.828040	0.521902	-4.837460
C	0.557059	-1.599779	-2.288804
H	3.869517	1.569248	0.315951
H	2.622154	1.952343	-2.163253
H	4.104526	-2.688668	3.054180
H	1.931431	0.239232	5.412080
H	2.941212	-1.248293	-0.202859
H	0.682633	2.063020	2.314284
H	-2.235072	2.788820	-3.965359
H	-1.596021	-1.491916	-4.038339
H	-0.083952	3.378502	-1.062797

H	-4.936609	-0.369676	-3.514942
H	-1.370181	1.261296	-5.368609
H	-3.678804	0.316473	-5.579122
C	-4.204548	-0.083442	-0.906542
H	-3.475004	-0.369829	-0.116808
C	0.071520	1.747883	-3.100300
H	0.456409	1.556903	-2.079447
C	1.093557	1.053521	-3.999605
C	2.326978	1.681451	-4.276329
C	0.893737	-0.260801	-4.480401
C	3.310119	1.038858	-5.047503
H	2.516103	2.689218	-3.877076
C	1.873083	-0.903923	-5.259796
H	-0.041269	-0.790296	-4.240670
C	3.083519	-0.252470	-5.556769
H	4.262373	1.553896	-5.252561
H	1.686791	-1.923698	-5.633744
H	3.849341	-0.753629	-6.169454
C	-0.004589	3.268007	-3.232808
C	-0.119272	4.052552	-2.065191
C	-0.045187	3.912227	-4.487253
C	-0.286363	5.444973	-2.148791
H	-0.081639	3.558169	-1.081374
C	-0.201343	5.305729	-4.573445
H	0.060243	3.312850	-5.405609
C	-0.327457	6.077372	-3.403908
H	-0.384278	6.039885	-1.226974
H	-0.226392	5.793315	-5.561334
H	-0.453837	7.169673	-3.471220
C	-5.064494	-1.333479	-1.125330
C	-4.401002	-2.538793	-1.437178
C	-6.463707	-1.342005	-0.964419
C	-5.120591	-3.735382	-1.558401
H	-3.304535	-2.545262	-1.531856
C	-7.188256	-2.541814	-1.101159
H	-6.991918	-0.410137	-0.711812
C	-6.519301	-3.743236	-1.392324
H	-4.569143	-4.666160	-1.763919
H	-8.282416	-2.535123	-0.968997
H	-7.086799	-4.683571	-1.485800
C	-5.017060	1.089240	-0.356721
C	-5.190524	1.205985	1.038859
C	-5.612163	2.053394	-1.195065
C	-5.933125	2.263079	1.585447
H	-4.719903	0.464156	1.699927
C	-6.354159	3.117724	-0.649388
H	-5.478692	1.982125	-2.285719
C	-6.516134	3.228079	0.742480
H	-6.048211	2.337732	2.678820
H	-6.804776	3.867896	-1.319040
H	-7.092136	4.064770	1.169170
C	2.760931	3.450545	2.457213
C	3.085545	4.174176	3.626172
C	3.774506	3.202193	1.510554
C	4.403055	4.601541	3.861672
H	2.295070	4.414393	4.355309
C	5.092913	3.625853	1.747199
H	3.521939	2.678124	0.576818
C	5.414957	4.320425	2.925527
H	4.639329	5.162836	4.780040
H	5.871814	3.407402	0.999383
H	6.448785	4.653457	3.110770
C	0.310441	4.001681	2.551405
H	0.767526	-1.506550	-1.201006
N	-2.839022	-0.712514	1.844707
H	-3.219314	0.007498	2.473736
H	-2.314393	-1.743646	2.558457
O	-6.665982	-3.119754	-1.519593
C	-8.046194	-2.819955	-1.413408
H	-8.250281	-1.732852	-1.558378
H	-8.556128	-3.389846	-2.214086
H	-8.471652	-3.128685	-0.428657
C	1.060735	3.885870	-2.796575
C	1.907618	4.769797	-2.094546
C	1.476756	3.408506	-4.057106
C	3.153123	5.142408	-2.622442
H	1.587481	5.148155	-1.110227
C	2.725610	3.779913	-4.589127
H	0.825016	2.719330	-4.617420
C	3.572069	4.640935	-3.869791
H	3.808528	5.820272	-2.052545
H	3.039137	3.388170	-5.570093
H	4.555059	4.922706	-4.279122
C	1.631351	2.879686	4.034668
C	1.520734	3.124719	5.418773
C	2.490735	3.695532	3.267978
C	2.259579	4.155919	6.024439
H	0.834293	2.508786	6.021545
C	3.229311	4.727082	3.869979
H	2.576242	3.512394	2.183460
C	3.117913	4.959323	5.253208
H	2.160687	4.335611	7.107169
H	3.892797	5.357039	3.255772
H	3.694821	5.769156	5.727613
C	5.007523	-0.987358	0.202702
C	5.215951	-0.513219	-1.109762
C	6.073070	-0.910488	1.122827
C	6.456452	0.015939	-1.498850
H	4.386337	-0.550061	-1.829655
C	7.316900	-0.378642	0.738104
H	5.928479	-1.265636	2.154460
C	7.514530	0.085599	-0.574626
H	6.590531	0.376779	-2.531245
H	8.136971	-0.324971	1.472105
H	8.488868	0.503855	-0.874090
C	1.923156	-1.602486	-3.004219
C	2.791451	-2.696918	-2.781105
C	2.345151	-0.577592	-3.875855
C	4.041868	-2.763775	-3.412470
H	2.481535	-3.505872	-2.101673
C	3.601603	-0.643039	-4.508647
H	1.687091	0.282445	-4.072511
C	4.452413	-1.738221	-4.284687
H	4.702820	-3.618535	-3.201786
H	3.910984	0.172092	-5.182411
H	5.436673	-1.787854	-4.776307
C	-1.347438	4.520220	-2.353701
C	-2.266149	4.780469	-1.316037
C	-1.478558	5.223853	-3.570754
C	-3.312451	5.698652	-1.502443
H	-2.149417	4.253809	-0.357267
C	-2.523541	6.145201	-3.756588
H	-0.751913	5.049365	-4.380212
C	-3.449453	6.380483	-2.724340
H	-4.026879	5.877408	-0.683007
H	-2.612684	6.684735	-4.713283

C	0.079793	5.041526	1.626600
C	-0.404533	4.003604	3.766046
C	-0.869048	6.040101	1.891243
H	0.654225	5.056966	0.686576
C	-1.354658	5.006283	4.036189
H	-0.234108	3.195081	4.494829
C	-1.596498	6.022759	3.096480
H	-1.047590	6.837136	1.151534
H	-1.913134	4.987832	4.985832
H	-2.347369	6.801785	3.302476
C	-0.424674	-3.067173	2.554076
C	0.817789	-3.423377	1.981259
C	-1.045749	-3.980930	3.431446
C	1.450537	-4.631000	2.319732
H	1.287989	-2.736559	1.260161
C	-0.427443	-5.204799	3.755644
H	-2.021352	-3.723896	3.871976
C	0.832457	-5.529917	3.215302
H	2.434546	-4.870372	1.883945
H	-0.924209	-5.897697	4.454170
H	1.335061	-6.469389	3.498553
C	-2.483282	-1.568996	2.589301
C	-3.381081	-2.290474	1.767169
C	-2.984655	-0.857994	3.697882
C	-4.752123	-2.316982	2.068115
H	-2.988008	-2.850770	0.897067
C	-4.361151	-0.885344	3.996820
H	-2.292501	-0.289557	4.340047
C	-5.246132	-1.620641	3.188160
H	-5.437709	-2.869505	1.406027
H	-4.742252	-0.325766	4.866373
H	-6.323433	-1.634175	3.417459
H	-4.270736	7.100359	-2.870546
C	-0.476085	1.418857	3.950172
C	-1.412387	2.476068	4.028489
C	-0.884359	0.133550	4.358543
C	-2.710621	2.257110	4.511863
H	-1.115071	3.478511	3.684876
C	-2.178647	-0.084908	4.867247
H	-0.206192	-0.723681	4.245705
C	-3.098140	0.973364	4.945902
H	-3.425300	3.094875	4.555506
H	-2.468109	-1.104937	5.162428
H	-4.114860	0.801474	5.334613
C	3.621651	-3.127809	0.426396
C	4.699303	-3.869660	-0.095269
C	2.409473	-3.789975	0.717498
C	4.556966	-5.248976	-0.341392
H	5.647420	-3.364623	-0.335089
C	2.267949	-5.163367	0.473413
H	1.554439	-3.219749	1.118047
C	3.340726	-5.898638	-0.065889
H	5.404952	-5.816826	-0.757910
H	1.299780	-5.632973	0.706339
H	3.231864	-6.976494	-0.268553
C	-0.122413	-2.959092	-2.454305
C	-0.310114	-3.548658	-3.725407
C	-0.499951	-3.685822	-1.309333
C	-0.913540	-4.811103	-3.848200
H	0.049717	-3.024540	-4.625657
C	-1.074439	-4.963513	-1.430203
H	-0.301404	-3.266246	-0.311429
C	-1.302650	-5.524542	-2.698029
H	-1.058356	-5.253033	-4.847143
H	-1.291516	-5.530029	-0.510113
H	-1.749890	-6.527134	-2.795076
Zero-point correction=		1.232105 (Hartree/Particle)	
Thermal correction to Energy=		1.312120	
Thermal correction to Enthalpy=		1.313064	
Thermal correction to Gibbs Free Energy=		1.111102	
Sum of electronic and zero-point Energies=		-4429.443401	
Sum of electronic and thermal Energies=		-4429.363387	
Sum of electronic and thermal Enthalpies=		-4429.362442	
Sum of electronic and thermal Free Energies=		-4429.564404	
SCF Done (in solvent): -4431.4372135			
Zero-point correction=		1.228788 (Hartree/Particle)	
Thermal correction to Energy=		1.308285	
Thermal correction to Enthalpy=		1.309229	
Thermal correction to Gibbs Free Energy=		1.108193	
Sum of electronic and zero-point Energies=		-4429.440545	
Sum of electronic and thermal Energies=		-4429.361047	
Sum of electronic and thermal Enthalpies=		-4429.360103	
Sum of electronic and thermal Free Energies=		-4429.561140	
SCF Done (in solvent): -4431.436459			

[Pd(IPr*)(allyl)Cl]-X (adduct)			
158			
StI6+KCO3H+NH SCF Done: -4430.64653174 A.U.			
Pd	1.057127	0.788833	-0.523509
C	0.189295	2.477142	0.009866
O	-0.544929	3.115460	-0.741635
C	1.190720	4.044350	3.924235
C	0.636061	4.883090	2.939211
H	1.846065	2.018213	4.404516
C	1.422906	2.685934	3.637822
C	0.310705	4.366751	1.676110
C	0.535550	3.003539	1.383172
C	1.100962	2.174024	2.374955
H	-0.108750	5.013114	0.892497
H	1.259314	1.107849	2.146481
H	1.442439	4.451087	4.916886
H	0.456584	5.947739	3.157413
K	6.029850	-0.210491	0.741188
C	3.922394	2.200122	-0.753406

[Pd(IPr*)(allyl)Cl]-X			
152			
StI6+NH SCF Done: -3566.31560386 A.U.			
Pd	0.675579	0.566890	-1.189040
C	0.053564	-0.867405	-2.410859
O	0.473932	-2.003375	-2.297065
C	-2.705351	0.183859	-5.569151
C	-2.263292	-1.145760	-5.415113
H	-2.601156	2.222467	-4.783418
C	-2.252454	1.182215	-4.688865
C	-1.370167	-1.477113	-4.386811
C	-0.906411	-0.474448	-3.502905
C	-1.355621	0.851035	-3.661264
H	-1.026341	-2.512543	-4.239639
H	-1.010297	1.616413	-2.951213
H	-3.409865	0.438626	-6.377396
H	-2.623952	-1.929594	-6.100374
C	3.173523	1.367371	-2.570787
C	3.916775	1.077322	-3.754032

C	5.167842	2.053794	-1.462546
C	4.023682	2.799685	0.543476
C	6.397546	2.429466	-0.902450
H	5.149254	1.623980	-2.478207
C	5.256643	3.161640	1.112330
H	3.106077	2.957927	1.124323
C	6.467258	2.961443	0.406475
H	7.332489	2.318833	-1.476434
H	5.254878	3.604369	2.119812
C	3.400795	-1.125959	-0.342610
O	4.457529	-1.736199	-0.627191
O	3.469960	-0.382078	0.842601
O	2.300916	-1.106887	-0.982176
N	2.738152	1.777199	-1.283559
H	2.894792	1.314396	-2.188413
H	2.632555	0.149413	0.905979
O	7.736560	3.227051	0.901747
C	7.824751	3.922500	2.130107
H	7.410508	3.332293	2.984828
H	8.901157	4.104479	2.318188
H	7.293194	4.902803	2.097626
N	-1.189843	-0.957032	-1.352773
C	-1.012839	1.109230	-3.370359
H	-0.703147	1.423434	-2.349816
C	-0.432668	-0.289134	-3.601306
C	-0.489370	-1.268048	-2.579143
C	-0.674148	-0.226684	-0.304741
C	0.099413	-2.551616	-2.714472
C	0.095150	-3.538428	-1.541881
H	0.351678	-2.917525	-0.654685
C	0.191299	-0.650063	-4.811915
H	0.257574	0.093507	-5.619441
C	0.734660	-1.931315	-4.988461
H	1.211804	-2.194497	-5.945719
C	0.698859	-2.869576	-3.946864
H	1.165522	-3.858121	-4.071429
C	-2.476327	-1.418302	-1.070065
C	-2.774219	-1.006032	0.194040
H	-3.658781	-1.172394	0.810708
H	-3.048912	-2.014742	-1.782374
N	-1.671060	-0.265680	0.644145
C	-1.543935	0.237899	1.987845
C	-2.220245	1.432527	2.351531
C	-0.817291	-0.534060	2.926857
C	-2.059391	1.901878	3.667057
C	-0.768763	-0.072803	4.259534
C	-1.343443	1.153605	4.614422
H	-2.527395	2.854033	3.955023
H	-0.293578	-0.703358	5.025637
H	-1.257284	1.522264	5.648367
C	-3.217239	2.069179	1.379256
H	-2.764315	2.028622	0.366341
C	-0.233647	-1.893878	2.551617
H	-0.474203	-2.062915	1.481889
C	1.286885	-2.051361	2.647763
C	1.899567	-3.024021	1.823206
C	2.098518	-1.364724	3.573179
C	3.260063	-3.338624	1.947279
H	1.299611	-3.563344	1.074568
C	3.463459	-1.680714	3.708781
H	1.666600	-0.576295	4.205052
C	4.044453	-2.680032	2.911495
H	3.700829	-4.088286	1.272889
C	3.913973	1.446133	-1.358520
C	5.294189	0.843592	-3.713546
H	3.382780	1.011788	-4.716892
C	5.292101	1.190674	-1.305820
H	3.383452	1.704424	-0.429552
C	5.998840	0.879126	-2.487505
H	5.858005	0.608619	-4.629712
H	5.797932	1.244255	-0.331094
N	1.797542	1.561058	-2.559850
H	1.423177	1.629544	-3.515458
O	7.344983	0.612240	-2.553228
C	8.077563	0.601484	-1.343544
H	7.691562	-0.160098	-0.624387
H	9.122216	0.345307	-1.607663
H	8.070767	1.596080	-0.836615
N	0.222409	0.127210	1.707617
C	2.095876	-2.054140	1.785617
H	0.986132	-2.060768	1.808354
C	2.533566	-0.611149	2.028227
C	1.608220	0.447494	1.914907
C	-0.307870	-0.035932	0.449863
C	1.993679	1.809936	1.951887
C	0.930419	2.883375	1.716072
H	0.299710	2.495087	0.885693
C	3.880169	-0.275992	2.279115
H	4.618612	-1.085477	2.383827
C	4.279809	1.065321	2.365359
H	5.337020	1.309152	2.554652
C	3.348273	2.104220	2.184220
H	3.671731	3.155964	2.200756
C	-0.720841	-0.115075	2.709464
C	-1.877772	-0.464845	2.069555
H	-2.857171	-0.747494	2.461091
H	-0.487712	0.018453	3.769336
N	-1.602810	-0.431865	0.696929
C	-2.539947	-0.673908	-0.368251
C	-2.663595	-1.989106	-0.891195
C	-3.261235	0.426232	-0.886059
C	-3.533051	-2.173538	-1.979576
C	-4.120797	0.189412	-1.976759
C	-4.249029	-1.093402	-2.520548
H	-3.629026	-3.175476	-2.421968
H	-4.676041	1.026935	-2.420012
H	-4.901971	-1.253987	-3.391650
C	-1.869668	-3.147173	-0.271354
H	-0.801410	-2.834875	-0.279065
C	-3.145213	1.807172	-0.233249
H	-2.250669	1.762989	0.422067
C	-2.857644	2.926478	-1.231069
C	-1.540822	3.413389	-1.357797
C	-3.859997	3.490172	-2.051036
C	-1.213507	4.402111	-2.299609
H	-0.743412	2.978447	-0.736232
C	-3.540474	4.477864	-2.998098
H	-4.907050	3.170521	-1.928334
C	-2.214264	4.931175	-3.132498
H	-0.171106	4.748936	-2.373106
H	-4.335225	4.902488	-3.632145
H	-1.966618	5.705612	-3.875649
C	-4.313629	2.099390	0.720852
C	-5.047590	1.053309	1.320673
C	-4.610598	3.426985	1.100898
C	-6.038414	1.323162	2.280410

H	4.071799	-1.138684	4.451419
H	5.108605	-2.943645	3.032783
C	-0.999380	-2.999303	3.311840
C	-2.413317	-2.967397	3.313777
C	-0.353534	-4.068811	3.963026
C	-3.158430	-3.982665	3.930931
H	-2.938567	-2.131337	2.827053
C	-1.099894	-5.087339	4.585415
H	0.745371	-4.113129	3.978223
C	-2.503426	-5.052943	4.568804
H	-4.259127	-3.936964	3.912276
H	-0.573437	-5.915485	5.086236
H	-3.085878	-5.852603	5.053109
C	-3.545108	3.535662	1.662467
C	-2.917914	4.548764	0.909188
C	-4.474260	3.907849	2.658845
C	-3.191737	5.903719	1.163718
H	-2.200483	4.262005	0.124209
C	-4.744093	5.262230	2.918216
H	-5.002151	3.127217	3.229099
C	-4.100202	6.266649	2.172991
H	-2.691495	6.680935	0.563483
H	-5.470018	5.534288	3.701262
H	-4.315900	7.328659	2.371858
C	-4.493787	1.215553	1.330717
C	-5.207644	1.125813	0.119529
C	-4.950921	0.476640	2.442839
C	-6.335341	0.299853	0.007057
H	-4.842572	1.672315	-0.761338
C	-6.085249	-0.349661	2.334829
H	-4.395226	0.516382	3.392993
C	-6.777354	-0.447857	1.114611
H	-6.854863	0.226863	-0.961818
H	-6.422395	-0.928398	3.209796
H	-7.654780	-1.108037	1.026312
C	1.186596	-4.617738	-1.621691
C	0.883936	-5.994971	-1.648887
C	2.543838	-4.223762	-1.623374
C	1.912160	-6.956405	-1.668593
H	-0.165654	-6.325583	-1.644536
C	3.568091	-5.182398	-1.634301
H	2.796807	-3.154495	-1.616712
C	3.258205	-6.555666	-1.655884
H	1.653225	-8.027418	-1.688227
H	4.615330	-4.840274	-1.625095
H	4.061859	-7.309754	-1.664305
C	-1.282150	-4.145854	-1.288975
C	-1.699477	-4.413551	0.030457
C	-2.152524	-4.466091	-2.351036
C	-2.971948	-4.944261	0.292321
H	-1.026332	-4.193199	0.872877
C	-3.428443	-4.999984	-2.095415
H	-1.831989	-4.268968	-3.386604
C	-3.846444	-5.230817	-0.772010
H	-3.277364	-5.118839	1.335808
H	-4.102151	-5.232919	-2.935757
H	-4.850266	-5.637785	-0.571013
C	-0.415206	2.158128	-4.309503
C	0.735456	2.872549	-3.915526
C	-0.975661	2.411457	-5.579818
C	1.321555	3.809693	-4.783584
H	1.172329	2.703134	-2.917798
C	-0.387461	3.346427	-6.448821
H	-4.845301	0.011211	1.027710
C	-5.606135	3.699674	2.054425
H	-4.051283	4.258902	0.645804
C	-6.322774	2.648145	2.653059
H	-6.596425	0.489131	2.735374
H	-5.819208	4.743933	2.333815
H	-7.102697	2.861177	3.401065
C	-1.955307	-4.445413	-1.083720
C	-0.979488	-4.720698	-2.065576
C	-3.005067	-5.370800	-0.896808
C	-1.057624	-5.886480	-2.846406
H	-0.158546	-4.005722	-2.216135
C	-3.086275	-6.534319	-1.681543
H	-3.766500	-5.184789	-0.123771
C	-2.112485	-6.797260	-2.661278
H	-0.281781	-6.083304	-3.604015
H	-3.913847	-7.243736	-1.519987
H	-2.173127	-7.712008	-3.272444
C	-2.265931	-3.380550	1.187751
C	-1.297699	-3.798841	2.122322
C	-3.593796	-3.195656	1.629190
C	-1.636036	-4.002051	3.469854
H	-0.260537	-3.958358	1.789678
C	-3.939365	-3.403321	2.976372
H	-4.358573	-2.858494	0.910602
C	-2.958842	-3.799165	3.903665
H	-0.856198	-4.316612	4.181232
H	-4.979939	-3.249200	3.304473
H	-3.226143	-3.954076	4.961009
C	1.513832	4.195989	1.201304
C	1.719929	5.307821	2.041276
C	1.892448	4.281017	-0.157949
C	2.299259	6.485908	1.534743
H	1.416150	5.251437	3.098668
C	2.472212	5.456228	-0.661009
H	1.737793	3.421879	-0.836105
C	2.678295	6.563245	0.183498
H	2.452165	7.349516	2.201781
H	2.766218	5.502183	-1.721808
H	3.131805	7.485965	-0.212367
C	-0.008035	3.012999	2.914291
C	-1.372116	3.303117	2.703182
C	0.440890	2.792321	4.232758
C	-2.276870	3.332295	3.775636
H	-1.731603	3.494174	1.679379
C	-0.459131	2.836164	5.312890
H	1.502819	2.558862	4.410541
C	-1.822524	3.093429	5.085669
H	-3.342971	3.523872	3.579052
H	-0.092843	2.656744	6.336571
H	-2.532316	3.107290	5.927982
C	2.492989	-2.563069	0.392706
C	2.124272	-3.871292	0.005134
C	3.186277	-1.762022	-0.532965
C	2.465064	-4.366660	-1.262930
H	1.585304	-4.520840	0.714345
C	3.525158	-2.250848	-1.806178
H	3.465911	-0.732325	-0.278080
C	3.171260	-3.557984	-2.172853
H	2.165743	-5.388998	-1.543527
H	4.049539	-1.583051	-2.508367
H	3.429645	-3.944178	-3.171615
C	2.541216	-2.958539	2.935338

H	-1.887466	1.872709	-5.884924
C	0.766295	4.047424	-6.053793
H	2.217289	4.362110	-4.456850
H	-0.836204	3.532314	-7.438078
H	1.226104	4.784147	-6.732096
C	-2.539412	1.169770	-3.383442
C	-3.158779	2.348779	-2.908718
C	-3.348132	0.143974	-3.909043
C	-4.550136	2.508120	-2.990999
H	-2.525848	3.145290	-2.486305
C	-4.747323	0.291995	-3.968819
H	-2.874928	-0.777561	-4.284541
C	-5.352510	1.477836	-3.521499
H	-5.014818	3.439328	-2.629094
H	-5.364979	-0.521508	-4.382497
H	-6.445510	1.601808	-3.581820

Zero-point correction= 1.230106 (Hartree/Particle)
Thermal correction to Energy= 1.310938
Thermal correction to Enthalpy= 1.311882
Thermal correction to Gibbs Free Energy= 1.106999
Sum of electronic and zero-point Energies= -4429.416426
Sum of electronic and thermal Energies= -4429.335594
Sum of electronic and thermal Enthalpies= -4429.334650
Sum of electronic and thermal Free Energies= -4429.539532

SCF Done (in solvent): -4431.4112976

C	3.712282	-3.740388	2.871778
C	1.773772	-2.980532	4.119888
C	4.107438	-4.524801	3.970106
H	4.305202	-3.745216	1.943449
C	2.163042	-3.766706	5.216339
H	0.854754	-2.373236	4.172333
C	3.334738	-4.542569	5.144527
H	5.023888	-5.132939	3.904173
H	1.547788	-3.776786	6.130574
H	3.642116	-5.163350	6.001031

Zero-point correction= 1.201343 (Hartree/Particle)
Thermal correction to Energy= 1.275962
Thermal correction to Enthalpy= 1.276906
Thermal correction to Gibbs Free Energy= 1.085353
Sum of electronic and zero-point Energies= -3565.114261
Sum of electronic and thermal Energies= -3565.039642
Sum of electronic and thermal Enthalpies= -3565.038698
Sum of electronic and thermal Free Energies= -3565.230251

SCF Done (in solvent): -3566.9842351

[Pd(IPr*)(allyl)Cl]-X-XI

152

StI6--PROD SCF Done: -3566.30910785 A.U.

Pd	-0.223896	-0.297754	-1.442867
C	-1.272464	1.210810	-2.389024
O	-2.378418	1.537148	-1.978332
C	1.139221	3.839483	-4.838185
C	-0.141139	4.230640	-4.403345
H	2.655836	2.271426	-4.788028
C	1.648083	2.580637	-4.469493
C	-0.913478	3.366464	-3.613337
C	-0.405991	2.101155	-3.236917
C	0.883680	1.721320	-3.668165
H	-1.914122	3.660592	-3.266586
H	1.292846	0.752019	-3.343772
H	1.743966	4.520217	-5.458672
H	-0.541855	5.218879	-4.680044
C	-2.461996	-1.256986	-3.126115
C	-3.558964	-0.932397	-3.966391
C	-2.690602	-2.183535	-2.078215
C	-4.818659	-1.503638	-3.760537
H	-3.416492	-0.200094	-4.777918
C	-3.951352	-2.751658	-1.856442
H	-1.859720	-2.449210	-1.404499
C	-5.033373	-2.404044	-2.691817
H	-5.674437	-1.243052	-4.401945
H	-4.076426	-3.432990	-1.003860
N	-1.211668	-0.629951	-3.238462
H	-0.983566	-0.287395	-4.178120
O	-6.315342	-2.861785	-2.535657
C	-6.566746	-3.786153	-1.489524
H	-6.330297	-3.352599	-0.490758
H	-7.647401	-4.023603	-1.533576
H	-5.984791	-4.728994	-1.619004
N	0.175290	-0.807657	1.453331
C	-2.565059	-1.038425	2.356486
H	-1.929180	-0.137885	2.220200

[Pd(IPr*)(allyl)Cl]-XI

152

StI6+PROD SCF Done: -3566.32886186 A.U.

Pd	-0.554169	-0.218182	1.087857
C	-0.624071	-1.773867	3.408966
O	-0.722753	-2.994415	3.314892
C	2.661781	-0.001620	5.594915
C	2.233574	-1.315706	5.861148
H	2.348940	1.780402	4.366403
C	2.001916	0.764949	4.615965
C	1.155373	-1.865861	5.150427
C	0.486378	-1.100769	4.169120
C	0.921270	0.218801	3.910426
H	0.821360	-2.899620	5.327529
H	0.458267	0.780193	3.077271
H	3.522052	0.418878	6.139915
H	2.752716	-1.921192	6.620886
C	-2.899371	-1.450611	2.434966
C	-4.078977	-1.088120	3.112801
C	-2.977667	-2.301825	1.317571
C	-5.327563	-1.506004	2.637256
H	-4.018950	-0.450141	4.006671
C	-4.223504	-2.734676	0.843555
H	-2.062016	-2.586568	0.779275
C	-5.410456	-2.309460	1.479561
H	-6.259948	-1.202658	3.136580
H	-4.248241	-3.362259	-0.055720
N	-1.632055	-0.898147	2.858717
H	-1.746109	-0.015780	3.386442
O	-6.670100	-2.586984	1.030117
C	-6.800738	-3.180230	-0.255008
H	-7.885585	-3.225686	-0.469097
H	-6.299710	-2.564681	-1.037414
H	-6.385864	-4.214180	-0.284144
N	0.083106	-0.157785	-1.805124
C	0.968928	-2.878753	-1.658858
H	1.364858	-2.066454	-1.011076

C	-1.810218	-2.213846	1.736469	C	-0.490706	-2.536296	-1.956204
C	-0.483949	-2.073362	1.269669	C	-0.901994	-1.187377	-2.007202
C	0.335756	0.087374	0.418875	C	0.371956	0.315545	-0.539262
C	0.192956	-3.121147	0.585030	C	-2.258299	-0.817031	-2.183364
C	1.591193	-2.923166	-0.011294	C	-2.656436	0.649748	-2.014643
H	1.626390	-1.869438	-0.378222	H	-2.143698	0.960668	-1.072195
C	-2.447572	-3.458985	1.565307	C	-1.462551	-3.533877	-2.176621
H	-3.484855	-3.576743	1.913853	H	-1.164111	-4.591687	-2.111882
C	-1.786169	-4.519834	0.935916	C	-2.794041	-3.185507	-2.446206
H	-2.296307	-5.486869	0.804629	H	-3.538655	-3.974639	-2.638111
C	-0.484192	-4.345746	0.438132	C	-3.193028	-1.837989	-2.430030
H	0.014690	-5.166770	-0.097527	H	-4.250250	-1.569380	-2.574304
C	0.713036	-0.314276	2.646713	C	0.843305	0.471089	-2.791313
C	1.231410	0.919653	2.357310	C	1.632740	1.384304	-2.146278
H	1.735315	1.654818	2.988532	H	2.351321	2.112903	-2.532254
H	0.658456	-0.873286	3.584664	H	0.741360	0.227361	-3.851430
N	0.982958	1.149721	1.001466	N	1.342342	1.271450	-0.776794
C	1.536713	2.191429	0.174430	C	1.982715	2.029887	0.260467
C	0.750103	3.317415	-0.171612	C	3.345308	1.764797	0.563300
C	2.822226	1.959043	-0.365220	C	1.247850	3.038070	0.935973
C	1.298449	4.225081	-1.096676	C	3.953706	2.523917	1.581580
C	3.326543	2.885723	-1.296423	C	1.920833	3.813933	1.901626
C	2.569948	4.010597	-1.653148	C	3.254250	3.545995	2.239501
H	0.703536	5.091615	-1.416906	H	5.005395	2.329333	1.837442
H	4.302960	2.693877	-1.768299	H	1.389215	4.656769	2.369927
H	2.958332	4.719025	-2.400362	H	3.760980	4.152275	3.006764
C	-0.660330	3.455947	0.413091	C	4.136946	0.680498	-0.181379
H	-1.221182	2.568466	0.048673	H	3.703095	0.615484	-1.203039
C	3.622734	0.734850	0.075991	C	-0.216806	3.324486	0.608438
H	2.896418	-0.011500	0.454877	H	-0.473589	2.705118	-0.273990
C	4.300810	0.012847	-1.088528	C	-1.209572	2.913310	1.700946
C	5.687520	-0.210905	-1.165108	C	-2.530757	2.578144	1.316462
C	3.463228	-0.554587	-2.075532	C	-0.903680	2.915095	3.076254
C	6.224564	-0.997207	-2.203326	C	-3.502780	2.238394	2.267441
H	6.349175	0.205161	-0.390013	H	-2.805121	2.584054	0.250572
C	3.992661	-1.346534	-3.103261	C	-1.869466	2.559702	4.036385
H	2.368832	-0.401977	-1.994703	H	0.112675	3.158272	3.413595
C	5.381657	-1.572115	-3.169619	C	-3.174047	2.223916	3.636710
H	7.311625	-1.172396	-2.246037	H	-4.514812	1.964293	1.933590
H	3.314905	-1.813595	-3.834809	H	-1.594355	2.550782	5.102960
H	5.802328	-2.202813	-3.968662	H	-3.936098	1.963786	4.388228
C	4.529395	1.048896	1.264460	C	-0.380576	4.782233	0.159046
C	4.489450	0.209432	2.396948	C	0.242619	5.181442	-1.044640
C	5.416150	2.146725	1.268599	C	-1.114898	5.735880	0.889986
C	5.321812	0.449936	3.502438	C	0.132917	6.500366	-1.508691
H	3.792173	-0.641599	2.409199	H	0.813217	4.436098	-1.622883
C	6.250185	2.390610	2.373304	C	-1.224621	7.061109	0.427001
H	5.452303	2.822685	0.400352	H	-1.611387	5.435582	1.825723
C	6.207287	1.541871	3.494492	C	-0.603656	7.447951	-0.771746
H	5.274904	-0.224980	4.371952	H	0.623355	6.792454	-2.451342
H	6.936609	3.252402	2.359217	H	-1.804708	7.794633	1.009517
H	6.860089	1.734878	4.360743	H	-0.692884	8.484261	-1.134208
C	-1.442035	4.686557	-0.049344	C	3.972003	-0.727218	0.405686
C	-2.631612	4.523487	-0.788048	C	3.011134	-1.025282	1.390038
C	-1.026917	5.995753	0.281719	C	4.739981	-1.787197	-0.131170
C	-3.376095	5.640928	-1.206843	C	2.814465	-2.348868	1.822334
H	-2.963170	3.506504	-1.047433	H	2.386568	-0.225769	1.810713
C	-1.765462	7.112812	-0.140668	C	4.543023	-3.108265	0.298336
H	-0.113460	6.143893	0.878361	H	5.494011	-1.572608	-0.905474
C	-2.943623	6.939646	-0.890388	C	3.576320	-3.393969	1.278138
H	-4.302096	5.490909	-1.785001	H	2.035023	-2.563712	2.566737
H	-1.421798	8.126068	0.122710	H	5.134675	-3.922366	-0.149017
H	-3.525073	7.815763	-1.219336	H	3.387312	-4.433436	1.587330

C	-0.652847	3.383141	1.942579
C	-1.645808	2.645704	2.619018
C	0.342070	4.036829	2.699714
C	-1.624736	2.535668	4.019563
H	-2.433106	2.139239	2.035580
C	0.355620	3.942894	4.101959
H	1.140013	4.590933	2.179713
C	-0.622707	3.181454	4.765537
H	-2.384363	1.927162	4.532173
H	1.144468	4.454076	4.677027
H	-0.605308	3.088578	5.862977
C	1.781692	-3.779729	-1.265853
C	2.508139	-4.987580	-1.257165
C	1.162918	-3.371837	-2.466700
C	2.622831	-5.761767	-2.426413
H	2.994815	-5.322319	-0.327764
C	1.272610	-4.142311	-3.633668
H	0.579292	-2.431265	-2.489872
C	2.008425	-5.341866	-3.618759
H	3.198274	-6.701145	-2.403017
H	0.779887	-3.799921	-4.557579
H	2.100931	-5.948664	-4.533611
C	2.734081	-3.036675	0.998714
C	4.063198	-2.870651	0.542298
C	2.520893	-3.278221	2.370538
C	5.143836	-2.947257	1.432003
H	4.247334	-2.684381	-0.526324
C	3.605523	-3.355158	3.265543
H	1.494073	-3.419002	2.743120
C	4.920765	-3.193452	2.799656
H	6.166572	-2.796871	1.053081
H	3.416774	-3.547269	4.333952
H	5.769258	-3.247628	3.499533
C	-3.833913	-0.780879	1.539419
C	-3.712369	-0.054399	0.337434
C	-5.092158	-1.318576	1.884630
C	-4.817566	0.136979	-0.505462
H	-2.729434	0.331402	0.022341
C	-6.203874	-1.119197	1.045870
H	-5.207069	-1.886021	2.822232
C	-6.069505	-0.394464	-0.152922
H	-4.668050	0.669275	-1.456343
H	-7.182781	-1.537311	1.331903
H	-6.933472	-0.268660	-0.823680
C	-2.753198	-1.164632	3.869090
C	-3.654820	-0.312080	4.545957
C	-1.971597	-2.052464	4.637722
C	-3.767222	-0.344248	5.945257
H	-4.277478	0.383320	3.961342
C	-2.078983	-2.084728	6.039964
H	-1.271764	-2.734696	4.129613
C	-2.976752	-1.230213	6.700524
H	-4.477817	0.329873	6.449846
H	-1.457921	-2.787834	6.617925
H	-3.065255	-1.256471	7.798106

Zero-point correction= 1.201448 (Hartree/Particle)
Thermal correction to Energy= 1.274817
Thermal correction to Enthalpy= 1.275762
Thermal correction to Gibbs Free Energy= 1.090049
Sum of electronic and zero-point Energies= -3565.107659
Sum of electronic and thermal Energies= -3565.034291
Sum of electronic and thermal Enthalpies= -3565.033346
Sum of electronic and thermal Free Energies= -3565.219059

SCF Done (in solvent): -3566.9748578

C	5.593417	1.104283	-0.376724
C	5.933272	1.938400	-1.462173
C	6.608747	0.730571	0.529205
C	7.250612	2.391444	-1.641722
H	5.148100	2.238816	-2.176134
C	7.927553	1.184922	0.355826
H	6.358467	0.065098	1.370490
C	8.253715	2.016854	-0.729941
H	7.496247	3.038045	-2.499354
H	8.707498	0.882319	1.072868
H	9.288428	2.368412	-0.868480
C	-4.152916	0.816613	-1.760180
C	-5.039144	1.293261	-2.746607
C	-4.674314	0.428258	-0.505285
C	-6.419989	1.375804	-2.488760
H	-4.643176	1.604378	-3.725879
C	-6.052079	0.508989	-0.247563
H	-3.985837	0.045389	0.265254
C	-6.930782	0.982378	-1.240190
H	-7.099302	1.751239	-3.270910
H	-6.440493	0.184910	0.729426
H	-8.011845	1.045148	-1.037527
C	-2.126720	1.544944	-3.130219
C	-1.804963	2.890760	-2.858174
C	-1.956292	1.062700	-4.444284
C	-1.298620	3.728124	-3.864656
H	-1.951119	3.294326	-1.843914
C	-1.451764	1.898057	-5.456760
H	-2.203729	0.012164	-4.665883
C	-1.113980	3.232142	-5.168119
H	-1.045811	4.771851	-3.621077
H	-1.318246	1.502254	-6.476458
H	-0.712118	3.885898	-5.958549
C	1.080366	-4.143766	-0.807094
C	0.474006	-4.118960	0.468956
C	1.780530	-5.296873	-1.203474
C	0.553757	-5.222118	1.328605
H	-0.030161	-3.198156	0.808912
C	1.867968	-6.407551	-0.340340
H	2.276795	-5.324046	-2.185730
C	1.253680	-6.375738	0.923172
H	0.087320	-5.152196	2.322779
H	2.425269	-7.302541	-0.661354
H	1.326146	-7.245576	1.595825
C	1.790848	-2.861413	-2.945246
C	2.959221	-2.077376	-3.018514
C	1.398607	-3.592028	-4.087840
C	3.726419	-2.028136	-4.194174
H	3.262810	-1.501233	-2.133475
C	2.164090	-3.549683	-5.265571
H	0.477301	-4.194763	-4.055532
C	3.331951	-2.766771	-5.323477
H	4.635873	-1.406585	-4.226110
H	1.843217	-4.128303	-6.146732
H	3.929546	-2.730321	-6.248362

Zero-point correction= 1.203269 (Hartree/Particle)
Thermal correction to Energy= 1.277378
Thermal correction to Enthalpy= 1.278322
Thermal correction to Gibbs Free Energy= 1.088695
Sum of electronic and zero-point Energies= -3565.125593
Sum of electronic and thermal Energies= -3565.051484
Sum of electronic and thermal Enthalpies= -3565.050539
Sum of electronic and thermal Free Energies= -3565.240167

SCF Done (in solvent): -3567.0168099

[Pd(SIPr)(allyl)Cl]				[Pd(SIPr)(allyl)Cl]-I			
77				83			
SI-PREallyl SCF Done: -1865.95512008 A.U.				SI-PREallyl+K2CO3 SCF Done: -3329.72888860 A.U.			
Cl	1.063700	-2.623969	0.881649	Cl	0.203348	-2.321307	1.021685
N	1.224548	0.265605	-1.066779	N	-2.534758	-0.143577	0.509286
C	2.479749	0.557816	-0.430645	C	-3.042168	-1.180142	-0.345530
N	-0.949968	0.060028	-1.304037	N	-1.289372	1.573289	1.097079
C	2.588366	1.726451	0.377852	C	-3.219267	-0.883199	-1.729824
C	3.847246	2.020524	0.938237	C	-3.748727	-1.893983	-2.555096
H	3.963822	2.916905	1.566049	H	-3.895399	-1.698094	-3.627598
C	4.958632	1.198448	0.702051	C	-4.107530	-3.145375	-2.031317
H	5.934133	1.451454	1.147214	H	-4.525706	-3.919332	-2.694637
C	4.825992	0.052548	-0.091899	C	-3.932005	-3.411167	-0.667964
H	5.699616	-0.595927	-0.260155	H	-4.209563	-4.398126	-0.267230
C	3.587777	-0.298043	-0.667032	C	-3.388380	-2.442890	0.201352
C	1.414544	2.682539	0.597336	C	-2.912605	0.504507	-2.297600
H	0.476610	2.105755	0.467335	H	-2.032960	0.898001	-1.749393
C	1.365950	3.260617	2.022830	C	-2.523490	0.496197	-3.784655
H	1.435820	2.454672	2.781580	H	-1.722330	-0.243771	-3.988506
H	0.413020	3.807841	2.180226	H	-2.152066	1.498640	-4.082587
H	2.189021	3.981069	2.214786	H	-3.383991	0.257808	-4.445649
C	1.426824	3.812322	-0.454301	C	-4.090737	1.470155	-2.047468
H	2.352115	4.421132	-0.369480	H	-5.009458	1.113608	-2.559886
H	0.555744	4.487359	-0.319994	H	-3.854898	2.486339	-2.428391
H	1.389132	3.409993	-1.487383	H	-4.324747	1.560939	-0.967870
C	3.474229	-1.555301	-1.523879	C	-3.218675	-2.754725	1.685028
H	2.391005	-1.769203	-1.641129	H	-2.488765	-2.020593	2.086717
C	4.093878	-2.788057	-0.837616	C	-2.619103	-4.150864	1.938757
H	5.198985	-2.704494	-0.757072	H	-3.326502	-4.962840	1.665280
H	3.875056	-3.701900	-1.428636	H	-2.384753	-4.271362	3.017149
H	3.664654	-2.922954	0.173985	H	-1.680750	-4.280908	1.365627
C	4.110456	-1.330838	-2.914080	C	-4.567835	-2.604393	2.424195
H	3.692354	-0.442554	-3.432940	H	-5.033470	-1.611658	2.256026
H	3.957085	-2.216450	-3.566361	H	-4.438855	-2.745428	3.518332
H	5.205383	-1.164398	-2.822613	H	-5.292584	-3.367412	2.067124
C	0.068464	0.000952	-0.411389	C	-1.300255	0.412128	0.396466
C	0.993264	0.606292	-2.491431	C	-3.380134	0.584381	1.485401
H	1.167485	1.693935	-2.648375	H	-4.410309	0.711402	1.097863
C	-0.479177	0.201632	-2.695249	C	-2.618272	1.908839	1.658099
H	-1.072310	0.959467	-3.245013	H	-2.532167	2.227554	2.715130
C	-2.333750	0.033188	-0.931277	C	-0.172244	2.481594	1.066959
C	-3.004763	1.277933	-0.791691	C	-0.201059	3.568170	0.151727
C	-4.351069	1.255876	-0.376113	C	0.941120	4.390297	0.072601
H	-4.898486	2.204560	-0.257770	H	0.948785	5.241880	-0.625710
C	-4.999747	0.042407	-0.101378	C	2.078586	4.115360	0.843414
H	-6.050102	0.044676	0.231121	H	2.977824	4.742752	0.740321
C	-4.315666	-1.173321	-0.251105	C	2.086172	3.032758	1.735805
H	-4.835885	-2.119930	-0.037295	H	2.999590	2.816199	2.305729
C	-2.970689	-1.207705	-0.672914	C	0.957139	2.203477	1.886430
C	-2.312510	2.606923	-1.098473	C	-1.426424	3.870429	-0.712733
H	-1.240088	2.392139	-1.286677	H	-2.077023	2.972491	-0.697685
C	-2.900382	3.241786	-2.377192	C	-2.221164	5.054804	-0.117441
H	-2.864509	2.538727	-3.235451	H	-2.470871	4.888849	0.950943
H	-2.342333	4.160236	-2.656808	H	-3.167108	5.223414	-0.675024

H	-3.964313	3.524261	-2.228640
C	-2.358625	3.594555	0.083401
H	-3.400286	3.841496	0.377358
H	-1.858250	4.547030	-0.189893
H	-1.841212	3.182578	0.972010
C	-2.250151	-2.536198	-0.879461
H	-1.161324	-2.332337	-0.930901
C	-2.445516	-3.510646	0.295467
H	-2.150880	-3.032362	1.250807
H	-1.792536	-4.396224	0.162657
H	-3.494929	-3.866984	0.378548
C	-2.683821	-3.169317	-2.219545
H	-3.769284	-3.408150	-2.216824
H	-2.126732	-4.111712	-2.404989
H	-2.497657	-2.484731	-3.073995
C	-1.381581	0.800485	2.450109
H	-2.216180	1.256881	1.893941
H	-0.670333	1.511715	2.905838
C	-1.599697	-0.481980	3.057484
H	-2.551999	-1.009167	2.861505
C	-0.514427	-1.200008	3.603507
H	0.355793	-0.678255	4.038865
Pd	-0.165108	-0.672977	1.468049
H	-0.632711	-2.260208	3.875722
H	-0.584273	-0.771638	-3.224203
H	1.686990	0.049406	-3.149118

Zero-point correction= 0.647575 (Hartree/Particle)
Thermal correction to Energy= 0.686215
Thermal correction to Enthalpy= 0.687159
Thermal correction to Gibbs Free Energy= 0.578143
Sum of electronic and zero-point Energies= -1865.307545
Sum of electronic and thermal Energies= -1865.268905
Sum of electronic and thermal Enthalpies= -1865.267961
Sum of electronic and thermal Free Energies= -1865.376977

SCF Done (in solvent): -1866.2177549

H	-1.622421	5.988962	-0.170006
C	-1.102115	4.135938	-2.195362
H	-0.479838	5.045191	-2.330393
H	-2.040704	4.295023	-2.767204
H	-0.565427	3.284029	-2.655493
C	0.938895	1.050602	2.892130
H	0.504740	0.167519	2.373657
C	2.335363	0.642453	3.385224
H	3.031916	0.449471	2.540743
H	2.248998	-0.273324	4.010588
H	2.786233	1.421599	4.037587
C	0.030628	1.386729	4.096205
H	0.419697	2.270948	4.645051
H	-0.005029	0.531739	4.803942
H	-1.010506	1.611976	3.793251
C	0.810987	0.961558	-2.020675
H	0.831901	2.027712	-1.746862
H	0.174776	0.706441	-2.888257
C	1.976958	0.175463	-1.724548
H	2.833531	0.618067	-1.179509
C	1.905029	-1.227836	-1.844133
H	1.220543	-1.712243	-2.565424
Pd	0.294477	-0.441966	-0.505061
H	2.725468	-1.837402	-1.424180
O	4.773569	-1.929606	-0.361654
C	4.733214	-0.602294	-0.134303
O	4.232099	-0.176527	0.971000
O	5.152103	0.197721	-1.063278
K	3.220577	-2.353602	1.617983
K	5.697487	-1.557539	-2.617563
H	-3.435055	0.012975	2.436587
H	-3.081478	2.740792	1.086065

Zero-point correction= 0.665147 (Hartree/Particle)
Thermal correction to Energy= 0.712275
Thermal correction to Enthalpy= 0.713220
Thermal correction to Gibbs Free Energy= 0.579990
Sum of electronic and zero-point Energies= -3329.063742
Sum of electronic and thermal Energies= -3329.016613
Sum of electronic and thermal Enthalpies= -3329.015669
Sum of electronic and thermal Free Energies= -3329.148899

SCF Done (in solvent): -3330.0418648

[Pd(SIPr)(allyl)Cl]-I-II			
83			
SI-PREallyl--K2CO3 SCF Done: -3329.70653414 A.U.			
Cl	1.228676	0.150336	-2.088069
N	-1.053529	1.928489	0.399157
C	0.256417	2.489630	0.574539
N	-2.712238	0.531223	0.080918
C	1.052788	2.137086	1.707739
C	2.287223	2.800845	1.877368
H	2.919973	2.549342	2.740883
C	2.724779	3.779462	0.967453
H	3.679526	4.303497	1.139949
C	1.947224	4.081081	-0.160628
H	2.305325	4.830268	-0.884974
C	0.711757	3.436210	-0.387052
C	0.599069	1.082951	2.716262
H	0.116561	0.280874	2.114600
C	1.751437	0.422561	3.492011
H	2.566876	0.055336	2.831657
H	1.361409	-0.448773	4.058280
H	2.203505	1.111647	4.238495

[Pd(SIPr)(allyl)Cl]-II			
83			
SI-PREallyl--K2CO3post SCF Done: -3329.77276183 A.U.			
Cl	-1.463991	-1.009564	1.820348
N	0.043789	2.082585	0.543701
C	-1.268973	2.362607	0.053728
N	2.017119	1.162546	0.726432
C	-1.525236	2.349114	-1.350705
C	-2.813535	2.727589	-1.791401
H	-3.029733	2.729867	-2.871246
C	-3.813491	3.118506	-0.885155
H	-4.802877	3.432067	-1.256243
C	-3.546991	3.111236	0.494499
H	-4.336186	3.410813	1.202925
C	-2.282351	2.723658	0.990609
C	-0.457621	1.992038	-2.383238
H	0.391739	1.530424	-1.841310
C	-0.949491	0.929118	-3.384542
H	-1.332320	0.026561	-2.863487
H	-0.109722	0.614183	-4.038561
H	-1.753650	1.315184	-4.047291

C	-0.461550	1.648872	3.683514	C	0.057060	3.260998	-3.093367
H	-0.053265	2.500769	4.268719	H	-0.752687	3.766433	-3.662578
H	-0.787055	0.865009	4.398125	H	0.864384	3.000720	-3.809225
H	-1.364470	2.003759	3.147864	H	0.465304	3.996167	-2.368064
C	-0.088566	3.776582	-1.643873	C	-2.029733	2.706187	2.497073
H	-0.932855	3.057504	-1.699734	H	-1.052351	2.202247	2.651145
C	0.736420	3.583028	-2.932108	C	-3.080378	1.874542	3.259673
H	1.596308	4.285706	-2.979931	H	-4.102997	2.296210	3.152435
H	0.103167	3.780144	-3.822956	H	-2.842994	1.862529	4.344129
H	1.112386	2.541842	-2.992954	H	-3.072814	0.823687	2.907073
C	-0.656893	5.211689	-1.571623	C	-1.959023	4.142404	3.062163
H	-1.242477	5.389510	-0.645144	H	-1.225435	4.772488	2.517289
H	-1.314967	5.419858	-2.441439	H	-1.674714	4.131026	4.135386
H	0.162838	5.961519	-1.584419	H	-2.945067	4.648309	2.980485
C	-1.354131	0.615600	0.154234	C	0.737859	0.918695	0.321365
C	-2.268699	2.751076	0.624605	C	0.929194	3.210271	0.930979
H	-2.404701	2.929808	1.715884	H	1.105609	3.865308	0.046014
C	-3.365882	1.855202	0.040596	C	2.198854	2.474261	1.376655
H	-3.614448	2.118715	-1.013906	H	3.134759	2.964894	1.040450
C	-3.430159	-0.671095	-0.225960	C	3.107248	0.256893	0.523552
C	-4.164542	-1.289923	0.822496	C	3.943107	0.471750	-0.604329
C	-4.876292	-2.467213	0.521575	C	5.011704	-0.422469	-0.814934
H	-5.446620	-2.979155	1.310952	H	5.667661	-0.286947	-1.689819
C	-4.862485	-3.004827	-0.775695	C	5.241635	-1.490325	0.065288
H	-5.426163	-3.926538	-0.992473	H	6.080467	-2.181275	-0.115891
C	-4.136096	-2.373300	-1.793933	C	4.400269	-1.684003	1.171293
H	-4.135194	-2.803352	-2.807799	H	4.584802	-2.529406	1.853088
C	-3.403645	-1.193387	-1.544587	C	3.316615	-0.818684	1.423495
C	-4.113792	-0.725190	2.243126	C	3.685117	1.611617	-1.588439
H	-4.061933	0.382068	2.159601	H	2.822544	2.196272	-1.207074
C	-5.355078	-1.056698	3.088263	C	4.892378	2.565587	-1.685045
H	-6.296161	-0.778192	2.569849	H	5.183272	2.954877	-0.686763
H	-5.317236	-0.510557	4.053696	H	4.658905	3.431361	-2.340308
H	-5.408623	-2.138602	3.333983	H	5.780648	2.054725	-2.113636
C	-2.819784	-1.176703	2.953613	C	3.265428	1.078183	-2.972544
H	-2.801954	-2.281631	3.060851	H	4.057072	0.442033	-3.421803
H	-2.749945	-0.728254	3.966816	H	3.069599	1.918679	-3.671138
H	-1.924715	-0.882131	2.372172	H	2.344009	0.470109	-2.891621
C	-2.636234	-0.512531	-2.675005	C	2.401598	-1.053191	2.621702
H	-1.965582	0.247627	-2.224809	H	1.544297	-0.355629	2.532692
C	-1.721445	-1.496420	-3.427960	C	1.803126	-2.473497	2.601885
H	-1.063431	-2.032454	-2.714053	H	1.300224	-2.638091	1.624352
H	-1.062329	-0.943879	-4.127165	H	1.044695	-2.579016	3.405280
H	-2.303341	-2.241211	-4.012690	H	2.578582	-3.255890	2.747647
C	-3.605141	0.211180	-3.633865	C	3.133185	-0.756446	3.946435
H	-4.291506	-0.508271	-4.130394	H	3.996730	-1.440359	4.093177
H	-3.043024	0.747833	-4.427139	H	2.447760	-0.884991	4.810919
H	-4.235325	0.951111	-3.096500	H	3.524627	0.282402	3.967940
C	-0.114224	-2.482900	1.223275	C	1.259106	-1.750921	-1.783446
H	-1.021278	-3.111443	1.178677	H	2.329947	-1.758175	-1.505176
H	0.132558	-2.122928	2.238987	H	1.059914	-1.286595	-2.769435
C	0.955746	-2.746114	0.292666	C	0.386236	-2.807508	-1.341254
H	0.819235	-3.501984	-0.503271	H	0.854613	-3.594428	-0.708640
C	2.165039	-1.973305	0.325633	C	-0.689837	-3.337242	-2.267203
H	2.207771	-1.146381	1.049895	H	-0.350246	-4.246052	-2.813798
Pd	-0.029878	-0.866382	-0.151771	Pd	0.137260	-0.943289	-0.245041
H	2.609897	-1.755825	-0.661837	H	-0.992145	-2.569032	-3.008013
O	5.242593	-1.655778	-0.390675	O	-3.655926	-3.080323	-0.387299
C	4.560785	-1.600371	0.712972	C	-2.910489	-2.830467	-1.387698
O	3.760468	-2.684296	0.986015	O	-1.867696	-3.768196	-1.532884
O	4.480378	-0.572227	1.443791	O	-2.977310	-1.861829	-2.180739
K	4.485507	-3.933716	-1.051261	K	-1.661451	-3.869167	1.122507
K	3.828630	0.861501	-0.613648	K	-3.693773	-0.391328	-0.192263

H -4.305537 1.864987 0.628639	H 2.252186 2.345021 2.482458
H -2.196329 3.734720 0.125404	H 0.480416 3.828452 1.731424
Zero-point correction= 0.664407 (Hartree/Particle) Thermal correction to Energy= 0.710698 Thermal correction to Enthalpy= 0.711642 Thermal correction to Gibbs Free Energy= 0.583824 Sum of electronic and zero-point Energies= -3329.042127 Sum of electronic and thermal Energies= -3328.995837 Sum of electronic and thermal Enthalpies= -3328.994892 Sum of electronic and thermal Free Energies= -3329.122710	Zero-point correction= 0.665821 (Hartree/Particle) Thermal correction to Energy= 0.712308 Thermal correction to Enthalpy= 0.713252 Thermal correction to Gibbs Free Energy= 0.585431 Sum of electronic and zero-point Energies= -3329.106941 Sum of electronic and thermal Energies= -3329.060454 Sum of electronic and thermal Enthalpies= -3329.059510 Sum of electronic and thermal Free Energies= -3329.187331
SCF Done (in solvent): -3330.0077407	SCF Done (in solvent): -3330.0676522

[Pd(SIPr)(allyl)Cl]-III	**[Pd(SIPr)(allyl)Cl]-I'**
81 SI-PREallyl+KCO3menysKClISOMERopen SCF Done: -2269.51221114 A.U.	81 SI-PREallyl+KCO3menysKCl SCF Done: -2269.50275813 A.U.
N -0.795666 1.036191 1.320223	N -0.165228 1.524866 1.039731
C -2.098614 1.266441 0.773332	C -1.091508 2.397405 0.372016
N 1.331506 0.522409 1.406310	N 1.406590 0.015061 1.315214
C -2.239718 2.216648 -0.289445	C -0.629648 3.192303 -0.711033
C -3.529195 2.414352 -0.826023	C -1.550495 4.067753 -1.321762
H -3.672933 3.137317 -1.642234	H -1.221573 4.695766 -2.165049
C -4.643123 1.714679 -0.326958	C -2.874344 4.154725 -0.869611
H -5.642625 1.897431 -0.753641	H -3.579544 4.843369 -1.362177
C -4.482140 0.787264 0.711746	C -3.303010 3.364481 0.206173
H -5.355387 0.232801 1.088261	H -4.346690 3.432810 0.549470
C -3.210707 0.532700 1.275090	C -2.426303 2.468430 0.847138
C -1.034073 2.991407 -0.828270	C 0.816593 3.154636 -1.204503
H -0.200818 2.251151 -0.926454	H 1.329577 2.307718 -0.706037
C -1.235836 3.579312 -2.231895	C 0.895111 2.876246 -2.716905
H -1.556699 2.801410 -2.955658	H 0.317792 1.962707 -2.966182
H -0.277044 3.998719 -2.599630	H 1.949321 2.722095 -3.029893
H -1.982466 4.402160 -2.247704	H 0.488789 3.718396 -3.315612
C -0.572188 4.079294 0.162559	C 1.571488 4.444554 -0.823394
H -1.364103 4.844487 0.309880	H 1.114840 5.335418 -1.304983
H 0.336234 4.590551 -0.218385	H 2.632656 4.389063 -1.147644
H -0.323884 3.654239 1.154464	H 1.554976 4.615815 0.273529
C -3.068059 -0.493130 2.398762	C -2.898136 1.646904 2.042578
H -1.990995 -0.753656 2.470523	H -2.140079 0.851442 2.205455
C -3.814834 -1.813057 2.127936	C -4.245788 0.945916 1.795621
H -4.914833 -1.662574 2.075149	H -5.069896 1.681018 1.665776
H -3.626794 -2.519854 2.962696	H -4.509147 0.321685 2.676861
H -3.464850 -2.301602 1.193306	H -4.200492 0.281020 0.907608
C -3.527122 0.132839 3.737512	C -2.966695 2.536950 3.305652
H -3.017367 1.094127 3.956722	H -2.010265 3.064521 3.508855
H -3.336221 -0.562570 4.581446	H -3.225381 1.933184 4.201576
H -4.618335 0.340546 3.711013	H -3.747376 3.319304 3.189342
C 0.234292 0.489655 0.610653	C 0.425763 0.442585 0.474194
C -0.408315 1.397107 2.708803	C 0.555372 1.988467 2.246004
H -0.841929 0.676250 3.432683	H 1.155673 2.892274 1.990350
C 1.125099 1.288775 2.654900	C 1.427038 0.771713 2.588083
H 1.624087 2.281703 2.574816	H 2.461004 1.035678 2.885167
C 2.648974 0.165468 0.953822	C 2.419468 -0.939926 0.970929
C 3.462375 1.176288 0.380884	C 3.700770 -0.435446 0.622829
C 4.781879 0.835589 0.019953	C 4.714542 -1.360358 0.298319
H 5.436444 1.598653 -0.430968	H 5.716237 -0.993319 0.022855
C 5.259955 -0.468423 0.206025	C 4.453189 -2.736090 0.292270
H 6.295956 -0.719121 -0.073239	H 5.252521 -3.447889 0.030895
C 4.413347 -1.466923 0.714864	C 3.167035 -3.209840 0.597463
H 4.793420 -2.494088 0.811623	H 2.973545 -4.291585 0.561445
C 3.084428 -1.181784 1.089819	C 2.120534 -2.331426 0.943723
C 2.906820 2.559838 0.046457	C 3.985322 1.063677 0.516320
H 1.892397 2.637802 0.486376	H 3.064310 1.610654 0.801606

C	3.752604	3.705078	0.632782
H	3.869802	3.601292	1.731822
H	3.277274	4.687370	0.426436
H	4.770624	3.732079	0.189787
C	2.722197	2.698958	-1.479365
H	3.695828	2.648831	-2.010940
H	2.241574	3.668478	-1.731319
H	2.073907	1.876530	-1.861558
C	2.118581	-2.277484	1.538168
H	1.161531	-2.102776	0.996938
C	2.570985	-3.695516	1.155252
H	2.875412	-3.756227	0.089920
H	1.719424	-4.389931	1.293368
H	3.423644	-4.049741	1.775105
C	1.805188	-2.222551	3.048078
H	2.727089	-2.356937	3.654205
H	1.091565	-3.029396	3.313095
H	1.338761	-1.262929	3.343657
C	0.609323	-0.830540	-3.356227
H	1.230770	-0.092857	-3.894235
H	-0.333701	-1.109230	-3.863009
C	1.200870	-1.725535	-2.442604
H	2.290593	-1.645808	-2.252610
C	0.610988	-3.064126	-2.041348
H	0.899954	-3.819308	-2.814615
Pd	0.347046	-0.091693	-1.333544
H	1.035080	-3.397439	-1.072184
O	-2.626407	-3.104124	-0.622403
C	-1.377502	-3.286203	-0.585391
O	-0.601376	-3.574686	0.328495
O	-0.807326	-3.049960	-1.935041
K	-2.641899	-1.036709	-1.995865
H	-0.774875	2.410252	2.970012
H	1.557561	0.758627	3.526161

Zero-point correction= 0.664101 (Hartree/Particle)
Thermal correction to Energy= 0.706441
Thermal correction to Enthalpy= 0.707385
Thermal correction to Gibbs Free Energy= 0.589973
Sum of electronic and zero-point Energies= -2268.848110
Sum of electronic and thermal Energies= -2268.805770
Sum of electronic and thermal Enthalpies= -2268.804826
Sum of electronic and thermal Free Energies= -2268.922238

SCF Done (in solvent): -2269.792829

C	5.110162	1.508655	1.471809
H	4.891671	1.221908	2.521884
H	5.246394	2.610024	1.434348
H	6.081080	1.043736	1.198697
C	4.283777	1.471775	-0.941264
H	5.197820	0.972668	-1.326657
H	4.439670	2.568828	-1.013542
H	3.440651	1.200923	-1.606245
C	0.711199	-2.842147	1.234945
H	0.002184	-2.173967	0.692742
C	0.434422	-4.248912	0.687765
H	0.680037	-4.320097	-0.391252
H	-0.649247	-4.457781	0.782377
H	0.994730	-5.040147	1.233033
C	0.376057	-2.775984	2.738547
H	1.035843	-3.450196	3.326840
H	-0.677133	-3.082372	2.910380
H	0.492683	-1.752306	3.143900
C	1.663453	-0.799465	-2.326303
H	2.571757	-1.121283	-1.791794
H	1.789984	0.084503	-2.976629
C	0.682215	-1.789909	-2.670693
H	0.787821	-2.812332	-2.263829
C	-0.562476	-1.399582	-3.206015
H	-0.655869	-0.493202	-3.829765
Pd	-0.160611	-0.468036	-1.214573
H	-1.391911	-2.121160	-3.243687
O	-3.983023	-1.591099	-0.203267
C	-2.718974	-1.557227	-0.458739
O	-2.142461	-0.372602	-0.563604
O	-2.017940	-2.645419	-0.605296
K	-4.037080	-4.019710	-0.335675
H	-0.151285	2.260508	3.052657
H	0.986012	0.153055	3.401284

Zero-point correction= 0.662841 (Hartree/Particle)
Thermal correction to Energy= 0.705625
Thermal correction to Enthalpy= 0.706569
Thermal correction to Gibbs Free Energy= 0.587418
Sum of electronic and zero-point Energies= -2268.839918
Sum of electronic and thermal Energies= -2268.797133
Sum of electronic and thermal Enthalpies= -2268.796189
Sum of electronic and thermal Free Energies= -2268.915340

SCF Done (in solvent): -2269.7851883

[Pd(SIPr)(allyl)Cl]-I'-III			
81			
SI-PREallyl+KCO3--C-O SCF Done: -2269.47389272 A.U.			
N	-0.151235	1.190103	1.445438
C	-1.425225	1.751605	1.092919
N	1.787234	0.191938	1.207438
C	-1.463040	2.970623	0.371000
C	-2.724010	3.527934	0.077255
H	-2.781019	4.473648	-0.485287
C	-3.902394	2.876355	0.459551
H	-4.880971	3.315080	0.208328
C	-3.843254	1.644182	1.129538
H	-4.782196	1.129964	1.378746
C	-2.608896	1.055112	1.462596
C	-0.192685	3.637121	-0.149759
H	0.669773	3.009534	0.152309
C	-0.188983	3.657841	-1.691455
H	-0.361877	2.635569	-2.083639
H	0.786898	4.022306	-2.076214

[Pd(SIPr)(allyl)Cl]-IV			
68			
SIPr-Pd SCF Done: -1288.52607176 A.U.			
Pd	-0.003333	-0.110622	-1.828071
N	-1.098199	-0.151632	0.913238
N	1.096261	-0.255476	0.911059
C	-0.001653	-0.163954	0.099103
C	-0.766805	-0.362034	2.339192
C	0.761626	-0.175196	2.348370
C	-2.452945	0.009226	0.470717
C	-3.288052	-1.134410	0.393958
C	-4.645608	-0.940565	0.066060
C	-5.144661	0.343072	-0.194318
C	-4.287110	1.454840	-0.167704
C	-2.923791	1.316362	0.158170
C	-2.702169	-2.539555	0.519490
H	-6.209350	0.478603	-0.443591
C	-1.963513	2.506258	0.131465
C	2.444799	-0.049606	0.468054

H	-0.984529	4.319844	-2.093615
C	0.016036	5.042130	0.447424
H	-0.800411	5.734288	0.150084
H	0.972426	5.481962	0.093018
H	0.038348	5.012527	1.557248
C	-2.527735	-0.302171	2.162164
H	-1.690684	-0.842957	1.669489
C	-3.797185	-1.151330	1.974758
H	-4.660568	-0.740428	2.540420
H	-3.626811	-2.172403	2.387442
H	-4.085106	-1.218077	0.903175
C	-2.207018	-0.161165	3.665210
H	-1.247538	0.361788	3.839158
H	-2.135057	-1.159276	4.149006
H	-3.003653	0.413075	4.184695
C	0.576379	0.398797	0.595399
C	0.666390	1.713578	2.558309
H	1.042958	2.735674	2.315623
C	1.801655	0.682700	2.599340
H	1.581118	-0.155820	3.302975
C	2.812672	-0.639001	0.657562
C	3.966768	-0.009729	0.115067
C	4.940882	-0.829123	-0.487651
H	5.839094	-0.374323	-0.931140
C	4.780045	-2.223213	-0.540482
H	5.550131	-2.845777	-1.023452
C	3.649920	-2.824607	0.029467
H	3.544927	-3.921079	-0.000555
C	2.647067	-2.047525	0.645063
C	4.108535	1.513648	0.146702
H	3.636310	1.865544	1.089022
C	5.569348	1.995396	0.167583
H	6.157449	1.502074	0.969353
H	5.607888	3.091792	0.335188
H	6.081022	1.800931	-0.798965
C	3.323596	2.167611	-1.009853
H	3.747359	1.863757	-1.989892
H	3.370873	3.275029	-0.939474
H	2.261321	1.857489	-0.994250
C	1.451966	-2.725930	1.311959
H	0.758409	-1.929574	1.651679
C	0.659458	-3.599990	0.321621
H	0.265991	-2.969159	-0.504768
H	-0.193671	-4.085320	0.847941
H	1.282449	-4.413209	-0.107012
C	1.903380	-3.524731	2.552676
H	2.584803	-4.356529	2.273210
H	1.029580	-3.966051	3.078800
H	2.446716	-2.877298	3.272092
C	1.197400	0.129568	-2.687703
H	2.209238	-0.313134	-2.632217
H	1.209544	1.209460	-2.927767
C	0.136970	-0.687389	-3.265680
H	0.326457	-1.763997	-3.431354
C	-1.115585	-0.167689	-3.685815
H	-1.229357	0.922009	-3.789534
Pd	-0.070970	-0.327134	-1.115110
H	-1.747902	-0.767612	-4.355351
O	-4.044173	-1.637809	-1.405107
C	-2.907930	-1.074425	-1.597280
O	-2.742496	-0.158359	-2.498565
O	-1.880009	-1.469246	-0.837497
K	-3.070523	-3.543763	-0.182464
C	2.916059	1.277097	0.286720
C	4.254507	1.446969	-0.121549
C	5.090923	0.341078	-0.333197
C	4.603524	-0.961651	-0.143211
C	3.273687	-1.183228	0.265129
C	2.004726	2.488848	0.473061
H	6.134041	0.495017	-0.653003
C	2.701572	-2.591594	0.399625
H	-1.304736	0.363647	2.982248
H	1.069787	0.815827	2.755159
H	-5.318611	-1.809149	-0.002976
H	-4.689672	2.448707	-0.412926
H	-1.763673	-2.467972	1.107476
H	-1.014929	2.114903	-0.299700
H	4.646499	2.463834	-0.283715
H	5.268639	-1.820352	-0.322375
H	1.041925	2.129777	0.889737
H	1.830216	-2.523978	1.086475
C	2.158049	-3.063936	-0.966698
H	2.982742	-3.141081	-1.707128
H	1.673025	-4.059495	-0.879541
H	1.409263	-2.336504	-1.360164
C	3.693711	-3.604716	0.996757
H	3.187624	-4.574738	1.183992
H	4.538439	-3.811059	0.305658
H	4.121241	-3.245528	1.956240
C	2.582398	3.509971	1.471719
H	3.516316	3.975657	1.091435
H	1.854958	4.329593	1.651751
H	2.817611	3.035996	2.447696
C	1.673830	3.135555	-0.886644
H	0.960972	3.977491	-0.756928
H	2.587406	3.529389	-1.380874
H	1.205114	2.379818	-1.556776
C	-1.654648	3.044765	1.543095
H	-0.906990	3.864652	1.492350
H	-2.571358	3.443305	2.028127
H	-1.239251	2.259014	2.203378
C	-2.422096	3.647198	-0.790537
H	-3.320165	4.172080	-0.399288
H	-1.616364	4.405292	-0.880324
H	-2.654721	3.276717	-1.810033
C	-3.625094	-3.533794	1.245388
H	-4.540792	-3.753905	0.656684
H	-3.103589	-4.501152	1.401288
H	-3.944820	-3.148106	2.236054
C	-2.300195	-3.045954	-0.883814
H	-1.814460	-4.043002	-0.821107
H	-3.192978	-3.132905	-1.539137
H	-1.586696	-2.334345	-1.360086
H	-1.068449	-1.384763	2.661508
H	1.296252	-0.959182	2.923220

H 0.084096 1.776223 3.498091 H 2.785004 1.114022 2.873563	
Zero-point correction= 0.662297 (Hartree/Particle) Thermal correction to Energy= 0.704383 Thermal correction to Enthalpy= 0.705327 Thermal correction to Gibbs Free Energy= 0.587142 Sum of electronic and zero-point Energies= -2268.811596 Sum of electronic and thermal Energies= -2268.769510 Sum of electronic and thermal Enthalpies= -2268.768565 Sum of electronic and thermal Free Energies= -2268.886751 SCF Done (in solvent): -2269.7491304	Zero-point correction= 0.575504 (Hartree/Particle) Thermal correction to Energy= 0.608667 Thermal correction to Enthalpy= 0.609611 Thermal correction to Gibbs Free Energy= 0.510409 Sum of electronic and zero-point Energies= -1287.950568 Sum of electronic and thermal Energies= -1287.917405 Sum of electronic and thermal Enthalpies= -1287.916461 Sum of electronic and thermal Free Energies= -1288.015663 SCF Done (in solvent): -1288.6905835

[Pd(SIPr)(allyl)Cl]-V			**[Pd(SIPr)(allyl)Cl]-V-VI**		
109			109		
SI5 SCF Done: -2265.74646729 A.U.			SI5-SI6 SCF Done: -2265.74300742 A.U.		
C	-1.348161	1.591809 -1.811716	C	-0.335816	1.307086 -1.465763
O	-0.999256	1.429029 -2.969753	O	-0.028254	0.973257 -2.601105
Pd	0.142286	0.157833 -0.202421	Pd	0.216738	-0.025493 0.141612
N	-0.452370	2.199548 -0.783916	N	0.957742	1.890342 -0.404432
C	-5.518399	1.036248 -0.790715	C	-3.946279	3.590465 -0.762324
C	-5.125041	1.502743 -2.057637	C	-3.319406	3.590206 -2.022164
H	-4.835910	0.324038 1.152701	H	-3.902122	2.797768 1.268384
C	-4.541056	0.718395 0.169951	C	-3.405806	2.824940 0.286120
C	-3.762874	1.670812 -2.350809	C	-2.149881	2.841515 -2.226038
C	-2.779895	1.380687 -1.378976	C	-1.598777	2.083008 -1.170395
C	-3.180025	0.877607 -0.122621	C	-2.245114	2.068444 0.078882
H	-3.435843	2.029295 -3.338707	H	-1.639551	2.835305 -3.201570
H	-2.412691	0.572872 0.607513	H	-1.828206	1.431510 0.872387
H	-6.587014	0.907270 -0.555108	H	-4.862083	4.181639 -0.601239
H	-5.882839	1.739656 -2.821453	H	-3.741791	4.182622 -2.849742
C	0.897153	2.613255 -1.179592	C	2.282344	1.672715 -0.857339
O	1.378203	2.491314 -2.284222	O	2.618233	0.763977 -1.599613
O	1.469986	3.184108 -0.099917	O	3.115651	2.593575 -0.309300
C	2.926085	3.451272 -0.084647	C	4.579080	2.395862 -0.357933
C	3.250947	4.586749 -1.063833	C	5.076993	2.486952 -1.807545
H	3.039079	4.278252 -2.104589	H	4.687620	1.644741 -2.408184
H	2.649700	5.487834 -0.825339	H	4.740517	3.438837 -2.266683
H	4.325096	4.852077 -0.981391	H	6.186355	2.464921 -1.824413
C	3.156579	3.881747 1.368500	C	5.097204	3.571913 0.478824
H	4.222851	4.141861 1.524751	H	6.204522	3.546476 0.530755
H	2.534006	4.764822 1.616498	H	4.784897	4.535557 0.028431
H	2.885606	3.058913 2.059535	H	4.690276	3.524258 1.508861
C	3.681525	2.155704 -0.401901	C	4.933117	1.051904 0.299246
H	3.577837	1.866931 -1.463217	H	4.542901	0.198799 -0.286868
H	4.758247	2.281280 -0.172101	H	6.035104	0.954786 0.382119
H	3.290384	1.323623 0.215781	H	4.501040	0.998870 1.319754
N	-0.437144	-2.707999 0.390377	N	0.238964	-2.902640 0.594542
N	1.699157	-2.371013 0.052355	C	1.198753	-3.190962 -2.152263
C	0.490242	-1.750063 0.113420	H	0.159777	-3.159227 -1.767958
C	0.130146	-4.073959 0.490944	C	2.139409	-2.994655 -0.966929
C	1.644272	-3.819489 0.342179	C	1.656471	-2.843798 0.359026
C	-1.828267	-2.486157 0.658314	C	-0.565572	-1.825041 0.390687
C	-2.777700	-2.871467 -0.324617	C	2.519827	-2.593485 1.457188
C	-4.141441	-2.840439 0.029882	C	1.953147	-2.299979 2.843632
C	-4.543135	-2.426404 1.307223	H	0.913101	-2.691793 2.861972
C	-3.593763	-1.962663 2.231061	C	3.531112	-2.907841 -1.168911
C	-2.218732	-1.965868 1.924427	H	3.933045	-3.002681 -2.189673
C	-2.326047	-3.189456 -1.749370	C	4.404789	-2.673369 -0.097854
H	-5.612635	-2.423600 1.571561	H	5.488705	-2.598723 -0.279625
C	-1.181838	-1.385921 2.886035	C	3.902133	-2.508964 1.202146
C	2.967831	-1.713808 -0.059643	H	4.595857	-2.294729 2.029937
C	3.623670	-1.300770 1.130581	C	-0.508081	-4.171583 0.701856
C	4.924906	-0.773987 1.015421	C	1.862818	-0.773435 3.051053

C	5.538679	-0.645130	-0.239909
C	4.852733	-1.016228	-1.406039
C	3.556283	-1.566579	-1.341774
C	2.892875	-1.315417	2.471417
H	6.555935	-0.228253	-0.312169
C	2.769343	-1.913730	-2.601553
H	-0.145144	-4.537016	1.461430
H	2.216013	-4.045328	1.270083
H	-4.903187	-3.135007	-0.706652
H	-3.931261	-1.582591	3.206987
H	-1.342956	-3.704172	-1.686687
H	-0.408958	-0.914306	2.237127
H	5.458256	-0.439803	1.918964
H	5.333941	-0.876067	-2.385928
H	2.032782	-2.009905	2.380285
H	2.000847	-2.662432	-2.309214
C	2.010551	-0.665297	-3.101634
H	2.712616	0.149002	-3.374683
H	1.388513	-0.903438	-3.988891
H	1.333138	-0.265454	-2.310912
C	3.633274	-2.537772	-3.711495
H	2.990091	-2.889149	-4.544854
H	4.342571	-1.800956	-4.145068
H	4.224556	-3.401669	-3.341084
C	3.759646	-1.803575	3.644690
H	4.586325	-1.097017	3.869510
H	3.146758	-1.889892	4.566420
H	4.210428	-2.795859	3.434609
C	2.298345	0.083773	2.742456
H	1.683950	0.084281	3.667883
H	3.104607	0.838575	2.859083
H	1.647021	0.394559	1.890240
C	-0.493264	-2.470084	3.737769
H	0.295828	-2.022751	4.378683
H	-1.224014	-2.983179	4.399132
H	-0.009884	-3.242699	3.107765
C	-1.740636	-0.261176	3.773081
H	-2.444940	-0.636887	4.546151
H	-0.909180	0.243673	4.308813
H	-2.267938	0.506326	3.169854
C	-3.281379	-4.119208	-2.515602
H	-4.245323	-3.617109	-2.744367
H	-2.833331	-4.408806	-3.488464
H	-3.505002	-5.046489	-1.947249
C	-2.088197	-1.868986	-2.516763
H	-1.726975	-2.069001	-3.546986
H	-3.024307	-1.276700	-2.582044
H	-1.331663	-1.236773	-2.004381
C	-1.080639	3.012527	0.255990
C	-0.944235	2.674724	1.612958
C	-1.839183	4.131318	-0.127502
C	-1.588416	3.448099	2.588952
H	-0.347241	1.784638	1.871154
C	-2.486583	4.901015	0.853538
H	-1.936025	4.380319	-1.195498
C	-2.365471	4.560075	2.211995
H	-1.489186	3.174135	3.651064
H	-3.093740	5.768812	0.551732
H	-2.878289	5.161132	2.979333
H	-0.275571	-4.723989	-0.314853
H	2.105670	-4.397084	-0.486577
Zero-point correction=			0.901335 (Hartree/Particle)
Thermal correction to Energy=			0.956244
Thermal correction to Enthalpy=			0.957188

H	1.378616	-0.521598	4.018017
H	2.869988	-0.306793	3.025579
H	1.260484	-0.302400	2.231775
C	2.733652	-2.980043	3.982622
H	2.224621	-2.813236	4.955004
H	2.821192	-4.074294	3.819759
H	3.761141	-2.570261	4.080542
C	1.322190	-2.036459	-3.165319
H	2.315283	-2.037304	-3.662771
H	0.550149	-2.140591	-3.957028
H	1.190353	-1.050867	-2.677363
C	1.402679	-4.568273	-2.815216
H	1.282437	-5.398520	-2.086947
H	0.668408	-4.717220	-3.634966
H	2.418351	-4.656811	-3.256304
C	-1.967834	-3.679672	0.822423
H	-2.667186	-4.198747	0.136791
H	-0.337654	-4.790834	-0.207512
N	-1.851375	-2.243570	0.469090
C	-2.985736	-1.398292	0.222592
C	-3.309055	-1.055571	-1.121406
C	-3.738611	-0.928978	1.330984
C	-4.459540	-0.267429	-1.325537
C	-4.888390	-0.159041	1.066598
C	-5.250373	0.158215	-0.249712
H	-4.736571	0.035078	-2.344913
H	-5.495873	0.221335	1.901353
H	-6.142522	0.775436	-0.439225
C	-2.424279	-1.493094	-2.292401
H	-1.373774	-1.324411	-1.970088
C	-3.246211	-1.152459	2.762709
H	-2.719581	-2.129375	2.793828
C	-2.583605	-2.992944	-2.620889
H	-1.899915	-3.278299	-3.447698
H	-2.345014	-3.645353	-1.759562
H	-3.623110	-3.220989	-2.939863
C	-2.625723	-0.659071	-3.566491
H	-1.839961	-0.917162	-4.304469
H	-3.611749	-0.854316	-4.041417
H	-2.535279	0.424042	-3.360036
C	-4.374399	-1.217148	3.806455
H	-3.965341	-1.508221	4.796188
H	-4.868512	-0.231658	3.940932
H	-5.155638	-1.953031	3.524004
C	-2.200614	-0.078072	3.138801
H	-1.353542	-0.074653	2.417628
H	-2.658238	0.933980	3.128764
H	-1.792989	-0.261149	4.155609
C	0.665921	3.062055	0.376957
C	0.522849	4.308192	-0.265303
C	0.450481	2.964160	1.764489
C	0.152861	5.441471	0.472979
H	0.683400	4.366893	-1.352390
C	0.080976	4.100363	2.501902
H	0.555747	1.980199	2.246947
C	-0.073770	5.341126	1.858549
H	0.028578	6.409146	-0.038518
H	-0.094554	4.013150	3.586053
H	-0.373985	6.230200	2.435332
H	-0.170841	-4.756528	1.582172
H	-2.364766	-3.792090	1.855795
Zero-point correction=			0.900604 (Hartree/Particle)
Thermal correction to Energy=			0.954939
Thermal correction to Enthalpy=			0.955883

Thermal correction to Gibbs Free Energy= 0.812461 Sum of electronic and zero-point Energies= -2264.845133 Sum of electronic and thermal Energies= -2264.790223 Sum of electronic and thermal Enthalpies= -2264.789279 Sum of electronic and thermal Free Energies= -2264.934007 SCF Done (in solvent): -2266.2160955	Thermal correction to Gibbs Free Energy= 0.813400 Sum of electronic and zero-point Energies= -2264.842404 Sum of electronic and thermal Energies= -2264.788068 Sum of electronic and thermal Enthalpies= -2264.787124 Sum of electronic and thermal Free Energies= -2264.929607 SCF Done (in solvent): -2266.2003899

[Pd(SIPr)(allyl)Cl]-VI			
109			
SI6 SCF Done: -2265.77016562 A.U.			
Pd	-0.214406	0.194588	0.152642
N	1.346866	2.641941	-0.069219
C	-0.161529	3.217915	-2.491154
H	0.647932	2.474455	-2.338451
C	-0.620526	3.682540	-1.113515
C	0.106999	3.357320	0.058281
C	1.434624	1.297166	0.011445
C	-0.354034	3.686978	1.360238
C	0.356566	3.171161	2.609273
H	1.344519	2.771075	2.300230
C	-1.813124	4.415607	-0.955357
H	-2.405581	4.676148	-1.845707
C	-2.270654	4.788161	0.316425
H	-3.210211	5.354340	0.417323
C	-1.555712	4.413357	1.464309
H	-1.948434	4.673861	2.459871
C	2.660634	3.309693	-0.127873
C	-0.436252	1.990352	3.209491
H	0.108695	1.532233	4.061408
H	-1.435343	2.316387	3.566819
H	-0.611069	1.192837	2.449908
C	0.616913	4.267401	3.658325
H	1.200710	3.858993	4.510121
H	1.185179	5.115914	3.224134
H	-0.329318	4.673219	4.074090
C	-1.288970	2.483365	-3.241393
H	-2.096495	3.181579	-3.550273
H	-0.885156	2.006753	-4.158014
H	-1.734888	1.698597	-2.598299
C	0.412267	4.391344	-3.312613
H	1.253970	4.892402	-2.788038
H	0.782756	4.036554	-4.297641
H	-0.364209	5.163485	-3.502422
C	3.627274	2.113744	-0.287867
H	4.463267	2.120349	0.440972
H	2.833545	3.890113	0.806473
N	2.742421	0.944295	-0.056521
C	3.241442	-0.386642	0.146798
C	3.773152	-1.104854	-0.956080
C	3.181823	-0.952217	1.456592
C	4.299984	-2.391327	-0.717327
C	3.719812	-2.240972	1.635176
C	4.283681	-2.951373	0.564035
H	4.713389	-2.968891	-1.558076
H	3.687478	-2.710738	2.628714
H	4.693528	-3.960108	0.730035
C	3.795121	-0.524185	-2.368265
H	3.091176	0.334707	-2.383475
C	2.514208	-0.211364	2.616970
H	1.595473	0.252828	2.195403
C	5.212936	-0.023264	-2.726236
H	5.608127	0.693946	-1.977272
H	5.925119	-0.874930	-2.767662

[Pd(SIPr)(allyl)Cl]-VII			
115			
SI6+K2CO3 SCF Done: -3729.60896701 A.U.			
Pd	-0.136454	-0.060283	-0.134949
N	-2.839620	-1.341861	-0.252031
C	-2.072332	-2.065071	-2.990147
H	-2.297619	-1.060580	-2.580130
C	-2.104632	-3.070233	-1.845547
C	-2.372225	-2.673104	-0.509839
C	-2.110311	-0.224730	0.005345
C	-2.283412	-3.579258	0.587214
C	-2.452564	-3.098195	2.025961
H	-2.141108	-2.035656	2.029007
C	-1.820385	-4.435486	-2.083297
H	-1.622482	-4.772386	-3.113626
C	-1.796146	-5.362466	-1.028656
H	-1.599533	-6.427548	-1.235075
C	-2.006518	-4.931877	0.295244
H	-1.947585	-5.660010	1.118691
C	-4.277106	-1.034740	-0.425649
C	-1.521715	-3.820373	3.015301
H	-1.563655	-3.315137	4.002141
H	-1.814177	-4.880608	3.178056
H	-0.469857	-3.781801	2.670204
C	-3.920164	-3.192710	2.492940
H	-4.024527	-2.795319	3.524118
H	-4.606281	-2.613148	1.843374
H	-4.271092	-4.247229	2.493624
C	-0.650235	-1.956690	-3.577839
H	-0.322182	-2.913080	-4.041779
H	-0.623577	-1.168440	-4.357109
H	0.084528	-1.666304	-2.798636
C	-3.120617	-2.389802	-4.072590
H	-4.144062	-2.451066	-3.645229
H	-3.120842	-1.602398	-4.854705
H	-2.910627	-3.359376	-4.574157
C	-4.391870	0.332750	0.254363
H	-4.777888	0.266659	1.296262
H	-4.511607	-0.987825	-1.513778
N	-2.979481	0.784075	0.272249
C	-2.636913	2.097003	0.745669
C	-2.955413	3.207413	-0.084341
C	-2.032044	2.259098	2.032459
C	-2.698543	4.502741	0.409294
C	-1.796225	3.580708	2.464825
C	-2.133468	4.690385	1.674202
H	-2.930029	5.375484	-0.220379
H	-1.333688	3.750268	3.446593
H	-1.935788	5.708616	2.045437
C	-3.558452	3.044274	-1.479665
H	-3.467448	1.973438	-1.757487
C	-1.610846	1.072931	2.906785
H	-1.018448	0.379935	2.263855
C	-5.050418	3.449508	-1.485502
H	-5.639856	2.917614	-0.709246
H	-5.160482	4.536352	-1.282833

H	5.218992	0.472612	-3.719743
C	3.294278	-1.522397	-3.430374
H	3.195124	-1.013334	-4.411102
H	4.000952	-2.368142	-3.566910
H	2.304509	-1.936440	-3.160969
C	3.399767	0.921917	3.172109
H	2.867425	1.477040	3.973161
H	4.340907	0.516699	3.600741
H	3.674057	1.653371	2.387029
C	2.039287	-1.138884	3.746282
H	1.422664	-1.972500	3.352684
H	2.885660	-1.571892	4.321106
H	1.415937	-0.568505	4.465409
C	0.271461	-0.763704	-1.509945
O	0.432597	-0.187383	-2.568424
N	-2.013592	-0.765172	0.489436
C	0.303091	-5.056146	-1.156023
C	-0.149972	-4.440315	-2.338599
H	1.093205	-4.745166	0.853081
C	0.752373	-4.271724	-0.079549
C	-0.145117	-3.042151	-2.450166
C	0.293648	-2.253257	-1.361917
C	0.731123	-2.874456	-0.174878
H	-0.485486	-2.540926	-3.369304
H	1.056928	-2.246187	0.665517
H	0.294941	-6.154466	-1.071022
H	-0.509083	-5.055624	-3.178968
C	-3.093569	-0.231435	-0.167968
O	-3.031091	0.758997	-0.906415
O	-4.264238	-0.882036	0.129328
C	-5.528758	-0.511677	-0.511593
C	-5.418795	-0.677084	-2.036464
H	-4.699004	0.049684	-2.456369
H	-5.076196	-1.703203	-2.284125
H	-6.410992	-0.519207	-2.507619
C	-6.511857	-1.534634	0.075075
H	-7.532453	-1.364329	-0.324421
H	-6.195661	-2.566076	-0.181474
H	-6.542682	-1.450330	1.180109
C	-5.927382	0.919499	-0.115157
H	-5.199832	1.648273	-0.517908
H	-6.938212	1.153406	-0.509345
H	-5.953033	1.014288	0.989919
C	-2.018840	-2.038116	1.090583
C	-1.334630	-2.214645	2.320005
C	-2.577782	-3.183741	0.468496
C	-1.199778	-3.485450	2.899438
H	-0.901790	-1.325470	2.804864
C	-2.445083	-4.449727	1.053607
H	-3.091992	-3.066026	-0.495300
C	-1.753281	-4.614750	2.269036
H	-0.661831	-3.592438	3.855918
H	-2.869755	-5.327670	0.540286
H	-1.647526	-5.614249	2.719488
H	4.064205	2.067358	-1.306483
H	2.699652	4.016046	-0.981829
Zero-point correction=			0.901378 (Hartree/Particle)
Thermal correction to Energy=			0.956754

H	-5.512577	3.242369	-2.473846
C	-2.791883	3.841294	-2.554396
H	-3.200998	3.608402	-3.559391
H	-2.890316	4.936950	-2.401856
H	-1.716513	3.585566	-2.559503
C	-2.815105	0.278569	3.455763
H	-2.455278	-0.553248	4.095641
H	-3.476345	0.927220	4.070026
H	-3.428990	-0.174900	2.655618
C	-0.680881	1.450183	4.070407
H	0.173695	2.067593	3.729080
H	-1.213188	2.006753	4.873062
H	-0.251550	0.521741	4.493389
C	-0.417586	1.235606	-1.615930
O	-1.137591	0.995900	-2.587759
N	1.992389	0.204259	-0.236863
C	1.787108	4.955824	-1.676655
C	1.746044	4.133507	-2.818819
H	1.155988	5.192232	0.397213
C	1.124569	4.558383	-0.502161
C	1.027061	2.927972	-2.789994
C	0.377383	2.517797	-1.605242
C	0.440755	3.334500	-0.459380
H	0.955303	2.286034	-3.681954
H	-0.059875	3.008120	0.461685
H	2.344549	5.906008	-1.700979
H	2.269284	4.440296	-3.739136
C	2.726412	-0.746557	-0.838415
O	2.305728	-1.625780	-1.617616
O	4.064541	-0.747968	-0.419186
C	5.119772	-1.373651	-1.217359
C	5.079905	-0.845262	-2.659548
H	4.127216	-1.121661	-3.149724
H	5.180067	0.259236	-2.670014
H	5.919502	-1.273826	-3.244351
C	6.402518	-0.908519	-0.510598
H	7.299615	-1.257137	-1.060986
H	6.426449	0.198325	-0.449982
H	6.459682	-1.319012	0.520161
C	5.000576	-2.907030	-1.166260
H	4.129874	-3.244847	-1.757925
H	5.917876	-3.377670	-1.577015
H	4.873403	-3.244697	-0.116620
K	1.223023	-3.591561	-0.328852
K	3.745937	-0.783565	2.470393
C	1.171774	-1.763140	2.050801
O	2.090238	-2.684528	1.910734
O	1.241441	-0.870224	2.960485
O	0.172392	-1.768646	1.171661
C	2.599742	1.330625	0.361609
C	2.158217	1.768754	1.635126
C	3.596898	2.089343	-0.302611
C	2.715627	2.911502	2.233123
H	1.387012	1.169449	2.145561
C	4.146851	3.228288	0.299448
H	3.903121	1.793219	-1.315747
C	3.716501	3.647967	1.574116
H	2.350859	3.232659	3.222958
H	4.902242	3.815984	-0.246836
H	4.143400	4.552179	2.036003
H	-4.911809	-1.816913	0.033623
H	-5.030370	1.039995	-0.304351
Zero-point correction=			0.919769 (Hartree/Particle)
Thermal correction to Energy=			0.982379

Thermal correction to Enthalpy= 0.957698 Thermal correction to Gibbs Free Energy= 0.811043 Sum of electronic and zero-point Energies= -2264.868787 Sum of electronic and thermal Energies= -2264.813411 Sum of electronic and thermal Enthalpies= -2264.812467 Sum of electronic and thermal Free Energies= -2264.959122 SCF Done (in solvent): -2266.2243848	Thermal correction to Enthalpy= 0.983323 Thermal correction to Gibbs Free Energy= 0.824176 Sum of electronic and zero-point Energies= -3728.689198 Sum of electronic and thermal Energies= -3728.626588 Sum of electronic and thermal Enthalpies= -3728.625644 Sum of electronic and thermal Free Energies= -3728.784791 SCF Done (in solvent): -3730.0805809

[Pd(SIPr)(allyl)Cl]-VII-VIII				**[Pd(SIPr)(allyl)Cl]-VIII**			
115				86			
SI6+K2CO3--KN SCF Done: -3729.57743221 A.U.				SI6+K2CO3menysKNisomer1 SCF Done: -2497.06653870 A.U.			
Pd	-0.194362	-0.430786	0.295828	Pd	0.014141	-0.843067	0.053801
N	-2.975894	-1.256398	0.227053	N	2.179171	1.102202	0.527772
C	-3.022665	-0.972001	-2.651327	C	2.303880	-0.412110	3.039882
H	-2.505661	-0.177193	-2.070440	H	1.534121	0.315810	2.712799
C	-2.681593	-2.300927	-1.972596	C	3.240427	-0.677676	1.865795
C	-2.649877	-2.415962	-0.550171	C	3.146597	0.049936	0.653031
C	-2.147391	-0.186271	0.379286	C	0.882947	0.917072	0.194001
C	-2.309340	-3.628747	0.107056	C	3.977071	-0.217443	-0.466307
C	-2.202070	-3.708662	1.627747	C	3.811112	0.530002	-1.787430
H	-2.116428	-2.667650	2.005786	H	3.005742	1.281754	-1.647428
C	-2.391872	-3.456700	-2.724946	C	4.226773	-1.681486	1.946026
H	-2.394924	-3.403413	-3.823115	H	4.325349	-2.267376	2.873670
C	-2.098994	-4.679781	-2.097069	C	5.073199	-1.953893	0.861213
H	-1.897604	-5.574696	-2.708353	H	5.833261	-2.747287	0.943808
C	-2.055350	-4.763247	-0.695820	C	4.943887	-1.233084	-0.335283
H	-1.809579	-5.722210	-0.212485	H	5.595290	-1.474636	-1.190255
C	-4.241655	-1.096198	0.973287	C	2.512781	2.520809	0.756740
C	-0.922425	-4.427924	2.096957	C	3.338427	-0.420565	-2.906590
H	-0.816964	-4.333992	3.196524	H	3.120157	0.154986	-3.832041
H	-0.935156	-5.512028	1.851965	H	4.125795	-1.164215	-3.154709
H	-0.019143	-3.963756	1.653443	H	2.429831	-0.980480	-2.602498
C	-3.455429	-4.381793	2.229973	C	5.091140	1.295101	-2.178380
H	-3.416890	-4.361899	3.339235	H	4.927844	1.882504	-3.106696
H	-4.394437	-3.886481	1.906750	H	5.412828	1.994283	-1.377422
H	-3.520445	-5.444490	1.910685	H	5.935315	0.599229	-2.370294
C	-2.516963	-0.854211	-4.097575	C	1.535563	-1.684813	3.447099
H	-3.065739	-1.529673	-4.788812	H	2.212254	-2.465170	3.856516
H	-2.673008	0.183110	-4.458721	H	0.779538	-1.440479	4.220870
H	-1.433460	-1.075189	-4.158198	H	0.999962	-2.108961	2.572665
C	-4.538973	-0.684475	-2.594946	C	3.064210	0.203900	4.231906
H	-4.925514	-0.662655	-1.558033	H	3.582563	1.142293	3.941617
H	-4.762614	0.300587	-3.055311	H	2.364987	0.437838	5.062259
H	-5.107203	-1.460026	-3.151000	H	3.835382	-0.493036	4.625201
C	-4.248157	0.413397	1.276551	C	1.295048	3.236623	0.141788
H	-4.946774	0.981153	0.624032	H	1.503673	3.634709	-0.877364
H	-5.108326	-1.434922	0.370837	H	3.473145	2.784907	0.269865
N	-2.849342	0.802485	0.988449	N	0.302436	2.141949	0.051752
C	-2.410208	2.166605	1.091730	C	-0.978777	2.350766	-0.558511
C	-2.695065	3.051081	0.016128	C	-2.034206	2.880439	0.232302
C	-1.724029	2.584267	2.263028	C	-1.152128	2.044078	-1.939324
C	-2.221168	4.373999	0.115209	C	-3.276365	3.114269	-0.392267
C	-1.256530	3.913226	2.300384	C	-2.416249	2.296960	-2.511532
C	-1.490080	4.795593	1.234629	C	-3.467791	2.829497	-1.750878
H	-2.411409	5.078641	-0.709326	H	-4.110675	3.518110	0.201728
H	-0.708188	4.265625	3.187381	H	-2.577031	2.070116	-3.577016
H	-1.105759	5.826945	1.282587	H	-4.446286	3.018768	-2.220598
C	-3.552738	2.624802	-1.176050	C	-1.839785	3.212419	1.709028
H	-3.685062	1.526060	-1.117082	H	-0.908551	2.704249	2.035378
C	-1.598173	1.663153	3.472380	C	-0.031190	1.481212	-2.811930
H	-1.687666	0.618855	3.113660	H	0.797839	1.162589	-2.149786
C	-4.951273	3.275141	-1.070116	C	-1.671137	4.736129	1.903476
H	-5.423324	3.086553	-0.083213				

H	-4.882044	4.376837	-1.194402
H	-5.627788	2.886065	-1.860477
C	-2.926579	2.914540	-2.552478
H	-3.623649	2.597694	-3.356871
H	-2.722050	3.995295	-2.699258
H	-1.973369	2.372550	-2.691319
C	-2.755389	1.955047	4.455915
H	-2.735100	1.241135	5.306198
H	-2.675846	2.983981	4.869094
H	-3.748195	1.877567	3.964658
C	-0.244242	1.746062	4.192949
H	0.585475	1.520150	3.498647
H	-0.066460	2.741434	4.655146
H	-0.200590	0.984440	4.996928
C	0.089254	-0.086451	-1.643054
O	0.169283	-1.043654	-2.428855
N	2.510300	0.193682	-0.314391
C	0.768816	3.914376	-3.127429
C	0.795865	2.813020	-4.007872
H	0.479057	4.564079	-1.063029
C	0.495404	3.716689	-1.763904
C	0.570545	1.518777	-3.519143
C	0.289604	1.313235	-2.147512
C	0.239614	2.424875	-1.281022
H	0.611318	0.640425	-4.181431
H	-0.000983	2.267455	-0.221014
H	0.965182	4.929111	-3.510062
H	1.006110	2.968991	-5.078494
C	3.447173	-0.671707	-0.678979
O	3.294695	-1.746126	-1.304274
O	4.733749	-0.369413	-0.138344
C	5.962657	-0.849600	-0.770717
C	5.932844	-0.569321	-2.281550
H	5.129952	-1.151135	-2.772411
H	5.754011	0.509462	-2.466356
H	6.906098	-0.842380	-2.738624
C	7.051608	-0.008746	-0.088590
H	8.054817	-0.267206	-0.485084
H	6.862631	1.070583	-0.256645
H	7.055335	-0.188737	1.007214
C	6.163078	-2.347825	-0.480268
H	5.327528	-2.930127	-0.911018
H	7.122387	-2.704442	-0.909917
H	6.202317	-2.530429	0.615810
K	1.134907	-3.090243	-1.058689
K	3.630089	-1.196677	2.317250
C	0.855089	-1.655635	2.447448
O	1.356955	-2.006303	1.265564
O	1.468342	-1.911536	3.521844
O	-0.260476	-0.963100	2.398613
C	2.790899	1.488018	0.116228
C	2.112530	1.997551	1.255693
C	3.638132	2.379877	-0.597314
C	2.268545	3.330258	1.665523
H	1.406044	1.328005	1.776758
C	3.788657	3.711073	-0.187258
H	4.147948	2.012226	-1.500036
C	3.108015	4.200658	0.946856
H	1.711251	3.689123	2.544994
H	4.436678	4.385795	-0.770816
H	3.224135	5.250834	1.257763
H	-4.211066	-1.699043	1.905590
H	-4.500590	0.638497	2.331227
H	-0.849713	5.149436	1.281673
H	-2.599817	5.273829	1.614949
H	-1.455164	4.977140	2.965742
C	-2.982334	2.678780	2.594662
H	-2.734493	2.832160	3.665167
H	-3.938989	3.208167	2.396850
H	-3.139517	1.594398	2.440099
C	0.523380	2.564887	-3.760528
H	1.380486	2.166879	-4.343461
H	-0.251810	2.903567	-4.480942
H	0.871854	3.459348	-3.202393
C	-0.469236	0.222893	-3.584345
H	-0.844618	-0.553490	-2.888657
H	-1.253226	0.451414	-4.337386
H	0.397178	-0.219000	-4.115262
C	-1.227232	-0.316111	1.492331
O	-0.992050	0.170000	2.593775
C	-5.193306	-1.776679	0.475873
C	-4.606231	-2.102759	1.715664
H	-4.966169	-0.648515	-1.382818
C	-4.502361	-0.937241	-0.425349
C	-3.342000	-1.585484	2.056170
C	-2.633884	-0.778054	1.140709
C	-3.220380	-0.459799	-0.104122
H	-2.880570	-1.813490	3.029916
H	-2.662550	0.167600	-0.815701
H	-6.196586	-2.156740	0.221915
H	-5.146428	-2.747379	2.428506
K	-2.711444	-4.063608	-1.036117
C	-0.075105	-2.973433	-1.364298
O	-0.786739	-2.750503	-0.228379
O	-0.385972	-3.943714	-2.103817
O	0.840230	-2.079552	-1.590985
H	0.917000	4.068010	0.767694
H	2.612286	2.706027	1.850090

Zero-point correction= 0.918322 (Hartree/Particle) Thermal correction to Energy= 0.980894 Thermal correction to Enthalpy= 0.981838 Thermal correction to Gibbs Free Energy= 0.821298 Sum of electronic and zero-point Energies= -3728.659110 Sum of electronic and thermal Energies= -3728.596538 Sum of electronic and thermal Enthalpies= -3728.595594 Sum of electronic and thermal Free Energies= -3728.756134 SCF Done (in solvent): -3730.0567553	Zero-point correction= 0.691621 (Hartree/Particle) Thermal correction to Energy= 0.738051 Thermal correction to Enthalpy= 0.738995 Thermal correction to Gibbs Free Energy= 0.610514 Sum of electronic and zero-point Energies= -2496.374917 Sum of electronic and thermal Energies= -2496.328488 Sum of electronic and thermal Enthalpies= -2496.327543 Sum of electronic and thermal Free Energies= -2496.456024 SCF Done (in solvent): -2497.4182449

[Pd(SIPr)(allyl)Cl]-IX				**[Pd(SIPr)(allyl)Cl]-IX-X**			
104				104			
SI6+KCO3+NH2 SCF Done: -2898.94932711 A.U.				SI6+KCO3+NH2--H SCF Done: -2898.95215414 A.U.			
Pd	0.163578	-0.490873	0.270731	Pd	-0.240664	-0.193858	-0.625591
C	-1.313094	0.634257	0.991390	C	0.529589	1.363519	-1.588324
O	-1.341146	1.166693	2.099695	O	-0.075958	2.082199	-2.382128
C	-4.775743	1.044471	-1.590575	C	4.785208	1.926812	-1.005230
C	-4.916806	1.120882	-0.191779	C	4.197593	2.189768	-2.257548
H	-3.386580	0.761091	-3.248203	H	4.439575	1.276735	1.048237
C	-3.508718	0.813902	-2.154685	C	3.987516	1.489163	0.067161
C	-3.792024	0.991988	0.635411	C	2.814417	2.024097	-2.432974
C	-2.517717	0.753973	0.075024	C	2.012454	1.566798	-1.363847
C	-2.390968	0.647958	-1.324173	C	2.611318	1.295167	-0.116475
H	-3.878683	1.056057	1.730808	H	2.329960	2.245725	-3.397202
H	-1.396632	0.446451	-1.751589	H	1.977454	0.939126	0.709309
H	-5.659498	1.154806	-2.239476	H	5.870655	2.059174	-0.867047
H	-5.913006	1.272141	0.253463	H	4.822187	2.530478	-3.099372
K	0.856109	-4.376483	-3.736090	K	1.439160	-5.120929	0.667994
C	-2.408663	-2.343406	0.573711	C	2.458802	-1.640939	-1.049003
C	-3.220876	-2.369608	-0.582586	C	2.627319	-1.909467	0.339505
C	-3.026520	-2.218978	1.830488	C	3.630721	-1.475202	-1.820960
C	-4.608203	-2.253611	-0.480051	C	3.898303	-2.001472	0.917080
H	-2.737150	-2.437982	-1.568760	H	1.729273	-1.965075	0.975920
C	-4.424354	-2.109336	1.944049	C	4.911382	-1.554286	-1.247071
H	-2.403483	-2.164359	2.737139	H	3.538057	-1.229154	-2.891041
C	-5.223901	-2.109107	0.782986	C	5.058997	-1.816599	0.131114
H	-5.246248	-2.233157	-1.375728	H	4.018062	-2.164046	2.000081
H	-4.868496	-1.994412	2.942593	H	5.786919	-1.377523	-1.887272
C	1.459067	-2.624855	-1.582472	C	-0.575111	-3.124921	0.486549
O	2.386587	-3.052899	-2.362881	O	-0.622104	-3.951167	1.452800
O	0.221775	-3.087792	-1.736242	O	-0.006728	-3.543849	-0.671332
O	1.723740	-1.737377	-0.669770	O	-0.991165	-1.911249	0.575009
N	2.524461	1.018676	1.154556	N	-2.989136	0.773538	-0.100393
N	1.257556	2.333870	-0.068472	N	-1.525751	2.127285	0.829237
C	1.390819	1.069002	0.415698	C	-1.670099	0.978107	0.116897
C	3.125181	2.354223	1.343941	C	-3.810082	1.925053	0.324460
C	2.449042	3.162478	0.228216	C	-2.832462	2.705593	1.219484
C	3.070578	-0.162440	1.763140	C	-3.563301	-0.409274	-0.679945
C	4.159870	-0.797688	1.109614	C	-4.114954	-1.378783	0.201219
C	4.691579	-1.956360	1.706491	C	-4.684327	-2.531435	-0.372131
C	4.159018	-2.463964	2.900476	C	-4.696733	-2.717591	-1.762545
C	3.084636	-1.815817	3.526692	C	-4.135960	-1.750633	-2.608155
C	2.516332	-0.649908	2.973877	C	-3.556166	-0.575871	-2.086999
C	4.779244	-0.228667	-0.164932	C	-4.130297	-1.181647	1.716109
H	4.585604	-3.376503	3.347515	H	-5.140460	-3.631162	-2.189979
C	1.371339	0.064761	3.686558	C	-2.945059	0.461696	-3.023073
C	0.360231	2.694765	-1.126680	C	-0.316871	2.472268	1.522095
C	-0.667674	3.635694	-0.852988	C	0.368821	3.657497	1.147807
C	-1.529808	3.995691	-1.906850	C	1.545503	3.989297	1.849108
C	-1.371556	3.448098	-3.186769	C	2.024928	3.172464	2.881101
C	-0.345241	2.525446	-3.436505	C	1.335292	2.001487	3.230978
C	0.540180	2.120576	-2.417094	C	0.153728	1.619391	2.564167
C	-0.805821	4.285758	0.521779	C	-0.161653	4.568696	0.043839

H	-2.060384	3.737012	-3.996478	H	2.951363	3.444140	3.411810
C	1.649599	1.115047	-2.725633	C	-0.573790	0.337987	2.970952
H	4.227206	2.314770	1.254380	H	-4.721720	1.591138	0.855786
H	3.082134	3.241677	-0.684708	H	-3.010555	2.529707	2.303718
H	5.529189	-2.478596	1.218575	H	-5.112239	-3.305342	0.284155
H	2.678809	-2.221095	4.467286	H	-4.141740	-1.910060	-3.698062
H	4.067982	0.522457	-0.569021	H	-3.439410	-0.344164	1.947644
H	0.942063	0.818902	2.997016	H	-2.405058	1.213001	-2.412713
H	-2.345349	4.710512	-1.717662	H	2.102614	4.896779	1.569967
H	-0.232349	2.098431	-4.445221	H	1.727403	1.362475	4.036863
H	-0.197849	3.682786	1.229045	H	-0.909153	3.980869	-0.530170
H	2.034823	0.709546	-1.769019	H	-1.164225	-0.017684	2.104090
C	1.140570	-0.112529	-3.503229	C	0.384509	-0.820779	3.302860
H	0.817293	0.148937	-4.534653	H	0.833358	-0.721011	4.315165
H	1.947233	-0.871157	-3.564282	H	-0.157906	-1.786120	3.243501
H	0.292214	-0.591035	-2.971760	H	1.210950	-0.862998	2.565952
C	2.825689	1.793214	-3.458036	C	-1.555086	0.595142	4.133130
H	3.228856	2.650852	-2.879830	H	-2.305688	1.370399	3.874315
H	3.650639	1.067001	-3.615671	H	-2.101974	-0.336720	4.386783
H	2.510200	2.181697	-4.450570	H	-1.017601	0.942269	5.041838
C	-2.248460	4.283407	1.058427	C	0.924829	5.007164	-0.954982
H	-2.274095	4.726982	2.075541	H	0.467197	5.592642	-1.779294
H	-2.930433	4.882787	0.418420	H	1.691413	5.653638	-0.476484
H	-2.645721	3.254322	1.126886	H	1.434330	4.133648	-1.402014
C	-0.244323	5.725647	0.483007	C	-0.860654	5.801974	0.660167
H	-0.865167	6.369044	-0.176833	H	-0.126449	6.437207	1.200662
H	-0.244397	6.179168	1.496848	H	-1.334048	6.424870	-0.128009
H	0.791986	5.759973	0.086508	H	-1.643056	5.516162	1.393816
C	4.991598	-1.280271	-1.268214	C	-3.619660	-2.408035	2.495205
H	5.371751	-0.784093	-2.187678	H	-3.585375	-2.175236	3.581311
H	5.755865	-2.030919	-0.970964	H	-4.298915	-3.279333	2.375794
H	4.049583	-1.811314	-1.516149	H	-2.605636	-2.706860	2.165589
C	6.108227	0.490275	0.165842	C	-5.546139	-0.785240	2.193466
H	6.864384	-0.239755	0.526310	H	-6.262174	-1.617475	2.023212
H	6.523187	0.988850	-0.735967	H	-5.547309	-0.553909	3.279882
H	5.993167	1.255773	0.962753	H	-5.943082	0.098567	1.650509
C	0.213311	-0.887933	4.034726	C	-1.888128	-0.166362	-3.951891
H	0.502613	-1.642441	4.797061	H	-2.342065	-0.856478	-4.695149
H	-0.650920	-0.312380	4.422498	H	-1.341313	0.627499	-4.499635
H	-0.126850	-1.418405	3.122738	H	-1.149591	-0.736529	-3.351244
C	1.888626	0.806131	4.937428	C	-4.038780	1.199539	-3.822278
H	1.067730	1.373462	5.425027	H	-3.590241	1.985264	-4.466214
H	2.304271	0.095556	5.684141	H	-4.600981	0.500535	-4.478431
H	2.696770	1.522174	4.677649	H	-4.774947	1.685633	-3.147568
N	-0.992596	-2.341247	0.438221	N	1.161508	-1.543073	-1.582221
H	-0.529444	-2.805130	1.230764	H	1.195501	-1.375657	-2.595950
H	-0.595993	-2.757757	-0.496477	H	0.475767	-2.603658	-1.227836
O	-6.586293	-1.949847	0.770433	O	6.259320	-1.885548	0.795554
C	-7.236465	-1.684995	1.999764	C	7.436780	-1.581866	0.069771
H	-6.851565	-0.755802	2.483212	H	7.407278	-0.553343	-0.361763
H	-8.310438	-1.549066	1.766515	H	8.276857	-1.645434	0.788377
H	-7.132531	-2.527277	2.724103	H	7.620903	-2.305298	-0.759925
H	2.866757	2.730562	2.359890	H	-4.121359	2.503649	-0.574450
H	2.160215	4.183840	0.541169	H	-2.855741	3.797069	1.037489

Zero-point correction= 0.839961 (Hartree/Particle)	Zero-point correction= 0.836010 (Hartree/Particle)
Thermal correction to Energy= 0.895136	Thermal correction to Energy= 0.890903
Thermal correction to Enthalpy= 0.896080	Thermal correction to Enthalpy= 0.891847
Thermal correction to Gibbs Free Energy= 0.750202	Thermal correction to Gibbs Free Energy= 0.746694
Sum of electronic and zero-point Energies= -2898.109366	Sum of electronic and zero-point Energies= -2898.116145
Sum of electronic and thermal Energies= -2898.054192	Sum of electronic and thermal Energies= -2898.061251
Sum of electronic and thermal Enthalpies= -2898.053247	Sum of electronic and thermal Enthalpies= -2898.060307
Sum of electronic and thermal Free Energies= -2898.199125	Sum of electronic and thermal Free Energies= -2898.205460
SCF Done (in solvent): -2899.421987	SCF Done (in solvent): -2899.4201289

[Pd(SIPr)(allyl)Cl]-X (adduct)				[Pd(SIPr)(allyl)Cl]-X			
104				98			
SI6+KCO3H+NH SCF Done: -2898.91483182 A.U.				SI6+NH SCF Done: -2034.60164377 A.U.			
Pd	-0.080663	0.579613	-0.269212	Pd	0.103600	-0.357287	-0.575486
C	1.256290	0.176090	1.128514	C	-0.884305	-1.590895	0.638596
O	1.244400	0.647195	2.260955	O	-0.715063	-1.612826	1.846936
C	4.597907	-2.191525	-0.278221	C	-3.669467	-4.325721	-1.228658
C	4.797005	-1.132478	0.626068	C	-3.230135	-4.541814	0.092322
H	3.126168	-3.385988	-1.357941	H	-3.530523	-3.047381	-2.988660
C	3.293620	-2.530836	-0.682823	C	-3.186661	-3.224266	-1.957441
C	3.695749	-0.420464	1.124773	C	-2.323163	-3.652813	0.685399
C	2.392378	-0.710726	0.668277	C	-1.839423	-2.539677	-0.041800
C	2.198101	-1.780285	-0.228971	C	-2.267906	-2.341978	-1.369842
H	3.830930	0.405343	1.836815	H	-1.964582	-3.807892	1.714479
H	1.176302	-2.039805	-0.544547	H	-1.881656	-1.470032	-1.919748
H	5.462251	-2.753431	-0.667452	H	-4.386458	-5.022765	-1.691545
H	5.816200	-0.847651	0.930756	H	-3.598150	-5.411055	0.660647
K	0.055665	-1.637685	-5.342950	C	2.453117	-2.031261	-1.258340
C	2.651495	1.719868	-1.278870	C	2.989732	-3.351849	-1.186000
C	3.607546	1.166350	-2.183793	C	3.346184	-0.962853	-0.962696
C	3.180511	2.410492	-0.155188	C	4.316994	-3.583872	-0.816583
C	4.983363	1.278178	-1.968483	H	2.330997	-4.208175	-1.408618
H	3.240139	0.603282	-3.059359	C	4.673014	-1.190033	-0.570887
C	4.562004	2.531418	0.068549	H	2.978054	0.074396	-1.035481
H	2.473922	2.845644	0.565120	C	5.173829	-2.507654	-0.492210
C	5.480314	1.951759	-0.830851	H	4.720075	-4.606782	-0.755866
H	5.708990	0.822450	-2.660500	H	5.305183	-0.321984	-0.338591
H	4.906628	3.068897	0.964237	N	0.184377	2.226816	0.815002
C	-1.148672	-0.138884	-3.084908	N	-1.908646	1.575330	0.680195
O	-1.700455	-0.315914	-4.201737	C	-0.630984	1.251061	0.335230
O	0.055524	-0.892181	-2.924875	C	-0.531739	3.203971	1.657015
O	-1.502326	0.587485	-2.123212	C	-1.996712	2.927840	1.272257
N	-2.601655	0.667822	1.290852	C	1.614970	2.213123	0.694990
N	-1.576808	-1.226024	1.720126	C	2.197189	2.956072	-0.367202
C	-1.535273	-0.097029	0.959734	C	3.601989	2.981273	-0.463205
C	-3.443147	0.074316	2.351316	C	4.396663	2.298552	0.470606
C	-2.635772	-1.174680	2.756033	C	3.798776	1.546847	1.490972
C	-2.932617	1.933032	0.692181	C	2.396532	1.474157	1.619946
C	-3.935383	1.968591	-0.314085	C	1.321168	3.607949	-1.433347
C	-4.274930	3.222993	-0.855904	H	5.494581	2.334592	0.385706
C	-3.637356	4.394414	-0.422161	C	1.769417	0.586942	2.690008
C	-2.641886	4.331157	0.562759	C	-3.055206	0.871433	0.184101
C	-2.266483	3.102084	1.141969	C	-3.832495	0.105244	1.094798
C	-4.655717	0.705145	-0.777802	C	-4.918190	-0.629822	0.579222
H	-3.912486	5.365554	-0.864050	C	-5.228452	-0.597262	-0.786890
C	-1.185601	3.056572	2.217766	C	-4.467793	0.190193	-1.662144
C	-0.839698	-2.422125	1.433606	C	-3.367711	0.939898	-1.200856
C	0.129116	-2.886990	2.361889	C	-3.548737	0.123953	2.594990
C	0.820717	-4.078533	2.059482	H	-6.069581	-1.193507	-1.173724
C	0.563921	-4.782619	0.879185	C	-2.591859	1.825298	-2.176605
C	-0.400234	-4.310661	-0.025786	H	-0.203207	4.239574	1.435584
C	-1.126879	-3.130262	0.225122	H	-2.378070	3.644613	0.507983
C	0.403125	-2.160766	3.676771	H	4.082548	3.535876	-1.283526
H	1.122352	-5.705500	0.655534	H	4.432229	0.977556	2.188564
C	-2.193001	-2.642211	-0.759952	H	0.314473	3.762427	-0.988079
H	-3.566712	0.797506	3.182821	H	0.675661	0.545918	2.509061
H	-3.232838	-2.109246	2.754010	H	-5.522540	-1.249312	1.258949
H	-5.045330	3.280445	-1.640545	H	-4.727961	0.216789	-2.732244
H	-2.138128	5.254622	0.888139	H	-2.508354	0.491459	2.724662
H	-4.061491	-0.157155	-0.412504	H	-1.712731	2.238577	-1.641005
H	-0.890908	1.999734	2.375164	C	-2.043290	1.037556	-3.380982
H	1.585897	-4.449652	2.757917	H	-2.853507	0.543872	-3.957377
H	-0.588521	-4.880879	-0.946977	H	-1.505107	1.714031	-4.076204

H 0.019355 -1.125335 3.566635	H -1.324834 0.258822 -3.048152
H -2.065724 -1.543609 -0.863191	C -3.463552 3.017309 -2.628029
C -2.053602 -3.233734 -2.173535	H -3.837027 3.597261 -1.758095
H -2.332809 -4.309052 -2.206211	H -2.883208 3.703938 -3.280111
H -2.720278 -2.685948 -2.870283	H -4.349889 2.673597 -3.202574
H -1.014693 -3.122476 -2.542841	C -3.622554 -1.263555 3.255371
C -3.619484 -2.902515 -0.228967	H -3.339560 -1.188848 4.325965
H -3.807268 -2.390610 0.733741	H -4.647631 -1.689377 3.216042
H -4.375708 -2.533009 -0.952625	H -2.923743 -1.968231 2.768861
H -3.790383 -3.989028 -0.072883	C -4.514557 1.106782 3.297336
C 1.902831 -2.038898 4.004264	H -5.560950 0.740336 3.225410
H 2.042305 -1.385152 4.889618	H -4.262976 1.209649 4.374117
H 2.355451 -3.023967 4.246584	H -4.493869 2.116914 2.837574
H 2.462211 -1.592648 3.161662	C 1.145240 2.633392 -2.618146
C -0.341408 -2.864623 4.835204	H 0.470212 3.059684 -3.389469
H 0.069111 -3.884794 4.994660	H 2.123637 2.410757 -3.093227
H -0.221390 -2.298594 5.783118	H 0.712504 1.664759 -2.283648
H -1.426441 -2.978568 4.634100	C 1.838581 4.978444 -1.904609
C -4.739102 0.575346 -2.310243	H 2.790943 4.888849 -2.468533
H -5.171911 -0.411645 -2.582112	H 1.103831 5.454542 -2.586882
H -5.402492 1.350088 -2.751132	H 2.014134 5.664480 -1.050192
H -3.737966 0.658362 -2.773226	C 2.276211 -0.864104 2.573477
C -6.067877 0.623047 -0.154275	H 3.356714 -0.947009 2.816190
H -6.712186 1.440156 -0.543682	H 1.711921 -1.519440 3.266511
H -6.555993 -0.342803 -0.405590	H 2.127247 -1.249173 1.544998
H -6.048973 0.724094 0.951046	C 2.000731 1.163929 4.101904
C 0.092586 3.790376 1.772473	H 1.503239 0.532555 4.867783
H -0.050617 4.891020 1.723256	H 3.083622 1.202430 4.348230
H 0.915570 3.583634 2.486564	H 1.603212 2.197169 4.194024
H 0.409661 3.434887 0.770962	N 1.130469 -1.769486 -1.588470
C -1.723104 3.602042 3.557062	H 0.637182 -2.627268 -1.869708
H -0.948153 3.528103 4.349072	O 6.457134 -2.840779 -0.126477
H -2.018071 4.669781 3.466312	C 7.335681 -1.794193 0.233372
H -2.618637 3.039361 3.897204	H 6.959956 -1.208533 1.106969
N 1.280366 1.596631 -1.459684	H 8.297933 -2.267813 0.510391
H 1.087414 1.343027 -2.437673	H 7.516512 -1.083848 -0.608861
H 0.405781 -0.688556 -2.002955	H -0.327127 2.995442 2.732232
O 6.852625 1.977388 -0.689916	H -2.685716 2.947362 2.138144
C 7.383306 2.612162 0.454305	
H 7.030615 2.138860 1.403017	
H 8.485003 2.509518 0.394515	
H 7.128339 3.698562 0.495686	
H -4.451488 -0.169048 1.955042	
H -2.179553 -1.063289 3.761114	
Zero-point correction= 0.838301 (Hartree/Particle) Thermal correction to Energy= 0.894122 Thermal correction to Enthalpy= 0.895067 Thermal correction to Gibbs Free Energy= 0.746505 Sum of electronic and zero-point Energies= -2898.076531 Sum of electronic and thermal Energies= -2898.020709 Sum of electronic and thermal Enthalpies= -2898.019765 Sum of electronic and thermal Free Energies= -2898.168327	Zero-point correction= 0.810029 (Hartree/Particle) Thermal correction to Energy= 0.859451 Thermal correction to Enthalpy= 0.860395 Thermal correction to Gibbs Free Energy= 0.726333 Sum of electronic and zero-point Energies= -2033.791615 Sum of electronic and thermal Energies= -2033.742193 Sum of electronic and thermal Enthalpies= -2033.741248 Sum of electronic and thermal Free Energies= -2033.875311
SCF Done (in solvent): -2899.399905	SCF Done (in solvent): -2034.9713931

[Pd(SIPr)(allyl)Cl]-X-XI	**[Pd(SIPr)(allyl)Cl]-XI**
98	98
SI6--PROD SCF Done: -2034.59193636 A.U.	SI6+PROD SCF Done: -2034.60959097 A.U.
Pd -0.048608 0.101008 -0.779561	Pd 0.091377 0.375289 -0.377296
C 0.153079 1.927528 0.174688	C 0.339108 3.037466 0.108706
O -0.488731 2.155249 1.187000	O -0.254557 3.484802 1.087471
C 3.610830 4.267178 -0.946243	C 4.633762 3.494778 -0.223889
C 2.765524 4.687036 0.098670	C 3.887240 4.223390 0.719148
H 3.987881 2.735293 -2.451048	H 4.554723 1.998546 -1.811067

C	3.322995	3.079313	-1.643194	C	3.978622	2.601997	-1.093872
C	1.641583	3.923863	0.447336	C	2.494128	4.064322	0.791054
C	1.354954	2.724032	-0.245195	C	1.828814	3.172810	-0.078812
C	2.203722	2.312166	-1.292715	C	2.588978	2.436194	-1.019738
H	0.963003	4.241806	1.253922	H	1.891809	4.614398	1.529545
H	1.977047	1.361280	-1.800496	H	2.106971	1.655889	-1.634949
H	4.496199	4.865546	-1.214694	H	5.728434	3.609877	-0.272403
H	2.984452	5.619264	0.643972	H	4.394354	4.916595	1.409029
C	-2.336206	2.056448	-1.217632	C	-1.797020	2.326078	-1.084007
C	-2.949492	3.294149	-1.556103	C	-2.390777	2.381122	-2.362539
C	-3.121246	1.109437	-0.513432	C	-2.606048	2.072281	0.043110
C	-4.282601	3.553476	-1.226970	C	-3.763392	2.157147	-2.520171
H	-2.362121	4.060062	-2.089760	H	-1.765574	2.569763	-3.250910
C	-4.454513	1.369296	-0.164626	C	-3.981868	1.857956	-0.112545
H	-2.666420	0.141857	-0.243567	H	-2.156442	2.013742	1.040871
C	-5.050792	2.597693	-0.522684	C	-4.571011	1.882191	-1.395869
H	-4.759682	4.508292	-1.496402	H	-4.233267	2.177369	-3.514527
H	-5.011802	0.595106	0.382189	H	-4.573375	1.631128	0.783449
N	0.076544	-2.580215	0.382457	N	-0.497610	-2.191941	0.939841
N	2.063959	-1.664825	0.560058	N	1.589500	-2.126021	0.276703
C	0.790856	-1.443651	0.145973	C	0.433475	-1.410094	0.325963
C	0.854518	-3.624675	1.076779	C	0.045734	-3.474145	1.433419
C	2.291561	-3.062021	0.997229	C	1.443405	-3.510597	0.772663
C	-1.356074	-2.606045	0.271241	C	-1.797681	-1.714959	1.314312
C	-1.939561	-3.011900	-0.956951	C	-2.893800	-1.966200	0.447463
C	-3.343599	-2.970853	-1.065473	C	-4.171600	-1.541322	0.859187
C	-4.137290	-2.557538	0.015091	C	-4.350968	-0.876790	2.081821
C	-3.539324	-2.167550	1.222142	C	-3.247657	-0.596208	2.900730
C	-2.138147	-2.174342	1.375072	C	-1.949383	-1.009153	2.536388
C	-1.066339	-3.379815	-2.152495	C	-2.671058	-2.554627	-0.941555
H	-5.233236	-2.526020	-0.090526	H	-5.359284	-0.555351	2.390225
C	-1.504196	-1.688001	2.674639	C	-0.750506	-0.631444	3.402472
C	3.067465	-0.637721	0.603605	C	2.770519	-1.664786	-0.391261
C	3.007523	0.333227	1.644465	C	3.797324	-1.066094	0.385849
C	3.998451	1.335549	1.647807	C	4.961900	-0.638007	-0.280133
C	5.007511	1.365601	0.675206	C	5.098420	-0.796666	-1.668118
C	5.038981	0.403980	-0.343428	C	4.061576	-1.369108	-2.419566
C	4.062341	-0.609058	-0.407528	C	2.878039	-1.817263	-1.797660
C	1.894476	0.312760	2.697273	C	3.589776	-0.795826	1.873499
H	5.762192	2.167010	0.697324	H	6.018557	-0.457763	-2.171170
C	4.009550	-1.577001	-1.590560	C	1.725707	-2.370691	-2.633057
H	0.742633	-4.604104	0.567786	H	0.097929	-3.465859	2.546347
H	2.833625	-3.093101	1.963182	H	2.257816	-3.767507	1.481725
H	-3.824264	-3.255044	-2.014351	H	-5.037655	-1.718308	0.202626
H	-4.171113	-1.826369	2.057416	H	-3.394186	-0.038972	3.839806
H	-0.048490	-3.591990	-1.759701	H	-1.687836	-3.073514	-0.925641
H	-0.404061	-1.701249	2.540044	H	0.150014	-1.111013	2.965118
H	3.972887	2.120754	2.415560	H	5.768108	-0.155063	0.292400
H	5.817872	0.459244	-1.118599	H	4.170706	-1.466568	-3.511591
H	0.946191	0.130725	2.148291	H	2.832254	-1.523462	2.238162
H	3.500428	-2.501880	-1.248806	H	0.963809	-2.771966	-1.932034
C	3.138378	-0.990079	-2.722532	C	1.042355	-1.227741	-3.411959
H	3.586796	-0.052309	-3.114562	H	1.745421	-0.752522	-4.129131
H	3.047842	-1.706633	-3.566091	H	0.164426	-1.602702	-3.978560
H	2.116078	-0.752643	-2.354771	H	0.685077	-0.452154	-2.689665
C	5.398058	-1.990420	-2.110161	C	2.162468	-3.522263	-3.558019
H	6.044192	-2.373255	-1.293095	H	2.651515	-4.338994	-2.986800
H	5.301851	-2.785906	-2.878158	H	1.285562	-3.947633	-4.089799
H	5.928369	-1.141465	-2.591265	H	2.880319	-3.178613	-4.332530
C	1.720042	1.644226	3.443298	C	2.987707	0.613917	2.061278
H	0.799000	1.605706	4.059093	H	2.783592	0.816870	3.133437
H	2.571660	1.852348	4.126557	H	3.682127	1.393767	1.683724
H	1.608176	2.492712	2.743186	H	2.035479	0.712848	1.495095

C	2.073253	-0.828927	3.721331
H	3.024131	-0.712029	4.283398
H	1.238320	-0.819011	4.453036
H	2.081769	-1.828783	3.248606
C	-0.942862	-2.172792	-3.104730
H	-0.262615	-2.393990	-3.953661
H	-1.933643	-1.877881	-3.508550
H	-0.532723	-1.277628	-2.569803
C	-1.555845	-4.636477	-2.895738
H	-2.532195	-4.465547	-3.396358
H	-0.832434	-4.925389	-3.686591
H	-1.676747	-5.496662	-2.205043
C	-1.885385	-0.226453	2.976480
H	-2.974836	-0.116016	3.161939
H	-1.354822	0.126143	3.886175
H	-1.606514	0.446709	2.141786
C	-1.839892	-2.627225	3.851025
H	-1.320436	-2.295198	4.774621
H	-2.930348	-2.632572	4.063032
H	-1.536810	-3.674877	3.640802
N	-1.007343	1.772923	-1.520996
H	-0.549425	2.481424	-2.104997
O	-6.346604	2.955196	-0.239263
C	-7.144390	2.040107	0.486029
H	-6.717534	1.814397	1.492369
H	-8.134687	2.518255	0.618214
H	-7.282797	1.075561	-0.058701
H	0.495137	-3.740404	2.124356
H	2.911211	-3.603790	0.248066

Zero-point correction= 0.809381 (Hartree/Particle)
Thermal correction to Energy= 0.857936
Thermal correction to Enthalpy= 0.858880
Thermal correction to Gibbs Free Energy= 0.727547
Sum of electronic and zero-point Energies= -2033.782555
Sum of electronic and thermal Energies= -2033.734001
Sum of electronic and thermal Enthalpies= -2033.733056
Sum of electronic and thermal Free Energies= -2033.864390

SCF Done (in solvent): -2034.961645

C	4.863321	-0.985058	2.715928
H	5.624918	-0.208890	2.489644
H	4.625773	-0.894873	3.796419
H	5.329101	-1.978211	2.544636
C	-2.559474	-1.398533	-1.959740
H	-2.339258	-1.782713	-2.978074
H	-3.500211	-0.810145	-1.998663
H	-1.740603	-0.699324	-1.659858
C	-3.739908	-3.580827	-1.356822
H	-4.735160	-3.106912	-1.493905
H	-3.470196	-4.046753	-2.327628
H	-3.850293	-4.388602	-0.603203
C	-0.509510	0.890030	3.336921
H	-1.379314	1.457206	3.730643
H	0.382465	1.176311	3.931692
H	-0.333974	1.208365	2.288034
C	-0.892184	-1.135998	4.851479
H	0.026479	-0.911416	5.433334
H	-1.740600	-0.646364	5.375084
H	-1.065368	-2.232322	4.886416
N	-0.361846	2.409397	-0.985066
H	0.095834	2.556782	-1.894191
O	-5.893430	1.637269	-1.647473
C	-6.741030	1.348975	-0.547172
H	-6.791974	2.196885	0.175073
H	-7.750697	1.174403	-0.966169
H	-6.414351	0.436272	0.003099
H	-0.603770	-4.321762	1.130956
H	1.495054	-4.228198	-0.078135

Zero-point correction= 0.811252 (Hartree/Particle)
Thermal correction to Energy= 0.860222
Thermal correction to Enthalpy= 0.861166
Thermal correction to Gibbs Free Energy= 0.728909
Sum of electronic and zero-point Energies= -2033.798339
Sum of electronic and thermal Energies= -2033.749369
Sum of electronic and thermal Enthalpies= -2033.748425
Sum of electronic and thermal Free Energies= -2033.880682

SCF Done (in solvent): -2034.9987472

[Pd(IMes)(allyl)Cl]			
57			
MesI-PREallyl SCF Done: -1629.03758852 A.U.			
Cl	0.647873	1.711773	2.106949
N	1.176602	-1.494131	0.172121
C	2.522883	-1.014197	-0.014953
N	-0.983452	-1.576867	0.275753
C	2.969574	-0.779959	-1.334753
C	4.280202	-0.295209	-1.504939
H	4.647902	-0.103025	-2.526727
C	5.129824	-0.054890	-0.406247
C	4.645632	-0.324971	0.889850
H	5.300249	-0.145804	1.758947
C	3.342030	-0.805750	1.117595
C	0.059263	-0.704117	0.094411
C	0.837165	-2.831402	0.395538
H	1.600296	-3.610640	0.483949

[Pd(IMes)(allyl)Cl]-I			
63			
MesI-PREallyl+K2CO3 SCF Done: -3092.82404595 A.U.			
Cl	-1.062920	-1.983626	1.052877
N	-2.646374	1.319686	0.514687
C	-3.672144	0.395528	0.106150
N	-0.718832	2.268839	0.796129
C	-4.035294	0.350011	-1.258131
C	-5.026350	-0.575726	-1.639589
H	-5.323504	-0.627639	-2.700375
C	-5.646449	-1.428079	-0.705578
C	-5.261390	-1.334303	0.647591
H	-5.735553	-1.996785	1.390836
C	-4.272997	-0.433077	1.082082
C	-1.310762	1.156456	0.249514
C	-2.882016	2.509939	1.208916
H	-3.891336	2.815757	1.500524

C	-0.530811	-2.883880	0.462120
H	-1.220223	-3.717502	0.626648
C	-2.360414	-1.164913	0.189337
C	-3.013666	-1.288429	-1.056688
C	-4.338291	-0.819295	-1.149695
H	-4.865943	-0.899459	-2.114743
C	-5.000676	-0.249216	-0.043617
C	-4.312332	-0.165976	1.184816
H	-4.822610	0.267850	2.060979
C	-2.986428	-0.616859	1.332736
C	-0.836221	1.519132	-2.124780
H	-1.584119	0.813607	-2.520097
H	0.071778	1.638831	-2.744514
C	-1.293051	2.620207	-1.325212
H	-2.358192	2.666985	-1.031899
C	-0.353682	3.436303	-0.658076
H	0.651494	3.611018	-1.080057
Pd	-0.121017	1.295792	-0.106894
H	-0.686136	4.146052	0.115122
C	-6.411116	0.283834	-0.167816
H	-6.917609	-0.095842	-1.077624
H	-7.028850	0.008032	0.711832
H	-6.410713	1.394506	-0.225651
C	6.519034	0.508808	-0.606172
H	6.521649	1.610012	-0.449493
H	7.243620	0.077567	0.114868
H	6.897435	0.320264	-1.631191
C	2.060064	-1.042822	-2.511545
H	1.658616	-2.078680	-2.491056
H	1.181835	-0.364654	-2.482874
H	2.588518	-0.894120	-3.473044
C	2.816467	-1.055610	2.507894
H	1.969178	-0.361348	2.707661
H	2.436884	-2.092160	2.628638
H	3.600592	-0.883298	3.270222
C	-2.246333	-0.506245	2.640752
H	-1.434460	0.255071	2.576654
H	-2.928594	-0.220846	3.464726
H	-1.753969	-1.464280	2.909759
C	-2.303851	-1.906874	-2.238907
H	-1.280273	-1.493770	-2.355732
H	-2.187043	-3.005012	-2.111380
H	-2.862014	-1.734964	-3.179934
C	-1.660385	3.106668	1.388602
H	-1.373377	4.041839	1.878788
C	0.697852	2.511802	0.668314
C	1.135170	3.366784	-0.367235
C	2.520412	3.423440	-0.622598
H	2.883489	4.065455	-1.443364
C	3.439512	2.637881	0.102789
C	2.960467	1.830185	1.155955
H	3.649142	1.153220	1.689008
C	1.592109	1.764738	1.469557
C	0.607545	0.570779	-2.281080
H	0.924171	1.620627	-2.196764
H	-0.079457	0.343265	-3.118514
C	1.484535	-0.450499	-1.787094
H	2.403777	-0.173949	-1.226498
C	1.013366	-1.785287	-1.732691
H	0.266431	-2.160387	-2.455871
Pd	-0.289971	-0.385870	-0.583361
H	1.605259	-2.523281	-1.164080
O	3.500444	-2.640289	0.176490
C	3.903606	-1.437083	0.609837
O	3.663969	-1.093563	1.824714
O	4.500407	-0.649059	-0.240115
K	1.784844	-2.733616	2.048867
K	4.662040	-2.346479	-1.979784
C	4.907753	2.589545	-0.239417
H	5.136786	3.120970	-1.185909
H	5.522543	3.044733	0.567183
H	5.201093	1.518455	-0.317780
C	-6.679046	-2.444277	-1.139925
H	-6.229980	-3.460037	-1.199131
H	-7.520875	-2.505187	-0.419295
H	-7.096972	-2.207715	-2.139120
C	-3.372893	1.253638	-2.271308
H	-3.296066	2.297467	-1.901025
H	-2.333620	0.917188	-2.472020
H	-3.928791	1.261000	-3.228986
C	-3.839422	-0.368625	2.526037
H	-2.744226	-0.539263	2.594212
H	-4.057802	0.619324	2.984073
H	-4.348809	-1.144764	3.129333
C	1.098125	0.906768	2.610924
H	0.343634	0.165384	2.270948
H	1.950299	0.362323	3.059900
H	0.608534	1.526884	3.393149
C	0.137027	4.122451	-1.215833
H	-0.621539	3.434651	-1.650936
H	-0.426602	4.876419	-0.625635
H	0.638734	4.653166	-2.048706
Zero-point correction=			0.456716 (Hartree/Particle)
Thermal correction to Energy=			0.487209
Thermal correction to Enthalpy=			0.488153
Thermal correction to Gibbs Free Energy=			0.393863
Sum of electronic and zero-point Energies=			-1628.580872
Sum of electronic and thermal Energies=			-1628.550380
Sum of electronic and thermal Enthalpies=			-1628.549436
Sum of electronic and thermal Free Energies=			-1628.643726
SCF Done (in solvent): -1629.2577763			
Zero-point correction=			0.474322 (Hartree/Particle)
Thermal correction to Energy=			0.513992
Thermal correction to Enthalpy=			0.514936
Thermal correction to Gibbs Free Energy=			0.399136
Sum of electronic and zero-point Energies=			-3092.349724
Sum of electronic and thermal Energies=			-3092.310054
Sum of electronic and thermal Enthalpies=			-3092.309110
Sum of electronic and thermal Free Energies=			-3092.424910
SCF Done (in solvent): -3093.085896			

[Pd(IMes)(allyl)Cl]-I-II	**[Pd(IMes)(allyl)Cl]-II**
63	63
MesI-PREallyl--K2CO3 SCF Done: -3092.78577301 A.U.	MesI-PREallyl--K2CO3post SCF Done: -3092.85086883 A.U.
Cl -0.683042 0.171729 -2.190213	

N	0.858140	-2.508126	0.265484
C	-0.559790	-2.753878	0.282678
N	2.761182	-1.489236	0.127673
C	-1.289079	-2.475799	1.464525
C	-2.679357	-2.700869	1.449693
H	-3.264953	-2.465274	2.353246
C	-3.337553	-3.215480	0.310954
C	-2.571923	-3.477035	-0.845952
H	-3.070628	-3.869545	-1.748866
C	-1.180923	-3.238707	-0.891517
C	1.408658	-1.247905	0.148910
C	1.846166	-3.498234	0.319158
H	1.598727	-4.559725	0.419360
C	3.052042	-2.852180	0.229635
H	4.079198	-3.230016	0.229539
C	3.714820	-0.420417	0.004899
C	4.256938	0.138484	1.183101
C	5.156038	1.212181	1.043969
H	5.587742	1.666411	1.951694
C	5.503716	1.728361	-0.221899
C	4.915722	1.155287	-1.368108
H	5.159168	1.564892	-2.362802
C	4.009210	0.080791	-1.282728
C	0.727524	1.730134	1.740595
H	1.746113	2.130394	1.896650
H	0.294483	1.254294	2.640906
C	-0.147718	2.428144	0.824921
H	0.244994	3.273604	0.229153
C	-1.496282	1.986564	0.607245
H	-1.816589	1.074736	1.136686
Pd	0.460670	0.512109	0.034934
H	-1.851713	2.080575	-0.435207
O	-4.418507	2.679864	-0.432827
C	-3.945929	2.212073	0.682844
O	-2.945786	2.952682	1.272514
O	-4.234668	1.078314	1.156822
K	-3.048387	4.753669	-0.451401
K	-3.546926	-0.053291	-1.047764
C	-4.827096	-3.486869	0.348364
H	-5.380070	-2.658698	0.839960
H	-5.247107	-3.635370	-0.667619
H	-5.047841	-4.407072	0.931854
C	-0.392995	-3.411696	-2.165246
H	-0.067980	-2.406617	-2.516504
H	0.517539	-4.028237	-2.020011
H	-1.007866	-3.877688	-2.959844
C	-0.593707	-1.926526	2.684223
H	0.286388	-2.544438	2.960793
H	-0.204855	-0.908999	2.463871
H	-1.278568	-1.868847	3.551550
C	3.813635	-0.368700	2.534099
H	2.719532	-0.210115	2.654365
H	3.990223	-1.459292	2.646176
H	4.337964	0.154429	3.357262
C	3.313470	-0.479099	-2.499188
H	3.356492	-1.588173	-2.522696
H	2.233650	-0.205680	-2.482700
H	3.759324	-0.090589	-3.435399
C	6.501927	2.858190	-0.348077
H	6.310538	3.475063	-1.249712
H	6.480407	3.525913	0.537465
H	7.538874	2.464220	-0.435143
Cl	0.669449	0.787097	2.097187
N	0.308921	-2.487600	0.015834
C	1.728155	-2.323032	-0.110881
N	-1.810083	-2.114027	0.159333
C	2.278556	-2.009317	-1.379318
C	3.682513	-1.910387	-1.480190
H	4.125247	-1.663125	-2.459399
C	4.530137	-2.123370	-0.370477
C	3.938015	-2.408232	0.880456
H	4.582380	-2.555013	1.764050
C	2.537706	-2.503154	1.038666
C	-0.611692	-1.456160	-0.028017
C	-0.303439	-3.733206	0.213992
H	0.271014	-4.663871	0.258386
C	-1.647847	-3.492641	0.305714
H	-2.497443	-4.166695	0.453791
C	-3.071086	-1.423744	0.148085
C	-3.764645	-1.315806	-1.079096
C	-4.974273	-0.599292	-1.086559
H	-5.525170	-0.492914	-2.036270
C	-5.489649	-0.002220	0.084179
C	-4.762305	-0.134442	1.283357
H	-5.149547	0.332353	2.204634
C	-3.543258	-0.839862	1.342894
C	-1.413149	1.223338	-1.982221
H	-2.488294	0.965723	-1.932861
H	-0.926659	0.910935	-2.928914
C	-0.935926	2.408891	-1.315501
H	-1.707036	3.001956	-0.773915
C	0.138992	3.263432	-1.955482
H	-0.299325	4.098355	-2.548359
Pd	-0.455751	0.563025	-0.273460
H	0.790162	2.658461	-2.619109
O	2.589450	3.598721	0.546904
C	2.183605	3.282777	-0.617196
O	0.966947	3.913607	-0.953882
O	2.697482	2.474961	-1.425199
K	0.174324	3.656515	1.573005
K	3.307717	0.997957	0.587745
C	1.907551	-2.711850	2.394371
H	1.312416	-3.647316	2.442133
H	2.675303	-2.751829	3.191626
H	1.214367	-1.868926	2.610688
C	1.384072	-1.742707	-2.561691
H	0.607366	-2.528280	-2.668141
H	0.834241	-0.787502	-2.395129
H	1.962041	-1.673020	-3.502980
C	6.034629	-2.067541	-0.527956
H	6.544826	-1.874763	0.437828
H	6.426058	-3.032808	-0.917519
H	6.343383	-1.281802	-1.248176
C	-2.732767	-0.933458	2.611441
H	-2.451649	-1.983304	2.839276
H	-1.778408	-0.370050	2.503612
H	-3.289011	-0.526127	3.478453
C	-3.167203	-1.903202	-2.334385
H	-2.158604	-1.469418	-2.508121
H	-3.031959	-3.002601	-2.251228
H	-3.798450	-1.697018	-3.220247
C	-6.798502	0.755568	0.038216
H	-7.648126	0.075518	-0.188939
H	-7.018968	1.258041	1.001278
H	-6.787047	1.531047	-0.756892

Zero-point correction= 0.473380 (Hartree/Particle) Thermal correction to Energy= 0.512682 Thermal correction to Enthalpy= 0.513627 Thermal correction to Gibbs Free Energy= 0.396657 Sum of electronic and zero-point Energies= -3092.312393 Sum of electronic and thermal Energies= -3092.273091 Sum of electronic and thermal Enthalpies= -3092.272146 Sum of electronic and thermal Free Energies= -3092.389116 SCF Done (in solvent): -3093.0484939	Zero-point correction= 0.475820 (Hartree/Particle) Thermal correction to Energy= 0.514792 Thermal correction to Enthalpy= 0.515736 Thermal correction to Gibbs Free Energy= 0.401980 Sum of electronic and zero-point Energies= -3092.375049 Sum of electronic and thermal Energies= -3092.336077 Sum of electronic and thermal Enthalpies= -3092.335133 Sum of electronic and thermal Free Energies= -3092.448889 SCF Done (in solvent): -3093.1050688

[Pd(IMes)(allyl)Cl]-III			**[Pd(IMes)(allyl)Cl]-I'**		
61			61		
MesI-PREallyl+KCO3menysKClISOMERopen SCF Done: -2032.59700635 A.U.			MesI-PREallyl+KCO3menysKCl SCF Done: -2032.58737150 A.U.		
N	0.803816	-1.889316	0.645558	N	-1.066844	-1.340183	-1.266505
C	2.180123	-1.571784	0.379564	C	-2.417489	-1.293493	-0.761775
N	-1.349508	-1.736877	0.720488	N	1.090203	-1.216154	-1.397369
C	2.719670	-1.886877	-0.891223	C	-2.785554	-2.247427	0.216448
C	4.056401	-1.514055	-1.148438	C	-4.101785	-2.208454	0.709712
H	4.496222	-1.755001	-2.131063	H	-4.406875	-2.945302	1.471726
C	4.842710	-0.853720	-0.177386	C	-5.035455	-1.256832	0.249872
C	4.260943	-0.560533	1.074845	C	-4.623606	-0.331908	-0.726746
H	4.850602	-0.021705	1.834177	H	-5.338472	0.426708	-1.087250
C	2.927354	-0.904575	1.383690	C	-3.313344	-0.315483	-1.247507
C	-0.246544	-1.152617	0.143102	C	0.036399	-0.925241	-0.566424
C	0.363673	-2.898785	1.506413	C	-0.709319	-1.883180	-2.502411
H	1.057369	-3.588027	1.997644	H	-1.461290	-2.269012	-3.197379
C	-1.003339	-2.797534	1.555616	C	0.656434	-1.801338	-2.589081
H	-1.753943	-3.375913	2.103154	H	1.355580	-2.093719	-3.378388
C	-2.677915	-1.219091	0.509809	C	2.461908	-0.988956	-1.030182
C	-3.395018	-1.630602	-0.635901	C	3.192320	-2.075593	-0.494939
C	-4.666872	-1.067002	-0.847289	C	4.514804	-1.837981	-0.080924
H	-5.243843	-1.374752	-1.735579	H	5.097063	-2.669670	0.350020
C	-5.213939	-0.116440	0.039668	C	5.103123	-0.558857	-0.185079
C	-4.458005	0.266453	1.166191	C	4.334855	0.493099	-0.719644
H	-4.870509	1.011296	1.867095	H	4.779747	1.499214	-0.799390
C	-3.180114	-0.267508	1.427076	C	3.004911	0.308845	-1.153717
C	-0.672509	2.224305	-2.316463	C	1.487669	-1.032885	2.391010
H	-1.216670	1.919665	-3.227867	H	2.403183	-1.450583	1.941182
H	0.240557	2.822765	-2.497156	H	0.867847	-1.755555	2.954686
C	-1.352081	2.337320	-1.086789	C	1.492184	0.350842	2.777095
H	-2.431936	2.085529	-1.055601	H	2.350579	0.982517	2.482214
C	-0.898815	3.195911	0.081286	C	0.299007	0.977180	3.199405
H	-1.237232	4.246253	-0.099123	H	-0.485434	0.409503	3.730616
Pd	-0.379035	0.432354	-1.113064	Pd	0.103748	0.081565	1.174367
H	-1.375597	2.842067	1.020220	H	0.251984	2.074556	3.269352
O	2.308871	2.479001	1.392433	O	-1.798982	3.348340	-0.483374
C	1.052888	2.534654	1.452310	C	-0.953327	2.573039	0.112988
O	0.241902	2.103087	2.283694	O	-1.347039	1.351591	0.402680
O	0.515755	3.214848	0.257173	O	0.254433	2.969285	0.404487
K	2.491594	1.816508	-0.989738	K	-0.215592	5.198933	-0.515541
C	-2.772862	-2.584992	-1.626179	C	-2.904349	0.757840	-2.221753
H	-1.938061	-2.075426	-2.159112	H	-2.700839	1.698201	-1.655203
H	-2.334252	-3.474141	-1.127107	H	-1.978589	0.505858	-2.774286
H	-3.509651	-2.930083	-2.377228	H	-3.711220	0.955484	-2.957756
C	-2.347846	0.189661	2.596651	C	-1.785142	-3.259265	0.726560
H	-1.956000	-0.666584	3.184872	H	-1.251803	-3.766316	-0.105525
H	-1.458806	0.771812	2.259069	H	-1.005811	-2.755073	1.339004
H	-2.933596	0.835791	3.278876	H	-2.275759	-4.032873	1.349044
C	1.871385	-2.559693	-1.944500	C	-6.434603	-1.204220	0.823095
H	1.316709	-3.425122	-1.526857	H	-6.488581	-0.473844	1.660464
H	1.097545	-1.857451	-2.330522	H	-7.177406	-0.882986	0.064148
H	2.485388	-2.909173	-2.797199	H	-6.753723	-2.187985	1.224100

C 2.299786 -0.518911 2.697459	C 2.179805 1.455968 -1.673265
H 1.880574 -1.398530 3.228851	H 1.539666 1.885614 -0.860681
H 3.037342 -0.025710 3.357282	H 2.829181 2.265390 -2.064441
H 1.468633 0.206008 2.542353	H 1.490947 1.133658 -2.480647
C -6.566016 0.504275 -0.235626	C 2.527647 -3.420344 -0.317893
H -6.467340 1.381214 -0.913007	H 1.597249 -3.313953 0.281018
H -7.253152 -0.212612 -0.730179	H 2.225398 -3.863964 -1.290260
H -7.051590 0.862166 0.694699	H 3.196281 -4.138736 0.194837
C 6.286063 -0.493332 -0.456301	C 6.535665 -0.337701 0.247823
H 6.971621 -1.266706 -0.045696	H 6.767523 -0.885405 1.184836
H 6.492203 -0.417836 -1.543452	H 7.245810 -0.704928 -0.525645
H 6.565632 0.468984 0.020163	H 6.754227 0.736233 0.414733
Zero-point correction= 0.472832 (Hartree/Particle) Thermal correction to Energy= 0.508380 Thermal correction to Enthalpy= 0.509324 Thermal correction to Gibbs Free Energy= 0.402641 Sum of electronic and zero-point Energies= -2032.124174 Sum of electronic and thermal Energies= -2032.088626 Sum of electronic and thermal Enthalpies= -2032.087682 Sum of electronic and thermal Free Energies= -2032.194365 SCF Done (in solvent): -2032.8363738	Zero-point correction= 0.472805 (Hartree/Particle) Thermal correction to Energy= 0.508117 Thermal correction to Enthalpy= 0.509061 Thermal correction to Gibbs Free Energy= 0.403065 Sum of electronic and zero-point Energies= -2032.114567 Sum of electronic and thermal Energies= -2032.079254 Sum of electronic and thermal Enthalpies= -2032.078310 Sum of electronic and thermal Free Energies= -2032.184306 SCF Done (in solvent): -2032.8270076

[Pd(IMes)(allyl)Cl]-I'-III	**[Pd(IMes)(allyl)Cl]-IV**
61	48
MesI-PREallyl+KCO3--C-O SCF Done: -2032.56057913 A.U.	Mes-Pd SCF Done: -1051.60758393 A.U.
N -0.347129 -1.909314 0.485598	Pd 0.001831 -0.000120 -1.694538
C -1.761537 -1.652840 0.522509	N -1.085697 0.010811 1.080466
N 1.785608 -1.690802 0.175003	N 1.084021 -0.007472 1.082741
C -2.309467 -0.844765 1.548721	C 0.000056 0.001140 0.222788
C -3.699673 -0.617593 1.529762	C -0.687286 0.007966 2.419339
H -4.132531 0.046042 2.294930	C 0.682791 -0.003307 2.420779
C -4.541597 -1.184221 0.554285	C -2.454726 0.009680 0.639582
C -3.956562 -1.985606 -0.451241	C -3.116334 -1.228271 0.489065
H -4.599456 -2.449519 -1.220837	C -4.462804 -1.205234 0.076656
C -2.564585 -2.216012 -0.497860	C -5.137997 0.003218 -0.187204
C 0.607608 -0.968058 0.125147	C -4.430200 1.215605 -0.041793
C 0.226715 -3.155159 0.756531	C -3.085354 1.245590 0.368685
H -0.373157 -4.014855 1.071212	C 2.453831 -0.008923 0.644370
C 1.574473 -3.016984 0.557610	C 3.119036 1.227891 0.497682
H 2.399055 -3.729647 0.657954	C 4.467215 1.202067 0.092252
C 3.078790 -1.096744 -0.026264	C 5.140719 -0.007986 -0.170517
C 3.821190 -0.710519 1.112237	C 4.431361 -1.218861 -0.023826
C 5.073575 -0.104254 0.904742	C 3.083911 -1.246003 0.379534
H 5.662043 0.214117 1.781437	H -1.414071 0.013597 3.237600
C 5.578098 0.132812 -0.390580	H 1.407835 -0.007992 3.240593
C 4.788677 -0.241708 -1.497250	H -4.995756 -2.162300 -0.050910
H 5.156664 -0.038670 -2.516908	H -4.939509 2.168616 -0.263690
C 3.531767 -0.857206 -1.341215	H 5.004101 2.157884 -0.028756
C 2.055067 1.992889 0.401891	H 4.941655 -2.173356 -0.236668
H 2.958707 1.837391 -0.216589	C 6.579606 -0.013657 -0.637837
H 2.248772 1.862436 1.485059	H 7.096564 0.936146 -0.393357
C 1.113958 3.027187 -0.006993	H 7.154415 -0.846106 -0.181518
H 1.192091 3.441312 -1.029342	H 6.636803 -0.147058 -1.740648
C 0.114625 3.569097 0.845545	C -6.592232 0.012933 -0.604081
H 0.214674 3.428846 1.932631	H -6.943755 -0.996046 -0.899032
Pd 0.344274 0.971603 -0.188957	H -7.242503 0.363637 0.227245
H -0.408283 4.485521 0.538024	H -6.764556 0.699731 -1.459049
O -3.643505 2.362664 -0.066796	C 2.371936 2.519517 0.722945
C -2.377472 2.220179 0.061599	H 1.514316 2.584361 0.017090
O -1.739324 2.780707 1.053356	H 1.943983 2.576373 1.746401
O -1.722337 1.462087 -0.814401	H 3.025381 3.400318 0.570143
K -3.783853 0.885296 -2.038467	C 2.299106 -2.530500 0.478992
	H 2.940402 -3.415920 0.302921

C	3.228378	-0.872650	2.490855
H	2.240656	-0.363527	2.535335
H	3.047517	-1.938229	2.746497
H	3.885394	-0.437969	3.268711
C	2.648854	-1.177157	-2.520974
H	2.233435	-2.204576	-2.457084
H	1.777686	-0.483036	-2.524134
H	3.193455	-1.073200	-3.479566
C	-1.458185	-0.184409	2.602767
H	-0.484163	-0.691530	2.739519
H	-1.256310	0.864600	2.286677
H	-1.991619	-0.150466	3.574196
C	-1.936973	-2.999296	-1.629166
H	-1.083878	-2.437360	-2.066134
H	-1.526821	-3.974257	-1.290670
H	-2.673178	-3.208469	-2.431002
C	-6.027026	-0.897206	0.576131
H	-6.213709	0.198544	0.554740
H	-6.555234	-1.363273	-0.281054
H	-6.497655	-1.279753	1.506652
C	6.939511	0.762339	-0.584606
H	7.167259	1.497594	0.214156
H	7.741076	-0.008717	-0.556364
H	7.016828	1.280722	-1.561736

Zero-point correction= 0.472013 (Hartree/Particle)
Thermal correction to Energy= 0.506663
Thermal correction to Enthalpy= 0.507607
Thermal correction to Gibbs Free Energy= 0.404422
Sum of electronic and zero-point Energies= -2032.088566
Sum of electronic and thermal Energies= -2032.053916
Sum of electronic and thermal Enthalpies= -2032.052972
Sum of electronic and thermal Free Energies= -2032.156157

SCF Done (in solvent): -2032.7856927

H	1.812282	-2.640173	1.471116
H	1.479940	-2.523848	-0.275427
C	-2.366113	-2.518571	0.711454
H	-1.937018	-2.575883	1.734378
H	-3.017718	-3.400618	0.557988
H	-1.508957	-2.580329	0.004660
C	-2.301088	2.530746	0.463727
H	-2.942797	3.415330	0.284958
H	-1.814216	2.643600	1.455444
H	-1.481928	2.521951	-0.290721

Zero-point correction= 0.385599 (Hartree/Particle)
Thermal correction to Energy= 0.411532
Thermal correction to Enthalpy= 0.412476
Thermal correction to Gibbs Free Energy= 0.324229
Sum of electronic and zero-point Energies= -1051.221985
Sum of electronic and thermal Energies= -1051.196052
Sum of electronic and thermal Enthalpies= -1051.195108
Sum of electronic and thermal Free Energies= -1051.283354

SCF Done (in solvent): -1051.7299556

[Pd(IMes)(allyl)Cl]-V

89

MesI5 SCF Done: -2028.82333005 A.U.

C	-0.743679	1.075439	-1.442582
O	-0.394071	0.703718	-2.567604
Pd	0.173908	-0.135197	0.286804
N	0.189918	1.891594	-0.546486
C	-4.981083	1.642151	-0.674438
C	-4.464760	1.620314	-1.981357
H	-4.522234	1.388572	1.441235
C	-4.121029	1.419115	0.416580
C	-3.091172	1.416137	-2.192559
C	-2.216531	1.234532	-1.099903
C	-2.753031	1.205332	0.205791
H	-2.664874	1.403166	-3.207166
H	-2.087310	0.981327	1.054922
H	-6.056375	1.810299	-0.504921
H	-5.134090	1.771976	-2.843473
C	1.611028	1.909778	-0.841063
O	2.167683	1.259827	-1.701798
O	2.200385	2.784545	0.006360
C	3.590488	2.552428	0.458939
C	4.585832	2.648887	-0.706507
H	4.474160	1.794389	-1.398340
H	4.424179	3.587162	-1.274802
H	5.620026	2.661319	-0.303010
C	3.801373	3.692168	1.461150
H	4.804408	3.610195	1.926370
H	3.723793	4.675250	0.954450

[Pd(IMes)(allyl)Cl]-V-VI

89

MesI5-I6 SCF Done: -2028.82182418 A.U.

C	-0.493489	0.920883	-1.172562
O	-0.159119	0.615848	-2.319534
Pd	0.160908	-0.359207	0.401077
N	0.648660	1.666363	-0.174415
C	-4.450313	2.568373	-0.494100
C	-3.884630	2.530346	-1.780592
H	-4.196877	2.011119	1.597353
C	-3.746884	2.017709	0.592524
C	-2.608543	1.976584	-1.971712
C	-1.884386	1.455251	-0.878257
C	-2.479036	1.454068	0.399938
H	-2.141621	1.944416	-2.968042
H	-1.935438	0.988204	1.238304
H	-5.447768	3.009766	-0.340001
H	-4.437549	2.941820	-2.640482
C	1.991938	1.640101	-0.651773
O	2.457888	0.768273	-1.363322
O	2.665438	2.713602	-0.173021
C	4.126192	2.829586	-0.363675
C	4.444108	2.993993	-1.856679
H	4.182008	2.077283	-2.416419
H	3.871978	3.845879	-2.277373
H	5.526046	3.202218	-1.987974
C	4.456273	4.107980	0.416532
H	5.541471	4.326228	0.352886
H	3.894495	4.969592	0.003221

H	3.032239	3.651001	2.258186
C	3.632346	1.180996	1.143118
H	3.365174	0.375864	0.432044
H	4.651686	0.970899	1.524732
H	2.919579	1.144440	1.992262
N	-0.992828	-2.935532	0.309571
N	1.163565	-2.955520	0.117040
C	0.099339	-2.099528	0.310608
C	-0.622612	-4.269011	0.121796
C	0.743474	-4.281049	0.000369
C	-2.353410	-2.468870	0.366288
C	-3.023055	-2.190793	-0.846451
C	-4.371266	-1.792078	-0.763795
C	-5.034170	-1.653701	0.469695
C	-4.310908	-1.898385	1.655834
C	-2.965433	-2.305710	1.629180
C	2.515281	-2.494728	-0.069084
C	3.400204	-2.532435	1.031886
C	4.712698	-2.063806	0.836282
C	5.133587	-1.545062	-0.405209
C	4.214703	-1.521674	-1.472942
C	2.895206	-1.996897	-1.338315
H	-1.362772	-5.074311	0.085702
H	1.450125	-5.099725	-0.166990
H	-4.909514	-1.553756	-1.695200
H	-4.806882	-1.761841	2.631651
H	5.415308	-2.074964	1.686236
H	4.524434	-1.103818	-2.444744
C	-0.351298	3.026775	0.181216
C	-0.303831	3.067306	1.585955
C	-0.940359	4.078994	-0.540321
C	-0.856429	4.159196	2.270041
H	0.161696	2.224299	2.121001
C	-1.501570	5.166691	0.149293
H	-0.974303	4.026270	-1.639129
C	-1.461487	5.209726	1.553663
H	-0.822000	4.188117	3.370620
H	-1.976023	5.983755	-0.416599
H	-1.904295	6.061954	2.092787
C	6.512717	-0.949850	-0.573377
H	7.213112	-1.292172	0.214871
H	6.951481	-1.200691	-1.561084
H	6.459708	0.160075	-0.516439
C	-6.485413	-1.236046	0.531799
H	-6.845206	-0.865767	-0.448416
H	-7.135331	-2.086210	0.834205
H	-6.640617	-0.428233	1.277605
C	2.912130	-3.006905	2.379894
H	2.047952	-2.391580	2.712853
H	2.554869	-4.058108	2.346304
H	3.708242	-2.938606	3.146600
C	1.916465	-1.912978	-2.481313
H	2.441762	-1.936196	-3.456350
H	1.173819	-2.735133	-2.456532
H	1.352947	-0.955621	-2.426866
C	-2.299056	-2.260556	-2.168294
H	-1.689793	-3.183211	-2.262606
H	-3.009926	-2.222549	-3.016199
H	-1.600527	-1.401182	-2.274915
C	-2.163536	-2.519377	2.890132
H	-2.784766	-2.382853	3.796630
H	-1.713564	-3.534263	2.925274
H	-1.317158	-1.798130	2.925730
H	4.177017	3.993907	1.483216
C	4.830201	1.610284	0.253368
H	4.579561	0.682119	-0.294009
H	5.928690	1.762815	0.224153
H	4.525629	1.485939	1.312563
N	0.538559	-3.272463	0.025207
C	2.592966	-2.546040	-1.111119
C	1.960475	-3.035929	0.056580
C	-0.363591	-2.247844	0.205447
C	2.644017	-3.210767	1.279775
C	3.964071	-2.242300	-1.019863
H	4.472625	-1.838331	-1.910488
C	4.691288	-2.410051	0.176151
C	4.016047	-2.895885	1.314004
H	4.568607	-3.021422	2.260193
C	-0.102368	-4.476544	-0.261163
C	-1.448836	-4.207998	-0.264385
H	-2.317079	-4.849404	-0.444526
H	0.453793	-5.401732	-0.440886
N	-1.584976	-2.847321	0.021378
C	-2.830739	-2.126092	0.038575
C	-3.356952	-1.652374	-1.183606
C	-3.465865	-1.899195	1.280415
C	-4.588043	-0.968840	-1.137155
C	-4.693567	-1.214865	1.270016
C	-5.275823	-0.753518	0.070915
H	-5.007057	-0.571457	-2.075514
H	-5.204731	-1.023225	2.228466
C	0.228511	2.813622	0.594101
C	-0.202940	3.979972	-0.066399
C	0.205553	2.752649	1.999060
C	-0.673601	5.071909	0.677432
H	-0.187447	4.006547	-1.166239
C	-0.259371	3.849802	2.741763
H	0.540034	1.824983	2.490651
C	-0.705844	5.009698	2.083018
H	-1.026608	5.975637	0.155935
H	-0.281211	3.795194	3.841860
H	-1.082138	5.865713	2.665175
C	-2.798483	-2.330003	2.563690
H	-2.513495	-3.403032	2.541375
H	-1.854925	-1.757172	2.706054
H	-3.452579	-2.159029	3.440683
C	1.893622	-3.650947	2.514520
H	1.118683	-2.898688	2.781112
H	1.358234	-4.610845	2.355605
H	2.572800	-3.772443	3.380686
C	1.809627	-2.272619	-2.369412
H	1.015472	-3.027247	-2.540641
H	1.316420	-1.278187	-2.290597
H	2.473328	-2.247571	-3.255563
C	-2.597075	-1.819813	-2.476355
H	-1.720643	-1.134783	-2.504566
H	-2.204877	-2.850488	-2.599459
H	-3.237106	-1.583782	-3.348553
C	-6.605970	-0.036584	0.093218
H	-6.786552	0.517639	-0.849009
H	-7.444951	-0.753787	0.230977
H	-6.657414	0.690295	0.930276
C	6.164166	-2.067531	0.226054
H	6.339999	-1.016788	-0.087843
H	6.583648	-2.192776	1.244219
H	6.750144	-2.711840	-0.464232

Zero-point correction= 0.710917 (Hartree/Particle) Thermal correction to Energy= 0.758567 Thermal correction to Enthalpy= 0.759511 Thermal correction to Gibbs Free Energy= 0.628759 Sum of electronic and zero-point Energies= -2028.112413 Sum of electronic and thermal Energies= -2028.064763 Sum of electronic and thermal Enthalpies= -2028.063819 Sum of electronic and thermal Free Energies= -2028.194571 SCF Done (in solvent): -2029.2475294	Zero-point correction= 0.710215 (Hartree/Particle) Thermal correction to Energy= 0.757397 Thermal correction to Enthalpy= 0.758342 Thermal correction to Gibbs Free Energy= 0.627727 Sum of electronic and zero-point Energies= -2028.111610 Sum of electronic and thermal Energies= -2028.064427 Sum of electronic and thermal Enthalpies= -2028.063483 Sum of electronic and thermal Free Energies= -2028.194098 SCF Done (in solvent): -2029.2407107

[Pd(IMes)(allyl)Cl]-VI			
89			
MesI6 SCF Done: -2028.84943844 A.U.			
Pd	0.165140	-0.364209	0.231723
N	0.353914	-3.302395	0.103399
C	2.506531	-2.715172	-0.938524
C	1.780537	-3.103829	0.211441
C	-0.511873	-2.238525	0.140939
C	2.368241	-3.191174	1.494491
C	3.873831	-2.432592	-0.769988
H	4.451421	-2.096819	-1.645974
C	4.506090	-2.511921	0.485714
C	3.739825	-2.897065	1.605094
H	4.217669	-2.950343	2.597416
C	-0.326857	-4.509804	-0.035605
C	-1.662900	-4.197989	-0.091878
H	-2.550873	-4.829127	-0.194047
H	0.197320	-5.469229	-0.082450
N	-1.754834	-2.808170	0.017494
C	-2.965570	-2.032211	-0.035724
C	-3.574322	-1.813213	-1.293295
C	-3.464114	-1.466995	1.160083
C	-4.702624	-0.972479	-1.330707
C	-4.598003	-0.640681	1.065036
C	-5.220501	-0.366557	-0.169773
H	-5.176011	-0.765843	-2.304457
H	-4.991552	-0.172476	1.982214
C	-1.033955	0.259984	-1.211151
O	-0.856331	-0.101818	-2.359363
N	1.198260	1.409268	0.397183
C	-3.848184	3.357055	-0.173531
C	-3.575690	3.058361	-1.524032
H	-3.437293	2.847520	1.905873
C	-3.237012	2.612638	0.849921
C	-2.678232	2.032501	-1.847962
C	-2.045293	1.295360	-0.819680
C	-2.344031	1.581854	0.526439
H	-2.438647	1.788514	-2.894202
H	-1.844115	0.993964	1.310656
H	-4.537755	4.178338	0.079668
H	-4.059936	3.638303	-2.325904
C	2.321750	1.456480	-0.388427
O	2.706538	0.523292	-1.105174
O	3.005409	2.639106	-0.249338
C	4.287486	2.856509	-0.921867
C	4.103130	2.821822	-2.448292
H	3.804981	1.810381	-2.780913
H	3.316109	3.542642	-2.751790
H	5.050024	3.108472	-2.951345
C	4.677015	4.265937	-0.454217
H	5.645556	4.568670	-0.901871
H	3.900434	4.998530	-0.753634
H	4.768653	4.294988	0.650298

[Pd(IMes)(allyl)Cl]-VII			
95			
MesI6+K2CO3 SCF Done: -3492.68833274 A.U.			
Pd	0.336718	-0.374781	-0.178791
N	2.535808	-2.541779	-0.135569
C	4.083153	-1.261647	-1.564375
C	3.659797	-1.650386	-0.271815
C	1.211730	-2.170967	-0.051965
C	4.319348	-1.230007	0.910872
C	5.193625	-0.393586	-1.651955
H	5.536126	-0.073752	-2.650376
C	5.883108	0.055241	-0.504510
C	5.434876	-0.376689	0.763621
H	5.962506	-0.036082	1.670505
C	2.699533	-3.908094	0.114586
C	1.454362	-4.412110	0.374182
H	1.114717	-5.419917	0.631201
H	3.686413	-4.380174	0.090793
N	0.565675	-3.341866	0.269030
C	-0.831539	-3.421246	0.609763
C	-1.730587	-3.959490	-0.337081
C	-1.242942	-2.948178	1.880823
C	-3.095306	-4.001203	0.007651
C	-2.624372	-2.980687	2.154374
C	-3.562750	-3.489492	1.234034
H	-3.817554	-4.385555	-0.730483
H	-2.975145	-2.589372	3.123935
C	-0.375402	-0.699933	-2.010164
O	0.375367	-0.777229	-2.983226
N	-0.795682	1.448892	-0.141782
C	-4.646166	-0.626297	-2.718062
C	-3.749055	-0.211343	-3.723574
H	-4.843477	-1.386338	-0.682336
C	-4.154160	-1.068160	-1.478651
C	-2.366441	-0.251981	-3.492111
C	-1.867736	-0.678863	-2.239310
C	-2.772149	-1.076336	-1.237287
H	-1.645680	0.048900	-4.268420
H	-2.376919	-1.385851	-0.262129
H	-5.732313	-0.597631	-2.902973
H	-4.134559	0.139486	-4.694874
C	-0.211662	2.576384	-0.592625
O	0.837424	2.639753	-1.260768
O	-0.851004	3.737769	-0.148063
C	-0.586356	5.041522	-0.761428
C	-0.837089	4.972104	-2.275638
H	-0.129937	4.269225	-2.754731
H	-1.872547	4.630520	-2.480194
H	-0.707416	5.976162	-2.729277
C	-1.626374	5.950198	-0.087327
H	-1.585566	6.972365	-0.514753
H	-2.646901	5.542107	-0.233948
H	-1.434339	6.034357	1.003645

C	5.318887	1.819379	-0.443025
H	5.017120	0.803762	-0.761045
H	6.318461	2.054676	-0.863859
H	5.391998	1.839874	0.663957
C	0.618699	2.557718	0.976074
C	0.236732	2.531710	2.338771
C	0.289953	3.701424	0.206825
C	-0.463014	3.605593	2.911478
H	0.492067	1.638171	2.930866
C	-0.408680	4.771587	0.781646
H	0.568979	3.718595	-0.857000
C	-0.793257	4.731757	2.135846
H	-0.752576	3.562714	3.974355
H	-0.673385	5.642445	0.160281
H	-1.348584	5.572179	2.581429
C	1.821938	-2.494085	-2.262364
H	0.989492	-3.205751	-2.433774
H	1.391466	-1.468671	-2.275488
H	2.538202	-2.571828	-3.103079
C	1.520600	-3.522904	2.700778
H	0.716795	-2.764878	2.831598
H	1.012865	-4.505300	2.596311
H	2.126965	-3.545424	3.626835
C	-2.758786	-1.692013	2.475008
H	-2.500088	-2.760631	2.626619
H	-1.796810	-1.132091	2.492785
H	-3.376517	-1.352883	3.328872
C	-3.006890	-2.433421	-2.546969
H	-3.136629	-3.536902	-2.553773
H	-3.501466	-2.027857	-3.450364
H	-1.920308	-2.225078	-2.630717
C	5.962076	-2.129978	0.627928
H	6.377734	-2.430569	1.610494
H	6.583752	-2.591904	-0.167129
H	6.082258	-1.028816	0.532948
C	-6.371194	0.607220	-0.248349
H	-5.975288	1.645821	-0.292398
H	-6.989733	0.446372	-1.154005
H	-7.029537	0.541881	0.642034

Zero-point correction= 0.710487 (Hartree/Particle)
Thermal correction to Energy= 0.758612
Thermal correction to Enthalpy= 0.759556
Thermal correction to Gibbs Free Energy= 0.624985
Sum of electronic and zero-point Energies= -2028.138952
Sum of electronic and thermal Energies= -2028.090827
Sum of electronic and thermal Enthalpies= -2028.089883
Sum of electronic and thermal Free Energies= -2028.224453

SCF Done (in solvent): -2029.2611686

C	0.840044	5.516252	-0.433266
H	1.583653	4.922707	-0.995224
H	0.956239	6.587540	-0.699175
H	1.044295	5.397372	0.650924
K	2.876529	1.931685	0.130840
K	-0.999407	3.177089	2.671917
C	0.976335	1.219959	2.361494
O	1.426308	2.435794	2.220711
O	0.050772	0.926219	3.193526
O	1.487802	0.276472	1.566332
C	-2.137947	1.423427	0.295084
C	-2.494804	0.629089	1.416004
C	-3.175292	2.093440	-0.406743
C	-3.835632	0.517358	1.818923
H	-1.694059	0.113635	1.968003
C	-4.509410	1.980184	0.005402
H	-2.922042	2.669047	-1.307804
C	-4.854290	1.191836	1.121369
H	-4.081452	-0.115704	2.687086
H	-5.297320	2.488735	-0.573516
H	-5.906701	1.094214	1.431591
C	-5.040205	-3.427082	1.548075
H	-5.269707	-3.879296	2.536126
H	-5.378918	-2.368307	1.591777
H	-5.649877	-3.945319	0.781433
C	7.101930	0.943957	-0.633287
H	7.035196	1.608795	-1.519020
H	7.248245	1.576021	0.266556
H	8.023878	0.333898	-0.755101
C	3.354923	-1.747860	-2.787485
H	3.234321	-2.851669	-2.768160
H	2.326620	-1.319351	-2.829998
H	3.891924	-1.470099	-3.715112
C	3.793002	-1.621592	2.266773
H	2.791438	-1.145259	2.393972
H	3.666378	-2.719818	2.363753
H	4.463076	-1.272760	3.076110
C	-0.265944	-2.405656	2.892675
H	0.739021	-2.859047	2.782899
H	-0.123620	-1.302096	2.795081
H	-0.627336	-2.596836	3.922888
C	-1.247960	-4.363232	-1.708645
H	-0.840376	-3.478000	-2.243835
H	-0.431470	-5.113978	-1.666145
H	-2.072304	-4.779577	-2.318942

Zero-point correction= 0.729482 (Hartree/Particle)
Thermal correction to Energy= 0.784693
Thermal correction to Enthalpy= 0.785638
Thermal correction to Gibbs Free Energy= 0.639136
Sum of electronic and zero-point Energies= -3491.958851
Sum of electronic and thermal Energies= -3491.903639
Sum of electronic and thermal Enthalpies= -3491.902695
Sum of electronic and thermal Free Energies= -3492.049196

SCF Done (in solvent): -3493.1208867

[Pd(IMes)(allyl)Cl]-VII-VIII			
95			
MesI6+K2CO3--KN SCF Done: -3492.66076954 A.U.			
Pd	0.746995	-0.119273	-0.459379
N	3.606104	0.607201	-0.192920
C	4.097224	-1.301480	1.265046
C	3.915258	-0.791863	-0.039977
C	2.315905	1.076408	-0.295707

[Pd(IMes)(allyl)Cl]-VIII			
84			
I6+K2CO3menysKNisomer1 SCF Done: -2495.86298673 A.U.			
Pd	-0.040404	0.844449	-0.075083
N	2.245965	-1.059759	-0.527276
C	2.344047	0.374846	-3.083769
H	1.590024	-0.360079	-2.736927

C	3.973259	-1.605417	-1.197809
C	4.310691	-2.687826	1.400532
H	4.433881	-3.108396	2.412433
C	4.351341	-3.545429	0.281231
C	4.187504	-2.985842	-1.005303
H	4.228143	-3.641320	-1.891477
C	4.535623	1.644927	-0.260757
C	3.814423	2.800822	-0.410352
H	4.126483	3.844373	-0.514026
H	5.612598	1.460151	-0.205468
N	2.466294	2.435816	-0.425913
C	1.369262	3.363917	-0.528692
C	0.971422	4.059306	0.635241
C	0.732348	3.534812	-1.780091
C	-0.153325	4.900066	0.537864
C	-0.392138	4.381470	-1.814722
C	-0.869026	5.045302	-0.666826
H	-0.497188	5.429701	1.441162
H	-0.915100	4.520870	-2.775461
C	0.678312	-0.328541	1.519450
O	1.163176	-1.337479	2.054757
N	-2.034045	-0.623421	0.281429
C	-1.227684	2.570911	4.102972
C	-0.403429	1.564204	4.644614
H	-2.057563	3.431380	2.276280
C	-1.413271	2.652190	2.711143
C	0.207937	0.629694	3.796287
C	0.031700	0.712296	2.394668
C	-0.766653	1.743671	1.860956
H	0.827528	-0.188084	4.196100
H	-0.879293	1.830757	0.772043
H	-1.726282	3.292851	4.770198
H	-0.251993	1.502356	5.734564
C	-2.411358	-1.846240	0.621641
O	-1.725648	-2.718382	1.200803
O	-3.704170	-2.210694	0.119860
C	-4.489193	-3.280636	0.731585
C	-4.571683	-3.073380	2.252439
H	-3.568602	-3.157930	2.711745
H	-4.981478	-2.068032	2.480575
H	-5.241356	-3.832065	2.707265
C	-5.874139	-3.106244	0.089861
H	-6.590329	-3.851588	0.492081
H	-6.264498	-2.088101	0.290105
H	-5.818176	-3.245106	-1.010768
C	-3.896433	-4.656890	0.380258
H	-2.892140	-4.762240	0.830026
H	-4.554488	-5.469881	0.752355
H	-3.805820	-4.770856	-0.721361
K	0.664194	-3.286522	0.385905
K	-2.816825	-1.788757	-2.423729
C	-0.051871	-1.276936	-2.719031
O	-0.199839	-1.924978	-1.565679
O	-0.631055	-1.656490	-3.770323
O	0.662643	-0.174246	-2.631424
C	-2.882761	0.388027	-0.139753
C	-2.447289	1.261961	-1.182389
C	-4.137558	0.680246	0.474058
C	-3.236343	2.345647	-1.599887
H	-1.455335	1.088170	-1.637256
C	-4.912652	1.769217	0.054476
H	-4.479630	0.039250	1.299307
C	-4.476885	2.610392	-0.990861

C	3.267512	0.703846	-1.915934
C	3.190523	0.020315	-0.679608
C	0.937390	-0.861591	-0.174339
C	3.971889	0.365527	0.451867
C	3.794719	-0.317672	1.807072
H	2.976029	-1.060249	1.713614
C	4.225606	1.732882	-2.020331
H	4.321312	2.284843	-2.968678
C	5.045203	2.072818	-0.933963
H	5.784779	2.882886	-1.037459
C	4.911141	1.403536	0.291534
H	5.536197	1.703091	1.147517
C	2.583768	-2.413390	-0.485463
C	3.355362	0.689080	2.889612
H	3.158338	0.156193	3.844692
H	4.149164	1.440074	3.090212
H	2.433759	1.229038	2.587765
C	5.061880	-1.095639	2.214914
H	4.899105	-1.628647	3.175442
H	5.344017	-1.846384	1.446964
H	5.928226	-0.414026	2.352463
C	1.548980	1.616925	-3.531911
H	2.208573	2.400526	-3.962743
H	0.802247	1.330492	-4.300002
H	0.998399	2.053218	-2.672770
C	3.124722	-0.261998	-4.250941
H	3.656078	-1.181772	-3.927758
H	2.435211	-0.534610	-5.077419
H	3.884725	0.437652	-4.661003
C	1.458126	-3.086222	-0.086834
H	1.274957	-4.148763	0.094247
H	3.592411	-2.761692	-0.725783
N	0.461768	-2.122890	0.094461
C	-0.842030	-2.365391	0.658631
C	-1.846154	-2.944721	-0.154930
C	-1.063667	-1.981713	2.011042
C	-3.099268	-3.195965	0.443376
C	-2.337290	-2.249050	2.551593
C	-3.340735	-2.860335	1.781818
H	-3.902503	-3.646503	-0.159000
H	-2.546672	-1.969396	3.594531
H	-4.327445	-3.062432	2.228386
C	-1.594370	-3.288969	-1.620648
H	-0.705530	-2.709664	-1.946166
C	0.033980	-1.331466	2.853386
H	0.674935	-0.742675	2.166962
C	-1.284072	-4.792917	-1.783733
H	-0.410353	-5.106048	-1.176733
H	-2.150471	-5.410640	-1.463483
H	-1.065464	-5.035010	-2.845003
C	-2.761929	-2.871432	-2.535307
H	-2.474831	-3.007992	-3.597907
H	-3.669772	-3.486202	-2.355518
H	-3.024288	-1.805166	-2.394236
C	0.921580	-2.409272	3.510566
H	1.757239	-1.934379	4.065940
H	0.337247	-3.027696	4.225443
H	1.363146	-3.089023	2.752496
C	-0.496797	-0.317440	3.877576
H	-1.128742	0.446464	3.381510
H	-1.076881	-0.797841	4.695065
H	0.353506	0.223285	4.338179
C	-1.195845	0.274311	-1.566356

H	-2.863595	2.997607	-2.405286
H	-5.873220	1.972696	0.556920
H	-5.092970	3.462700	-1.318366
C	-2.149895	5.844160	-0.716857
H	-3.017915	5.167144	-0.550659
H	-2.182263	6.629081	0.065747
H	-2.297257	6.328461	-1.703932
C	4.609464	-5.027860	0.451336
H	4.242432	-5.400995	1.429800
H	4.131035	-5.625210	-0.352232
H	5.698970	-5.247689	0.409961
C	3.773488	-1.016798	-2.569733
H	4.055619	-1.737485	-3.361389
H	2.706930	-0.725935	-2.720881
H	4.374439	-0.093359	-2.704267
C	1.225194	2.832363	-3.018117
H	2.333899	2.825055	-3.067679
H	0.903283	1.765104	-3.033228
H	0.838752	3.324520	-3.932018
C	1.712136	3.875837	1.938388
H	2.731100	4.317689	1.897324
H	1.163984	4.344278	2.777662
H	1.829668	2.798479	2.178568
C	4.060783	-0.386421	2.464383
H	5.005653	0.193123	2.552566
H	3.233019	0.346116	2.389480
H	3.919810	-0.960030	3.400110

Zero-point correction= 0.728217 (Hartree/Particle)
Thermal correction to Energy= 0.783146
Thermal correction to Enthalpy= 0.784090
Thermal correction to Gibbs Free Energy= 0.636449
Sum of electronic and zero-point Energies= -3491.932552
Sum of electronic and thermal Energies= -3491.877624
Sum of electronic and thermal Enthalpies= -3491.876680
Sum of electronic and thermal Free Energies= -3492.024321

SCF Done (in solvent): -3493.0980796

O	-0.911026	-0.220623	-2.652139
C	-5.276570	1.503088	-0.694617
C	-4.664970	1.864583	-1.912448
H	-5.047244	0.394182	1.175717
C	-4.567561	0.711144	0.235000
C	-3.359487	1.426490	-2.204901
C	-2.635769	0.667002	-1.261260
C	-3.246199	0.317085	-0.036413
H	-2.879783	1.679189	-3.163624
H	-2.675156	-0.267039	0.701129
H	-6.310913	1.818547	-0.479945
H	-5.217823	2.472972	-2.647033
K	-2.988100	3.882626	0.998676
C	-0.339829	2.867184	1.462305
O	-0.958848	2.686303	0.266124
O	-0.752933	3.768340	2.238592
O	0.608968	2.010033	1.696184

Zero-point correction= 0.669780 (Hartree/Particle)
Thermal correction to Energy= 0.715433
Thermal correction to Enthalpy= 0.716377
Thermal correction to Gibbs Free Energy= 0.589859
Sum of electronic and zero-point Energies= -2495.193207
Sum of electronic and thermal Energies= -2495.147554
Sum of electronic and thermal Enthalpies= -2495.146609
Sum of electronic and thermal Free Energies= -2495.273127

SCF Done (in solvent): -2496.2126867

[Pd(IMes)(allyl)Cl]-IX

84

MesI6+KCO3+NH2 SCF Done: -2662.03753398 A.U.

Pd	-0.385993	-0.091496	-0.328079
C	0.802461	0.618145	-1.753675
O	0.414869	1.091055	-2.825206
C	5.058908	0.088918	-1.101719
C	4.582176	0.582738	-2.333219
H	4.517535	-0.593603	0.898391
C	4.155381	-0.204556	-0.065477
C	3.205506	0.762526	-2.531250
C	2.290560	0.462057	-1.496552
C	2.781601	-0.008558	-0.261406
H	2.803922	1.136240	-3.486531
H	2.065310	-0.228710	0.545224
H	6.140067	-0.067874	-0.952622
H	5.291566	0.819722	-3.143002
K	-4.558537	-3.356863	0.440891
C	1.222036	-2.706451	-0.561998
C	1.410214	-2.949563	0.820535
C	2.290077	-2.947832	-1.444157
C	2.649833	-3.380956	1.297586
H	0.576956	-2.743776	1.510585
C	3.540013	-3.384134	-0.970622
H	2.165289	-2.739159	-2.519140
C	3.733693	-3.582726	0.410751

[Pd(IMes)(allyl)Cl]-IX-X

84

MesI6+KCO3+NH2--H SCF Done: -2662.03080404 A.U.

Pd	-0.641747	0.009430	0.407520
C	0.239558	-1.140848	1.759701
O	-0.337204	-1.693648	2.698035
C	4.570199	-1.273261	1.554399
C	3.897973	-1.695439	2.719460
H	4.347346	-0.508169	-0.477640
C	3.833914	-0.840332	0.437813
C	2.496148	-1.670434	2.770370
C	1.750487	-1.221950	1.656550
C	2.433579	-0.821102	0.490660
H	1.946654	-1.990930	3.669704
H	1.843987	-0.500831	-0.381134
H	5.672055	-1.282193	1.520282
H	4.474803	-2.039954	3.593350
K	0.016536	5.095455	-1.270701
C	1.583702	2.072878	0.913538
C	1.894297	2.217604	-0.470882
C	2.640356	2.250041	1.835164
C	3.193139	2.519661	-0.894985
H	1.111228	1.998252	-1.216024
C	3.950102	2.542428	1.415205
H	2.441857	2.110796	2.910372
C	4.240533	2.678492	0.041747

H	2.817174	-3.550181	2.372246
H	4.359104	-3.525076	-1.688640
C	-2.296230	-1.944381	1.266666
O	-3.233906	-2.133244	2.119522
O	-2.177247	-2.772579	0.234728
O	-1.482599	-0.932591	1.385067
N	-2.283076	2.174477	0.185237
N	-0.261206	2.827291	0.605918
C	-0.980199	1.739949	0.179491
C	-2.371806	3.504240	0.603241
C	-1.094146	3.915842	0.875529
C	-3.428834	1.362987	-0.142938
C	-4.219453	0.844315	0.905484
C	-5.370431	0.107505	0.540134
C	-5.709922	-0.133866	-0.804123
C	-4.868687	0.381030	-1.815858
C	-3.730073	1.148987	-1.512181
C	1.154138	2.803325	0.867276
C	2.034434	3.418701	-0.052597
C	3.409395	3.378702	0.239682
C	3.905545	2.749570	1.398854
C	2.989439	2.148121	2.284114
C	1.601769	2.157850	2.042455
H	-3.333892	4.020471	0.672806
H	-0.697547	4.867251	1.242475
H	-6.013911	-0.283548	1.347315
H	-5.123098	0.206596	-2.874931
H	4.116388	3.832853	-0.473718
H	3.364951	1.642928	3.189395
N	-0.001680	-2.132663	-1.006161
H	-0.093753	-2.176106	-2.028469
H	-0.921031	-2.521525	-0.511232
O	4.924933	-3.944424	0.988572
C	6.062954	-4.047774	0.152493
H	6.277703	-3.089848	-0.378477
H	6.918164	-4.294027	0.811582
H	5.956114	-4.855429	-0.610058
C	-6.972692	-0.887804	-1.173103
H	-6.789756	-1.639845	-1.971306
H	-7.422141	-1.402881	-0.297829
H	-7.749099	-0.197825	-1.569603
C	5.393837	2.684703	1.648014
H	5.628893	2.320098	2.667932
H	5.870670	1.991330	0.921253
H	5.874306	3.676638	1.515193
C	1.514015	4.052991	-1.320092
H	0.764201	4.844758	-1.110868
H	2.337599	4.505246	-1.905554
H	1.012549	3.296963	-1.960736
C	0.627203	1.477237	2.973512
H	-0.226046	2.142424	3.223736
H	0.176570	0.573039	2.504469
H	1.119895	1.173404	3.917335
C	-3.851747	0.985595	2.358175
H	-3.432753	0.005241	2.684591
H	-3.086875	1.763567	2.537065
H	-4.745911	1.210441	2.975637
C	-2.860239	1.737624	-2.593855
H	-2.709977	2.826899	-2.435763
H	-1.841502	1.290138	-2.600526
H	-3.310771	1.592591	-3.595003
Zero-point correction=			0.649184 (Hartree/Particle)
Thermal correction to Energy=			0.696609
Thermal correction to Enthalpy=			0.697553

H	3.436183	2.591103	-1.967033
H	4.739458	2.635140	2.174315
C	-1.376019	2.641820	-1.193716
O	-1.481253	3.357737	-2.234591
O	-1.185128	3.275498	-0.008789
O	-1.377091	1.350526	-1.212500
N	-2.992998	-1.673262	-0.453592
N	-1.145770	-2.651145	-1.021353
C	-1.629593	-1.534651	-0.387394
C	-3.351391	-2.849296	-1.112697
C	-2.183533	-3.467736	-1.476940
C	-3.926399	-0.703421	0.066012
C	-4.478418	0.247935	-0.822385
C	-5.350029	1.208211	-0.274945
C	-5.665716	1.234287	1.098573
C	-5.104771	0.251852	1.938487
C	-4.228594	-0.734825	1.445708
C	0.252799	-2.887880	-1.263562
C	0.944548	-3.811393	-0.445591
C	2.313957	-4.004607	-0.700487
C	2.987615	-3.306345	-1.722651
C	2.255227	-2.401201	-2.515518
C	0.880282	-2.170787	-2.308163
H	-4.399260	-3.128814	-1.257942
H	-1.989546	-4.398339	-2.018733
H	-5.785575	1.968101	-0.945039
H	-5.354089	0.249199	3.012791
H	2.878428	-4.701588	-0.059476
H	2.769656	-1.844246	-3.316259
N	0.272469	1.743719	1.303365
H	0.191316	1.708163	2.327508
H	-0.574253	2.552102	0.722845
O	5.485412	2.935816	-0.479197
C	6.582508	2.980013	0.414999
H	6.701312	2.023630	0.977236
H	7.486773	3.148598	-0.201550
H	6.493989	3.812307	1.153311
C	-4.096628	0.265468	-2.281077
H	-3.040389	0.606823	-2.367817
H	-4.170423	-0.739938	-2.745835
H	-4.737149	0.963026	-2.854731
C	-3.614432	-1.776560	2.346792
H	-3.728453	-2.796860	1.922379
H	-2.520758	-1.611353	2.471750
H	-4.082792	-1.765358	3.350351
C	-6.562641	2.316291	1.658511
H	-5.983306	3.247816	1.843224
H	-7.379355	2.576740	0.953877
H	-7.020702	2.015705	2.622668
C	0.244875	-4.521601	0.688544
H	0.916952	-5.256008	1.172783
H	-0.085049	-3.796442	1.462468
H	-0.664399	-5.057745	0.344962
C	0.109088	-1.169028	-3.133124
H	-0.854817	-1.591061	-3.487243
H	-0.159358	-0.267674	-2.535880
H	0.692479	-0.843149	-4.016202
C	4.474007	-3.497044	-1.915298
H	4.742794	-4.572369	-1.980722
H	4.842532	-2.992732	-2.830903
H	5.027866	-3.075234	-1.048163
Zero-point correction=			0.645941 (Hartree/Particle)
Thermal correction to Energy=			0.693238
Thermal correction to Enthalpy=			0.694182

Thermal correction to Gibbs Free Energy= 0.566129 Sum of electronic and zero-point Energies= -2661.388350 Sum of electronic and thermal Energies= -2661.340925 Sum of electronic and thermal Enthalpies= -2661.339981 Sum of electronic and thermal Free Energies= -2661.471405 SCF Done (in solvent): -2662.4642583	Thermal correction to Gibbs Free Energy= 0.561695 Sum of electronic and zero-point Energies= -2661.384863 Sum of electronic and thermal Energies= -2661.337566 Sum of electronic and thermal Enthalpies= -2661.336622 Sum of electronic and thermal Free Energies= -2661.469109 SCF Done (in solvent): -2662.4602078

[Pd(IMes)(allyl)Cl]-X (adduct)				**[Pd(IMes)(allyl)Cl]-X**			
84				78			
MesI6+KCO3H+NH SCF Done: -2662.03826227 A.U.				MesI6+NH SCF Done: -1797.68287874 A.U.			
Pd	0.282549	-0.253480	0.036814	Pd	0.016934	0.210624	-0.559624
C	1.440538	-0.947305	-1.408764	C	0.845357	0.963820	1.069659
O	1.196109	-0.708497	-2.590277	O	0.391004	0.754824	2.186597
C	4.840259	-3.453664	-0.445854	C	4.315758	3.501273	0.587057
C	4.533673	-3.143353	-1.785702	C	3.835131	3.179964	1.871513
H	4.289643	-3.165873	1.642898	H	4.060065	3.218775	-1.558020
C	4.042565	-2.941511	0.593342	C	3.673766	2.985666	-0.553486
C	3.425520	-2.338069	-2.082375	C	2.706563	2.361137	2.013085
C	2.614756	-1.826524	-1.043759	C	2.052124	1.848390	0.869077
C	2.939653	-2.128460	0.293326	C	2.549056	2.160055	-0.412326
H	3.159146	-2.083253	-3.120000	H	2.305653	2.100686	3.004713
H	2.320553	-1.697216	1.096273	H	2.038169	1.728707	-1.290038
H	5.704907	-4.095880	-0.212044	H	5.194707	4.156886	0.476414
H	5.161152	-3.540063	-2.600200	H	4.340800	3.579524	2.765305
K	-3.659698	-0.299084	1.699744	C	-2.404110	1.959994	-0.998044
C	-1.848898	-2.346695	0.030264	C	-3.083663	3.116805	-1.480900
C	-2.633022	-3.317325	0.748798	C	-3.121092	1.130714	-0.092779
C	-2.575843	-1.548790	-0.915435	C	-4.396118	3.409817	-1.094796
C	-4.013417	-3.451832	0.551987	H	-2.562315	3.794365	-2.178422
H	-2.129977	-3.963332	1.487332	C	-4.430208	1.424591	0.308663
C	-3.962152	-1.682529	-1.111303	H	-2.619565	0.232768	0.302204
H	-2.017042	-0.811878	-1.512945	C	-5.088455	2.569236	-0.195860
C	-4.706253	-2.629361	-0.369119	H	-4.914482	4.302824	-1.477191
H	-4.589336	-4.201507	1.117831	H	-4.923173	0.747431	1.020675
H	-4.446368	-1.039283	-1.861444	N	-0.058464	-2.650694	0.240656
C	-1.015371	-0.135629	2.813200	N	2.025843	-2.085452	0.063087
O	-1.923504	-0.174551	3.664881	C	0.753521	-1.587379	-0.078645
O	0.206776	-0.679810	3.126956	C	0.686653	-3.784495	0.563656
O	-1.140776	0.372367	1.624756	C	2.006546	-3.427975	0.451367
N	0.081492	2.682256	-0.579987	C	-1.497677	-2.553893	0.218156
N	2.167903	2.179486	-0.293181	C	-2.162572	-2.659127	-1.026347
C	0.910035	1.629552	-0.262063	C	-3.557550	-2.485340	-1.036265
C	0.807125	3.853733	-0.805311	C	-4.284069	-2.220888	0.142965
C	2.127298	3.535991	-0.622043	C	-3.580905	-2.134741	1.360034
C	-1.355273	2.584771	-0.647586	C	-2.180536	-2.283774	1.425059
C	-2.110329	3.013830	0.465183	C	3.213192	-1.303183	-0.154998
C	-3.514403	2.889329	0.388609	C	3.926372	-0.824850	0.970214
C	-4.149985	2.328560	-0.739315	C	5.073765	-0.048850	0.732144
C	-3.350677	1.915056	-1.826005	C	5.512706	0.251861	-0.573125
C	-1.948944	2.045207	-1.813718	C	4.763669	-0.233408	-1.661970
C	3.366280	1.455277	0.041471	C	3.603532	-1.011530	-1.480663
C	4.211071	1.005759	-0.999406	H	0.210743	-4.732153	0.833743
C	5.354979	0.272877	-0.635130	H	2.927722	-3.999837	0.599125
C	5.662016	-0.010569	0.710418	H	-4.092732	-2.540728	-1.998582
C	4.799251	0.473367	1.713572	H	-4.131724	-1.912126	2.288768
C	3.644033	1.217461	1.406412	H	5.628111	0.355306	1.594560
H	0.315984	4.793594	-1.075370	H	5.085379	0.007040	-2.688887
H	3.036703	4.140983	-0.685926	N	-1.117050	1.622934	-1.398607
H	-4.123554	3.236397	1.241439	H	-0.700781	2.357618	-1.984667
H	-3.832924	1.482494	-2.718358	O	-6.374043	2.942471	0.124016
H	6.010958	-0.114611	-1.431432	C	-7.091715	2.131304	1.031554
H	5.029437	0.264837	2.771508	H	-6.598632	2.075949	2.031679

N	-0.514461	-2.156881	0.230188	H	-8.089905	2.596076	1.152810
H	-0.090936	-2.834830	0.871721	H	-7.226699	1.088905	0.653710
H	0.717368	-0.652436	2.273179	C	-1.418011	-2.076650	2.710126
O	-6.074449	-2.818111	-0.461750	H	-0.710928	-2.907558	2.914793
C	-6.759274	-2.139916	-1.494287	H	-0.815909	-1.143226	2.642632
H	-6.343996	-2.375690	-2.502800	H	-2.104086	-1.984978	3.574186
H	-7.814485	-2.473778	-1.452901	C	-1.384838	-2.875097	-2.302932
H	-6.736365	-1.029206	-1.362230	H	-0.873505	-1.933020	-2.603614
C	-5.652693	2.155959	-0.792273	H	-0.593515	-3.643607	-2.183121
H	-5.926603	1.083162	-0.904102	H	-2.049821	-3.179558	-3.134165
H	-6.148594	2.542625	0.120927	C	3.439729	-1.104616	2.371847
H	-6.091830	2.684826	-1.664366	H	3.488039	-2.186533	2.618900
C	6.892595	-0.816868	1.053646	H	4.045209	-0.556263	3.118792
H	6.952436	-1.040227	2.137416	H	2.380977	-0.794247	2.494365
H	6.890715	-1.781424	0.503874	C	2.775825	-1.472774	-2.655501
H	7.820314	-0.277408	0.765062	H	2.430075	-2.519782	-2.533324
C	3.888143	1.295234	-2.445476	H	1.857325	-0.849322	-2.741515
H	4.511363	0.676467	-3.119598	H	3.340795	-1.395148	-3.604733
H	2.824605	1.082170	-2.674270	C	6.741437	1.104855	-0.781269
H	4.072442	2.362636	-2.695818	H	6.996792	1.211621	-1.854261
C	2.726998	1.737099	2.487225	H	6.579174	2.122519	-0.365441
H	2.435879	2.792125	2.302238	H	7.623696	0.678707	-0.258576
H	1.782643	1.155413	2.530875	C	-5.774429	-1.981528	0.074786
H	3.204309	1.675153	3.484103	H	-6.228533	-1.906638	1.083087
C	-1.424049	3.530784	1.704011	H	-5.982904	-1.030213	-0.461198
H	-0.746991	2.743795	2.096762	H	-6.293728	-2.791652	-0.479159
H	-0.809176	4.431413	1.495450				
H	-2.155143	3.785799	2.495230				
C	-1.100922	1.618161	-2.983832				
H	-0.424965	2.438871	-3.305644				
H	-0.438397	0.761250	-2.726834				
H	-1.726388	1.323725	-3.848344				
Zero-point correction= 0.648211 (Hartree/Particle) Thermal correction to Energy= 0.696595 Thermal correction to Enthalpy= 0.697539 Thermal correction to Gibbs Free Energy= 0.564679 Sum of electronic and zero-point Energies= -2661.390051 Sum of electronic and thermal Energies= -2661.341667 Sum of electronic and thermal Enthalpies= -2661.340723 Sum of electronic and thermal Free Energies= -2661.473583 SCF Done (in solvent): -2662.4605565				Zero-point correction= 0.619641 (Hartree/Particle) Thermal correction to Energy= 0.661601 Thermal correction to Enthalpy= 0.662545 Thermal correction to Gibbs Free Energy= 0.542675 Sum of electronic and zero-point Energies= -1797.063237 Sum of electronic and thermal Energies= -1797.021278 Sum of electronic and thermal Enthalpies= -1797.020334 Sum of electronic and thermal Free Energies= -1797.140203 SCF Done (in solvent): -1798.010824				

[Pd(IMes)(allyl)Cl]-X-XI				**[Pd(IMes)(allyl)Cl]-XI**			
78				78			
MesI6--PROD SCF Done: -1797.68272437 A.U.				Mes6+PROD SCF Done: -1797.68299799 A.U.			
Pd	0.014386	0.212084	-0.558106	Pd	0.199796	0.130543	-0.567130
C	0.848960	0.965409	1.068212	C	-0.315772	1.867872	0.932120
O	0.398428	0.757826	2.186924	O	-1.116773	1.574218	1.829961
C	4.327159	3.488326	0.564946	C	3.642749	3.300611	1.994716
C	3.857729	3.162661	1.852333	C	2.673022	3.013815	2.971372
H	4.038661	3.228979	-1.579548	H	4.085654	3.328814	-0.141040
C	3.666497	2.987631	-0.571398	C	3.328399	3.128169	0.632550
C	2.724657	2.351282	2.001342	C	1.399719	2.560616	2.591589
C	2.056478	1.847331	0.861485	C	1.076427	2.378275	1.228084
C	2.540661	2.165108	-0.423252	C	2.060395	2.667781	0.250761
H	2.332493	2.087733	2.995657	H	0.623999	2.332049	3.337625
H	2.018370	1.741354	-1.297928	H	1.863425	2.473123	-0.816160
H	5.213793	4.132244	0.448877	H	4.644372	3.650707	2.291478
H	4.376846	3.551843	2.742985	H	2.909926	3.144277	4.039525
C	-2.407527	1.962678	-0.990573	C	-2.183928	2.063829	-0.742924
C	-3.087252	3.120543	-1.470683	C	-2.763874	3.144434	-1.436882
C	-3.124080	1.131624	-0.086604	C	-2.994762	0.984755	-0.344731
C	-4.399568	3.412694	-1.083474	C	-4.130957	3.140838	-1.742482

H	-2.566201	3.799578	-2.166992
C	-4.433045	1.424587	0.315938
H	-2.622251	0.232829	0.306076
C	-5.091552	2.570192	-0.186085
H	-4.918101	4.306478	-1.463820
H	-4.925822	0.745933	1.026652
N	-0.059658	-2.652264	0.230106
N	2.024593	-2.085090	0.059290
C	0.752349	-1.587007	-0.082654
C	0.685347	-3.787263	0.549075
C	2.005254	-3.429499	0.441052
C	-1.498813	-2.554829	0.209285
C	-2.165317	-2.658943	-1.034372
C	-3.560286	-2.484965	-1.042308
C	-4.285145	-2.221259	0.138123
C	-3.580272	-2.135640	1.354276
C	-2.179814	-2.284611	1.417211
C	3.212447	-1.300657	-0.148458
C	3.918503	-0.828348	0.981063
C	5.070976	-0.052898	0.752437
C	5.518300	0.250833	-0.546764
C	4.773827	-0.230255	-1.643483
C	3.612109	-1.004575	-1.472307
H	0.209332	-4.736304	0.814086
H	2.926514	-4.001393	0.588155
H	-4.096772	-2.539579	-2.003945
H	-4.129764	-1.913138	2.283824
H	5.622825	0.342984	1.619968
H	5.104272	0.011005	-2.667677
N	-1.120967	1.626021	-1.393009
H	-0.705569	2.361522	-1.978671
O	-6.377175	2.942489	0.134755
C	-7.094349	2.129424	1.040961
H	-6.600892	2.072186	2.040798
H	-8.092581	2.593765	1.163512
H	-7.229273	1.087733	0.661118
C	6.738925	1.112346	-0.768636
H	6.437659	2.154248	-1.012924
H	7.380740	1.159762	0.133554
H	7.354216	0.741530	-1.614317
C	-5.775525	-1.981343	0.072202
H	-5.984165	-1.028007	-0.460188
H	-6.295590	-2.789322	-0.484129
H	-6.228658	-1.909802	1.081198
C	-1.388790	-2.874020	-2.311816
H	-0.871798	-1.933733	-2.608367
H	-0.602089	-3.647794	-2.195162
H	-2.055441	-3.171065	-3.144396
C	-1.415046	-2.076435	2.700782
H	-0.704888	-2.905323	2.902987
H	-0.815830	-1.141097	2.632890
H	-2.099428	-1.987556	3.566485
C	2.789803	-1.462950	-2.652079
H	2.453507	-2.514181	-2.539354
H	1.865758	-0.847145	-2.733273
H	3.354917	-1.372065	-3.600031
C	3.426904	-1.114210	2.379711
H	4.027216	-0.565796	3.130812
H	2.366453	-0.808529	2.499072
H	3.478941	-2.196675	2.623824
Zero-point correction=			0.619567 (Hartree/Particle)
Thermal correction to Energy=			0.660646
Thermal correction to Enthalpy=			0.661590
Thermal correction to Gibbs Free Energy=			0.544619

H	-2.140411	3.999718	-1.746511
C	-4.366225	0.981773	-0.634862
H	-2.544441	0.134467	0.186360
C	-4.946568	2.060731	-1.338276
H	-4.595135	3.973873	-2.291087
H	-4.963720	0.118973	-0.313427
N	0.217199	-2.661969	0.427565
N	2.229514	-2.114991	-0.153764
C	0.942420	-1.627192	-0.124297
C	1.027018	-3.755565	0.734828
C	2.303917	-3.408885	0.367131
C	-1.184959	-2.521906	0.728412
C	-2.129953	-2.861765	-0.265259
C	-3.492866	-2.665391	0.029395
C	-3.914808	-2.140407	1.267325
C	-2.935898	-1.799605	2.222862
C	-1.560707	-1.975255	1.978589
C	3.345790	-1.309035	-0.572387
C	3.971085	-0.480633	0.386749
C	5.042053	0.321671	-0.046349
C	5.477190	0.323466	-1.387479
C	4.806449	-0.500501	-2.314404
C	3.731757	-1.325649	-1.929838
H	0.625291	-4.668597	1.185104
H	3.249599	-3.956554	0.427252
H	-4.243425	-2.910701	-0.740299
H	-3.248237	-1.355328	3.182227
H	5.531433	0.985647	0.684688
H	5.119473	-0.492878	-3.371924
N	-0.773457	2.060199	-0.456349
H	-0.268168	2.808380	-0.948499
O	-6.270463	2.145882	-1.672562
C	-7.129956	1.089838	-1.276834
H	-7.152912	0.960175	-0.169372
H	-8.144226	1.362672	-1.626641
H	-6.839848	0.116897	-1.738752
C	-5.381537	-1.926517	1.570586
H	-5.738270	-2.630260	2.353857
H	-5.565565	-0.900031	1.952023
H	-6.014813	-2.078481	0.672997
C	6.644611	1.187700	-1.810379
H	6.615909	2.179987	-1.313492
H	7.612338	0.715845	-1.530776
H	6.661383	1.352445	-2.906604
C	3.440521	-0.411027	1.796003
H	2.414376	0.016615	1.783262
H	3.364729	-1.415631	2.262671
H	4.070116	0.235546	2.436126
C	2.954516	-2.150750	-2.926209
H	2.893767	-3.216811	-2.621409
H	1.907358	-1.779306	-2.985153
H	3.403971	-2.101026	-3.936943
C	-1.666538	-3.326217	-1.623624
H	-1.135160	-2.493823	-2.137654
H	-0.944124	-4.166026	-1.551891
H	-2.516068	-3.645370	-2.257953
C	-0.528509	-1.494218	2.967327
H	0.403339	-2.092596	2.935392
H	-0.266621	-0.441808	2.721152
H	-0.926154	-1.507407	4.001339
Zero-point correction=			0.621097 (Hartree/Particle)
Thermal correction to Energy=			0.662807
Thermal correction to Enthalpy=			0.663751
Thermal correction to Gibbs Free Energy=			0.544101

Sum of electronic and zero-point Energies= -1797.063157 Sum of electronic and thermal Energies= -1797.022078 Sum of electronic and thermal Enthalpies= -1797.021134 Sum of electronic and thermal Free Energies= -1797.138105 SCF Done (in solvent): -1798.0108657	Sum of electronic and zero-point Energies= -1797.061901 Sum of electronic and thermal Energies= -1797.020191 Sum of electronic and thermal Enthalpies= -1797.019247 Sum of electronic and thermal Free Energies= -1797.138897 SCF Done (in solvent): -1798.0302931

[Pd(IPr)(cin)Cl]				**[Pd(IPr)(cin)Cl]-I**			
85				91			
I-PREcin SCF Done: -2095.66186438 A.U.				I-PREcin+K2CO3 SCF Done: -3559.45321193 A.U.			
Cl	0.639671	-2.374120	0.281877	Cl	-0.493943	1.310949	2.023191
N	-2.126172	0.168282	0.904218	N	0.668790	-2.091085	1.070797
C	-3.121001	-0.536714	0.134111	C	2.008709	-1.604745	1.272328
N	-0.279513	1.158595	1.457311	N	-1.348585	-2.271104	0.305268
C	-3.732240	0.148842	-0.950062	C	2.865064	-1.529365	0.136709
C	-4.737215	-0.536988	-1.658646	C	4.171151	-1.050095	0.350467
H	-5.241732	-0.044910	-2.503331	H	4.859771	-0.961350	-0.499860
C	-5.105532	-1.845296	-1.304858	C	4.613165	-0.685992	1.632619
H	-5.898342	-2.361005	-1.869932	H	5.641476	-0.316406	1.771876
C	-4.457479	-2.504707	-0.252470	C	3.746944	-0.776062	2.732051
H	-4.737010	-3.539816	-0.004073	H	4.104913	-0.486777	3.732708
C	-3.437077	-1.869676	0.486917	C	2.414626	-1.222587	2.576164
C	-3.316859	1.574042	-1.316515	C	2.394442	-2.000698	-1.240979
H	-2.226885	1.644845	-1.117604	H	1.340610	-1.670234	-1.347610
C	-3.515523	1.908057	-2.803935	C	3.151456	-1.368457	-2.417072
H	-3.055116	1.141276	-3.459460	H	3.069792	-0.257299	-2.393606
H	-3.046728	2.886258	-3.038930	H	2.699025	-1.709551	-3.371533
H	-4.589742	1.989812	-3.074686	H	4.219884	-1.683447	-2.439399
C	-4.022004	2.615490	-0.420732	C	2.414224	-3.543947	-1.322001
H	-5.122475	2.578663	-0.567197	H	3.451127	-3.931884	-1.225871
H	-3.675293	3.641450	-0.667788	H	2.009446	-3.884371	-2.298696
H	-3.813123	2.441750	0.653811	H	1.799980	-4.010080	-0.525021
C	-2.719361	-2.594671	1.621636	C	1.482269	-1.320592	3.783183
H	-1.770855	-2.051200	1.815152	H	0.446540	-1.414856	3.395573
C	-2.318785	-4.030357	1.236613	C	1.506224	-0.057797	4.664960
H	-3.202556	-4.688527	1.092510	H	2.505931	0.122896	5.114482
H	-1.700706	-4.476129	2.042907	H	0.786121	-0.168274	5.502040
H	-1.707190	-4.026933	0.313080	H	1.193706	0.828729	4.078239
C	-3.574662	-2.576952	2.906793	C	1.818215	-2.575226	4.619961
H	-3.820173	-1.543658	3.227976	H	1.786316	-3.503530	4.013652
H	-3.036595	-3.073415	3.741474	H	1.102583	-2.690721	5.460846
H	-4.534656	-3.114849	2.751656	H	2.840020	-2.499221	5.049832
C	-0.843697	0.375845	0.479896	C	-0.277677	-1.409016	0.348532
C	-2.357990	0.791848	2.134525	C	0.190474	-3.339795	1.485813
H	-3.328378	0.737493	2.635833	H	0.803572	-4.030888	2.070505
C	-1.188798	1.416005	2.484557	C	-1.089780	-3.446711	1.009046
H	-0.923918	2.017072	3.358917	H	-1.833397	-4.241506	1.112969
C	1.066759	1.673635	1.349101	C	-2.548301	-1.927429	-0.421826

C	1.275544	2.827722	0.545909
C	2.598359	3.293190	0.415220
H	2.805278	4.180818	-0.200285
C	3.661437	2.637841	1.057488
H	4.689015	3.016638	0.938800
C	3.423353	1.496928	1.834226
H	4.266855	0.979178	2.314113
C	2.120445	0.978280	1.990206
C	0.107761	3.539687	-0.134653
H	-0.622640	2.754156	-0.422208
C	-0.604674	4.499036	0.843901
H	-0.981297	3.966133	1.739007
H	-1.473473	4.985448	0.352196
H	0.089862	5.295471	1.185913
C	0.505421	4.283066	-1.421454
H	1.107217	5.191950	-1.208005
H	-0.403247	4.617113	-1.963889
H	1.096538	3.640464	-2.105302
C	1.868224	-0.275548	2.819815
H	0.923140	-0.728572	2.453714
C	2.961903	-1.340889	2.627212
H	3.117483	-1.554965	1.551409
H	2.650737	-2.287573	3.113661
H	3.929094	-1.035575	3.082005
C	1.695300	0.090708	4.309855
H	2.619431	0.558555	4.712665
H	1.481270	-0.817316	4.911838
H	0.862022	0.806388	4.467293
C	-0.005837	0.851377	-2.721517
H	-0.306661	1.907057	-2.637003
H	-0.686262	0.221248	-3.323777
C	1.372468	0.505107	-2.596381
H	2.088794	1.281242	-2.268668
C	1.768151	-0.866830	-2.588654
H	1.209602	-1.583075	-3.217960
C	3.068264	-1.326025	-2.064075
C	3.825437	-0.540996	-1.155775
C	3.555675	-2.610671	-2.399892
C	5.030973	-1.017183	-0.625588
H	3.442202	0.434424	-0.817081
C	4.764493	-3.087234	-1.868306
H	2.967328	-3.245601	-3.081865
C	5.511481	-2.292137	-0.981367
H	5.588595	-0.393712	0.091694
H	5.122056	-4.092756	-2.142162
H	6.455241	-2.669497	-0.556709
Pd	0.274401	-0.400802	-0.993499

Zero-point correction= 0.704559 (Hartree/Particle)
Thermal correction to Energy= 0.747125
Thermal correction to Enthalpy= 0.748069
Thermal correction to Gibbs Free Energy= 0.629536
Sum of electronic and zero-point Energies= -2094.957305
Sum of electronic and thermal Energies= -2094.914739
Sum of electronic and thermal Enthalpies= -2094.913795
Sum of electronic and thermal Free Energies= -2095.032328

SCF Done (in solvent): -2095.9687431

C	-2.632087	-2.300383	-1.788817
C	-3.753022	-1.845988	-2.511660
H	-3.855733	-2.102831	-3.576198
C	-4.732815	-1.049577	-1.897738
H	-5.592092	-0.690797	-2.486518
C	-4.621859	-0.701861	-0.543780
H	-5.391945	-0.069337	-0.078251
C	-3.524891	-1.132769	0.229636
C	-1.553263	-3.164779	-2.442100
H	-0.587539	-2.903371	-1.956091
C	-1.821863	-4.664745	-2.183224
H	-1.884872	-4.895914	-1.102602
H	-1.012509	-5.289200	-2.616908
H	-2.781930	-4.970626	-2.650577
C	-1.390687	-2.922778	-3.953808
H	-2.253443	-3.320077	-4.529143
H	-0.484761	-3.444081	-4.326183
H	-1.289933	-1.845839	-4.197212
C	-3.408936	-0.793280	1.712702
H	-2.329749	-0.782544	1.971658
C	-3.944916	0.602796	2.064160
H	-3.451532	1.382679	1.452177
H	-3.725018	0.830608	3.126579
H	-5.045084	0.680872	1.927295
C	-4.094651	-1.893419	2.553099
H	-5.181643	-1.943853	2.327571
H	-3.978447	-1.684134	3.637332
H	-3.662908	-2.895775	2.350368
C	-0.246952	0.406545	-2.395434
H	-0.466234	-0.538866	-2.914649
H	0.774450	0.827733	-2.533863
C	-1.332204	1.287879	-2.097011
H	-2.370648	0.956017	-2.288426
C	-1.051774	2.428851	-1.301390
H	-0.009068	2.828774	-1.329993
Pd	-0.472818	0.497115	-0.269713
O	3.876283	2.100863	-0.751310
C	2.788192	2.374370	-1.472210
O	1.846362	3.078373	-0.947457
O	2.708173	1.898877	-2.684329
K	2.366695	2.278318	1.349401
K	5.131340	1.624922	-2.808187
C	-2.066048	3.254911	-0.628534
C	-1.626036	4.360803	0.142140
C	-3.456523	2.980457	-0.669455
C	-2.539862	5.163463	0.840229
H	-0.545414	4.570606	0.183414
C	-4.369876	3.787187	0.024708
H	-3.826699	2.110492	-1.234441
C	-3.917872	4.882912	0.784169
H	-2.175320	6.015607	1.436610
H	-5.446192	3.553399	-0.018100
H	-4.636708	5.512189	1.333006

Zero-point correction= 0.721446 (Hartree/Particle)
Thermal correction to Energy= 0.772632
Thermal correction to Enthalpy= 0.773576
Thermal correction to Gibbs Free Energy= 0.634167
Sum of electronic and zero-point Energies= -3558.731766
Sum of electronic and thermal Energies= -3558.680580
Sum of electronic and thermal Enthalpies= -3558.679636
Sum of electronic and thermal Free Energies= -3558.819045

SCF Done (in solvent): -3559.799395

[Pd(IPr)(cin)Cl]-I-II				**[Pd(IPr)(cin)Cl]-II**			
91				91			
I-PREcin--K2CO3 SCF Done: -3559.42223871 A.U.				I-PREcin--K2CO3post SCF Done: -3559.47027570 A.U.			
Cl	-0.495375	1.183051	2.193042	Cl	0.661665	-1.440900	-2.212385
N	1.777972	1.711258	-0.787366	N	2.787008	0.200741	0.443091
C	0.654107	2.544905	-1.135280	C	2.897021	-1.127662	0.973869
N	3.010073	0.070875	-0.088221	N	1.990190	2.081316	-0.256828
C	-0.169785	2.159843	-2.230532	C	2.255302	-1.422465	2.211035
C	-1.227211	3.024424	-2.585288	C	2.453981	-2.710576	2.756063
H	-1.893155	2.748315	-3.414807	H	1.976796	-2.964723	3.715330
C	-1.440674	4.230704	-1.894517	C	3.257857	-3.663105	2.106859
H	-2.258254	4.901524	-2.205371	H	3.415291	-4.653803	2.563483
C	-0.618386	4.579348	-0.811286	C	3.860190	-3.352504	0.875783
H	-0.796977	5.521723	-0.270232	H	4.481065	-4.107389	0.367613
C	0.436016	3.736380	-0.393652	C	3.683050	-2.085176	0.275063
C	0.110642	0.889181	-3.031719	C	1.414276	-0.398609	2.971554
H	0.437355	0.122391	-2.301145	H	1.212437	0.447701	2.286049
C	-1.129099	0.327585	-3.744208	C	0.036535	-0.962415	3.365704
H	-1.996969	0.225869	-3.060237	H	-0.507143	-1.347582	2.477705
H	-0.892646	-0.672325	-4.166718	H	-0.580253	-0.159930	3.821343
H	-1.448517	0.961048	-4.599434	H	0.111930	-1.782328	4.111703
C	1.275478	1.127586	-4.018169	C	2.195979	0.149413	4.183061
H	1.026581	1.941923	-4.731603	H	2.427003	-0.652101	4.917616
H	1.477772	0.207547	-4.605216	H	1.599202	0.926714	4.704910
H	2.212463	1.403788	-3.491832	H	3.156833	0.608696	3.868904
C	1.313823	4.135970	0.791236	C	4.333150	-1.779369	-1.073780
H	1.896869	3.238628	1.086115	H	3.901799	-0.825062	-1.440402
C	0.496424	4.561819	2.025626	C	4.009116	-2.849127	-2.135812
H	-0.116949	5.466826	1.827285	H	4.411488	-3.847659	-1.860338
H	1.181288	4.810213	2.863302	H	4.466756	-2.568730	-3.107419
H	-0.159107	3.732165	2.355218	H	2.914243	-2.919882	-2.295564
C	2.295995	5.257002	0.382975	C	5.859953	-1.603892	-0.920658
H	2.862763	5.007871	-0.536969	H	6.118207	-0.822047	-0.177520
H	3.028086	5.451756	1.194340	H	6.320552	-1.319261	-1.889702
H	1.749358	6.203748	0.183853	H	6.336036	-2.549771	-0.583894
C	1.692226	0.454482	-0.220868	C	1.602856	0.784753	0.025890
C	3.111015	2.092009	-0.987576	C	3.857221	1.106365	0.420973
H	3.376637	3.053127	-1.435712	H	4.866132	0.822715	0.733509
C	3.887924	1.060846	-0.534240	C	3.351100	2.294208	-0.031346
H	4.974323	0.937446	-0.492184	H	3.822694	3.267763	-0.195646
C	3.394071	-1.222143	0.417875	C	1.034880	3.129444	-0.502465
C	3.845464	-2.201021	-0.504776	C	0.657248	3.939918	0.597439
C	4.140328	-3.481319	0.007104	C	-0.292290	4.954749	0.361493
H	4.486431	-4.273031	-0.673952	H	-0.611274	5.601554	1.194340
C	3.993630	-3.764786	1.373540	C	-0.848495	5.138895	-0.912666
H	4.223936	-4.774370	1.750050	H	-1.591106	5.935848	-1.077448
C	3.564880	-2.768874	2.262715	C	-0.473079	4.302085	-1.975157
H	3.466060	-3.001066	3.333753	H	-0.928200	4.448455	-2.967127
C	3.260249	-1.470446	1.806718	C	0.471203	3.271416	-1.793341
C	3.946735	-1.902840	-2.002827	C	1.222283	3.720872	2.001132
H	4.194177	-0.826139	-2.118078	H	1.891825	2.837520	1.968033
C	5.059958	-2.696545	-2.709540	C	2.073202	4.925131	2.452343
H	6.032463	-2.600200	-2.183746	H	2.892931	5.131200	1.733015
H	5.190865	-2.328508	-3.748307	H	2.526777	4.735679	3.448031
H	4.817426	-3.778237	-2.779522	H	1.458229	5.846822	2.532310
C	2.584995	-2.117901	-2.696318	C	0.114576	3.390425	3.020835
H	2.251331	-3.171211	-2.582628	H	-0.607992	4.226339	3.133173
H	2.658335	-1.891021	-3.780471	H	0.557269	3.194192	4.020088
H	1.807150	-1.465597	-2.255465	H	-0.449410	2.490205	2.709624
C	2.874349	-0.362753	2.780732	C	0.864397	2.355356	-2.948363
H	2.274686	0.386945	2.228851	H	1.390306	1.477219	-2.522573
C	1.984717	-0.846616	3.937072	C	-0.369672	1.798725	-3.682905
H	1.174753	-1.503789	3.559718	H	-1.064845	1.348478	-2.943354

H	1.496877	0.022916	4.419903	H	-0.059211	1.007185	-4.395741
H	2.559687	-1.394791	4.714959	H	-0.912986	2.582951	-4.252283
C	4.148926	0.345721	3.288386	C	1.833961	3.072880	-3.909390
H	4.806348	-0.362179	3.837630	H	1.360167	3.968066	-4.367063
H	3.883891	1.177062	3.975026	H	2.147222	2.393755	-4.730515
H	4.735354	0.767731	2.444979	H	2.747449	3.411890	-3.377369
C	-0.340174	-2.174424	-0.708675	C	-1.713116	1.156045	0.714995
H	0.419253	-2.972626	-0.781262	H	-1.644069	2.232214	0.466430
H	-0.671388	-1.775160	-1.688154	H	-1.716248	0.950889	1.803995
C	-1.295652	-2.253086	0.375304	C	-2.440395	0.258826	-0.149504
H	-1.210226	-3.062791	1.122565	H	-2.914856	0.718754	-1.044909
C	-2.400869	-1.358163	0.483164	C	-3.283479	-0.852768	0.457610
H	-2.386738	-0.470247	-0.167879	Pd	-0.286031	0.096855	-0.321673
Pd	0.093409	-0.525755	0.485799	H	-2.841204	-1.145765	1.436270
O	-4.250026	-1.143759	-2.991320	O	-2.036773	-3.759401	-1.100946
C	-3.978824	-0.827321	-1.780564	C	-2.297770	-3.028371	-0.094683
O	-3.837852	-1.860933	-0.912431	O	-3.249895	-2.032745	-0.392287
O	-3.770648	0.373254	-1.372982	O	-1.788902	-3.066646	1.049842
K	-3.314536	-3.421283	-2.742663	K	-2.225566	-1.741293	-2.814291
K	-2.836925	1.928792	0.344732	K	0.448296	-3.654409	-0.105364
C	-3.180168	-1.246831	1.753103	C	-4.750211	-0.479739	0.668294
C	-4.564710	-0.945059	1.734015	C	-5.109044	0.831385	1.051369
C	-2.532812	-1.358299	3.008088	C	-5.773859	-1.441860	0.524278
C	-5.277075	-0.769615	2.932399	C	-6.452385	1.169828	1.288320
C	-3.250188	-1.192600	4.203705	C	-7.118432	-1.102258	0.755226
C	-4.624711	-0.897591	4.173115	C	-7.464839	0.205259	1.138964
H	-5.059512	-0.880647	0.753989	H	-4.322076	1.593122	1.162571
H	-1.444957	-1.516489	3.037993	H	-5.501048	-2.464655	0.224817
H	-6.355496	-0.544355	2.895546	H	-6.710260	2.198769	1.587954
H	-2.722277	-1.273239	5.167381	H	-7.902134	-1.868233	0.635555
H	-5.184826	-0.763242	5.112673	H	-8.518532	0.471952	1.320237
Zero-point correction= 0.720816 (Hartree/Particle) Thermal correction to Energy= 0.771308 Thermal correction to Enthalpy= 0.772252 Thermal correction to Gibbs Free Energy= 0.634967 Sum of electronic and zero-point Energies= -3558.702670 Sum of electronic and thermal Energies= -3558.652178 Sum of electronic and thermal Enthalpies= -3558.651234 Sum of electronic and thermal Free Energies= -3558.788519				Zero-point correction= 0.722053 (Hartree/Particle) Thermal correction to Energy= 0.772857 Thermal correction to Enthalpy= 0.773802 Thermal correction to Gibbs Free Energy= 0.635425 Sum of electronic and zero-point Energies= -3558.748223 Sum of electronic and thermal Energies= -3558.697418 Sum of electronic and thermal Enthalpies= -3558.696474 Sum of electronic and thermal Free Energies= -3558.834851			
SCF Done (in solvent): -3559.7630889				SCF Done (in solvent): -3559.8117207			

[Pd(IPr)(cin)Cl]-III				**[Pd(IPr)(cin)Cl]-I'**			
89 I-PREcin+KCO3menysKClISOMERopen SCF Done: -2499.20243816 A.U.				89 I-PREcin+KCO3menysKCl SCF Done: -2499.22104425 A.U.			
N	2.523236	-0.096229	0.986340	N	1.683634	1.491455	0.792155
C	2.956444	1.237992	0.663397	C	1.230627	2.704120	0.151612
N	1.321098	-1.891477	1.062151	N	2.114424	-0.605045	1.143882
C	4.061306	1.389917	-0.211283	C	1.655777	2.945764	-1.178998
C	4.464030	2.703661	-0.527112	C	1.239502	4.149733	-1.782589
H	5.315435	2.864839	-1.204950	H	1.555212	4.373213	-2.813863
C	3.780740	3.809610	-0.003034	C	0.435773	5.064573	-1.088461
H	4.104412	4.829111	-0.267121	H	0.120508	6.000201	-1.577564
C	2.676947	3.628279	0.844921	C	0.022686	4.788317	0.222716
H	2.145225	4.511267	1.226801	H	-0.626009	5.502635	0.751197
C	2.236055	2.339119	1.203312	C	0.401179	3.597367	0.871984
C	4.718716	0.172419	-0.863060	C	2.557274	1.979162	-1.946083
H	4.670085	-0.666831	-0.136101	H	2.631043	1.041197	-1.360504
C	3.906495	-0.259611	-2.105397	C	1.949035	1.588025	-3.305157
H	2.842700	-0.449671	-1.845820	H	0.923476	1.189620	-3.161228
H	4.335798	-1.180496	-2.554620	H	2.564473	0.803642	-3.794027
H	3.924599	0.542725	-2.873390	H	1.892937	2.450789	-4.001738
C	6.202327	0.383239	-1.210615	C	3.983747	2.545981	-2.088918

H	6.333218	1.114433	-2.036511	H	3.988359	3.490510	-2.673863
H	6.653433	-0.571099	-1.553206	H	4.644008	1.820275	-2.609992
H	6.784656	0.747088	-0.338267	H	4.427513	2.763665	-1.095032
C	1.026453	2.121872	2.116841	C	-0.049020	3.306548	2.300532
H	0.411148	1.340970	1.619185	H	0.040817	2.209499	2.451182
C	0.126322	3.357995	2.257801	C	-1.520814	3.681361	2.551399
H	0.637174	4.195688	2.780175	H	-1.676290	4.781227	2.503899
H	-0.753308	3.094587	2.886891	H	-1.818534	3.358778	3.571650
H	-0.252818	3.715024	1.279851	H	-2.195097	3.176258	1.830173
C	1.442571	1.602835	3.510773	C	0.870578	4.025025	3.314695
H	2.030950	0.666192	3.454036	H	1.939361	3.755512	3.190989
H	0.542219	1.390902	4.127559	H	0.576260	3.775259	4.356051
H	2.053262	2.358728	4.049983	H	0.793143	5.127118	3.194684
C	1.383413	-0.656579	0.439294	C	1.290632	0.227894	0.422363
C	3.153668	-0.961067	1.888429	C	2.728902	1.445876	1.715984
H	4.076480	-0.687369	2.409565	H	3.186577	2.356509	2.111197
C	2.389643	-2.097478	1.939776	C	2.994790	0.122937	1.948105
H	2.501775	-3.021597	2.514885	H	3.730559	-0.369862	2.590379
C	0.191054	-2.759546	0.890314	C	2.230727	-2.020629	0.897545
C	0.191641	-3.690412	-0.177440	C	3.317938	-2.453715	0.099085
C	-0.962603	-4.482444	-0.347092	C	3.413202	-3.834437	-0.176362
H	-1.003236	-5.206319	-1.176031	H	4.243225	-4.206850	-0.797394
C	-2.061472	-4.355845	0.516195	C	2.450815	-4.730299	0.306700
H	-2.952560	-4.985995	0.365594	H	2.534286	-5.803877	0.073434
C	-2.033202	-3.424696	1.566172	C	1.373636	-4.265661	1.079438
H	-2.904322	-3.329249	2.234046	H	0.623049	-4.982904	1.441559
C	-0.909781	-2.599153	1.769664	C	1.234967	-2.900058	1.398421
C	1.363372	-3.789342	-1.149451	C	4.331340	-1.482818	-0.508431
H	2.197038	-3.191975	-0.723894	H	4.081630	-0.458758	-0.164679
C	1.861904	-5.237285	-1.318650	C	5.764208	-1.782459	-0.025751
H	2.120717	-5.697801	-0.342190	H	5.828685	-1.759023	1.081991
H	2.766254	-5.260765	-1.962029	H	6.477536	-1.033106	-0.428645
H	1.099122	-5.882269	-1.804636	H	6.108315	-2.784547	-0.359407
C	0.991894	-3.139706	-2.498764	C	4.235997	-1.464273	-2.047044
H	0.145858	-3.673479	-2.982565	H	4.476686	-2.455400	-2.486279
H	1.857491	-3.158345	-3.194019	H	4.946533	-0.723730	-2.470407
H	0.697026	-2.077061	-2.326863	H	3.215717	-1.184033	-2.373144
C	-0.911104	-1.525419	2.855633	C	0.078648	-2.375138	2.241825
H	0.110073	-1.097104	2.910660	H	-0.291096	-1.439087	1.766471
C	-1.849891	-0.368326	2.456694	C	-1.140115	-3.306866	2.271335
H	-1.561700	0.045726	1.467746	H	-1.484826	-3.545049	1.244197
H	-1.785614	0.443082	3.216726	H	-1.974452	-2.785207	2.780578
H	-2.903839	-0.720343	2.396082	H	-0.944280	-4.257585	2.814280
C	-1.251178	-2.089146	4.247408	C	0.550054	-2.038306	3.672928
H	-2.288247	-2.485423	4.291583	H	0.900141	-2.949779	4.204735
H	-1.167091	-1.294522	5.018729	H	-0.284171	-1.594804	4.255719
H	-0.563847	-2.913705	4.527717	H	1.381058	-1.303942	3.672291
C	0.391859	0.974494	-2.925190	C	0.536292	-1.823245	-2.031664
H	1.194432	0.446255	-3.465463	H	1.204509	-2.596333	-1.620961
H	0.544983	2.055732	-2.760459	H	0.934498	-1.274370	-2.903625
C	-0.898581	0.430651	-2.850929	C	-0.877368	-1.998864	-1.894473
H	-1.085178	-0.552927	-3.324447	H	-1.253599	-2.828532	-1.268656
C	-2.167383	1.250805	-2.697307	C	-1.771512	-0.969346	-2.278019
H	-2.566338	1.433330	-3.723768	H	-1.424250	-0.224508	-3.018689
Pd	0.154538	0.066660	-0.968559	Pd	-0.261821	-0.282269	-0.738367
O	-2.301980	3.885365	-0.402283	O	-3.368638	1.403011	1.233930
C	-1.911563	2.769574	-0.828854	C	-2.384130	0.669260	0.863732
O	-1.959522	2.598782	-2.210918	O	-1.435022	1.218569	0.113954
O	-1.554441	1.777221	-0.112432	O	-2.300361	-0.592217	1.168101
K	-3.436159	2.396087	1.412047	K	-4.735462	-0.651164	1.533867
C	-3.293336	0.574100	-1.904186	C	-3.222269	-0.956283	-2.016513
C	-3.109721	-0.619009	-1.173476	C	-3.911056	0.284849	-2.000791
C	-4.545052	1.227371	-1.834754	C	-3.974598	-2.140215	-1.801111

C -4.145042 -1.136088 -0.375582 C -5.582210 0.716838 -1.030112 C -5.382136 -0.467769 -0.291297 H -2.118828 -1.111703 -1.183262 H -4.690323 2.163755 -2.398131 H -3.969461 -2.061936 0.193554 H -6.554548 1.235717 -0.992855 H -6.194456 -0.877285 0.331454	C -5.299125 0.338198 -1.798506 C -5.365594 -2.088151 -1.604105 C -6.039699 -0.847472 -1.607111 H -3.331758 1.215084 -2.105983 H -3.466612 -3.117089 -1.823515 H -5.806620 1.315799 -1.783020 H -5.933170 -3.024551 -1.473601 H -7.134173 -0.807662 -1.481400
Zero-point correction= 0.719540 (Hartree/Particle) Thermal correction to Energy= 0.766300 Thermal correction to Enthalpy= 0.767244 Thermal correction to Gibbs Free Energy= 0.638175 Sum of electronic and zero-point Energies= -2498.482898 Sum of electronic and thermal Energies= -2498.436139 Sum of electronic and thermal Enthalpies= -2498.435194 Sum of electronic and thermal Free Energies= -2498.564263 SCF Done (in solvent): -2499.5281348	Zero-point correction= 0.719611 (Hartree/Particle) Thermal correction to Energy= 0.766567 Thermal correction to Enthalpy= 0.767511 Thermal correction to Gibbs Free Energy= 0.639114 Sum of electronic and zero-point Energies= -2498.501433 Sum of electronic and thermal Energies= -2498.454477 Sum of electronic and thermal Enthalpies= -2498.453533 Sum of electronic and thermal Free Energies= -2498.581930 SCF Done (in solvent): -2499.5397451

[Pd(IPr)(cin)Cl]-I'-III	
89 I-PREcin+KCO3--C-O SCF Done: -2499.18037777 A.U. N 1.723100 1.763645 0.712858 C 0.691294 2.754349 0.534727 N 2.786157 -0.122437 0.706950 C 0.738880 3.562411 -0.625890 C -0.262773 4.541844 -0.780685 H -0.263951 5.180883 -1.677313 C -1.276503 4.686015 0.174265 H -2.061316 5.445717 0.032193 C -1.322925 3.841713 1.294127 H -2.156352 3.946146 2.002481 C -0.343506 2.851652 1.503506 C 1.747403 3.291747 -1.739207 H 2.564842 2.668806 -1.318171 C 1.057093 2.451247 -2.835769 H 0.603182 1.542091 -2.387497 H 1.784316 2.141854 -3.615866 H 0.244339 3.030927 -3.322177 C 2.389390 4.568751 -2.309845 H 1.644520 5.210072 -2.826802 H 3.166290 4.306914 -3.058429 H 2.866381 5.178157 -1.514040 C -0.407805 1.893111 2.694095 H -0.160253 0.888390 2.287088 C -1.816281 1.789331 3.304750 H -2.087234 2.700306 3.881483 H -1.848294 0.936992 4.018502 H -2.574728 1.639468 2.508742 C 0.618886 2.250935 3.790767 H 1.660254 2.230333 3.414808 H 0.554836 1.527510 4.631828 H 0.420532 3.265618 4.198096 C 1.583428 0.446627 0.321025 C 2.969600 2.006599 1.295810 H 3.260604 3.001408 1.646478 C 3.638762 0.810638 1.302564 H 4.627106 0.536702 1.684229 C 3.061345 -1.518468 0.510265 C 3.900209 -1.902425 -0.568196 C 4.066410 -3.282924 -0.796009 H 4.699067 -3.624978 -1.628408 C 3.429665 -4.233333 0.018769 H 3.566738 -5.307440 -0.185008	

C 2.632661 -3.822507 1.095924 H 2.152093 -4.578038 1.737768 C 2.436134 -2.453802 1.371562 C 4.553282 -0.852015 -1.469591 H 4.797840 0.022732 -0.828609 C 5.872097 -1.326321 -2.104128 H 6.576690 -1.727003 -1.345722 H 6.369006 -0.482081 -2.625414 H 5.702525 -2.117910 -2.864716 C 3.567037 -0.352860 -2.547638 H 3.296160 -1.178477 -3.239004 H 4.024894 0.463104 -3.145533 H 2.628061 0.022592 -2.096815 C 1.583892 -2.018800 2.563569 H 1.638301 -0.912541 2.630105 C 0.098876 -2.377190 2.355257 H -0.270757 -1.895642 1.419052 H -0.511404 -2.005654 3.207067 H -0.046189 -3.476243 2.275678 C 2.133351 -2.588366 3.887098 H 2.067175 -3.696922 3.916193 H 1.550661 -2.198561 4.748549 H 3.197429 -2.311239 4.037804 C 0.287467 -1.353214 -2.374064 H 1.025556 -2.174890 -2.366056 H 0.447704 -0.611696 -3.178885 C -1.055505 -1.647536 -1.939181 H -1.188840 -2.586375 -1.375658 C -2.250934 -0.900079 -2.256600 H -2.249115 -0.337381 -3.204097 Pd -0.001462 -0.430233 -0.499196 O -3.746529 1.262828 0.375027 C -2.709384 0.717499 -0.122856 O -2.460447 0.802457 -1.422917 O -1.906626 0.000029 0.634424 K -3.989272 -0.775982 1.817957 C -3.587504 -1.455316 -1.862680 C -3.736989 -2.684871 -1.174665 C -4.757713 -0.694932 -2.116568 C -5.003117 -3.132779 -0.748571 C -6.019232 -1.138100 -1.694302 C -6.151187 -2.358825 -1.002338 H -2.856124 -3.311023 -0.972224 H -4.646838 0.285012 -2.602352 H -5.091822 -4.103212 -0.232463 H -6.907877 -0.519254 -1.895646 H -7.143381 -2.710558 -0.676145	
Zero-point correction= 0.718875 (Hartree/Particle) Thermal correction to Energy= 0.764966 Thermal correction to Enthalpy= 0.765911 Thermal correction to Gibbs Free Energy= 0.637650 Sum of electronic and zero-point Energies= -2498.461502 Sum of electronic and thermal Energies= -2498.415411 Sum of electronic and thermal Enthalpies= -2498.414467 Sum of electronic and thermal Free Energies= -2498.542728 SCF Done (in solvent): -2499.4919674	

[Pd(IPr*)(cin)Cl]	**[Pd(IPr*)(cin)Cl]-I**
141 StI-PREcin SCF Done: -3628.57085686 A.U.	147 StI-PREcin+K2CO3 SCF Done: -5092.38002416 A.U.

Cl	-2.834778	0.473082	-1.256365
C	0.610190	-2.226271	-2.177556
H	1.367729	-2.617448	-1.485694
H	1.029967	-1.695709	-3.047814
C	-0.658880	-2.877508	-2.288337
H	-0.919209	-3.690684	-1.585887
C	-1.678400	-2.281985	-3.073562
H	-1.372409	-1.595605	-3.885663
Pd	-0.878996	-0.885632	-1.475438
N	0.194156	-0.355508	1.260511
C	-2.555103	-1.037684	1.991217
H	-2.413226	-0.413886	1.080190
C	-1.422982	-2.061176	2.030303
C	-0.102063	-1.714542	1.655111
C	0.082281	0.118054	-0.025888
C	0.961815	-2.653566	1.691774
C	2.376982	-2.239446	1.285548
H	2.263144	-1.548462	0.418190
C	-1.654460	-3.376374	2.482619
H	-2.676715	-3.663156	2.769844
C	-0.609470	-4.305258	2.572158
H	-0.808228	-5.321332	2.947892
C	0.687594	-3.946864	2.178823
H	1.505120	-4.680478	2.238865
C	0.723071	0.616793	2.116176
C	0.962840	1.721303	1.349981
H	1.343219	2.711947	1.612996
H	0.883771	0.426621	3.179916
N	0.568236	1.400822	0.041141
C	0.831359	2.244870	-1.103772
C	-0.083837	3.271911	-1.453485
C	2.057683	2.074747	-1.791170
C	0.230432	4.088614	-2.555911
C	2.352619	2.947909	-2.859555
C	1.437313	3.929951	-3.255189
H	-0.478539	4.878749	-2.844806
H	3.325504	2.856969	-3.367113
H	1.674815	4.596980	-4.098868
C	-1.300169	3.561135	-0.571429
H	-1.776700	2.578424	-0.355153
C	3.087078	1.032103	-1.363348
H	2.711962	0.570764	-0.426855
C	3.301440	-0.125087	-2.341303
C	3.987657	-1.265582	-1.867092
C	2.883204	-0.111338	-3.686333
C	4.238011	-2.366306	-2.698392
H	4.341525	-1.297140	-0.825190
C	3.147092	-1.206873	-4.531348
H	2.320762	0.748581	-4.077445
C	3.818848	-2.339111	-4.041294
H	4.752411	-3.247635	-2.285248
H	2.805748	-1.177102	-5.578363
H	4.010385	-3.200325	-4.700462
C	4.401810	1.737899	-0.994809
C	4.459370	2.498331	0.193955
C	5.543807	1.685664	-1.818381
C	5.629719	3.182887	0.555493
H	3.572404	2.545614	0.844787
C	6.716318	2.376906	-1.461684
H	5.516944	1.088791	-2.743415
C	6.765827	3.124659	-0.273360
H	5.654682	3.766876	1.489652
H	7.599734	2.324391	-2.117936

Cl	2.939643	0.005799	0.163260
N	-0.724856	-0.643698	1.348018
C	-0.710017	-2.066972	1.575284
N	-0.799665	1.328264	0.459015
C	-1.819081	-2.830048	1.127752
C	-1.923580	-4.172766	1.552454
H	-2.784071	-4.769804	1.211993
C	-0.949446	-4.737873	2.389668
H	-1.056737	-5.778137	2.736940
C	0.176480	-3.984482	2.767229
H	0.968449	-4.438451	3.382471
C	0.322936	-2.640413	2.361451
C	-2.866651	-2.259229	0.170627
H	-2.476183	-1.277560	-0.177494
C	1.556459	-1.828337	2.743007
H	1.774309	-1.151041	1.885034
C	-0.315044	0.052170	0.230273
C	-1.425776	0.185738	2.240939
H	-1.805006	-0.188237	3.194613
C	-1.471323	1.427466	1.678778
H	-1.910904	2.364005	2.031197
C	-0.764786	2.326056	-0.586843
C	-1.845578	2.348785	-1.498431
C	-1.743078	3.191657	-2.621809
H	-2.555425	3.198551	-3.364298
C	-0.623127	4.023953	-2.782659
H	-0.544382	4.668428	-3.672147
C	0.379400	4.072299	-1.797647
H	1.222000	4.772393	-1.897915
C	0.321549	3.229560	-0.671967
C	-3.130806	1.605247	-1.128579
H	-2.830377	0.652316	-0.646255
C	1.283442	3.318740	0.511245
H	1.645270	2.285671	0.705161
C	-0.247285	-0.266591	-3.049579
H	-1.259090	0.161579	-3.011332
H	-0.150183	-1.329805	-3.335664
C	0.855330	0.595303	-3.335514
H	0.704448	1.688854	-3.391903
C	2.150784	0.032505	-3.328788
H	2.274184	-1.054691	-3.536518
Pd	0.992354	-0.190816	-1.310131
O	3.054740	-3.769863	-1.389988
C	2.581753	-3.234091	-2.514834
O	3.407173	-2.692882	-3.343853
O	1.293108	-3.225004	-2.712269
K	4.844472	-1.928301	-1.397005
K	0.845595	-4.710365	-0.768626
C	3.387959	0.825851	-3.420711
C	4.536693	0.227659	-4.005305
C	3.482966	2.163150	-2.963328
C	5.732154	0.954084	-4.139362
H	4.457293	-0.815542	-4.353871
C	4.672472	2.890100	-3.114752
H	2.620249	2.624999	-2.459185
C	5.803822	2.290232	-3.700322
H	6.610776	0.478096	-4.605619
H	4.722371	3.927570	-2.750152
H	6.738515	2.863215	-3.811975
C	2.522498	4.184478	0.292916
C	2.447023	5.595501	0.298306
C	3.779930	3.572693	0.114574
C	3.599563	6.376797	0.115385

H	7.686111	3.660558	0.007934
C	-2.358952	4.409204	-1.280767
C	-3.118495	3.819026	-2.317008
C	-2.588018	5.762803	-0.960583
C	-4.077125	4.568329	-3.016004
H	-2.953875	2.756782	-2.557856
C	-3.549431	6.514156	-1.662544
H	-2.012542	6.236071	-0.150224
C	-4.296115	5.921019	-2.693593
H	-4.663818	4.089517	-3.816612
H	-3.715441	7.570577	-1.396270
H	-5.050266	6.508272	-3.241793
C	-0.831696	4.153840	0.757203
C	-1.440064	3.742546	1.958934
C	0.238317	5.073194	0.820990
C	-0.977468	4.211048	3.198700
H	-2.258497	3.008432	1.924043
C	0.701200	5.550691	2.059981
H	0.731316	5.395444	-0.109859
C	0.099528	5.113805	3.254678
H	-1.449799	3.843402	4.122504
H	1.542769	6.261411	2.091924
H	0.471677	5.474556	4.226931
C	3.251204	-3.391459	0.760300
C	4.624275	-3.477667	1.070599
C	2.713964	-4.347631	-0.133476
C	5.436447	-4.473786	0.497575
H	5.070422	-2.753948	1.768467
C	3.518423	-5.347830	-0.699919
H	1.642769	-4.318299	-0.381492
C	4.888946	-5.414103	-0.390457
H	6.506615	-4.514523	0.755790
H	3.070486	-6.076254	-1.394228
H	5.523843	-6.195771	-0.836530
C	3.047661	-1.427435	2.399982
C	3.924797	-0.371349	2.077618
C	2.798229	-1.700004	3.760872
C	4.522777	0.407741	3.080135
H	4.140730	-0.140688	1.024131
C	3.391075	-0.920219	4.769736
H	2.113876	-2.518115	4.034091
C	4.251079	0.140515	4.433751
H	5.192897	1.232717	2.791483
H	3.175045	-1.141938	5.827127
H	4.708691	0.755725	5.224579
C	-3.917095	-1.718841	1.820662
C	-4.303450	-2.176203	0.542472
C	-4.774459	-1.954326	2.916264
C	-5.524204	-2.846722	0.365065
H	-3.650274	-1.987673	-0.323224
C	-5.994195	-2.631991	2.740091
H	-4.485133	-1.598540	3.917717
C	-6.373361	-3.078409	1.462410
H	-5.808102	-3.180571	-0.643829
H	-6.652234	-2.806282	3.606798
H	-7.332331	-3.602324	1.320022
C	-2.535028	-0.083528	3.184978
C	-3.400197	1.033937	3.163414
C	-1.736570	-0.294260	4.326350
C	-3.473703	1.907754	4.258051
H	-4.033515	1.196789	2.276046
C	-1.796420	0.589574	5.420429
H	-1.064140	-1.166049	4.364188
H	1.475295	6.087228	0.463751
C	4.936551	4.355169	-0.052344
H	3.841794	2.472482	0.096673
C	4.851676	5.757717	-0.057367
H	3.522031	7.475949	0.120043
H	5.909872	3.858388	-0.191602
H	5.758307	6.369543	-0.190258
C	0.506755	3.769009	1.756163
C	0.846867	3.235696	3.014622
C	-0.583117	4.662600	1.672336
C	0.104101	3.562927	4.159457
H	1.675625	2.515558	3.084948
C	-1.327649	4.996079	2.817326
H	-0.889899	5.060199	0.692195
C	-0.990017	4.442402	4.064966
H	0.367152	3.101057	5.123407
H	-2.192643	5.671499	2.726260
H	-1.585031	4.686548	4.959302
C	2.779943	-2.741803	2.863974
C	3.364329	-3.085006	4.099360
C	3.296791	-3.316427	1.682116
C	4.440664	-3.992604	4.152445
H	2.976081	-2.638954	5.028496
C	4.358788	-4.233727	1.735012
H	2.869356	-3.063906	0.694251
C	4.938679	-4.574240	2.973430
H	4.888434	-4.248946	5.126219
H	4.716759	-4.683636	0.794114
H	5.774470	-5.290950	3.019348
C	1.363204	-0.937405	3.963617
C	0.365802	-1.163545	4.932149
C	2.275669	0.122647	4.162088
C	0.279751	-0.350209	6.077707
H	-0.346996	-1.992178	4.791573
C	2.204043	0.922492	5.312284
H	3.050403	0.304084	3.399070
C	1.202816	0.690278	6.274948
H	-0.507473	-0.539302	6.825155
H	2.924684	1.743961	5.452812
H	1.143789	1.320504	7.176609
C	-2.915684	-3.156782	-1.072110
C	-3.930097	-4.107504	-1.307548
C	-1.839489	-3.072942	-1.980374
C	-3.874316	-4.937413	-2.443197
H	-4.775911	-4.194454	-0.607517
C	-1.776477	-3.900595	-3.114478
H	-1.014263	-2.367133	-1.788012
C	-2.803344	-4.834900	-3.350853
H	-4.678284	-5.670324	-2.619120
H	-0.900386	-3.811028	-3.777420
H	-2.766702	-5.485793	-4.239086
C	-4.218228	-1.959695	0.818414
C	-4.384298	-1.936585	2.218448
C	-5.317074	-1.594691	0.005387
C	-5.610853	-1.556288	2.793342
H	-3.541129	-2.215763	2.869128
C	-6.545143	-1.227333	0.576934
H	-5.201876	-1.575692	-1.088735
C	-6.697214	-1.203328	1.975322
H	-5.715676	-1.538451	3.889888
H	-7.381830	-0.936899	-0.077306
H	-7.657703	-0.905843	2.424612
C	-4.017606	1.214480	-2.307501

C	-2.668790	1.689765	5.393362
H	-4.155694	2.772196	4.221555
H	-1.163131	0.408227	6.303783
H	-2.724903	2.376139	6.253273
C	-3.083931	-2.731377	-3.120547
C	-4.083172	-1.831086	-3.567152
C	-3.477141	-4.039672	-2.746660
C	-5.424482	-2.231212	-3.650936
C	-4.818143	-4.442350	-2.842899
C	-5.798229	-3.541505	-3.299427
H	-3.794253	-0.798992	-3.816786
H	-2.719649	-4.762521	-2.405044
H	-6.186955	-1.512460	-3.990664
H	-5.100365	-5.468816	-2.559498
H	-6.850737	-3.857821	-3.373632

Zero-point correction= 1.118211 (Hartree/Particle)
Thermal correction to Energy= 1.186619
Thermal correction to Enthalpy= 1.187563
Thermal correction to Gibbs Free Energy= 1.009287
Sum of electronic and zero-point Energies= -3627.452646
Sum of electronic and thermal Energies= -3627.384238
Sum of electronic and thermal Enthalpies= -3627.383293
Sum of electronic and thermal Free Energies= -3627.561570

SCF Done (in solvent): -3629.1817629

C	-4.979013	2.095405	-2.844915
C	-3.882852	-0.068276	-2.881128
C	-5.774278	1.707178	-3.937643
H	-5.116626	3.089000	-2.389907
C	-4.679649	-0.462592	-3.968418
H	-3.152292	-0.780082	-2.467561
C	-5.628045	0.427720	-4.503060
H	-6.520888	2.407825	-4.344631
H	-4.556820	-1.472880	-4.389767
H	-6.256296	0.123430	-5.355190
C	-3.881782	2.413948	-0.055750
C	-3.840563	3.823510	-0.015783
C	-4.611744	1.734427	0.941259
C	-4.516823	4.533432	0.992846
H	-3.256241	4.374775	-0.768483
C	-5.284382	2.439197	1.950623
H	-4.633014	0.636954	0.938401
C	-5.239124	3.845213	1.982359
H	-4.469018	5.634124	1.007882
H	-5.837255	1.877749	2.720341
H	-5.758565	4.401463	2.778759

Zero-point correction= 1.136446 (Hartree/Particle)
Thermal correction to Energy= 1.212920
Thermal correction to Enthalpy= 1.213864
Thermal correction to Gibbs Free Energy= 1.019528
Sum of electronic and zero-point Energies= -5091.243578
Sum of electronic and thermal Energies= -5091.167104
Sum of electronic and thermal Enthalpies= -5091.166160
Sum of electronic and thermal Free Energies= -5091.360496

SCF Done (in solvent): -5093.0148613

[Pd(IPr*)(cin)Cl]-I-II

147

StI-PREcin--K2CO3 SCF Done: -5092.34752390 A.U.

Cl	1.159188	-2.972274	0.662216
N	0.695833	0.896102	1.437550
C	0.660743	-0.045384	2.528961
N	0.502135	1.776691	-0.524298
C	-0.582148	-0.253166	3.172915
C	-0.632948	-1.164373	4.247037
H	-1.590801	-1.325141	4.767367
C	0.529997	-1.841292	4.654768
H	0.485201	-2.547020	5.500135
C	1.750018	-1.625004	3.994763
H	2.649921	-2.178153	4.300981
C	1.841862	-0.724659	2.915712
C	-1.797678	0.562106	2.729877
H	-1.729005	0.624618	1.622398
C	3.140395	-0.526059	2.125549
H	2.862472	-0.789637	1.082940
C	0.426804	0.556668	0.125202
C	0.898917	2.271198	1.594192
H	1.097409	2.722998	2.567453
C	0.795249	2.826928	0.352215
H	0.886613	3.861694	0.011796
C	0.236028	1.940099	-1.923484
C	-1.025631	2.450603	-2.317135
C	-1.286287	2.566250	-3.695680
H	-2.256746	2.959981	-4.030434
C	-0.325613	2.178582	-4.641661
H	-0.547364	2.268645	-5.716696
C	0.923370	1.692131	-4.225841
H	1.677182	1.414389	-4.975491

[Pd(IPr*)(cin)Cl]-II

147

StI-PREcin--K2CO3post SCF Done: -5092.38991160 A.U.

Cl	-0.667739	-2.853369	0.486333
N	-1.637450	0.461915	-0.746308
C	-1.488520	-0.122018	-2.050894
N	-1.160379	1.299556	1.189704
C	-0.453937	0.357682	-2.901718
C	-0.417286	-0.108758	-4.233263
H	0.354948	0.290769	-4.908380
C	-1.338150	-1.056879	-4.696265
H	-1.293903	-1.407896	-5.739585
C	-2.323995	-1.557553	-3.827535
H	-3.036871	-2.314583	-4.187653
C	-2.428006	-1.097497	-2.497151
C	0.576061	1.393471	-2.450399
H	0.480624	1.493001	-1.348543
C	-3.539860	-1.610213	-1.567795
H	-3.096277	-1.643502	-0.549584
C	-0.659233	0.430370	0.239710
C	-2.698488	1.315959	-0.403286
H	-3.547547	1.491911	-1.066893
C	-2.406288	1.822035	0.830776
H	-2.961412	2.497588	1.487053
C	-0.442197	1.757278	2.348116
C	0.112424	3.061219	2.328100
C	0.679448	3.546040	3.526082
H	1.114523	4.555793	3.542685
C	0.717272	2.753881	4.681144
H	1.156754	3.156192	5.607430
C	0.221186	1.439747	4.654136
H	0.293464	0.801014	5.547948

C	1.232265	1.566819	-2.858454	C	-0.354413	0.913896	3.483761
C	-2.047315	2.901209	-1.272104	C	0.155606	3.897115	1.043925
H	-1.672735	2.537111	-0.292640	H	-0.337793	3.301061	0.251857
C	2.614458	1.119810	-2.381004	C	-0.868691	-0.518704	3.391708
H	2.534669	1.017880	-1.280303	H	-0.641694	-0.840901	2.341777
C	-1.400710	-0.867539	-2.206230	C	2.783156	0.083730	0.865853
H	-1.190637	-0.129305	-2.998565	H	2.778196	0.684909	1.794488
H	-2.319954	-0.651087	-1.629987	H	3.135404	0.642688	-0.020146
C	-1.009369	-2.234482	-2.438659	C	2.988585	-1.334482	0.963910
H	-0.421690	-2.463457	-3.344910	H	3.175174	-1.750284	1.976971
C	-1.406449	-3.316484	-1.598740	C	3.677055	-2.106880	-0.139766
H	-1.819300	-3.068442	-0.612646	Pd	0.939986	-0.798971	0.534033
Pd	0.036566	-1.221763	-0.734816	H	3.279942	-1.759581	-1.114766
O	-5.123479	-2.748595	-0.839307	O	1.888347	-5.104432	-0.662681
C	-4.027938	-3.412490	-0.742096	C	2.554497	-4.098064	-1.044347
O	-3.385853	-3.708617	-1.891584	O	3.312177	-3.514057	-0.007673
O	-3.487851	-3.751101	0.375070	O	2.577061	-3.560422	-2.182074
K	-4.444411	-1.805835	-3.105549	K	1.556674	-4.250862	1.857815
K	-1.488424	-3.780365	1.874300	K	0.028170	-3.757367	-2.317316
C	-0.770090	-4.653341	-1.705588	C	5.192188	-1.988369	-0.243730
C	-1.412418	-5.797900	-1.172679	C	5.923879	-1.010028	0.455986
C	0.513308	-4.803987	-2.278880	C	5.872618	-2.812397	-1.168664
C	-0.780992	-7.051348	-1.209944	C	7.305260	-0.853683	0.236947
C	1.140312	-6.058958	-2.319135	C	7.249375	-2.656492	-1.391023
C	0.498521	-7.189050	-1.782548	C	7.973060	-1.672522	-0.689089
H	-2.424514	-5.674998	-0.757523	H	5.400042	-0.351351	1.165219
H	1.044914	-3.918306	-2.653653	H	5.296067	-3.565559	-1.728497
H	-1.298092	-7.933820	-0.798712	H	7.862274	-0.081495	0.792480
H	2.146670	-6.148854	-2.759775	H	7.762957	-3.302722	-2.121496
H	0.992010	-8.174028	-1.810058	H	9.053452	-1.546253	-0.865473
C	-2.107711	4.429746	-1.131144	C	2.037165	0.974774	-2.649781
C	-3.168337	5.028353	-0.414699	C	3.040770	1.906608	-2.298688
C	-1.083693	5.263577	-1.627679	C	2.444948	-0.311401	-3.049860
C	-3.199614	6.414852	-0.194823	C	4.399770	1.564507	-2.350612
H	-3.982363	4.397012	-0.025146	H	2.746076	2.907861	-1.954893
C	-1.110273	6.652258	-1.404841	C	3.808939	-0.654547	-3.117819
H	-0.255679	4.822540	-2.204422	H	1.703487	-1.088400	-3.277033
C	-2.167242	7.234503	-0.686026	C	4.794724	0.278305	-2.762906
H	-4.038308	6.857949	0.365886	H	5.151130	2.307137	-2.039560
H	-0.298798	7.282423	-1.802582	H	4.082063	-1.684574	-3.390800
H	-2.190979	8.322118	-0.514073	H	5.857383	-0.010722	-2.767865
C	-3.421554	2.253321	-1.444251	C	0.224806	2.764687	-3.042524
C	-3.768766	1.150000	-0.636554	C	0.888739	3.301743	-4.163936
C	-4.376372	2.735191	-2.367201	C	-0.802667	3.525029	-2.444024
C	-5.030407	0.535374	-0.733020	C	0.551357	4.575727	-4.654282
H	-3.032577	0.764180	0.084972	H	1.700100	2.725885	-4.635585
C	-5.636331	2.121295	-2.482077	C	-1.140593	4.799152	-2.925738
H	-4.147231	3.627095	-2.972076	H	-1.341516	3.111928	-1.577090
C	-5.968929	1.023270	-1.663364	C	-0.458004	5.333383	-4.033345
H	-5.263016	-0.341822	-0.108313	H	1.089762	4.983627	-5.524903
H	-6.372990	2.519343	-3.198760	H	-1.924688	5.382890	-2.417729
H	-6.964612	0.555445	-1.734487	H	-0.710077	6.337366	-4.410124
C	-3.131970	-0.114890	3.032659	C	-4.739190	-0.658692	-1.518790
C	-3.650162	-1.052871	2.115140	C	-5.460203	-0.525072	-0.314156
C	-3.857185	0.149327	4.213794	C	-5.140333	0.102725	-2.636513
C	-4.865942	-1.717392	2.355182	C	-6.549907	0.353808	-0.222393
H	-3.105501	-1.278543	1.180998	H	-5.134162	-1.086761	0.573654
C	-5.070113	-0.516944	4.465962	C	-6.235520	0.982149	-2.548647
H	-3.473619	0.891294	4.932338	H	-4.570632	0.032129	-3.576708
C	-5.577725	-1.446405	3.538587	C	-6.942702	1.112820	-1.340815
H	-5.225600	-2.425859	1.590259	H	-7.085019	0.457271	0.735039
H	-5.627768	-0.299488	5.391477	H	-6.530317	1.575594	-3.428887
H	-6.534857	-1.955898	3.735027	H	-7.793656	1.808632	-1.269016

C	-1.718991	2.001529	3.246130
C	-1.016206	2.336176	4.421589
C	-2.342184	3.034291	2.514285
C	-0.913477	3.675492	4.839986
H	-0.519404	1.541920	5.000523
C	-2.231905	4.372226	2.921245
H	-2.914252	2.781069	1.607392
C	-1.511141	4.698847	4.085037
H	-0.353499	3.919258	5.757115
H	-2.695391	5.165008	2.314806
H	-1.416405	5.749930	4.400601
C	3.616622	0.924346	2.109772
C	4.172953	1.460871	0.931180
C	3.517683	1.751778	3.247726
C	4.574517	2.804742	0.868208
H	4.285244	0.814986	0.045700
C	3.936910	3.092998	3.197899
H	3.070056	1.347127	4.170278
C	4.452352	3.626935	2.003581
H	4.976986	3.208043	-0.073750
H	3.845026	3.728449	4.093533
H	4.762385	4.682944	1.956407
C	4.264544	-1.484027	2.532905
C	5.156500	-1.176951	3.582830
C	4.410132	-2.716017	1.859639
C	6.162739	-2.083239	3.959436
H	5.072081	-0.212645	4.107146
C	5.420025	-3.619639	2.231669
H	3.700165	-2.970513	1.057278
C	6.298908	-3.309223	3.284468
H	6.850119	-1.824760	4.781057
H	5.518199	-4.575453	1.692120
H	7.091238	-4.017671	3.575018
C	3.679191	2.206795	-2.579523
C	5.050664	1.869985	-2.601295
C	3.326833	3.573690	-2.605288
C	6.037920	2.868992	-2.645176
H	5.347542	0.810202	-2.574010
C	4.312101	4.574746	-2.648557
H	2.263378	3.859197	-2.585248
C	5.674186	4.227433	-2.668325
H	7.101271	2.581424	-2.655667
H	4.011586	5.634665	-2.665243
H	6.448116	5.010362	-2.701339
C	3.018067	-0.266247	-2.880374
C	3.437741	-0.511191	-4.206219
C	2.978350	-1.350429	-1.980728
C	3.771752	-1.811380	-4.623715
H	3.537035	0.327577	-4.913687
C	3.316773	-2.651229	-2.388581
H	2.662431	-1.185570	-0.939431
C	3.705786	-2.887414	-3.717617
H	4.095418	-1.983955	-5.662734
H	3.248270	-3.470138	-1.655952
H	3.965327	-3.905818	-4.048255

Zero-point correction= 1.135363 (Hartree/Particle)
Thermal correction to Energy= 1.211401
Thermal correction to Enthalpy= 1.212345
Thermal correction to Gibbs Free Energy= 1.018650
Sum of electronic and zero-point Energies= -5091.212161
Sum of electronic and thermal Energies= -5091.136123
Sum of electronic and thermal Enthalpies= -5091.135179
Sum of electronic and thermal Free Energies= -5091.328874

SCF Done (in solvent): -5092.9830729

C	-3.988189	-3.038663	-1.908559
C	-3.391683	-4.138511	-1.252788
C	-4.972460	-3.295069	-2.889026
C	-3.738154	-5.457694	-1.598299
H	-2.646048	-3.947493	-0.462657
C	-5.318267	-4.612802	-3.236173
H	-5.482568	-2.452158	-3.381147
C	-4.695991	-5.701315	-2.599195
H	-3.262492	-6.300097	-1.069667
H	-6.086395	-4.789433	-4.006134
H	-4.969485	-6.733668	-2.869460
C	1.576915	4.164349	0.520370
C	1.737802	5.047907	-0.573079
C	2.722351	3.540571	1.049925
C	3.011158	5.324456	-1.093704
H	0.851502	5.520426	-1.023020
C	3.999847	3.812731	0.527033
H	2.618948	2.828559	1.879811
C	4.152376	4.716452	-0.536314
H	3.109288	6.011147	-1.949009
H	4.877912	3.301730	0.952085
H	5.152329	4.932235	-0.944621
C	-0.654134	5.192796	1.172567
C	-0.108781	6.339136	1.791126
C	-1.966573	5.269768	0.662591
C	-0.864689	7.514674	1.925112
H	0.934986	6.319161	2.142174
C	-2.725513	6.446839	0.788304
H	-2.394699	4.395880	0.148265
C	-2.179361	7.572716	1.427473
H	-0.419316	8.397397	2.411285
H	-3.747257	6.484301	0.377444
H	-2.770397	8.496908	1.527142
C	-2.380188	-0.619221	3.562963
C	-3.089038	0.220342	4.447123
C	-3.095905	-1.594112	2.831702
C	-4.480192	0.085997	4.605356
H	-2.544479	0.992576	5.013653
C	-4.482054	-1.742754	3.006280
H	-2.546180	-2.237281	2.124490
C	-5.182049	-0.900042	3.889594
H	-5.017957	0.753888	5.297480
H	-5.019770	-2.525779	2.446894
H	-6.270290	-1.012380	4.020070
C	-0.052439	-1.520364	4.208139
C	-0.640678	-2.597805	4.902392
C	1.362346	-1.444515	4.165036
C	0.156666	-3.575708	5.529996
H	-1.737464	-2.678954	4.945672
C	2.160854	-2.409481	4.801953
H	1.834952	-0.619112	3.612563
C	1.560584	-3.487899	5.485560
H	-0.327057	-4.406952	6.068136
H	3.258888	-2.319292	4.761462
H	2.183459	-4.243196	5.991538

Zero-point correction= 1.136467 (Hartree/Particle)
Thermal correction to Energy= 1.212587
Thermal correction to Enthalpy= 1.213532
Thermal correction to Gibbs Free Energy= 1.019220
Sum of electronic and zero-point Energies= -5091.253445
Sum of electronic and thermal Energies= -5091.177324
Sum of electronic and thermal Enthalpies= -5091.176380
Sum of electronic and thermal Free Energies= -5091.370691

SCF Done (in solvent): -5093.022194

[Pd(IPr*)(cin)Cl]-III				**[Pd(IPr*)(cin)Cl]-I'**			
145				145			
StI-PREcin+KCO3menysKClISOMERopen SCF Done: -4032.12197151 A.U.				StI-PREcin+KCO3menysKCl SCF Done: -4032.15005627 A.U.			
N	1.257322	1.268472	0.045082	N	0.765725	1.202768	-0.751560
C	1.255973	1.887304	-1.251491	C	0.299864	1.478562	-2.089088
N	0.786781	-0.150784	1.609502	N	1.090256	0.354881	1.218000
C	2.152020	1.417635	-2.242598	C	0.656345	0.613977	-3.153755
C	2.067037	1.990889	-3.525112	C	0.247456	0.963299	-4.453358
H	2.757180	1.651087	-4.311665	H	0.521263	0.300835	-5.288251
C	1.116365	2.988035	-3.804974	C	-0.526502	2.109470	-4.686470
H	1.051443	3.409570	-4.820564	H	-0.854326	2.354297	-5.708836
C	0.271406	3.471153	-2.794004	C	-0.906318	2.924544	-3.613393
H	-0.457190	4.269149	-3.005593	H	-1.566479	3.790231	-3.778427
C	0.347509	2.938856	-1.492707	C	-0.488633	2.636363	-2.298130
C	3.253150	0.436806	-1.832565	C	1.447726	-0.665603	-2.899590
H	2.758568	-0.366450	-1.237113	H	1.055346	-1.073397	-1.931489
C	-0.406061	3.534221	-0.308101	C	-0.902526	3.556679	-1.149460
H	-0.639177	2.691082	0.375364	H	-0.810359	2.974821	-0.207096
C	0.453760	0.164824	0.298728	C	0.482467	0.093088	0.011149
C	2.018605	1.645330	1.156023	C	1.530169	2.127474	-0.029194
H	2.691212	2.506420	1.138485	H	1.865735	3.068625	-0.470079
C	1.722881	0.750851	2.144642	C	1.704641	1.610017	1.219736
H	2.076096	0.669653	3.176396	H	2.212353	2.006136	2.100585
C	0.457903	-1.385278	2.262411	C	1.205625	-0.587677	2.300917
C	1.487027	-2.344335	2.438394	C	2.466020	-1.201645	2.519722
C	1.197538	-3.499188	3.192252	C	2.579744	-2.113847	3.587981
H	1.990068	-4.244327	3.357374	H	3.547343	-2.607609	3.765095
C	-0.087666	-3.714001	3.708696	C	1.471420	-2.409930	4.395177
H	-0.296787	-4.616157	4.304920	H	1.574736	-3.124014	5.227487
C	-1.122561	-2.806345	3.426512	C	0.227383	-1.809630	4.142418
H	-2.148028	-3.012884	3.768361	H	-0.643050	-2.058663	4.767817
C	-0.871519	-1.635344	2.688604	C	0.064636	-0.888780	3.088266
C	2.811007	-2.203206	1.680869	C	3.662072	-0.880586	1.617751
H	2.935543	-1.124959	1.446664	H	3.256372	-0.734618	0.590511
C	-1.986421	-0.709067	2.217851	C	-1.284294	-0.260287	2.752036
H	-1.821127	-0.625281	1.106687	H	-1.489214	-0.489644	1.675938
C	-0.394432	-1.332122	-2.915129	C	0.668652	-3.141979	0.194761
H	0.608777	-1.786277	-2.882487	H	1.227287	-3.068691	1.139623
H	-0.516129	-0.459454	-3.583056	H	1.274630	-3.350870	-0.705039
C	-1.507516	-2.090192	-2.497397	C	-0.685933	-3.590729	0.257161
H	-1.285986	-3.102952	-2.117920	H	-1.142772	-3.716054	1.254602
C	-2.918962	-1.937804	-3.039283	C	-1.509528	-3.579460	-0.893997
H	-2.891343	-2.221869	-4.118736	H	-1.027331	-3.642139	-1.886977
Pd	-0.862979	-0.735351	-0.914722	Pd	-0.615219	-1.538417	-0.448114
O	-4.834640	0.818594	-2.120843	O	-4.270099	-0.147639	-1.508618
C	-3.871260	0.022386	-1.962712	C	-3.179537	-0.420153	-0.903331
O	-3.411778	-0.578874	-3.123691	O	-2.042258	-0.476039	-1.585745
O	-3.322493	-0.266616	-0.846297	O	-3.133443	-0.648604	0.378766
K	-5.370426	0.749114	0.374892	K	-5.552592	-0.881859	0.573501
C	0.524251	4.472004	0.467075	C	-2.460405	-0.904250	3.485631
C	1.332298	5.419072	-0.197616	C	-3.021497	-0.357222	4.657674
C	0.608315	4.383329	1.872315	C	-3.027137	-2.086644	2.957854
C	2.198248	6.258750	0.523537	C	-4.121950	-0.971867	5.285390
H	1.292079	5.488825	-1.295923	H	-2.601134	0.572073	5.073596
C	1.472797	5.221535	2.596568	C	-4.123002	-2.704821	3.581520
H	0.005703	3.630938	2.401221	H	-2.628514	-2.483123	2.013701
C	2.273006	6.162392	1.924866	C	-4.679316	-2.146849	4.750282
H	2.823809	6.989322	-0.014122	H	-4.547927	-0.525597	6.198519
H	1.528156	5.128412	3.693112	H	-4.549404	-3.623133	3.144703
H	2.957439	6.815056	2.490028	H	-5.540268	-2.627951	5.242026

C	-1.757540	4.140229	-0.674042	C	-1.310703	1.260805	2.866164
C	-2.110567	5.467949	-0.360241	C	-0.536139	1.962708	3.811902
C	-2.717332	3.309771	-1.297010	C	-2.197601	1.983249	2.035624
C	-3.397870	5.955899	-0.655818	C	-0.665742	3.357291	3.948975
H	-1.373349	6.122852	0.129118	H	0.172490	1.409225	4.450156
C	-3.998248	3.797196	-1.604499	C	-2.337048	3.372709	2.180044
H	-2.448336	2.269450	-1.546378	H	-2.773378	1.427903	1.275807
C	-4.344288	5.123884	-1.277639	C	-1.576601	4.063753	3.143570
H	-3.657206	6.996392	-0.401445	H	-0.056182	3.892918	4.694803
H	-4.707496	3.122875	-2.109244	H	-3.026643	3.920459	1.518587
H	-5.347387	5.510270	-1.521056	H	-1.684927	5.154545	3.254295
C	4.237381	1.149002	-0.894037	C	0.015405	4.772559	-0.989844
C	4.496729	2.531218	-1.007852	C	0.319662	5.233305	0.311003
C	4.884098	0.430836	0.132654	C	0.562680	5.464737	-2.089586
C	5.345718	3.181933	-0.095127	C	1.141114	6.354600	0.508025
H	3.999185	3.113518	-1.798316	H	-0.090001	4.691298	1.177196
C	5.740336	1.072454	1.041201	C	1.386340	6.588670	-1.895530
H	4.702976	-0.648492	0.222091	H	0.355722	5.116209	-3.112416
C	5.965567	2.457101	0.938279	C	1.679217	7.039129	-0.596937
H	5.513555	4.266717	-0.187523	H	1.367117	6.690931	1.532785
H	6.221489	0.483922	1.838455	H	1.806110	7.112574	-2.769345
H	6.623318	2.969179	1.658548	H	2.328194	7.916574	-0.446259
C	3.944575	-0.290024	-2.991073	C	-2.391490	3.918663	-1.209962
C	5.347272	-0.345188	-3.115725	C	-3.315887	2.871285	-1.410826
C	3.162958	-0.999526	-3.929304	C	-2.875447	5.221147	-0.976576
C	5.951807	-1.103363	-4.136132	C	-4.695724	3.113109	-1.356399
H	5.979134	0.201357	-2.399774	H	-2.957521	1.852628	-1.622178
C	3.760830	-1.749311	-4.952280	C	-4.261651	5.465425	-0.923182
H	2.067686	-0.967724	-3.845560	H	-2.166866	6.049332	-0.822067
C	5.162752	-1.811756	-5.057017	C	-5.176011	4.413183	-1.105331
H	7.050828	-1.136443	-4.209110	H	-5.375404	2.262468	-1.522374
H	3.125575	-2.298655	-5.665411	H	-4.626210	6.488877	-0.737799
H	5.636031	-2.406157	-5.854779	H	-6.259808	4.609452	-1.062418
C	2.765643	-2.901987	0.310159	C	2.935538	-0.436567	-2.670217
C	3.954496	-3.010564	-0.450725	C	3.602461	0.724979	-3.110240
C	1.560508	-3.345035	-0.272400	C	3.687197	-1.424916	-1.992163
C	3.940930	-3.523889	-1.755779	C	4.984566	0.884220	-2.897301
H	4.911826	-2.690396	-0.010330	H	3.029719	1.510544	-3.627738
C	1.551820	-3.892901	-1.568692	C	5.067384	-1.275747	-1.785240
H	0.611524	-3.249417	0.274728	H	3.177658	-2.332084	-1.630274
C	2.734085	-3.974366	-2.319462	C	5.722952	-0.117047	-2.242252
H	4.871693	-3.550480	-2.343607	H	5.487540	1.799404	-3.249017
H	0.599397	-4.236125	-2.001988	H	5.625261	-2.057384	-1.246649
H	2.717924	-4.371019	-3.346248	H	6.803613	0.009530	-2.072107
C	4.019049	-2.575569	2.535178	C	1.098124	-1.772595	-3.895241
C	4.514241	-3.895341	2.605690	C	2.055845	-2.444214	-4.677651
C	4.651978	-1.576593	3.305038	C	-0.261818	-2.159470	-3.996552
C	5.604466	-4.209189	3.435475	C	1.670840	-3.494522	-5.534432
H	4.050660	-4.677763	1.983928	H	3.114664	-2.148673	-4.615103
C	5.744862	-1.885377	4.132124	C	-0.641609	-3.208442	-4.846671
H	4.284521	-0.539627	3.239945	H	-1.020907	-1.612738	-3.407913
C	6.223356	-3.206021	4.202570	C	0.324632	-3.885030	-5.617495
H	5.978301	-5.244802	3.477482	H	2.433967	-4.009914	-6.139769
H	6.228629	-1.089331	4.720840	H	-1.702426	-3.501483	-4.907767
H	7.081657	-3.451377	4.848012	H	0.025722	-4.710098	-6.283617
C	-1.941541	0.714214	2.748470	C	4.334415	0.436861	2.007074
C	-1.529896	1.025056	4.058740	C	4.439070	0.845548	3.351634
C	-2.446151	1.750163	1.929993	C	4.860365	1.271746	0.998203
C	-1.679463	2.331967	4.561761	C	5.038236	2.075497	3.681266
H	-1.104785	0.228624	4.691248	H	4.027780	0.204508	4.147362
C	-2.619422	3.049166	2.434835	C	5.459878	2.497364	1.324873
H	-2.674326	1.517231	0.873900	H	4.775870	0.962779	-0.055005
C	-2.247688	3.340205	3.762160	C	5.545328	2.908208	2.668579

H	-1.358423	2.561032	5.590712	H	5.102669	2.386335	4.736360
H	-3.001050	3.844399	1.774479	H	5.851172	3.142815	0.522378
H	-2.368682	4.360708	4.157896	H	6.005287	3.875781	2.925067
C	-3.380285	-1.316468	2.360861	C	4.672616	-2.028614	1.490373
C	-4.268674	-0.942994	3.394996	C	6.037257	-1.866726	1.802217
C	-3.814017	-2.261500	1.400753	C	4.249372	-3.273210	0.971847
C	-5.568658	-1.484917	3.457512	C	6.955563	-2.911408	1.585980
H	-3.944208	-0.209113	4.149586	H	6.391422	-0.905624	2.203207
C	-5.109241	-2.801582	1.460780	C	5.160931	-4.316291	0.753538
H	-3.143106	-2.530357	0.569167	H	3.189142	-3.420365	0.726598
C	-5.994955	-2.410364	2.486020	C	6.524362	-4.137895	1.055642
H	-6.247987	-1.182320	4.271111	H	8.018661	-2.759003	1.831989
H	-5.429035	-3.513277	0.685413	H	4.805224	-5.272369	0.337562
H	-7.012582	-2.831158	2.528028	H	7.244190	-4.952825	0.879466
C	-3.978893	-2.860541	-2.419258	C	-2.973159	-3.761337	-0.876269
C	-3.659533	-4.086301	-1.797322	C	-3.661016	-4.366102	0.207524
C	-5.347338	-2.535309	-2.579750	C	-3.736779	-3.301867	-1.978748
C	-4.668675	-4.970602	-1.373271	C	-5.057376	-4.511884	0.185633
C	-6.356232	-3.411083	-2.145783	C	-5.132836	-3.440559	-1.998852
C	-6.023538	-4.641637	-1.550046	C	-5.803951	-4.050769	-0.920028
H	-2.608958	-4.373738	-1.646820	H	-3.092891	-4.755822	1.066662
H	-5.616790	-1.584049	-3.063539	H	-3.223251	-2.781670	-2.800885
H	-4.388624	-5.924126	-0.897517	H	-5.567066	-5.010658	1.026581
H	-7.413688	-3.135449	-2.290219	H	-5.700827	-3.056288	-2.860302
H	-6.813145	-5.336308	-1.222130	H	-6.897734	-4.186691	-0.948368
Zero-point correction= 1.134215 (Hartree/Particle)				Zero-point correction= 1.134115 (Hartree/Particle)			
Thermal correction to Energy= 1.206293				Thermal correction to Energy= 1.206465			
Thermal correction to Enthalpy= 1.207238				Thermal correction to Enthalpy= 1.207409			
Thermal correction to Gibbs Free Energy= 1.022321				Thermal correction to Gibbs Free Energy= 1.022276			
Sum of electronic and zero-point Energies= -4030.987757				Sum of electronic and zero-point Energies= -4031.015942			
Sum of electronic and thermal Energies= -4030.915678				Sum of electronic and thermal Energies= -4030.943591			
Sum of electronic and thermal Enthalpies= -4030.914734				Sum of electronic and thermal Enthalpies= -4030.942647			
Sum of electronic and thermal Free Energies= -4031.09965				Sum of electronic and thermal Free Energies= -4031.127780			
SCF Done (in solvent): -4032.741225				SCF Done (in solvent): -4032.7585755			

[Pd(IPr*)(cin)Cl]-I'-III			
145			
StI-PREcin+KCO3--C-O SCF Done: -4032.10654746 A.U.			
N	1.038393	1.457781	-0.633840
C	0.649328	1.609454	-2.008688
N	1.168253	0.745050	1.407990
C	1.266055	0.813737	-2.999993
C	0.908876	1.040422	-4.343807
H	1.373066	0.426656	-5.130683
C	-0.055085	2.001224	-4.680846
H	-0.330646	2.154881	-5.735945
C	-0.693031	2.743992	-3.675928
H	-1.491136	3.457750	-3.932390
C	-0.350139	2.560921	-2.322905
C	2.316480	-0.230003	-2.619228
H	2.110470	-0.524752	-1.567105
C	-1.037316	3.346410	-1.207564
H	-1.010433	2.699028	-0.304928
C	0.624687	0.408498	0.178649
C	1.804477	2.395890	0.064090
H	2.201897	3.291989	-0.418985
C	1.879246	1.955280	1.354213
H	2.353677	2.383370	2.241452
C	1.135707	-0.039058	2.610840
C	2.344663	-0.636647	3.047345
C	2.399101	-1.128464	4.367686
H	3.350241	-1.530004	4.750549
C	1.255726	-1.123360	5.181025

H	1.312974	-1.506502	6.211994
C	0.027355	-0.675923	4.666452
H	-0.889064	-0.753067	5.272021
C	-0.056308	-0.125833	3.372958
C	3.483624	-0.867105	2.051615
H	3.298460	-0.193074	1.195216
C	-1.387534	0.274261	2.743751
H	-1.290273	-0.029093	1.664133
C	0.443672	-2.960646	-0.455969
H	1.054057	-3.253470	0.411966
H	0.987163	-2.980803	-1.415394
C	-0.960582	-3.266237	-0.414907
H	-1.369754	-3.587518	0.558434
C	-1.854473	-3.385042	-1.545224
H	-1.389936	-3.606648	-2.517873
Pd	-0.561740	-1.121335	-0.209247
O	-4.457096	-0.746728	-1.803642
C	-3.260649	-1.047188	-1.503097
O	-2.504125	-1.761470	-2.319354
O	-2.750462	-0.657209	-0.344181
K	-5.079060	-0.442713	0.627452
C	-0.285675	4.623374	-0.838210
C	0.217899	5.499916	-1.821322
C	-0.093256	4.949601	0.521202
C	0.890907	6.679206	-1.455212
H	0.089414	5.250572	-2.886239
C	0.576888	6.127007	0.890288
H	-0.459662	4.260062	1.295989
C	1.071868	6.997909	-0.097413
H	1.280746	7.350586	-2.237077
H	0.718072	6.360355	1.957879
H	1.602733	7.919675	0.189625
C	-2.525411	3.559463	-1.494947
C	-3.138768	4.826838	-1.514224
C	-3.324161	2.412372	-1.700185
C	-4.527806	4.943190	-1.720164
H	-2.530191	5.729301	-1.350689
C	-4.705819	2.524665	-1.914711
H	-2.854900	1.417302	-1.687221
C	-5.315455	3.795788	-1.917181
H	-4.994171	5.941673	-1.728771
H	-5.279148	1.601645	-2.099256
H	-6.399885	3.891944	-2.088881
C	3.698794	0.424010	-2.644880
C	4.351552	0.725335	-3.860373
C	4.332871	0.789358	-1.439480
C	5.609844	1.348375	-3.865100
H	3.869385	0.454516	-4.812782
C	5.594564	1.408863	-1.436228
H	3.822747	0.593539	-0.484880
C	6.239715	1.687698	-2.652469
H	6.105894	1.568715	-4.823986
H	6.071663	1.662687	-0.476174
H	7.230816	2.168496	-2.658373
C	2.183680	-1.532945	-3.411031
C	3.307711	-2.327032	-3.717237
C	0.899445	-2.026239	-3.743450
C	3.161302	-3.574734	-4.350905
H	4.313946	-1.967701	-3.451329
C	0.755207	-3.266693	-4.385557
H	-0.001288	-1.451345	-3.472779
C	1.883740	-4.048103	-4.693420
H	4.055225	-4.177647	-4.578628

H	-0.254182	-3.624837	-4.644462
H	1.766864	-5.020952	-5.196909
C	3.447509	-2.288426	1.465034
C	3.854391	-2.478772	0.125731
C	3.046707	-3.419169	2.207051
C	3.856003	-3.755767	-0.455700
H	4.167175	-1.614251	-0.478766
C	3.063045	-4.703052	1.631486
H	2.691056	-3.299490	3.240887
C	3.465035	-4.876502	0.296999
H	4.141955	-3.868480	-1.512344
H	2.739160	-5.569926	2.229290
H	3.456235	-5.877663	-0.161549
C	4.858840	-0.481748	2.596858
C	5.682401	-1.399093	3.281107
C	5.321348	0.840473	2.419458
C	6.928947	-0.998345	3.793886
H	5.351934	-2.444170	3.391931
C	6.569168	1.241684	2.923895
H	4.691891	1.558541	1.867865
C	7.376623	0.322699	3.618745
H	7.560516	-1.728745	4.324588
H	6.915767	2.276113	2.768779
H	8.356998	0.633302	4.013394
C	-1.722662	1.754067	2.746659
C	-1.310682	2.631237	3.768754
C	-2.586755	2.238377	1.737081
C	-1.792320	3.954346	3.807390
H	-0.623081	2.265100	4.548254
C	-3.088595	3.548257	1.787407
H	-2.847458	1.566965	0.899421
C	-2.697318	4.408827	2.831462
H	-1.463858	4.631758	4.612046
H	-3.757091	3.906610	0.989680
H	-3.076099	5.442224	2.865549
C	-2.546692	-0.584141	3.250245
C	-3.666045	-0.051069	3.926256
C	-2.520420	-1.973921	2.980732
C	-4.743338	-0.881210	4.302461
H	-3.699061	1.026217	4.152391
C	-3.589182	-2.802491	3.357419
H	-1.649179	-2.387686	2.446977
C	-4.713285	-2.258310	4.013139
H	-5.605292	-0.446681	4.834792
H	-3.551836	-3.879802	3.129824
H	-5.551911	-2.908370	4.309690
C	-3.198795	-3.978550	-1.331180
C	-3.871161	-3.824786	-0.093851
C	-3.872905	-4.645200	-2.379349
C	-5.167023	-4.331028	0.092682
C	-5.165451	-5.158231	-2.192804
C	-5.821419	-5.002583	-0.956948
H	-3.371265	-3.284508	0.722066
H	-3.374394	-4.745684	-3.356288
H	-5.665265	-4.207813	1.069760
H	-5.672075	-5.677007	-3.022146
H	-6.837424	-5.403775	-0.813628
Zero-point correction=		1.133070 (Hartree/Particle)	
Thermal correction to Energy=		1.204838	
Thermal correction to Enthalpy=		1.205782	
Thermal correction to Gibbs Free Energy=		1.021339	
Sum of electronic and zero-point Energies=		-4030.973478	
Sum of electronic and thermal Energies=		-4030.901709	
Sum of electronic and thermal Enthalpies=		-4030.900765	
Sum of electronic and thermal Free Energies=		-4031.085209	

SCF Done (in solvent): -4032.7148579	

[Pd(SIPr)(cin)Cl]				**[Pd(SIPr)(cin)Cl]-I**			
87				93			
SI-PREcin SCF Done: -2096.86259440 A.U.				SI-PREcin+K2CO3 SCF Done: -3560.65767698 A.U.			
Cl	0.588868	-2.310440	0.481478	Cl	0.236794	1.450130	1.915811
N	-2.085010	0.163136	0.935172	N	-0.960415	-1.824491	1.172452
C	-3.105692	-0.483054	0.159474	C	0.443415	-2.135858	1.139939
N	-0.192016	1.169670	1.429301	N	-2.872835	-0.945799	0.545318
C	-3.693766	0.241438	-0.919184	C	1.052911	-2.468752	-0.104912
C	-4.743295	-0.375106	-1.625940	C	2.437249	-2.737167	-0.108546
H	-5.220210	0.153870	-2.464087	H	2.956635	-2.900428	-1.064378
C	-5.197416	-1.657466	-1.276766	C	3.177103	-2.727347	1.082363
H	-6.028008	-2.116047	-1.836799	H	4.259396	-2.928011	1.053021
C	-4.583813	-2.360140	-0.233154	C	2.550315	-2.433286	2.304497
H	-4.927629	-3.376222	0.015453	H	3.140476	-2.434507	3.235015
C	-3.514806	-1.797676	0.496404	C	1.177795	-2.110417	2.357268
C	-3.197482	1.639773	-1.290785	C	0.253979	-2.597771	-1.402821
H	-2.095675	1.620425	-1.163659	H	-0.644536	-1.953972	-1.314223
C	-3.461543	2.025137	-2.755231	C	1.026061	-2.111607	-2.641351
H	-3.095479	1.246952	-3.455326	H	1.509623	-1.127951	-2.456126
H	-2.938865	2.974410	-2.996122	H	0.336657	-2.047215	-3.510569
H	-4.541480	2.188493	-2.958738	H	1.845248	-2.804349	-2.923810
C	-3.753905	2.718918	-0.338543	C	-0.234178	-4.052647	-1.580583
H	-4.861634	2.768802	-0.401007	H	0.628820	-4.744266	-1.686519
H	-3.348030	3.719153	-0.599987	H	-0.860708	-4.143422	-2.493189
H	-3.484300	2.517294	0.716625	H	-0.835973	-4.402302	-0.715076
C	-2.835782	-2.599625	1.602895	C	0.517016	-1.781901	3.695269
H	-1.889895	-2.077358	1.859405	H	-0.467311	-1.321077	3.465254
C	-2.421597	-4.005545	1.127212	C	1.305391	-0.746918	4.520465
H	-3.301129	-4.640602	0.887000	H	2.305837	-1.127642	4.818371
H	-1.846507	-4.519038	1.925378	H	0.756990	-0.503703	5.454804
H	-1.764987	-3.936942	0.238104	H	1.425857	0.192305	3.945676
C	-3.736554	-2.680126	2.854728	C	0.294873	-3.071616	4.517799
H	-4.048344	-1.675957	3.211547	H	-0.259582	-3.844062	3.944877
H	-3.210776	-3.194980	3.686255	H	-0.269458	-2.858899	5.450534
H	-4.664981	-3.250909	2.637369	H	1.268575	-3.522794	4.805879
C	-0.824302	0.396546	0.511337	C	-1.527330	-0.792460	0.495290
C	-2.311260	0.658530	2.313715	C	-1.969399	-2.821294	1.606470
H	-3.272203	1.206926	2.383530	H	-1.916691	-3.715410	0.945152
C	-1.074313	1.548655	2.554226	C	-3.284870	-2.041401	1.444519
H	-1.311028	2.633878	2.504002	H	-4.103487	-2.640929	0.999230
C	1.140777	1.682576	1.245250	C	-3.799954	-0.156372	-0.206190
C	1.337008	2.797456	0.379087	C	-4.303429	-0.706284	-1.415385
C	2.653722	3.257018	0.182205	C	-5.188244	0.082999	-2.176868
H	2.836888	4.111156	-0.486990	H	-5.591511	-0.312347	-3.122923
C	3.738262	2.646242	0.830641	C	-5.549404	1.371357	-1.753995
H	4.760885	3.018881	0.660565	H	-6.236956	1.977253	-2.365498
C	3.521174	1.561312	1.688601	C	-5.035475	1.891365	-0.556554
H	4.377390	1.082806	2.187502	H	-5.326338	2.903858	-0.235176
C	2.224905	1.050285	1.909632	C	-4.151365	1.140796	0.245438
C	0.162338	3.508212	-0.289545	C	-3.906566	-2.103349	-1.895103
H	-0.652370	2.763888	-0.400957	H	-3.175497	-2.517549	-1.170261
C	-0.362029	4.654091	0.604186	C	-5.128915	-3.044927	-1.922298
H	-0.642558	4.295418	1.614595	H	-5.644051	-3.073451	-0.939208
H	-1.255242	5.133712	0.150758	H	-4.824122	-4.079856	-2.184661

H	0.418446	5.433456	0.736098
C	0.487693	4.045193	-1.695494
H	1.148661	4.936769	-1.655940
H	-0.444207	4.355593	-2.212477
H	0.992571	3.282880	-2.321325
C	2.020891	-0.131760	2.850265
H	1.023044	-0.563307	2.626353
C	3.047604	-1.255604	2.615852
H	3.068461	-1.554094	1.549814
H	2.767828	-2.150337	3.208857
H	4.071008	-0.956188	2.929383
C	2.047351	0.342693	4.320504
H	3.046663	0.750971	4.584837
H	1.832367	-0.501335	5.009275
H	1.306401	1.146498	4.516379
C	-0.107105	0.614812	-2.796832
H	-0.387237	1.678499	-2.812547
H	-0.827044	-0.062857	-3.292453
C	1.270861	0.259048	-2.700061
H	2.014661	1.052205	-2.497854
C	1.653273	-1.109123	-2.562606
H	1.064057	-1.881409	-3.089335
C	2.972997	-1.522263	-2.047437
C	3.734979	-0.679828	-1.195679
C	3.478658	-2.811401	-2.335513
C	4.963252	-1.106602	-0.675652
H	3.335640	0.299784	-0.887277
C	4.710655	-3.237785	-1.814316
H	2.888099	-3.488754	-2.973500
C	5.462170	-2.386535	-0.985092
H	5.523083	-0.440028	-0.000189
H	5.083350	-4.247217	-2.051200
H	6.424087	-2.724348	-0.567917
Pd	0.232946	-0.454457	-0.961851
H	-2.351569	-0.197967	3.019232
H	-0.582729	1.346269	3.525769
H	-5.874714	-2.713476	-2.675718
C	-3.188532	-2.075690	-3.258922
H	-3.825427	-1.629059	-4.051163
H	-2.928337	-3.106389	-3.578485
H	-2.249118	-1.492873	-3.204900
C	-3.619107	1.708829	1.557838
H	-2.796793	1.052351	1.907795
C	-3.001758	3.107105	1.377214
H	-2.220900	3.076343	0.591337
H	-2.507301	3.432738	2.314176
H	-3.760725	3.870105	1.101372
C	-4.724461	1.703507	2.634779
H	-5.572629	2.360405	2.344561
H	-4.326968	2.069202	3.604937
H	-5.133294	0.682893	2.791283
C	-1.177819	0.866440	-2.307624
H	-2.254502	0.770522	-2.523399
H	-0.517861	0.172385	-2.856920
C	-0.667766	2.164516	-1.947507
H	-1.361818	3.013878	-1.808245
C	0.680648	2.262972	-1.546999
H	1.392893	1.477141	-1.880677
Pd	-0.550617	0.781212	-0.280025
O	4.940702	-0.164957	-0.467151
C	4.054107	-0.400794	-1.440102
O	2.943087	0.257927	-1.440679
O	4.325565	-1.301443	-2.333401
K	3.125107	0.894292	1.017829
K	6.615207	-1.545522	-1.607318
C	1.320641	3.435256	-0.928299
C	2.730030	3.564493	-1.043986
C	0.611939	4.407067	-0.179997
C	3.401594	4.645718	-0.449066
H	3.281980	2.781275	-1.591414
C	1.285026	5.486720	0.408996
H	-0.471293	4.290528	-0.026901
C	2.681579	5.613991	0.276201
H	4.495625	4.732086	-0.553181
H	0.718200	6.227817	0.995116
H	3.207188	6.460822	0.746104
H	-3.649169	-1.614110	2.406237
H	-1.786713	-3.150287	2.646582
Zero-point correction=	0.726816 (Hartree/Particle)		
Thermal correction to Energy=	0.770014		
Thermal correction to Enthalpy=	0.770958		
Thermal correction to Gibbs Free Energy=	0.651492		
Sum of electronic and zero-point Energies=	-2096.135778		
Sum of electronic and thermal Energies=	-2096.092580		
Sum of electronic and thermal Enthalpies=	-2096.091636		
Sum of electronic and thermal Free Energies=	-2096.211102		
SCF Done (in solvent): -2097.1707625			
Zero-point correction=	0.743329 (Hartree/Particle)		
Thermal correction to Energy=	0.795424		
Thermal correction to Enthalpy=	0.796368		
Thermal correction to Gibbs Free Energy=	0.654855		
Sum of electronic and zero-point Energies=	-3559.914348		
Sum of electronic and thermal Energies=	-3559.862253		
Sum of electronic and thermal Enthalpies=	-3559.861309		
Sum of electronic and thermal Free Energies=	-3560.002822		
SCF Done (in solvent): -3561.0034239			

[Pd(SIPr)(cin)Cl]-I-II			
93			
SI-PREcin--K2CO3 SCF Done: -3560.62632237 A.U.			
Cl	-0.885211	1.264914	2.176950
N	1.813588	1.894639	-0.240505
C	0.776540	2.689189	-0.832891
N	2.898349	0.095604	0.396110
C	0.216024	2.285562	-2.083236
C	-0.770746	3.113406	-2.661599
H	-1.228648	2.818741	-3.617344
C	-1.177198	4.305786	-2.038468

[Pd(SIPr)(cin)Cl]-II			
93			
SI-PREcin--K2CO3post SCF Done: -3560.67435575 A.U.			
Cl	0.597497	-1.448660	-2.228490
N	2.775086	0.147556	0.356622
C	2.864405	-1.150389	0.945081
N	1.943151	2.072967	-0.252915
C	2.230415	-1.410698	2.197631
C	2.421542	-2.683044	2.781736
H	1.942854	-2.905457	3.748373
C	3.221540	-3.660338	2.166045

H	-1.936940	4.944244	-2.518168	H	3.371727	-4.637372	2.653512
C	-0.615969	4.681592	-0.807455	C	3.832818	-3.387034	0.930494
H	-0.942617	5.614744	-0.322036	H	4.457135	-4.157508	0.449782
C	0.359755	3.879962	-0.175231	C	3.660251	-2.137844	0.293343
C	0.685106	1.030526	-2.820738	C	1.400579	-0.364540	2.939528
H	1.061654	0.322241	-2.055210	H	1.212242	0.475771	2.242165
C	-0.449578	0.307310	-3.566829	C	0.014223	-0.906005	3.336511
H	-1.342582	0.151485	-2.928503	H	-0.527666	-1.303719	2.453163
H	-0.090013	-0.680010	-3.927369	H	-0.597442	-0.090582	3.775837
H	-0.790204	0.863204	-4.465491	H	0.080146	-1.713651	4.096651
C	1.850396	1.372412	-3.774174	C	2.177125	0.188012	4.152695
H	1.526522	2.098306	-4.550175	H	2.383105	-0.605782	4.902835
H	2.213584	0.458937	-4.289683	H	1.589709	0.985185	4.654630
H	2.709641	1.821424	-3.234777	H	3.153290	0.621781	3.848691
C	0.957619	4.317114	1.159803	C	4.325129	-1.874310	-1.056478
H	1.488396	3.435201	1.576677	H	3.942147	-0.897996	-1.420578
C	-0.113433	4.720545	2.191477	C	3.933547	-2.923907	-2.115888
H	-0.669941	5.630491	1.879597	H	4.249386	-3.948267	-1.822331
H	0.366206	4.950258	3.165877	H	4.426615	-2.693080	-3.083493
H	-0.825846	3.887783	2.353097	H	2.838497	-2.908097	-2.290705
C	1.965021	5.471041	0.950279	C	5.860244	-1.786248	-0.908196
H	2.746576	5.220775	0.202868	H	6.163277	-1.046709	-0.137713
H	2.469128	5.732564	1.904417	H	6.332619	-1.496255	-1.870192
H	1.445168	6.381648	0.582415	H	6.288423	-2.766167	-0.606017
C	1.657418	0.598701	0.158148	C	1.606658	0.776402	0.004949
C	3.239250	2.287372	-0.361613	C	3.906100	1.094900	0.526001
H	3.510249	2.406121	-1.434380	H	4.063787	1.295227	1.611471
C	3.967668	1.106970	0.309414	C	3.396156	2.328121	-0.229048
H	4.827556	0.730964	-0.281276	H	3.788321	2.382466	-1.270802
C	3.162093	-1.292253	0.635692	C	0.992446	3.113441	-0.504665
C	3.538715	-2.096507	-0.474170	C	0.631262	3.953376	0.581817
C	3.794175	-3.462301	-0.242701	C	-0.305812	4.978256	0.342601
H	4.089655	-4.109768	-1.084028	H	-0.611977	5.638131	1.170408
C	3.669721	-4.011280	1.042955	C	-0.865414	5.158723	-0.930733
H	3.871335	-5.082227	1.205420	H	-1.598491	5.963548	-1.100196
C	3.283924	-3.199959	2.119720	C	-0.500172	4.309876	-1.986945
H	3.176373	-3.642319	3.122704	H	-0.952524	4.456739	-2.980467
C	3.022730	-1.825594	1.941967	C	0.431685	3.269082	-1.798239
C	3.664986	-1.517344	-1.882969	C	1.208060	3.748139	1.981628
H	3.323557	-0.462702	-1.844176	H	1.891393	2.875304	1.936863
C	5.132626	-1.522786	-2.359492	C	2.030898	4.969779	2.438323
H	5.796743	-1.000007	-1.640050	H	2.827416	5.220632	1.706680
H	5.230243	-1.023576	-3.346669	H	2.510577	4.777568	3.421315
H	5.515656	-2.560111	-2.466177	H	1.389311	5.869687	2.550021
C	2.749215	-2.234576	-2.894735	C	0.113303	3.386694	3.004904
H	3.004022	-3.311534	-2.988183	H	-0.633477	4.201833	3.111922
H	2.853045	-1.779930	-3.902097	H	0.560662	3.207795	4.005433
H	1.687445	-2.155356	-2.591332	H	-0.424974	2.470082	2.696247
C	2.569708	-0.968843	3.119825	C	0.814731	2.349881	-2.954059
H	2.374755	0.054316	2.737541	H	1.356317	1.480085	-2.530163
C	1.234522	-1.484626	3.693500	C	-0.426021	1.777028	-3.665069
H	0.472323	-1.532552	2.885143	H	-1.102136	1.321419	-2.911855
H	0.849009	-0.791133	4.467872	H	-0.121354	0.986999	-4.382055
H	1.343402	-2.493413	4.146333	H	-0.987503	2.555586	-4.224533
C	3.663654	-0.871014	4.202272	C	1.757537	3.069412	-3.940511
H	3.887390	-1.864351	4.646947	H	1.260558	3.947588	-4.406551
H	3.335018	-0.203018	5.025881	H	2.072340	2.383411	-4.755432
H	4.612240	-0.469280	3.787630	H	2.671485	3.438519	-3.429257
C	-0.133479	-2.106913	-0.593809	C	-1.713699	1.158580	0.714062
H	0.701556	-2.826425	-0.513008	H	-1.645507	2.232452	0.456570
H	-0.326420	-1.744910	-1.624063	H	-1.714248	0.961810	1.804128
C	-1.242999	-2.237726	0.329335	C	-2.442454	0.255810	-0.141868
H	-1.208100	-3.018976	1.109603	H	-2.916081	0.708337	-1.041291

C -2.414731 -1.428875 0.228157	C -3.282455 -0.853402 0.472209
H -2.352241 -0.554971 -0.435507	Pd -0.285088 0.094272 -0.322752
Pd -0.015451 -0.394437 0.581004	H -2.835955 -1.144507 1.449494
O -3.491708 -1.405787 -3.481820	O -2.058159 -3.776499 -1.078559
C -3.556524 -1.032755 -2.260339	C -2.305493 -3.035350 -0.076344
O -3.551099 -2.021213 -1.326700	O -3.254309 -2.036097 -0.374591
O -3.557549 0.190231 -1.863137	O -1.787502 -3.066463 1.063955
K -2.294075 -3.492266 -2.885074	K -2.283045 -1.788057 -2.816602
K -2.920804 1.855751 -0.098849	K 0.441185 -3.662446 -0.103355
C -3.388736 -1.323557 1.351782	C -4.748411 -0.480481 0.689911
C -4.747253 -1.003443 1.104124	C -5.107572 0.833984 1.060773
C -2.961893 -1.453423 2.695364	C -5.770603 -1.447030 0.565963
C -5.644934 -0.819758 2.168901	C -6.449833 1.171425 1.305603
C -3.864814 -1.279233 3.756734	C -7.113970 -1.108570 0.804908
C -5.209209 -0.958630 3.500563	C -7.460722 0.202401 1.176589
H -5.077095 -0.934841 0.057408	H -4.321850 1.599099 1.156269
H -1.900200 -1.641292 2.909255	H -5.497530 -2.472461 0.275837
H -6.699151 -0.578832 1.954881	H -6.707907 2.203098 1.595457
H -3.505935 -1.373614 4.794138	H -7.896534 -1.878021 0.701187
H -5.914899 -0.815293 4.334801	H -8.513527 0.468021 1.364392
H 3.432464 3.252052 0.145371	H 3.631238 3.285092 0.278821
H 4.335064 1.355160 1.330677	H 4.847985 0.686645 0.111635
Zero-point correction= 0.743010 (Hartree/Particle) Thermal correction to Energy= 0.794184 Thermal correction to Enthalpy= 0.795128 Thermal correction to Gibbs Free Energy= 0.657007 Sum of electronic and zero-point Energies= -3559.883313 Sum of electronic and thermal Energies= -3559.832138 Sum of electronic and thermal Enthalpies= -3559.831194 Sum of electronic and thermal Free Energies= -3559.969315	Zero-point correction= 0.744262 (Hartree/Particle) Thermal correction to Energy= 0.795624 Thermal correction to Enthalpy= 0.796568 Thermal correction to Gibbs Free Energy= 0.657348 Sum of electronic and zero-point Energies= -3559.930094 Sum of electronic and thermal Energies= -3559.878732 Sum of electronic and thermal Enthalpies= -3559.877787 Sum of electronic and thermal Free Energies= -3560.017008
SCF Done (in solvent): -3560.9679852	SCF Done (in solvent): -3561.0162516

[Pd(SIPr)(cin)Cl]-III	**[Pd(SIPr)(cin)Cl]-I'**
91 SI-PREcin+KCO3menysKClISOMERopen SCF Done: -2500.40370497 A.U.	91 SI-PREcin+KCO3menysKCl SCF Done: -2500.42270345 A.U.
N 2.523074 -0.055089 0.888751	N 1.632267 1.470594 0.810247
C 2.867671 1.301863 0.586335	C 1.242381 2.672596 0.123987
N 1.390677 -1.929875 0.938220	N 2.049298 -0.663243 1.141781
C 3.884161 1.558485 -0.366496	C 1.684270 2.879253 -1.210363
C 4.266880 2.897582 -0.589852	C 1.331188 4.090685 -1.839562
H 5.061492 3.120449 -1.320107	H 1.661235 4.277774 -2.873841
C 3.626882 3.946651 0.080745	C 0.575841 5.061617 -1.168625
H 3.930660 4.988773 -0.107819	H 0.310179 6.001836 -1.678066
C 2.571899 3.676712 0.968658	C 0.154428 4.834988 0.148961
H 2.050773 4.518126 1.447738	H -0.449033 5.596789 0.665774
C 2.166820 2.356696 1.242702	C 0.471540 3.638974 0.820692
C 4.500382 0.434094 -1.195011	C 2.548298 1.868381 -1.963309
H 3.969784 -0.503439 -0.929746	H 2.586066 0.934882 -1.366679
C 4.243465 0.658781 -2.699006	C 1.928210 1.485770 -3.319836
H 3.158722 0.781508 -2.887690	H 0.885671 1.135675 -3.175620
H 4.606453 -0.208488 -3.290365	H 2.510181 0.670169 -3.798579
H 4.765797 1.563798 -3.075446	H 1.911966 2.342176 -4.026166
C 6.000152 0.248250 -0.890674	C 3.994313 2.380762 -2.121748
H 6.580640 1.153971 -1.168451	H 4.028509 3.312266 -2.726055
H 6.419206 -0.606529 -1.462927	H 4.627671 1.623100 -2.630051
H 6.176315 0.061558 0.189605	H 4.452814 2.608390 -1.136585
C 0.988140 2.052463 2.169884	C 0.023561 3.422635 2.262314
H 0.394845 1.270782 1.646284	H 0.138489 2.338271 2.475086
C 0.041790 3.244970 2.377926	C -1.457157 3.778400 2.489403
H 0.521124 4.077922 2.936151	H -1.637792 4.867364 2.356949
H -0.820148 2.915346 3.001520	H -1.746970 3.528627 3.532483
H -0.350294 3.632464 1.415368	H -2.121872 3.208672 1.808427

C	1.448765	1.490531	3.530983	C	0.926003	4.223679	3.230318
H	2.063269	0.577177	3.416834	H	2.006620	4.011269	3.084792
H	0.573530	1.222021	4.161332	H	0.669150	3.999734	4.287563
H	2.053701	2.238535	4.087035	H	0.789052	5.315382	3.073836
C	1.416107	-0.673295	0.380942	C	1.270871	0.212763	0.449685
C	3.386874	-0.955241	1.681457	C	2.834781	1.475901	1.674242
H	4.282543	-1.261593	1.093954	H	3.720061	1.782635	1.070693
C	2.442279	-2.144321	1.951368	C	2.905938	0.014537	2.139089
H	2.010091	-2.115606	2.979731	H	2.478014	-0.125257	3.156560
C	0.223766	-2.755084	0.844914	C	2.151315	-2.067395	0.866530
C	0.183460	-3.784563	-0.132017	C	3.250770	-2.503782	0.080371
C	-0.996316	-4.547439	-0.243173	C	3.358269	-3.880802	-0.203763
H	-1.061469	-5.335828	-1.009212	H	4.200079	-4.245393	-0.813945
C	-2.092273	-4.313042	0.601471	C	2.392072	-4.785464	0.255530
H	-3.005011	-4.921817	0.500040	H	2.483183	-5.856954	0.015545
C	-2.025921	-3.305242	1.575220	C	1.301948	-4.327726	1.012265
H	-2.887674	-3.133729	2.241021	H	0.545746	-5.048710	1.356452
C	-0.874644	-2.504311	1.711258	C	1.156555	-2.965027	1.342515
C	1.351581	-3.995551	-1.089148	C	4.273568	-1.529047	-0.502530
H	2.233227	-3.494748	-0.634570	H	3.983504	-0.504401	-0.193507
C	1.701511	-5.479979	-1.298002	C	5.692265	-1.798666	0.037527
H	1.869919	-6.002777	-0.333124	H	5.716770	-1.780456	1.147311
H	2.623217	-5.575481	-1.909393	H	6.408029	-1.036981	-0.337297
H	0.897828	-6.021899	-1.840640	H	6.064681	-2.794520	-0.284065
C	1.066895	-3.275459	-2.424851	C	4.242608	-1.534951	-2.043972
H	0.178950	-3.717410	-2.926516	H	4.514209	-2.529218	-2.456704
H	1.933466	-3.361179	-3.114541	H	4.961205	-0.792969	-2.450621
H	0.861542	-2.197081	-2.233090	H	3.233221	-1.274421	-2.416909
C	-0.831647	-1.391175	2.754729	C	-0.010609	-2.472415	2.190471
H	0.134632	-0.863159	2.642067	H	-0.296255	-1.460168	1.832541
C	-1.926173	-0.337995	2.496891	C	-1.282555	-3.319446	2.040504
H	-1.826356	0.068030	1.469238	H	-1.584257	-3.393690	0.976394
H	-1.817117	0.494834	3.227881	H	-2.111745	-2.816865	2.576149
H	-2.943062	-0.772124	2.613837	H	-1.171343	-4.343972	2.458497
C	-0.898471	-1.948609	4.189821	C	0.405271	-2.372200	3.674004
H	-1.866376	-2.458584	4.383627	H	0.648623	-3.374369	4.089520
H	-0.791975	-1.130794	4.934244	H	-0.417192	-1.935278	4.278503
H	-0.091202	-2.687845	4.373067	H	1.300822	-1.732371	3.809874
C	0.321941	0.663491	-3.008768	C	0.501755	-1.797710	-2.048884
H	1.052957	0.025852	-3.532556	H	1.161887	-2.585951	-1.654501
H	0.551255	1.743578	-2.975010	H	0.901287	-1.240972	-2.914537
C	-0.996537	0.216789	-2.819963	C	-0.913004	-1.960841	-1.909914
H	-1.258933	-0.797372	-3.179865	H	-1.293339	-2.798897	-1.298557
C	-2.206742	1.123549	-2.696870	C	-1.802014	-0.920091	-2.272701
H	-2.605198	1.301600	-3.724181	H	-1.452823	-0.162772	-2.999381
Pd	0.095580	0.008595	-0.948782	Pd	-0.276621	-0.268285	-0.724561
O	-2.135708	3.828593	-0.480357	O	-3.353867	1.461131	1.263224
C	-1.829722	2.678553	-0.881979	C	-2.384846	0.709388	0.887440
O	-1.903331	2.471646	-2.255068	O	-1.430209	1.242660	0.133668
O	-1.537341	1.682778	-0.135825	O	-2.321857	-0.553334	1.189019
K	-3.360062	2.491533	1.388313	K	-4.759148	-0.567024	1.552834
H	3.745250	-0.457518	2.605821	C	-3.250514	-0.901280	-2.002479
H	2.933963	-3.130493	1.818377	C	-3.934279	0.342741	-1.985588
C	-3.365206	0.549563	-1.868268	C	-4.006702	-2.081360	-1.778690
C	-3.250834	-0.622890	-1.090744	C	-5.321061	0.402468	-1.776374
C	-4.571498	1.284385	-1.814545	C	-5.396201	-2.022962	-1.574415
C	-4.308005	-1.038445	-0.263048	C	-6.065548	-0.779633	-1.577890
C	-5.630382	0.875158	-0.980862	H	-3.351995	1.270295	-2.097630
C	-5.498746	-0.288703	-0.195385	H	-3.503343	-3.060583	-1.800055
H	-2.297758	-1.181646	-1.085728	H	-5.824588	1.382165	-1.761878
H	-4.662563	2.205018	-2.414033	H	-5.966640	-2.956697	-1.437593
H	-4.185500	-1.949641	0.342898	H	-7.159283	-0.735200	-1.447341
H	-6.566581	1.457365	-0.956187	H	2.721016	2.193494	2.508235

H -6.328453 -0.619119 0.450902	H 3.932261 -0.402872 2.138218
Zero-point correction= 0.742282 (Hartree/Particle) Thermal correction to Energy= 0.789477 Thermal correction to Enthalpy= 0.790421 Thermal correction to Gibbs Free Energy= 0.661494 Sum of electronic and zero-point Energies= -2499.661423 Sum of electronic and thermal Energies= -2499.614228 Sum of electronic and thermal Enthalpies= -2499.613284 Sum of electronic and thermal Free Energies= -2499.742211 SCF Done (in solvent): -2500.7309927	Zero-point correction= 0.741921 (Hartree/Particle) Thermal correction to Energy= 0.789472 Thermal correction to Enthalpy= 0.790416 Thermal correction to Gibbs Free Energy= 0.661252 Sum of electronic and zero-point Energies= -2499.680783 Sum of electronic and thermal Energies= -2499.633231 Sum of electronic and thermal Enthalpies= -2499.632287 Sum of electronic and thermal Free Energies= -2499.761451 SCF Done (in solvent): -2500.7427947

[Pd(SIPr)(cin)Cl]-I'-III	
91 SI-PREcin+KCO3--C-O SCF Done: -2500.38356178 A.U. N 1.471961 1.845525 0.622836 C 0.266267 2.622818 0.604495 N 2.864095 0.166322 0.390160 C -0.017699 3.429278 -0.523154 C -1.149967 4.267145 -0.472117 H -1.392869 4.904976 -1.337010 C -1.990750 4.264710 0.646246 H -2.880665 4.913355 0.668583 C -1.738396 3.393896 1.717837 H -2.454436 3.359065 2.550716 C -0.612600 2.549327 1.722509 C 0.803286 3.318151 -1.803602 H 1.543885 2.504746 -1.653850 C -0.104332 2.873963 -2.970014 H -0.714255 2.000935 -2.662291 H 0.503778 2.599938 -3.858166 H -0.800623 3.683842 -3.274901 C 1.566628 4.616379 -2.128649 H 0.865125 5.461004 -2.299692 H 2.178756 4.497181 -3.047932 H 2.243152 4.910910 -1.298790 C -0.381583 1.521760 2.833383 H -0.076741 0.589923 2.311044 C -1.663629 1.183074 3.613466 H -1.964810 2.003341 4.300619 H -1.490939 0.282537 4.242800 H -2.501714 0.995377 2.910282 C 0.742886 1.922357 3.808988 H 1.709383 2.073379 3.292592 H 0.898377 1.129832 4.572526 H 0.491347 2.865455 4.339901 C 1.563304 0.557956 0.175776 C 2.789047 2.429495 0.940793 H 3.166767 3.022928 0.074994 C 3.623467 1.162842 1.175262 H 3.644596 0.865105 2.251223 C 3.283877 -1.200135 0.310639 C 4.186402 -1.571069 -0.722275 C 4.556227 -2.926778 -0.818033 H 5.243158 -3.251816 -1.613582 C 4.055165 -3.877309 0.086677 H 4.351096 -4.934327 -0.009873 C 3.192528 -3.483396 1.118572 H 2.821542 -4.234813 1.834430 C 2.796946 -2.137214 1.260034 C 4.692400 -0.523603 -1.715853 H 4.827043 0.422807 -1.148386 C 6.053215 -0.873592 -2.341606 H 6.813325 -1.120535 -1.571240	

H 6.431443 -0.017428 -2.937926 H 5.976845 -1.738441 -3.034675 C 3.636158 -0.240311 -2.804929 H 3.452880 -1.151656 -3.412420 H 3.982933 0.563977 -3.488110 H 2.670820 0.065036 -2.355678 C 1.891493 -1.724528 2.419611 H 1.727070 -0.630899 2.349761 C 0.499141 -2.376547 2.314631 H 0.032012 -2.099457 1.343292 H -0.158072 -2.009360 3.132867 H 0.559909 -3.483822 2.387645 C 2.556186 -2.000827 3.783004 H 2.708991 -3.087988 3.953325 H 1.919778 -1.618345 4.609389 H 3.548270 -1.508319 3.856533 C 0.228502 -0.917508 -2.654706 H 1.013988 -1.659459 -2.878806 H 0.273260 -0.010070 -3.284346 C -1.047810 -1.416335 -2.206953 H -1.069435 -2.468482 -1.875277 C -2.316763 -0.729024 -2.281338 H -2.440817 0.000859 -3.097580 Pd 0.038149 -0.430756 -0.609112 O -3.727469 0.748329 0.824735 C -2.703271 0.396894 0.156500 O -2.567929 0.756047 -1.111593 O -1.790642 -0.385266 0.698223 K -3.666689 -1.457988 1.987396 H 2.733223 3.100208 1.820747 H 4.670553 1.250471 0.822440 C -3.568916 -1.449189 -1.897907 C -3.562725 -2.723890 -1.280338 C -4.818074 -0.801190 -2.065592 C -4.760625 -3.330079 -0.853200 C -6.011323 -1.399920 -1.638871 C -5.991392 -2.668860 -1.026854 H -2.611708 -3.256640 -1.133440 H -4.829693 0.210985 -2.496011 H -4.731486 -4.335716 -0.400710 H -6.966442 -0.868285 -1.773971 H -6.930015 -3.144025 -0.698904	
Zero-point correction= 0.741987 (Hartree/Particle) Thermal correction to Energy= 0.788375 Thermal correction to Enthalpy= 0.789320 Thermal correction to Gibbs Free Energy= 0.662256 Sum of electronic and zero-point Energies= -2499.641575 Sum of electronic and thermal Energies= -2499.595186 Sum of electronic and thermal Enthalpies= -2499.594242 Sum of electronic and thermal Free Energies= -2499.721306 SCF Done (in solvent): -2500.6978683	

[Pd(IMes)(cin)Cl]	**[Pd(IMes)(cin)Cl]-I**
67 MesI-PREcin SCF Done: -1859.94589840 A.U. Cl -0.140762 1.542507 1.718378 N 2.287527 -1.387380 0.486065 C 3.375399 -0.465077 0.282179	73 MesI-PREcin+K2CO3 SCF Done: -3323.73856655 A.U. Cl 0.122910 0.917983 -2.179030 N -0.829864 -2.481772 -0.835718 C -2.135929 -1.924152 -1.065652

N	0.293791	-2.230734	0.533379
C	3.967158	-0.399289	-0.998294
C	5.010725	0.526110	-1.189108
H	5.486920	0.594643	-2.181477
C	5.457808	1.362910	-0.146152
C	4.840726	1.253670	1.116985
H	5.180762	1.901454	1.942011
C	3.791153	0.347074	1.361374
C	0.982961	-1.087676	0.206516
C	2.414710	-2.689958	0.979130
H	3.386648	-3.105270	1.262600
C	1.150991	-3.223495	1.007624
H	0.783840	-4.205748	1.320442
C	-1.136070	-2.319829	0.362018
C	-1.638960	-2.679372	-0.910401
C	-3.030358	-2.610196	-1.106872
H	-3.442317	-2.864745	-2.097722
C	-3.906204	-2.214346	-0.073256
C	-3.363125	-1.923173	1.193297
H	-4.035409	-1.622284	2.013479
C	-1.976059	-1.962548	1.440961
C	0.091755	0.399156	-2.589399
H	0.155059	-0.574559	-3.100409
H	0.891857	1.116302	-2.851371
C	-1.192957	0.868950	-2.179809
H	-2.054746	0.178675	-2.241664
C	-1.316035	2.080155	-1.440802
H	-0.600375	2.897900	-1.642490
C	-2.543733	2.444272	-0.708086
C	-3.430212	1.452158	-0.215377
C	-2.845872	3.799925	-0.442753
C	-4.590034	1.807695	0.484048
H	-3.178671	0.387281	-0.337023
C	-4.008927	4.156218	0.259405
H	-2.154739	4.583184	-0.794380
C	-4.890899	3.163201	0.720634
H	-5.253745	1.016581	0.869619
H	-4.225352	5.219084	0.453029
H	-5.799286	3.442537	1.277722
Pd	0.026725	0.562479	-0.442252
C	3.472429	-1.287313	-2.115180
H	3.507383	-2.360320	-1.829799
H	2.412191	-1.058228	-2.351235
H	4.072364	-1.153832	-3.036040
C	3.102356	0.261853	2.699039
H	3.618041	0.882109	3.457317
H	2.051039	0.620637	2.605474
H	3.058068	-0.782491	3.074093
C	-1.400482	-1.571006	2.775152
H	-0.947937	-0.554173	2.695788
H	-2.182545	-1.544315	3.558337
H	-0.596310	-2.262648	3.100467
C	-0.702678	-3.122226	-2.008958
H	0.172673	-2.446284	-2.086352
H	-0.302141	-4.139278	-1.806263
H	-1.214314	-3.149859	-2.990691
C	-5.384827	-2.047584	-0.338650
H	-5.758949	-2.783593	-1.079315
H	-5.984651	-2.150382	0.587985
H	-5.587894	-1.034362	-0.751635
C	6.552722	2.379968	-0.379428
H	7.224642	2.465320	0.499280
H	7.171249	2.126113	-1.263837

N	1.266581	-2.678645	-0.336056
C	-2.969023	-1.635965	0.041411
C	-4.244370	-1.100060	-0.230070
H	-4.900516	-0.845989	0.615987
C	-4.686353	-0.838559	-1.541105
C	-3.813638	-1.125800	-2.613421
H	-4.135362	-0.912735	-3.646728
C	-2.530379	-1.669711	-2.403264
C	0.233881	-1.769175	-0.342418
C	-0.470654	-3.803503	-1.121869
H	-1.192427	-4.525757	-1.515393
C	0.857757	-3.926776	-0.806095
H	1.543653	-4.776857	-0.871852
C	2.578062	-2.319651	0.140575
C	2.900500	-2.607710	1.485243
C	4.125963	-2.126670	1.984334
H	4.385429	-2.322693	3.037834
C	5.016009	-1.389650	1.177153
C	4.670201	-1.163605	-0.171098
H	5.365071	-0.604014	-0.819376
C	3.454561	-1.615977	-0.719722
C	0.815836	0.148673	2.237363
H	1.191359	-0.760930	2.732282
H	-0.172494	0.537274	2.579426
C	1.770732	1.040425	1.659552
H	2.837299	0.745575	1.621153
C	1.288016	2.143575	0.906717
H	0.283789	2.544885	1.177160
Pd	0.536419	0.167855	0.106542
O	-3.641218	1.593583	1.297990
C	-2.442421	1.853706	1.819000
O	-1.654774	2.671122	1.215620
O	-2.100066	1.243000	2.923414
K	-2.504742	2.012833	-1.037297
K	-4.420795	0.828196	3.504257
C	2.114399	2.934044	-0.019178
C	1.637835	4.191273	-0.464867
C	3.351911	2.467821	-0.533187
C	2.382013	4.967085	-1.367705
H	0.666767	4.549539	-0.086140
C	4.095007	3.243598	-1.432828
H	3.715080	1.467260	-0.247320
C	3.617270	4.500538	-1.852754
H	1.994012	5.944340	-1.698513
H	5.051724	2.860196	-1.824209
H	4.200405	5.106869	-2.564345
C	1.938183	-3.383447	2.354102
H	0.910008	-2.971558	2.275954
H	1.878070	-4.448648	2.042683
H	2.244671	-3.358163	3.417863
C	3.078776	-1.311685	-2.147206
H	3.973860	-1.078556	-2.755961
H	2.536864	-2.156325	-2.618979
H	2.391313	-0.437219	-2.191827
C	6.298133	-0.821277	1.742362
H	6.196613	0.272254	1.917650
H	6.568132	-1.289989	2.709720
H	7.148270	-0.957777	1.042218
C	-1.580097	-1.910654	-3.550232
H	-0.662598	-1.300598	-3.397295
H	-1.271762	-2.974087	-3.627687
H	-2.036983	-1.615358	-4.514701
C	-2.511306	-1.818831	1.466738

H 6.120229 3.389342 -0.555916	H -1.679875 -2.543602 1.556656 H -2.157860 -0.846543 1.885233 H -3.350768 -2.177055 2.100178 C -6.058542 -0.244842 -1.775977 H -6.208080 0.046125 -2.835228 H -6.860381 -0.968095 -1.512098 H -6.215395 0.654732 -1.143199
Zero-point correction= 0.536158 (Hartree/Particle) Thermal correction to Energy= 0.572028 Thermal correction to Enthalpy= 0.572972 Thermal correction to Gibbs Free Energy= 0.466888 Sum of electronic and zero-point Energies= -1859.409740 Sum of electronic and thermal Energies= -1859.373870 Sum of electronic and thermal Enthalpies= -1859.372926 Sum of electronic and thermal Free Energies= -1859.479011 SCF Done (in solvent): -1860.2116523	Zero-point correction= 0.553076 (Hartree/Particle) Thermal correction to Energy= 0.597506 Thermal correction to Enthalpy= 0.598450 Thermal correction to Gibbs Free Energy= 0.471016 Sum of electronic and zero-point Energies= -3323.185491 Sum of electronic and thermal Energies= -3323.141061 Sum of electronic and thermal Enthalpies= -3323.140117 Sum of electronic and thermal Free Energies= -3323.267551 SCF Done (in solvent): -3324.0436552

[Pd(IMes)(cin)Cl]-I-II	**[Pd(IMes)(cin)Cl]-II**
73 MesI-PREcin--K2CO3 SCF Done: -3323.70689702 A.U. Cl -0.074753 -0.453734 -2.546205 N -1.149796 2.567581 -0.136970 C 0.255747 2.853520 -0.276945 N -3.023691 1.488112 -0.020809 C 1.105998 2.748524 0.849653 C 2.486578 2.948039 0.660695 H 3.165257 2.759582 1.508057 C 3.015862 3.300287 -0.596701 C 2.131499 3.427096 -1.691325 H 2.530511 3.700043 -2.684029 C 0.745867 3.184108 -1.563403 C -1.666600 1.289253 -0.110943 C -2.161252 3.529176 -0.066380 H -1.940297 4.601010 -0.077549 C -3.348081 2.847034 0.006795 H -4.383705 3.195178 0.070020 C -3.956763 0.398087 0.068664 C -4.382070 -0.016849 1.348823 C -5.270636 -1.106917 1.423364 H -5.613465 -1.448725 2.414394 C -5.721394 -1.773441 0.266333 C -5.259642 -1.329407 -0.990819 H -5.595828 -1.849471 -1.903526 C -4.371631 -0.245223 -1.120182 C -0.503362 -1.030278 1.845638 H -1.421137 -1.364444 2.364836 H 0.034701 -0.221407 2.376852 C 0.261596 -2.035582 1.128645 H -0.100537 -3.078825 1.094798 C 1.534612 -1.749501 0.547552 H 1.749718 -0.682963 0.380160 Pd -0.665679 -0.431498 -0.133310 O 3.480258 0.502766 2.864064 C 3.419859 -0.211796 1.796999 O 2.928491 -1.476862 1.944152 O 3.733301 0.188844 0.626196 K 2.042557 -1.042465 4.206389 K 2.850813 0.095044 -1.749746 C 2.157986 -2.707732 -0.417913 C 3.558775 -2.921113 -0.450947 C 1.350362 -3.363986 -1.380061 C 4.130763 -3.755501 -1.426771 C 1.927997 -4.200449 -2.350074	73 MesI-PREcin--K2CO3post SCF Done: -3323.75201022 A.U. Cl -1.098713 -0.310957 2.408770 N -2.802546 1.252167 -0.771715 C -3.380384 -0.055777 -0.888643 N -1.441589 2.886999 -0.417137 C -3.006452 -0.882221 -1.978730 C -3.628501 -2.143547 -2.091183 H -3.343756 -2.800227 -2.929964 C -4.602894 -2.583063 -1.167597 C -4.931149 -1.735899 -0.085439 H -5.676021 -2.069469 0.657130 C -4.326118 -0.470324 0.082072 C -1.500360 1.508782 -0.382335 C -3.513956 2.429439 -1.042686 H -4.555891 2.415640 -1.377796 C -2.647421 3.464709 -0.816978 H -2.772499 4.548414 -0.906498 C -0.231969 3.611089 -0.133070 C 0.618382 3.942023 -1.213256 C 1.817288 4.615123 -0.920352 H 2.499580 4.873485 -1.747662 C 2.173116 4.954359 0.403047 C 1.295400 4.601885 1.446978 H 1.562482 4.856341 2.486421 C 0.082605 3.924424 1.206373 C 1.650831 0.532087 -1.164480 H 1.985782 1.586585 -1.187250 H 1.473602 0.103462 -2.171582 C 2.124883 -0.338372 -0.115713 H 2.824445 0.121626 0.617764 C 2.482071 -1.782635 -0.433482 Pd 0.077824 0.329760 0.150345 H 1.845041 -2.140574 -1.273372 O 0.584377 -3.609111 1.904909 C 0.950909 -3.308602 0.725730 O 2.190308 -2.631899 0.710247 O 0.340829 -3.489585 -0.352469 K 1.601257 -1.414064 2.975615 K -1.817744 -2.867682 0.926289 C 3.950265 -1.997616 -0.801924 C 4.670751 -1.009165 -1.507617 C 4.607637 -3.205615 -0.479752 C 6.008249 -1.223007 -1.883377

C	3.319735	-4.397660	-2.381850
H	4.168792	-2.423895	0.315842
H	0.268802	-3.165748	-1.395594
H	5.221677	-3.913721	-1.432310
H	1.281619	-4.687534	-3.097553
H	3.771105	-5.050056	-3.146877
C	-0.172095	3.188096	-2.761267
H	-0.521467	2.148654	-2.955224
H	-1.071816	3.817860	-2.602222
H	0.351164	3.553871	-3.666552
C	0.594862	2.429294	2.233950
H	-0.402238	1.951234	2.216381
H	1.326588	1.761618	2.735744
H	0.520450	3.356422	2.843656
C	-3.835597	0.196798	-2.458582
H	-2.757033	-0.064849	-2.551360
H	-4.383855	-0.283817	-3.291897
H	-3.902943	1.298147	-2.581672
C	-3.857365	0.676179	2.583860
H	-2.746435	0.671056	2.584096
H	-4.167834	1.742308	2.621467
H	-4.214289	0.182089	3.508559
C	-6.681126	-2.939509	0.355910
H	-6.280249	-3.831524	-0.170590
H	-6.885486	-3.227373	1.406519
H	-7.654047	-2.694662	-0.122637
C	4.510836	3.466288	-0.750549
H	4.812885	3.595930	-1.810197
H	4.878021	4.350013	-0.186246
H	5.029465	2.578556	-0.327670

Zero-point correction= 0.552658 (Hartree/Particle)
Thermal correction to Energy= 0.596379
Thermal correction to Enthalpy= 0.597323
Thermal correction to Gibbs Free Energy= 0.472444
Sum of electronic and zero-point Energies= -3323.154239
Sum of electronic and thermal Energies= -3323.110518
Sum of electronic and thermal Enthalpies= -3323.109574
Sum of electronic and thermal Free Energies= -3323.234453

SCF Done (in solvent): -3324.0019726

C	5.946565	-3.418206	-0.850819
C	6.654398	-2.427799	-1.554722
H	4.173905	-0.060732	-1.763199
H	4.053586	-3.979058	0.072638
H	6.551292	-0.438009	-2.434731
H	6.440627	-4.367909	-0.587875
H	7.704192	-2.593726	-1.845695
C	-4.608734	0.387244	1.291772
H	-5.022007	1.379490	1.015959
H	-5.326121	-0.107252	1.975384
H	-3.659879	0.569299	1.843568
C	-1.943739	-0.438529	-2.949949
H	-2.124014	0.598488	-3.301448
H	-0.958154	-0.422689	-2.431841
H	-1.883426	-1.112839	-3.825504
C	0.253078	3.519723	-2.615678
H	0.105120	2.418685	-2.651284
H	-0.700560	3.981282	-2.949771
H	1.042975	3.793737	-3.341402
C	-0.831505	3.497519	2.327331
H	-1.883025	3.796536	2.133224
H	-0.835375	2.388162	2.422039
H	-0.517098	3.934816	3.295255
C	-5.287435	-3.920761	-1.348970
H	-5.752615	-4.278274	-0.407903
H	-6.096183	-3.850074	-2.108834
H	-4.579947	-4.698218	-1.704933
C	3.476705	5.670957	0.679133
H	3.536108	6.629336	0.120225
H	3.603281	5.898046	1.756505
H	4.345760	5.057361	0.357644

Zero-point correction= 0.554057 (Hartree/Particle)
Thermal correction to Energy= 0.598073
Thermal correction to Enthalpy= 0.599017
Thermal correction to Gibbs Free Energy= 0.472282
Sum of electronic and zero-point Energies= -3323.197953
Sum of electronic and thermal Energies= -3323.153937
Sum of electronic and thermal Enthalpies= -3323.152993
Sum of electronic and thermal Free Energies= -3323.279728

SCF Done (in solvent): -3324.0536661

[Pd(IMes)(cin)Cl]-III			
71			
MesI-PREcin+KCO3menysKClISOMERopen SCF Done: -2263.48106463 A.U.			
N	0.736613	-2.518713	-0.136272
C	-0.685446	-2.704976	-0.040739
N	2.698910	-1.623618	-0.251106
C	-1.325841	-2.531718	1.209007
C	-2.706325	-2.802756	1.282257
H	-3.218786	-2.661221	2.246644
C	-3.444525	-3.222780	0.156140
C	-2.779943	-3.323365	-1.087116
H	-3.345071	-3.630024	-1.984780
C	-1.398939	-3.062115	-1.207841
C	1.364792	-1.283014	-0.140231
C	1.651147	-3.574041	-0.232496
H	1.334112	-4.621839	-0.228002
C	2.895808	-3.003882	-0.304376
H	3.893275	-3.448970	-0.376300
C	3.741730	-0.632770	-0.225628
C	4.241272	-0.211671	1.028462
C	5.246372	0.771237	1.034801

[Pd(IMes)(cin)Cl]-I'			
71			
MesI-PREcin+KCO3menysKCl SCF Done: -2263.50524220 A.U.			
N	0.015307	-2.633265	0.758375
C	1.376265	-2.880151	0.347807
N	-1.975967	-1.792214	0.887193
C	1.582390	-3.401715	-0.953364
C	2.904508	-3.645622	-1.360252
H	3.085569	-4.052637	-2.369513
C	4.000685	-3.384437	-0.509420
C	3.745215	-2.868096	0.772410
H	4.591208	-2.644296	1.443509
C	2.438717	-2.593047	1.230183
C	-0.745880	-1.581012	0.318253
C	-0.724609	-3.483138	1.582628
H	-0.280312	-4.378202	2.028379
C	-1.984563	-2.949341	1.668811
H	-2.878436	-3.272585	2.210725
C	-3.115831	-0.950464	0.638168
C	-4.002992	-1.329919	-0.395241
C	-5.087901	-0.479349	-0.673325

H	5.640795	1.121593	2.003636	H	-5.787287	-0.751756	-1.481378
C	5.749187	1.330072	-0.160040	C	-5.290999	0.717384	0.047731
C	5.214034	0.887534	-1.385786	C	-4.377297	1.054419	1.065064
H	5.582002	1.328229	-2.327558	H	-4.521967	1.988950	1.632728
C	4.202766	-0.091597	-1.443402	C	-3.272532	0.236943	1.386194
C	1.419388	2.076185	1.371695	C	-1.507141	0.162300	-2.386488
H	2.471179	2.322291	1.143315	H	-2.587296	0.019882	-2.222569
H	1.225150	1.746151	2.409298	H	-1.064094	-0.467104	-3.180184
C	0.369625	2.632464	0.594420	C	-0.945322	1.449801	-2.103203
H	0.669627	3.301157	-0.236663	H	-1.579477	2.209113	-1.610680
C	-1.036442	2.910740	1.097827	C	0.458031	1.650495	-2.150827
H	-1.015797	3.793656	1.779281	H	1.060395	0.969500	-2.781130
Pd	0.643162	0.582384	0.054663	Pd	-0.126102	0.008834	-0.730403
O	-3.224643	0.333890	1.933648	O	2.453381	1.416729	2.107003
C	-2.229173	0.814903	1.336068	C	1.441665	1.178620	1.353335
O	-1.593021	1.880845	1.971734	O	1.519814	0.151067	0.520165
O	-1.801788	0.448978	0.187561	O	0.373261	1.921570	1.360386
K	-4.117922	0.019324	-0.511655	K	1.747951	3.801554	2.165764
C	3.635318	-0.752029	2.298667	C	2.235211	-1.963081	2.583898
H	2.565198	-0.449306	2.343167	H	2.568572	-0.901483	2.541653
H	3.653366	-1.861992	2.327531	H	1.172980	-1.954009	2.893703
H	4.155713	-0.367626	3.197072	H	2.827608	-2.489720	3.361364
C	3.553905	-0.498859	-2.743096	C	0.413944	-3.660083	-1.876896
H	3.555389	-1.600589	-2.881832	H	-0.389539	-4.239153	-1.374012
H	2.487521	-0.180115	-2.734457	H	-0.043523	-2.697966	-2.195561
H	4.056160	-0.035025	-3.614397	H	0.729893	-4.215498	-2.781480
C	-0.559325	-2.025425	2.400659	C	5.414091	-3.629172	-0.990658
H	0.364967	-2.615556	2.573743	H	5.721468	-2.852841	-1.725320
H	-0.225780	-0.980679	2.199210	H	6.144158	-3.604469	-0.156971
H	-1.178055	-2.032630	3.317297	H	5.507097	-4.610823	-1.501330
C	-0.690934	-3.131085	-2.541028	C	-2.271446	0.629755	2.437658
H	-0.124738	-2.193535	-2.726517	H	-1.343935	1.049255	1.966948
H	0.052592	-3.955768	-2.573134	H	-2.688530	1.397041	3.119778
H	-1.406329	-3.285433	-3.372764	H	-1.950461	-0.242381	3.044012
C	-4.911191	-3.582972	0.289111	C	-3.741046	-2.583335	-1.195905
H	-5.425186	-2.951750	1.044724	H	-2.713154	-2.566089	-1.617686
H	-5.454086	-3.494901	-0.675859	H	-3.805087	-3.495177	-0.564571
H	-5.031657	-4.635940	0.625877	H	-4.462244	-2.691195	-2.029235
C	6.827817	2.389825	-0.109445	C	-6.484367	1.598231	-0.250637
H	7.746328	2.007919	0.386179	H	-6.702844	1.635446	-1.337975
H	7.110556	2.740425	-1.122184	H	-7.398837	1.210509	0.250451
H	6.492957	3.274436	0.473864	H	-6.329228	2.636637	0.105670
C	-2.065740	3.219172	0.000603	C	1.172607	2.847947	-1.673746
C	-1.819033	3.023597	-1.374492	C	2.565296	2.759636	-1.413409
C	-3.364473	3.605192	0.403337	C	0.538000	4.100695	-1.474748
C	-2.843978	3.199719	-2.321527	C	3.297686	3.882404	-0.996351
C	-4.395774	3.777001	-0.538815	C	1.269740	5.226731	-1.062581
C	-4.139769	3.571098	-1.909531	C	2.658159	5.128779	-0.825814
H	-0.824829	2.679337	-1.696690	H	3.063132	1.782950	-1.514711
H	-3.570547	3.736546	1.477788	H	-0.540184	4.201505	-1.673112
H	-2.630877	3.040538	-3.391384	H	4.378452	3.784616	-0.804449
H	-5.400617	4.081309	-0.202596	H	0.757816	6.196657	-0.947871
H	-4.940351	3.717004	-2.653251	H	3.238970	6.019800	-0.535221
Zero-point correction= 0.551448 (Hartree/Particle)				Zero-point correction= 0.551519 (Hartree/Particle)			
Thermal correction to Energy= 0.591326				Thermal correction to Energy= 0.591538			
Thermal correction to Enthalpy= 0.592271				Thermal correction to Enthalpy= 0.592483			
Thermal correction to Gibbs Free Energy= 0.476305				Thermal correction to Gibbs Free Energy= 0.476134			
Sum of electronic and zero-point Energies= -2262.929616				Sum of electronic and zero-point Energies= -2262.953723			
Sum of electronic and thermal Energies= -2262.889738				Sum of electronic and thermal Energies= -2262.913704			
Sum of electronic and thermal Enthalpies= -2262.888794				Sum of electronic and thermal Enthalpies= -2262.912760			
Sum of electronic and thermal Free Energies= -2263.004760				Sum of electronic and thermal Free Energies= -2263.029108			
SCF Done (in solvent): -2263.7617532				SCF Done (in solvent): -2263.7823699			

[Pd(IMes)(cin)Cl]-I'-III	
71 MesI-PREcin+KCO3--C-O SCF Done: -2263.46656198 A.U. N 0.845186 -2.572935 0.112959 C -0.569927 -2.831691 0.133952 N 2.756845 -1.567043 0.032053 C -1.298655 -2.581879 1.319379 C -2.670323 -2.902441 1.323119 H -3.254361 -2.703349 2.235521 C -3.312250 -3.442187 0.189513 C -2.559940 -3.616605 -0.993862 H -3.051054 -4.015864 -1.898552 C -1.184845 -3.308782 -1.044795 C 1.401265 -1.313153 -0.030273 C 1.821541 -3.562983 0.255652 H 1.562991 -4.618474 0.387245 C 3.033499 -2.923968 0.205339 H 4.057495 -3.302998 0.281519 C 3.743721 -0.522924 -0.012699 C 4.135423 0.084986 1.200731 C 5.090173 1.115687 1.136967 H 5.404577 1.607944 2.072625 C 5.634571 1.549821 -0.090096 C 5.193042 0.932470 -1.277643 H 5.590817 1.276891 -2.246942 C 4.239921 -0.104644 -1.264605 C 1.715059 2.117453 0.040958 H 2.534636 2.236022 -0.689764 H 2.048865 2.172556 1.093985 C 0.397213 2.587904 -0.308594 H 0.209800 2.820004 -1.372751 C -0.663944 2.934865 0.614277 H -0.369763 3.379640 1.578610 Pd 0.477246 0.434876 -0.230557 O -3.340760 0.371646 1.458200 C -2.191647 0.682450 1.010044 O -1.421182 1.528873 1.678071 O -1.752995 0.182384 -0.128902 K -4.076477 -0.270769 -0.828824 C 3.463016 -0.311185 2.491549 H 2.381839 -0.051331 2.436645 H 3.514850 -1.405939 2.669479 H 3.909213 0.207722 3.361863 C 3.681616 -0.699844 -2.532901 H 3.737393 -1.808752 -2.531007 H 2.602454 -0.436049 -2.612808 H 4.209411 -0.321974 -3.430058 C -0.640259 -1.935669 2.509877 H 0.347958 -2.389038 2.731346 H -0.457245 -0.859605 2.291127 H -1.279549 -1.998213 3.410705 C -0.382660 -3.437171 -2.318126 H 0.096324 -2.465231 -2.565812 H 0.440140 -4.176551 -2.217487 H -1.019139 -3.747303 -3.170123 C -4.772699 -3.842976 0.252900 H -5.359976 -3.159354 0.902110 H -5.243983 -3.869700 -0.752363 H -4.886239 -4.861315 0.685022 C 6.628622 2.689485 -0.123932 H 7.400314 2.581602 0.666680 H 7.145741 2.758405 -1.102010	

H 6.118804 3.662011 0.052749 C -1.959897 3.419684 0.070921 C -2.416981 3.026340 -1.212427 C -2.822089 4.200800 0.875900 C -3.686859 3.415753 -1.673768 C -4.088475 4.590667 0.416092 C -4.530501 4.197334 -0.861395 H -1.772462 2.395423 -1.841876 H -2.492824 4.482198 1.888302 H -4.015681 3.119759 -2.684942 H -4.742012 5.198002 1.062331 H -5.524688 4.504225 -1.224477	
Zero-point correction= 0.550457 (Hartree/Particle) Thermal correction to Energy= 0.589928 Thermal correction to Enthalpy= 0.590873 Thermal correction to Gibbs Free Energy= 0.476087 Sum of electronic and zero-point Energies= -2262.916105 Sum of electronic and thermal Energies= -2262.876634 Sum of electronic and thermal Enthalpies= -2262.875689 Sum of electronic and thermal Free Energies= -2262.990475 SCF Done (in solvent): -2263.7362398	