Supporting Information

Suzuki–Miyaura Cross-Coupling of Esters by Selective O–C(O) Cleavage Mediated by Air- and Moisture-Stable [Pd(NHC)(μ-Cl)Cl]$_2$ Precatalysts: Catalyst Evaluation and Mechanism

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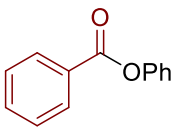
List of Known Compounds/General Methods

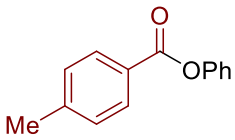
All starting materials reported in the manuscript have been previously described in literature or prepared by the method reported previously. Esters were prepared by standard methods.[1-3] All experiments were performed using standard Schlenk techniques under nitrogen or argon unless stated otherwise. 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 solvents were deoxygenated prior to use. 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 (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). Yields refer to isolated compounds, estimated to be >95% pure as determined by ^{1}H NMR. ^{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 (7.26 and 77.2 ppm, ^{1}H NMR and ^{13}C NMR, respectively). All coupling constants (J) are reported in Hertz (Hz). Abbreviations are as followed: s, singlet; d, doublet; t, triplet; q, quartet; qui, quintet; sex, sextet; sep, septet; brs, broad singlet; m, multiple peaks. 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 250 °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 15 min (splitless mode of injection, total run time of 22.0 min). High-resolution mass spectra (HRMS) were measured on a 7T Bruker Daltonics FT-MS instrument. 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. ^{1}H NMR and ^{13}C NMR data are given for all compounds in the SI for characterization purposes. ^{1}H NMR, ^{13}C NMR, and HRMS data are given for all new compounds.

Experimental Procedures and Characterization Data

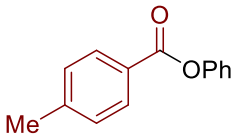
General Procedure for the Synthesis of Starting Materials. All esters used in this study were prepared by procedures reported in the literature.[1-3] **12a**, **12j-12w** are known compounds. Spectroscopic data matched those reported in the literature. (IPr)Pd(μ-Cl)Cl]$_2$ was prepared by our previously reported method.[19] (IPr)Pd(μ-Br)Br]$_2$ and [(IPr)Pd(μ-I)I]$_2$ were prepared according to the literature.[17-18] ^{1}H NMR and ^{13}C NMR data are given for all starting materials in the section below for characterization purposes.



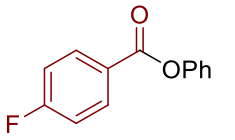
Phenyl benzoate (12a).[1] White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 (d, J = 7.5 Hz, 1H), 7.65 (t, J = 7.8 Hz, 1H), 7.53 (t, J = 7.8 Hz, 2H), 7.45 (t, J = 7.8 Hz, 2H), 7.29 (t, J = 7.5 Hz, 1H), 7.23 (d, J = 7.8 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.20, 150.98, 133.60, 130.19, 129.61, 129.51, 128.59, 125.91, 121.74.



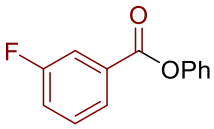
Phenyl 4-methylbenzoate (12j).[1] White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (d, J = 8.0 Hz, 2H), 7.34 (t, J = 8.0 Hz, 2H), 7.22 (d, J = 7.5 Hz, 2H), 7.19 (t, J = 8.0 Hz, 1H), 7.13 (d, J = 8.0 Hz, 2H), 2.37 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.26, 151.06, 144.42, 130.24, 129.47, 129.31, 126.85, 125.80, 121.79, 21.79.



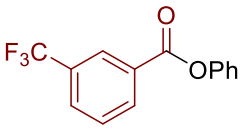
Phenyl 4-methoxylbenzoate (12k).[1] White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17 (d, J = 8.5 Hz, 2H), 7.43 (t, J = 8.0 Hz, 2H), 7.21 (d, J = 7.5 Hz, 1H), 6.99 (t, J = 8.5 Hz, 2H), 3.90 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.92, 163.90, 151.08, 132.30, 129.45, 125.73, 121.90, 121.82, 113.85, 55.53.



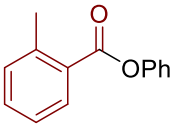
Phenyl 4-fluorobenzoate (12l).[1] White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 (dd, J = 9.0 Hz, 5.5 Hz, 2H), 7.44 (t, J = 8.0 Hz, 2H), 7.29 (t, J = 7.5 Hz, 1H), 7.24-7.16 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.14, 165.11 (d, J^F = 253.8 Hz), 164.17, 150.82, 132.80, 132.72, 129.49, 125.95, 125.82 (d, J^F = 3.0 Hz), 121.63, 115.75 (d, J^F = 22.0 Hz).



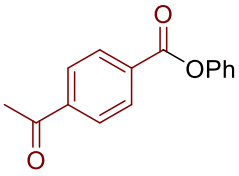
Phenyl 3-fluorobenzoate (12m).[4] Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (dt, J = 8.0 Hz, 1.5 Hz, 1H), 7.92 (ddd, J = 9.5 Hz, J = 2.5 Hz, 1.5 Hz, 1H), 7.53 (td, J = 8.0 Hz, J = 5.5 Hz, 1H), 7.47 (t , J = 8.0 Hz, 2H), 7.37 (td, J = 8.0 Hz, J = 5.5 Hz, 1H), 7.32 (t, J = 7.5 Hz, 1H), 7.25 (d, J = 8.0 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.62 (d, J^F = 246.2 Hz), 150.77, 131.77 (d, J^F = 7.3 Hz), 130.24 (d, J^F = 7.4 Hz), 129.56, 126.09, 125.92 (d, J^F = 3.1 Hz), 121.58, 120.69 (d, J^F = 21.2 Hz), 117.05 (d, J^F = 23.0 Hz).



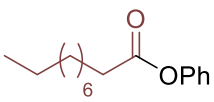
Phenyl 3-(trifluoromethyl) benzoate (12n).[5] White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (s, 1H), 8.40 (d, J = 8.0 Hz, 1H), 7.90 (d, J = 7.9 Hz, 1H), 7.67 (t, J = 7.8 Hz, 1H), 7.46 (t, J = 7.5 Hz, 2H), 7.31 (t, J = 7.5 Hz, 1H), 7.24 (d, J = 7.5 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.89, 150.67, 133.36, 131.35 (q, J^F = 32.9 Hz), 130.53, 130.08 (q, J^F = 3.6 Hz), 129.61, 129.30, 127.07 (q, J^F = 3.8 Hz), 126.22, 123.62 (q, J^F = 270.8 Hz), 121.56.



Phenyl 2-methylbenzoate (12o).[1] Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (d, J = 7.8 Hz, 1H), 7.52 (t, J = 7.5 Hz, 1H), 7.47 (t, J = 7.5 Hz, 2H), 7.36 (t, J = 8.0 Hz, 2H), 7.32-7.28 (m, 1H), 7.25 (d, J = 8.0 Hz, 2H), 2.71 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.84, 150.95, 141.32, 132.71, 131.97, 131.17, 129.49, 128.61, 125.93, 125.83, 121.84, 21.96.

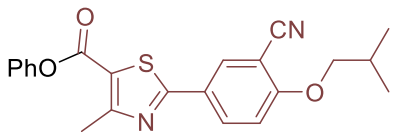


Phenyl 4-acetylbenzoate (12p).[6] White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (d, J = 8.0 Hz, 2H), 8.08 (d, J = 8.0 Hz, 2H), 7.45 (t, J = 8.0 Hz, 2H), 7.30 (t, J = 7.5 Hz, 1H), 2.68 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.47, 164.34, 150.75, 140.72, 133.35, 130.43, 129.60, 128.37, 126.17, 121.58, 26.96.

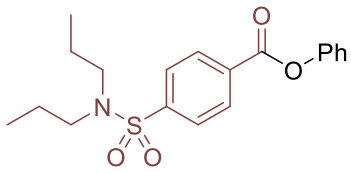


Phenyl decanoate (12q).[7] Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (t, J = 7.8 Hz, 2H), 7.22 (t, J = 7.4 Hz, 1H), 7.08 (d, J = 7.7 Hz, 2H), 2.56 (t, J = 7.5 Hz, 2H), 1.76 (m, 2H), 1.50-1.41 (m, 2H), 1.40-1.25 (m, 10H), 0.89 (t,

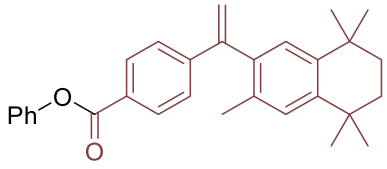
J = 6.7 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) 172.33, 150.78, 129.38, 125.69, 121.59, 34.44, 31.88, 29.44, 29.28, 29.13, 24.98, 22.69, 14.13.



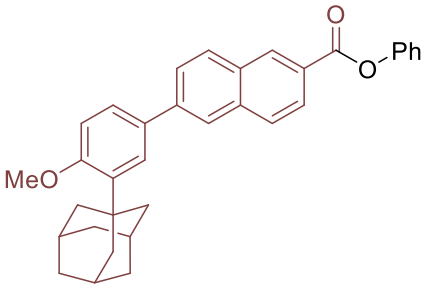
Phenyl 2-(3-cyano-4-isobutoxyphenyl)-4-methylthiazole-5-carboxylate (12r). Prepared according to the previous method[1] from phenol and the corresponding acid on 1.0 mmol scale using EDC and DMAP. CAS No. 1619982-03-4. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 (d, *J* = 2.5 Hz, 1H), 8.13 (dd, 9.0 Hz, 2.5 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.21 (d, *J* = 7.5 Hz, 2H), 7.03 (d, *J* = 9.0 Hz, 1H), 3.92 (d, *J* = 6.5 Hz, 2H), 2.83 (s, 3H), 2.22 (m, 1H), 1.10 (d, *J* = 7.0 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.14, 163.00, 162.68, 160.44, 150.24, 132.68, 132.24, 129.56, 126.24, 125.85, 121.62, 120.66, 115.35, 112.69, 103.10, 75.75, 28.17, 19.07, 17.71.



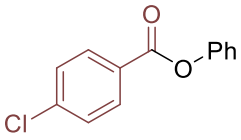
Phenyl 4-(*N*,*N*-dipropylsulfamoyl)benzoate (12s). Prepared according to the previous method[1] from phenol and the corresponding acid on 1.0 mmol scale using EDC and DMAP. CAS No. 70192-09-5. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.5 Hz, 2H), 7.95 (d, *J* = 8.5 Hz, 2H), 7.45 (t, *J* = 8.0 Hz, 2H), 7.30 (t, *J* = 7.5 Hz, 1H), 7.22 (d, *J* = 7.5 Hz, 2H), 3.13 (t, *J* = 7.5 Hz, 4H), 1.57 (sex, *J* = 7.5 Hz, 4H), 0.89 (t, *J* = 7.5 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.88, 150.64, 144.91, 132.87, 130.80, 129.63, 127.17, 126.26, 121.50, 49.95, 21.96, 11.19.



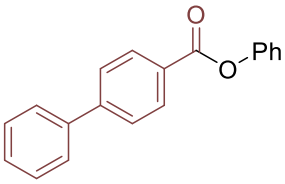
Phenyl 4-(1-(3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydro-naphthalen-2-yl) vinyl) benzoate (12t). Prepared according to the previous method[1] from phenol and the corresponding acid on 1.0 mmol scale using EDC and DMAP. CAS No. 2415156-25-9. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.5 Hz, 1H), 7.47-7.40 (m, 4H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.23 (t, *J* = 8.0 Hz, 2H), 7.18 (s, 1H), 7.12 (s, 1H), 5.88 (s, 1H), 5.39 (s, 1H), 2.00 (s, 3H), 1.74 (s, 4H), 1.33 (d, *J* = 11.5 Hz, 12H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.05, 151.03, 149.13, 146.30, 144.46, 142.41, 137.95, 132.74, 130.29, 129.49, 128.36, 128.11, 126.79, 125.86, 121.76, 117.19, 35.25, 35.23, 34.05, 33.95, 31.99, 31.93, 20.01.



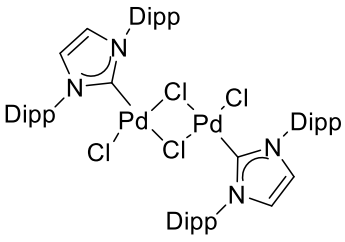
Phenyl 6-(3-(adamantan-1-yl)-4-methoxyphenyl)-2-naphthoate (12u). Prepared according to the previous method[1] from phenol and the corresponding acid on 1.0 mmol scale using EDC and DMAP. CAS No. 1996626-69-7. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.80 (s, 1H), 8.21 (d, *J* = 9.0 Hz, 1H), 8.07-8.02 (m, 2H), 7.98 (d, 9.0 Hz, 1H), 7.84 (d, *J* = 8.5 Hz, 1H), 7.63(s, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.32-7.27 (m, 3H), 7.01 (t, *J* = 7.5 Hz, 1H), 3.92 (s, 3H), 2.20 (s, 6H), 2.12 (s, 3H), 1.82 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.41, 158.98, 151.09, 141.76, 139.04, 136.26, 132.43, 131.69, 131.23, 129.83, 129.51, 128.43, 126.65, 126.24, 125.99, 125.87, 125.81, 125.75, 124.75, 121.79, 112.11, 55.17, 40.61, 37.12, 29.70, 29.10.



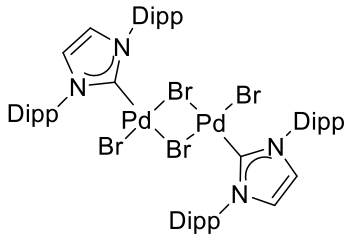
Phenyl 4-chlorobenzoate (12v).[8] White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.5 Hz, 2H), 7.49 (d, *J* = 9.0 Hz, 2H), 7.44 (t, *J* = 8.0 Hz, 2H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.21 (d, *J* = 7.5 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.35, 150.78, 140.14, 131.56, 129.55, 128.96, 128.04, 126.06, 121.62.



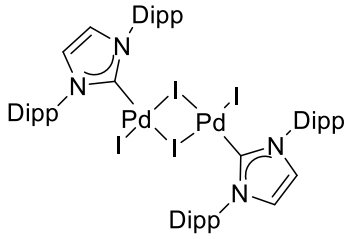
Phenyl [1,1'-biphenyl]-4-carboxylate (12w).[6] According to our previous report,[19] the reaction of **12v** (0.20 mmol), phenylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.05 mol%) in THF (0.5 M) for 12 h at room temperature, afforded after work-up and chromatography the corresponding ester in 83% yield (45 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.5 Hz, 2H), 7.66 (d, *J* = 8.5 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.45-7.32 (m, 5H), 7.23-7.13 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.09, 151.00, 146.34, 139.89, 130.72, 129.52, 129.00, 128.33, 128.29, 127.35, 127.25, 125.90, 121.75.



[Pd(IPr)(μ-Cl)Cl]$_2$ (1).[19] Yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (t, *J* = 7.7 Hz, 4H), 7.34-7.29 (m, 8H), 6.98 (s, 4H), 2.86 (brs, 4H), 2.60 (brs, 4H), 1.30 (d, *J* = 40.0 Hz, 24H), 0.99 (d, J = 27.5 Hz, 24H).



[Pd(IPr)(μ-Br)Br]₂ (2).[17] Yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (t, *J* = 7.7 Hz, 4H), 7.34 (d, *J* = 7.5 Hz, 4H), 7.28-7.26 (m, 4H), 7.01 (s, 4H), 3.11-2.95 (m, 4H), 2.71-2.58 (m, 4H), 1.41 (d, *J* = 7.0 Hz, 12H), 1.23 (d, *J* = 7.0 Hz, 12H), 1.05 (d, *J* = 6.8 Hz, 12H), 0.94 (d, *J* = 6.8 Hz, 12H).



[Pd(IPr)(μ-I)I]₂ (3).[18] Brown solid. ^{1}H NMR (500 MHz, $CDCl_3$) 7.51 (t, J = 7.7 Hz, 4H), 7.34 (d, *J* = 7.5 Hz, 4H), 7.27-7.22 (m, 4H), 7.09 (s, 4H), 3.34-3.24 (m, 4H), 2.90-2.59 (m, 4H), 1.47 (d, *J* = 6.5 Hz, 12H), 1.25 (d, *J* = 6.5 Hz, 12H), 1.08 (d, *J* = 6.9 Hz, 12H), 0.94 (d, *J* = 6.9 Hz, 12H).

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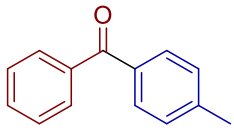
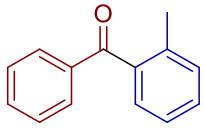
General Procedure for the Suzuki-Miyaura Cross-Coupling of Esters. An oven-dried vial equipped with a stir bar was charged with an ester substrate (neat, 1.0 equiv), K_2CO_3 (typically, 3.0 equiv), boronic acid (typically, 2.0 equiv), [(IPr)Pd(μ-Cl)Cl]$_2$ (typically, 0.25 mol%), placed under a positive pressure of argon, and subjected to three evacuation/backfilling cycles under high vacuum. THF (typically, 0.25 M) and H_2O (typically, 5.0 equiv) were added with vigorous stirring at room temperature, and the reaction mixture was stirred for an indicated time. After the indicated time, the reaction mixture was diluted with CH_2Cl_2 (10 mL), filtered, and concentrated. The sample was analyzed by ^{1}H NMR ($CDCl_3$, 500 MHz) and GC-MS to obtain conversion, selectivity and yield using internal standard and comparison with authentic samples. Purification by chromatography (EtOAc/hexanes) afforded the title product.

Phenyl(*p*-tolyl)methanone (14a).



According to the general procedure, the reaction of **1a** (0.20 mmol), 4-methylphenylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.25 mol%) in THF (0.25 M) for 12 h at room temperature afforded after work-up and chromatography the title product in 96% yield (38 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (d, J = 7.5 Hz, 2H), 7.72 (d, J = 7.5 Hz, 2H), 7.58 (t, J = 7.5 Hz, 1H), 7.48 (t, J = 7.5 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 2.46 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 196.52, 143.24, 137.96, 134.89, 132.16, 130.31, 129.94, 128.98, 128.21, 21.67. NMR data matched literature values.[1]

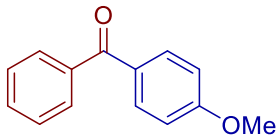
Phenyl(*o*-tolyl)methanone (14b).



According to the general procedure, the reaction of **1a** (0.20 mmol), 2-methylphenylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.25 mol%) in THF (0.25 M) for 12 h at room temperature afforded after work-up and chromatography the title product in 75% yield (29 mg). Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, J = 7.5 Hz,

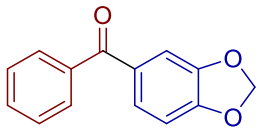
2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.33 (dd, *J* = 11.0 Hz, 7.5 Hz, 2H), 7.29-7.26 (m, 1H), 2.36 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.65, 138.62, 137.74, 136.75, 133.13, 131.00, 130.24, 130.14, 128.52, 128.46, 125.20, 20.00. NMR data matched literature values.[1]

(4-Methoxyphenyl)(phenyl)methanone (14c).



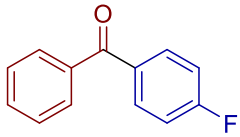
According to the general procedure, the reaction of **1a** (0.20 mmol), 4-methoxylphenylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.25 mol%) in THF (0.25 M) for 12 h at room temperature afforded after work-up and chromatography the title product in 99% yield (42 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.5 Hz, 2H), 7.76 (d, *J* = 7.5 Hz, 2H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 2H), 6.97 (d, *J* = 9.0 Hz, 2H), 3.89 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.57, 163.22, 138.30, 132.57, 131.89, 130.17, 129.74, 128.19, 113.56, 55.51. NMR data matched literature values.[1]

Benzo[*d*][1,3]dioxol-5-yl(phenyl)methanone (14d).



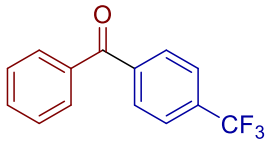
According to the general procedure, the reaction of **1a** (0.20 mmol), benzo[d][1,3]dioxol-5-ylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.25 mol%) run in THF (0.25 M) for 12 h at room temperature afforded after work-up and chromatography the title product in 95% yield (43 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.5 Hz, 2H), 7.57 (d, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.40-7.35 (m, 2H), 6.86 (d, *J* = 8.5 Hz, 1H), 6.07 (s, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.14, 151.52, 147.94, 138.13, 131.99, 131.92, 129.71, 128.21, 126.87, 109.92, 107.70, 101.85. NMR data matched literature values.[9]

(4-Fluorophenyl)(phenyl)methanone (14e).



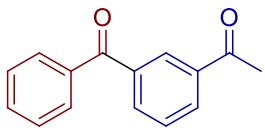
According to the general procedure, the reaction of **1a** (0.20 mmol), 4-fluorophenylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.25 mol%) in THF (0.25 M) for 12 h at room temperature afforded after work-up and chromatography the title product in 99% yield (39 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (dd, J = 9.0 Hz, 5.5 Hz, 2H), 7.77 (d, J = 8.0 Hz, 2H), 7.60 (t, J = 7.2 Hz, 1H), 7.49 (t, J = 7.8 Hz, 2H), 7.16 (d, J = 8.5 Hz, 2H), 2.46 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.28, 165.40 (d, J^F = 252.6 Hz), 137.51, 133.80 (d, J^F = 3.0 Hz), 132.68 (d, J^F = 9.1 Hz), 132.48, 129.88, 129.50, 128.36 (d, J^F = 21.6 Hz). NMR data matched literature values.[9]

Phenyl(4-(trifluoromethyl)phenyl)methanone (14f).



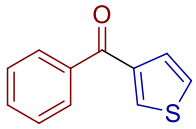
According to the general procedure, the reaction of **1a** (0.20 mmol), 4-trifluoromethyl phenylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.5 mol%) in THF (0.25 M) for 12 h at 60 °C afforded after work-up and chromatography the title product in 81% yield (41 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90 (d, J = 8.0 Hz, 2H), 7.81 (t, J = 7.5 Hz, 2H), 7.76 (d, J = 8.0 Hz, 2H), 7.63 (t, J = 7.5 Hz, 1H), 7.51 (t, J = 7.5 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.55, 140.73, 136.73, 133.73 (d, J^F = 32.5 Hz), 133.10, 130.13 (d, J^F = 4.3 Hz), 128.54, 125.36 (d, J^F = 3.8 Hz), 123.68 (d, J^F = 270 Hz). NMR data matched literature values.[1]

1-(3-Benzoylphenyl)ethan-1-one (14g).



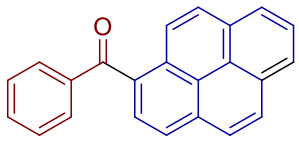
According to the general procedure, the reaction of **1a** (0.20 mmol), (3-acetylphenyl)boronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.5 mol%) in THF (0.25 M) for 12 h at 60 °C afforded after work-up and chromatography the title product in 73% yield (33 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (t, *J* = 1.8 Hz, 1H), 8.19 (dt, *J* = 7.5 Hz, 1.5 Hz, 1H), 7.99 (dt, *J* = 7.5 Hz, 1.5 Hz, 1H), 7.80 (d, *J* = 7.5 Hz, 2H), 7.66-7.58 (m, 2H), 7.51 (t, *J* = 7.5 Hz, 2H), 2.65 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.32, 195.88, 138.08, 137.19, 137.01, 134.27, 132.90, 131.77, 130.05, 129.72, 128.76, 128.52, 26.78. NMR data matched literature values.[1]

Phenyl(thiophen-3-yl)methanone (14h).



According to the general procedure, the reaction of **1a** (0.20 mmol), thiophen-3-ylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.25 mol%) in THF (0.25 M) for 12 h at room temperature afforded after work-up and chromatography the title product in 76% yield (29 mg). Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (dd, *J* = 3.0 Hz, *J* = 1.5 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 2H), 7.62-7.57 (m, 2H), 7.49 (t, *J* = 8.0 Hz, 2H), 7.39 (dd, *J* = 10.0 Hz, 7.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 190.02, 141.31, 138.64, 133.92, 132.31, 129.37, 128.62, 128.38, 126.20. NMR data matched literature values.[9]

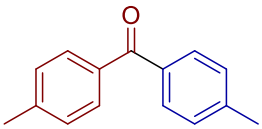
Phenyl(pyren-1-yl)methanone (14i).



According to the general procedure, the reaction of **1a** (0.20 mmol), pyren-1-ylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.25 mol%) in THF (0.25 M) for 12 h at room temperature afforded after work-up and chromatography the title product in 88% yield (53 mg). Colorless solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (d, *J* = 8.0 Hz, 1H), 8.25 (dd, *J* = 13.0 Hz, 7.5 Hz, 2H), 8.20 (t, *J* = 7.5 Hz, 2H), 8.14-8.04 (m, 4H), 7.90 (d, *J* = 7.5 Hz, 2H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.48,

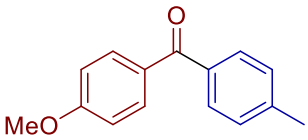
138.78, 133.19, 133.12, 133.09, 131.19, 130.69, 130.62, 129.76, 129.16, 128.90, 128.49, 127.23, 126.98, 126.43, 126.09, 125.95, 124.82, 124.75, 124.45, 123.79. NMR data matched literature values.[10]

Di-*p*-tolylmethanone (14j).



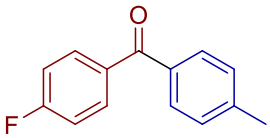
According to the general procedure, the reaction of **1n** (0.20 mmol), 4-methylphenylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.25 mol%) in THF (0.25 M) for 12 h at room temperature afforded after work-up and chromatography the title product in 83% yield (35 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (d, J = 8.0 Hz, 4H), 7.27 (d, J = 7.5 Hz, 4H), 2.44 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 196.28, 142.93, 135.22, 130.19, 128.91, 21.65. NMR data matched literature values.[14]

(4-Methoxyphenyl)(*p*-tolyl)methanone (14k).



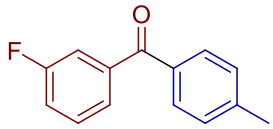
According to the general procedure, the reaction of **1m** (0.20 mmol), 4-methylphenylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.25 mol%) in THF (0.25 M) for 12 h at room temperature afforded after work-up and chromatography the title product in 61% yield (28 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (d, J = 8.5 Hz, 2H), 7.68 (t, J = 8.5 Hz, 2H), 7.27 (d, J = 7.5 Hz, 2H), 6.96 (t, J = 9.0 Hz, 2H), 3.89 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.40, 163.04, 142.63, 135.51, 132.44, 130.48, 130.01, 128.88, 113.49, 55.49, 21.63. NMR data matched literature values.[13]

(4-Fluorophenyl)(*p*-tolyl)methanone (14l).



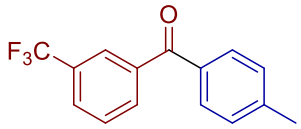
According to the general procedure, the reaction of **1j** (0.20 mmol), 4-methylphenylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.5 mol%) in THF (0.25 M) for 12 h at room temperature afforded after work-up and chromatography the title product in 99% yield (42 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (dd, J = 8.5 Hz, 5.5 Hz, 2H), 7.69 (d, J = 8.5 Hz, 2H), 7.29 (d, J = 8.0 Hz, 2H), 7.15 (t, J = 8.5 Hz, 2H), 2.45 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.06, 165.24 (d, J^F = 252.5 Hz), 143.33, 134.78, 134.13 (d, J^F = 3.1 Hz), 132.53 (d, J^F = 3.4 Hz), 130.14, 129.05, 115.37 (d, J^F = 22.5 Hz), 21.67. NMR data matched literature values.[9]

(3-Fluorophenyl)(*p*-tolyl)methanone (14m).



According to the general procedure, the reaction of **1k** (0.20 mmol), 4-methylphenylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.25 mol%) in THF (0.25 M) for 12 h at room temperature afforded after work-up and chromatography the title product in 99% yield (42 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (d, J = 8.0 Hz, 2H), 7.55 (d, J = 8.0 Hz, 1H), 7.50-7.42 (m, 2H), 7.32-7.25 (m, 3H), 2.45 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.03 (d, J^F = 2.3 Hz), 162.46 (d, J^F = 246.3 Hz), 143.70, 140.04 (d, J^F = 6.3 Hz), 134.33, 130.26, 129.89 (d, J^F = 7.6 Hz), 129.12, 125.67 (d, J^F = 3.1 Hz), 119.15, (d, J^F = 21.3 Hz) 116.67 (d, J^F = 22.5 Hz), 21.70. NMR data matched literature values.[11]

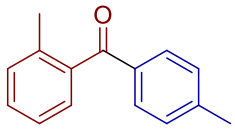
***p*-Tolyl(3-(trifluoromethyl)phenyl)methanone (14n)**.



According to the general procedure, the reaction of **1l** (0.20 mmol), 4-methylphenylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.25 mol%) in THF (0.25 M) for 12 h at room temperature afforded after work-up and chromatography the title product in 98% yield (51 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.96 (d, J

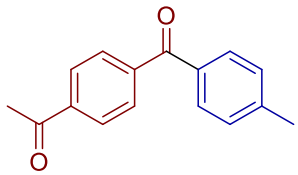
= 8.0 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 2H), 7.62 (t, *J* = 7.8 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 2.46 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.96, 143.99, 138.63, 134.07, 132.99, 130.89 (q, J^F = 32.6 Hz), 130.26, 129.26, 128.88, 128.60 (q, J^F = 3.8 Hz), 126.59 (q, J^F = 3.8 Hz), 123.72 (q, J^F = 270.0 Hz), 21.71. NMR data matched literature values.[12]

_o_-Tolyl(_p_-tolyl)methanone (14o).



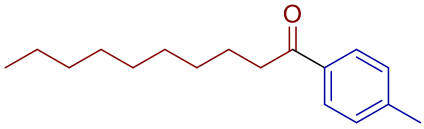
According to the general procedure, the reaction of **1o** (0.20 mmol), 4-methylphenylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.25 mol%) in THF (0.25 M) for 12 h at room temperature afforded after work-up and chromatography the title product in 56% yield (24 mg). Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.5 Hz, 2H), 7.41 (td, *J* = 7.5 Hz, *J* = 1.5 Hz, 1H), 7.34-7.27 (m, 5H), 2.46 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.38, 144.09, 138.98, 136.46, 135.15, 130.89, 130.31, 129.99, 129.18, 128.25, 125.16, 21.72, 19.91. NMR data matched literature values.[14]

1-(4-(4-Methylbenzoyl)phenyl)ethan-1-one (14p).



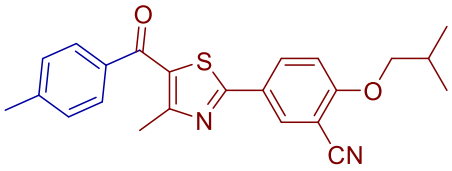
According to the general procedure, the reaction of **1p** (0.20 mmol), 4-methylphenylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.5 mol%) in THF (0.25 M) for 12 h at 60 °C afforded after work-up and chromatography the title product in 93% yield (44 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.0 Hz, 2H), 7.77 (d, *J* = 8.0 Hz, 2H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 2.59 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.71, 195.79, 144.03, 141.77, 139.38, 134.22, 130.36, 129.94, 129.20, 128.15, 26.92, 21.73. NMR data matched literature values.[15]

1-(*p*-Tolyl)decan-1-one (14q).



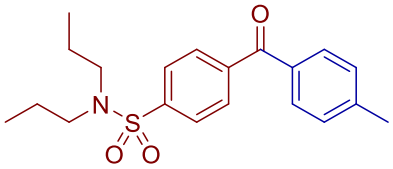
According to the general procedure, the reaction of **1q** (0.20 mmol), 4-methylphenylboronic acid (0.40 mmol), K_2CO_3 (0.60 mmol), H_2O (1.0 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.25 mol%) in THF (0.25 M) for 12 h at room temperature afforded after work-up and chromatography the title product in 93% yield (44 mg). Colourless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.0 Hz, 2H), 7.18 (d, *J* = 8.5 Hz, 2H), 2.87 (t, *J* = 7.5 Hz, 2H), 2.34 (s, 3H), 1.65 (m, 2H), 1.34-1.13 (m, 12H), 0.81 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 200.33, 143.56, 134.64, 129.21, 128.19, 38.56, 31.89, 29.51, 29.49, 29.43, 29.30, 24.54, 22.68, 21.62, 14.12. NMR data matched literature values.[16]

2-Isobutoxy-5-(4-methyl-5-(4-methylbenzoyl)thiazol-2-yl)benzonitrile (14r).



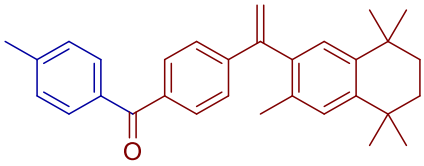
According to the general procedure, the reaction of **1r** (0.10 mmol), 4-methylphenylboronic acid (0.20 mmol), K_2CO_3 (0.30 mmol), H_2O (0.5 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (1.0 mol%) in THF (0.25 M) for 12 h at 60 °C afforded after work-up and chromatography the title product in 77% yield (30 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (d, *J* = 2.5 Hz, 1H), 8.11 (dd, 9.0 Hz, 2.5 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 9.0 Hz, 1H), 3.90 (d, *J* = 6.5 Hz, 2H), 2.64 (s, 3H), 2.46 (s, 3H), 2.21 (sep, *J* = 6.5 Hz, 1H), 1.09 (d, *J* = 6.5 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.14, 167.19, 162.52, 159.98, 143.78, 136.76, 132.59, 132.13, 129.26, 129.12, 125.95, 121.62, 112.64, 103.04, 75.72, 28.18, 21.72, 19.07, 18.43. HRMS calculated. for $C_{23}H_{23}N_2O_2S$ ($M + H^+$) 391.1475, found 391.1469.

4-(4-Methylbenzoyl)-*N*,*N*-dipropylbenzenesulfonamide (14s).



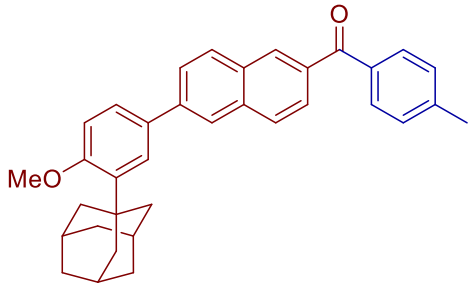
According to the general procedure, the reaction of **1s** (0.10 mmol), 4-methylphenylboronic acid (0.20 mmol), K_2CO_3 (0.30 mmol), H_2O (0.5 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.5 mol%) in THF (0.25 M) for 12 h at 40 °C afforded after work-up and chromatography the title product in 92% yield (33 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (d, J = 8.0 Hz, 2H), 7.86 (d, J = 8.0 Hz, 2H), 7.70 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 3.12 (t, J = 7.5 Hz, 4H), 2.45 (s, 3H), 1.57 (sex, J = 7.5 Hz, 4H), 0.88 (t, J = 7.5 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.28, 144.28, 143.25, 141.22, 133.92, 130.36, 130.24, 129.29, 126.92, 50.06, 22.05, 21.74, 11.18. HRMS calculated. for $C_{20}H_{26}NO_3S$ (M + H^+) 360.1628, found 360.1630.

(4-(1-(3,5,5,8,8-Pentamethyl-5,6,7,8-tetrahydronaphthalen-2-yl)vinyl)phenyl)(*p*-tolyl) methanone (14t).



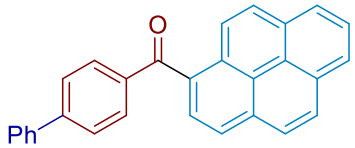
According to the general procedure, the reaction of **1t** (0.10 mmol), 4-methylphenylboronic acid (0.20 mmol), K_2CO_3 (0.30 mmol), H_2O (0.5 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.5 mol%) in THF (0.25 M) for 12 h at 40 °C afforded after work-up and chromatography the title product in 89% yield (36 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, J = 8.0 Hz, 2H), 7.36-7.31 (m, 4H), 7.18 (t, J = 7.5 Hz, 1H), 7.13 (d, J = 8.5 Hz, 2H), 7.07 (s, 1H), 7.02 (s, 1H), 5.77 (s, 1H), 5.29 (s, 1H), 1.89 (s, 3H), 1.63 (s, 4H), 1.22 (d, J = 12.0 Hz, 12H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.05, 151.02, 149.12, 146.30, 144.46, 142.40, 137.94, 132.73, 130.28, 129.49, 129.44, 128.34, 128.10, 126.78, 125.85, 121.75, 117.19, 35.23, 35.22, 34.04, 33.94, 31.97, 31.92, 20.00. HRMS calculated. for $C_{31}H_{35}O$ (M + H^+) 423.2682, found 423.2689.

(6-(3-(Adamantan-1-yl)-4-methoxyphenyl)naphthalen-2-yl)(*p*-tolyl)methanone (14u).



According to the general procedure, the reaction of **1u** (0.10 mmol), 4-methylphenylboronic acid (0.20 mmol), K_2CO_3 (0.30 mmol), H_2O (0.5 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.5 mol%) in THF (0.25 M) for 12 h at 40 °C afforded after work-up and chromatography the title product in 75% yield (36 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.26 (s, 1H), 7.93-7.98 (m, 3H), 7.82-7.77 (m, 3H), 7.61 (d, *J* = 2.0 Hz, 1H), 7.56 (dd, *J* = 7.8 Hz, 2.2 Hz, 1H), 7.33 (d, *J* = 7.5 Hz, 2H), 7.01 (d, *J* = 8.5 Hz, 1H), 3.91 (s, 3H), 2.48 (s, 3H), 2.19 (s, 6H), 2.11 (s, 3H), 1.81 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 196.49, 158.94, 143.09, 141.37, 139.04, 135.63, 135.33, 134.70, 132.56, 131.51, 130.99, 130.33, 129.73, 129.03, 128.30, 126.56, 126.23, 125.98, 125.73, 124.77, 112.13, 55.19, 40.62, 37.23, 37.14, 29.71, 29.12, 21.70. HRMS calculated. for $C_{35}H_{35}O_2$ (M + H^+) 487.2632, found 487.2636.

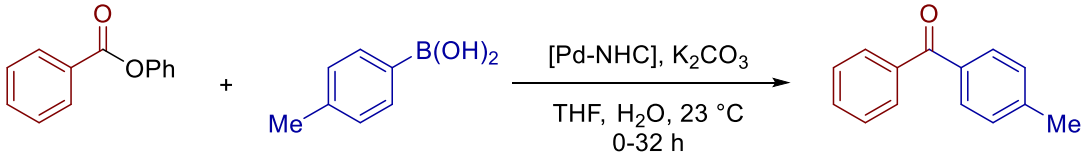
[1,1'-Biphenyl]-4-yl(pyren-1-yl)methanone (14w).



According to the general procedure, the reaction of **1w** (0.10 mmol), 4-methylphenylboronic acid (0.20 mmol), K_2CO_3 (0.30 mmol), H_2O (0.5 mmol) and [(IPr)Pd(μ-Cl)Cl]$_2$ (0.25 mol%) in THF (0.25 M) for 12 h at room temperature afforded after work-up and chromatography the title product in 86% yield (33 mg). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, *J* = 9.5 Hz, 1H), 8.29-8.19 (m, 5H), 8.16-8.11 (m, 3H), 8.08 (d, *J* = 8.0 Hz, 1H), 7.98 (d, *J* = 8.5 Hz, 2H), 7.70 (d, *J* = 8.5 Hz, 2H), 7.65 (d, *J* = 8.5 Hz, 2H), 7.48 (t, *J* = 8.5 Hz, 2H), 7.41 (t, *J* = 7.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.06, 145.93, 139.90, 137.41, 133.29, 133.06, 131.24, 131.21, 130.72, 129.70, 129.13, 128.99, 128.89, 128.30, 127.35, 127.24, 127.16, 126.85, 126.43,

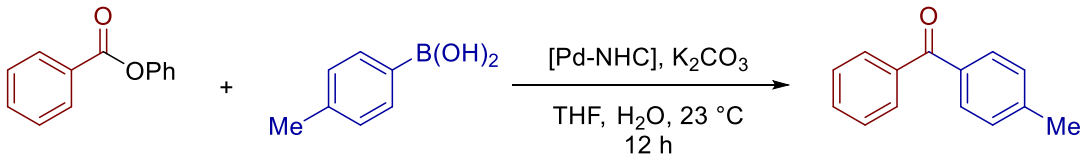
126.08, 125.94, 124.83, 124.78, 124.47, 123.85. HRMS calculated. for $C_{29}H_{19}O$ ($M + H^+$) 383.1430, found 383.1430.

Determination of Kinetic Profiles



An oven-dried vial equipped with a stir bar was charged with ester **1a** (0.10 mmol, 1.0 equiv), 4-methylphenylboronic acid (0.20 mmol, 2.0 equiv), K_2CO_3 (0.30 mmol, 3.0 equiv), and the corresponding Pd–NHC catalyst ([Pd], 0.5 mol%), placed under a positive pressure of argon, and subjected to three evacuation/backfilling cycles under high vacuum. THF (0.25 M) and H_2O (0.5 mmol) were added with vigorous stirring at room temperature and the reaction mixture was stirred for an indicated time (10 min, 30 min, 1 h, 2 h, 4 h, 6 h, 8 h, 12 h, 20 h and 32 h). After the indicated time, the reaction mixture was diluted with CH_2Cl_2 (5 mL), filtered, and concentrated. The sample was analyzed by ^{1}H NMR ($CDCl_3$, 500 MHz) and GC-MS to obtain conversion, selectivity and yield using internal standard and comparison with authentic samples.

Cross-Coupling using Various [Pd–NHC] Precatalysts



An oven-dried vial equipped with a stir bar was charged with ester **1a** (0.10 mmol, 1.0 equiv), 4-methylphenylboronic acid (0.20 mmol, 2.0 equiv), K_2CO_3 (0.30 mmol, 3.0 equiv), and the corresponding Pd–NHC catalyst ([Pd], 0.5 mol%), placed under a positive pressure of argon, and subjected to three evacuation/backfilling cycles under high vacuum. THF (0.25 M) and H_2O (0.5 mmol) were added with vigorous stirring at room temperature and the reaction mixture was stirred for 12 h at room temperature. After the indicated time, the reaction mixture was diluted with CH_2Cl_2 (5 mL), filtered, and concentrated. The sample was analyzed by ^{1}H NMR ($CDCl_3$, 500 MHz) and GC-MS to obtain conversion, selectivity and yield using internal standard and comparison with authentic samples.

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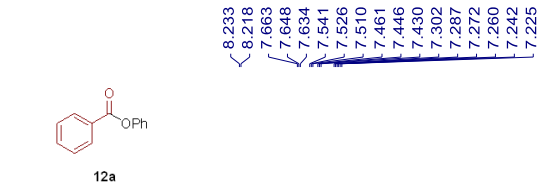
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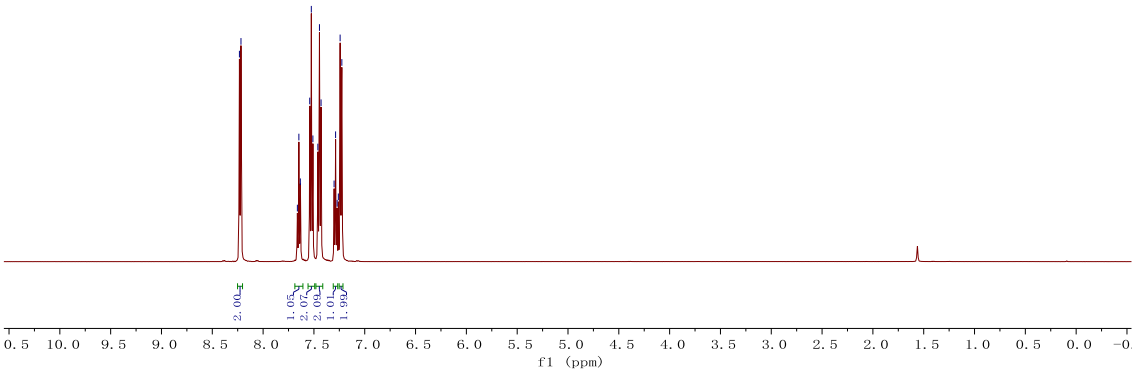
OPh

12a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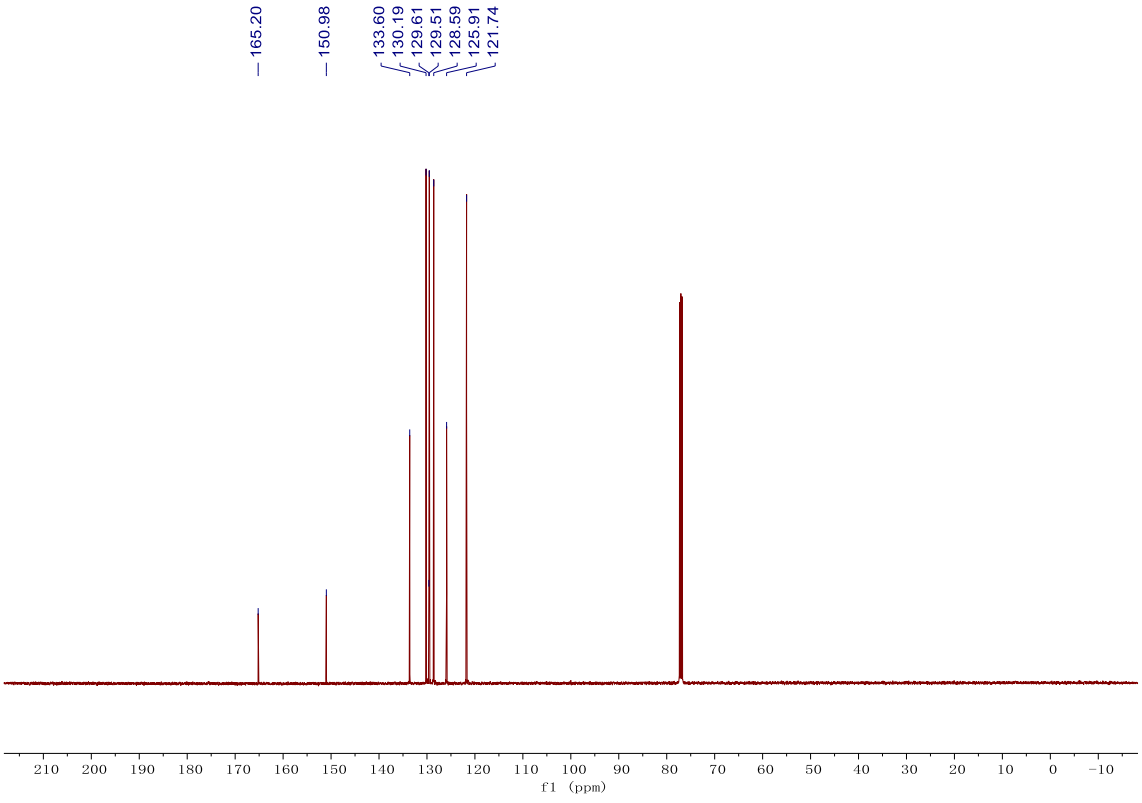
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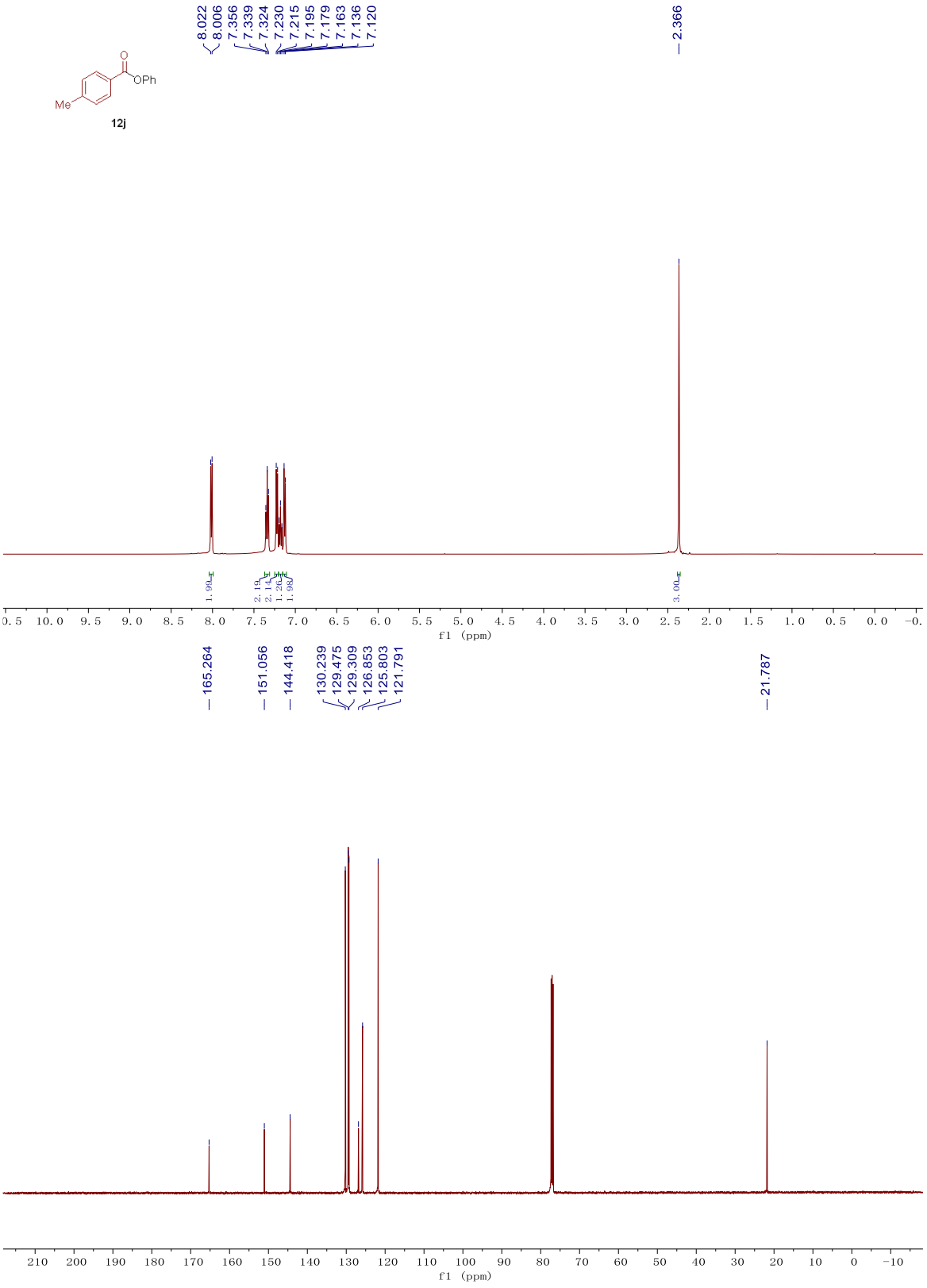
f1 (ppm)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Me
12j
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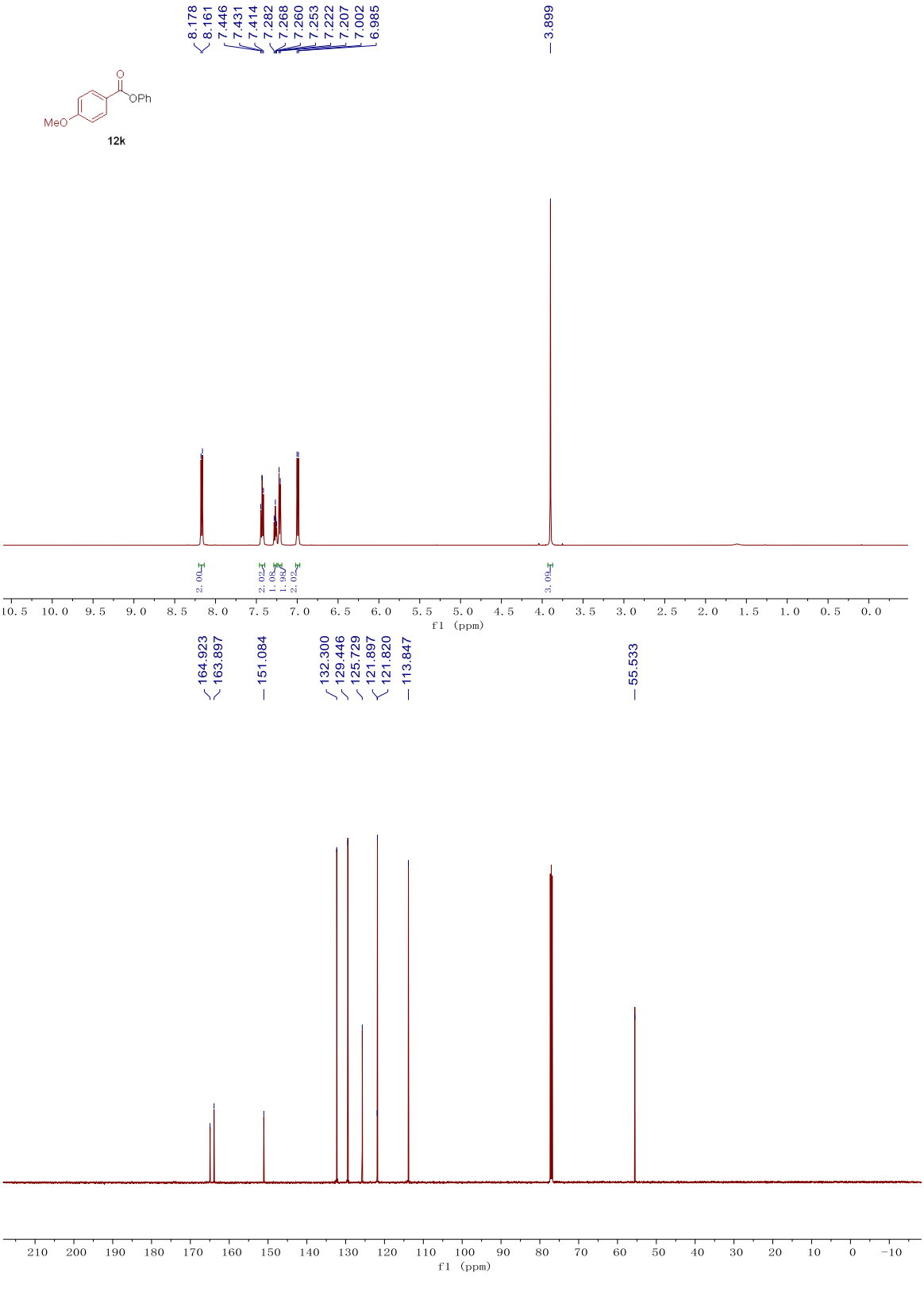
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2.02
3.09
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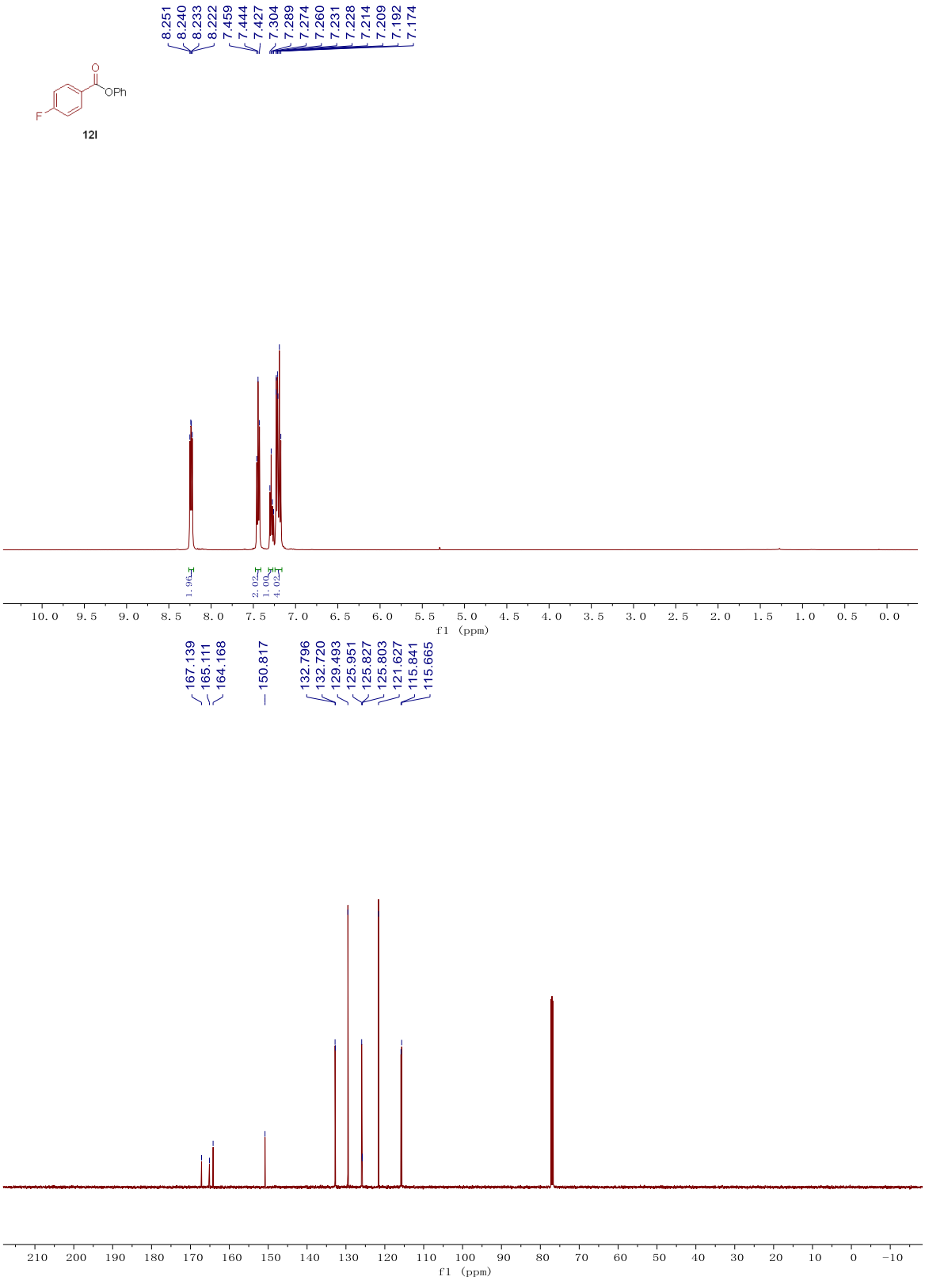
f1 (ppm)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f1 (ppm)


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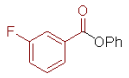
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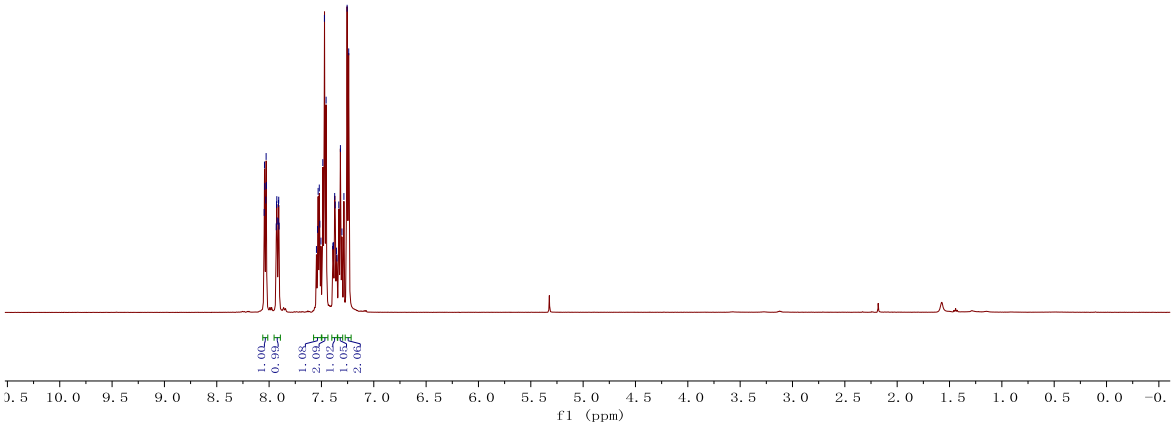
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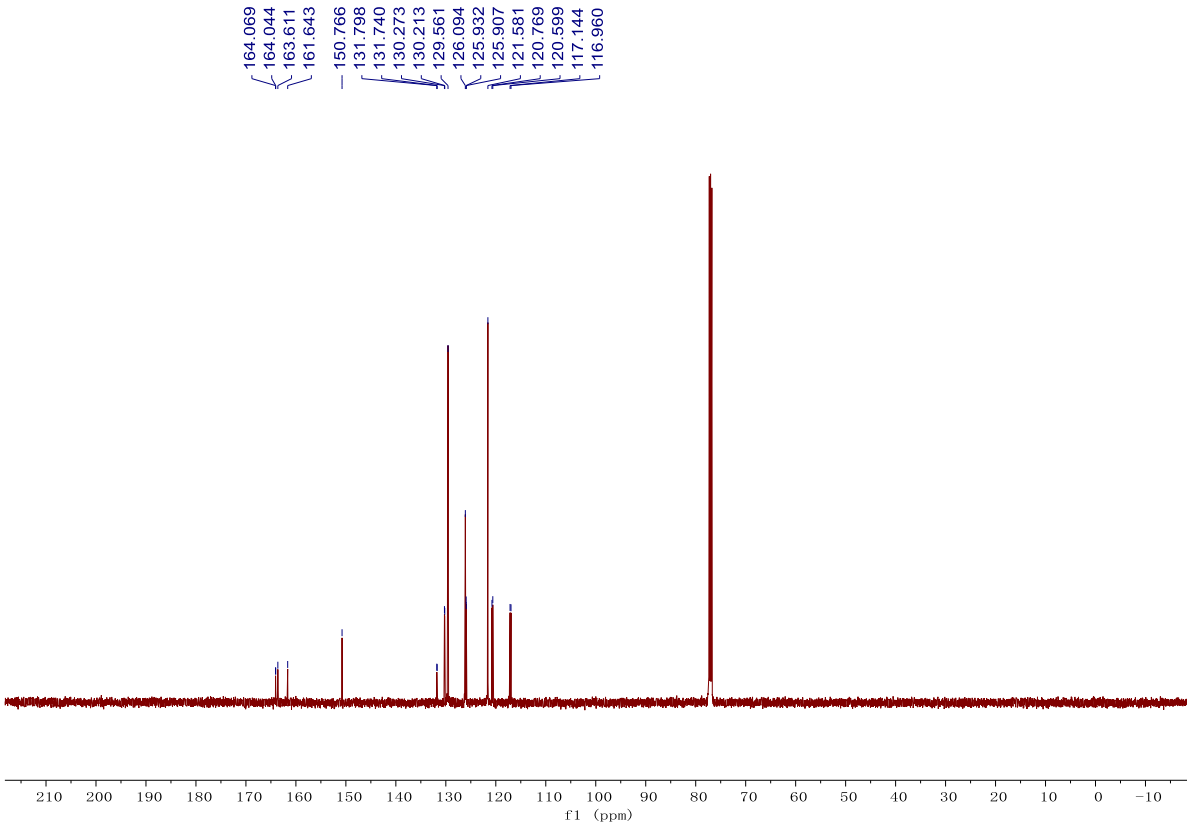
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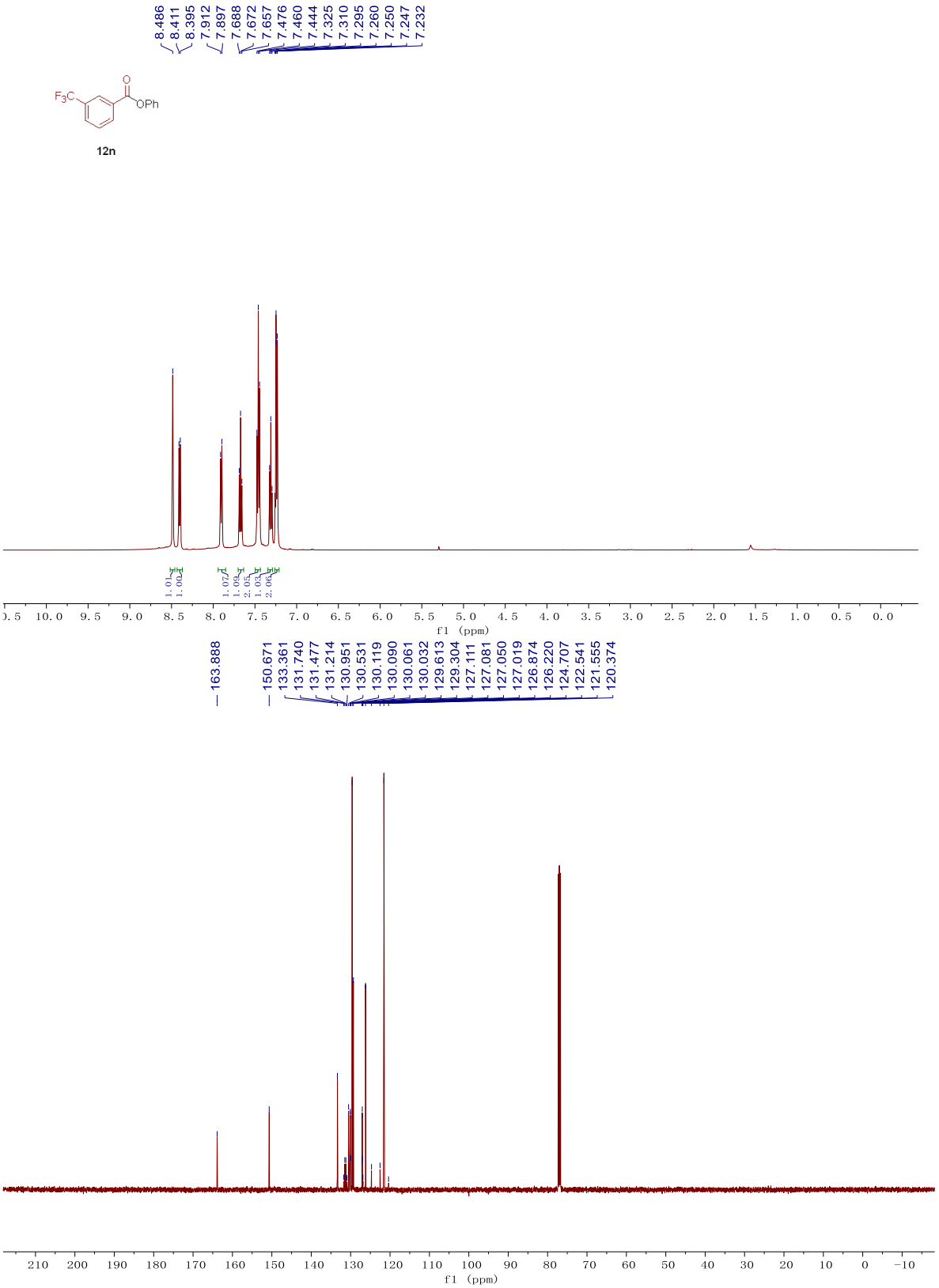
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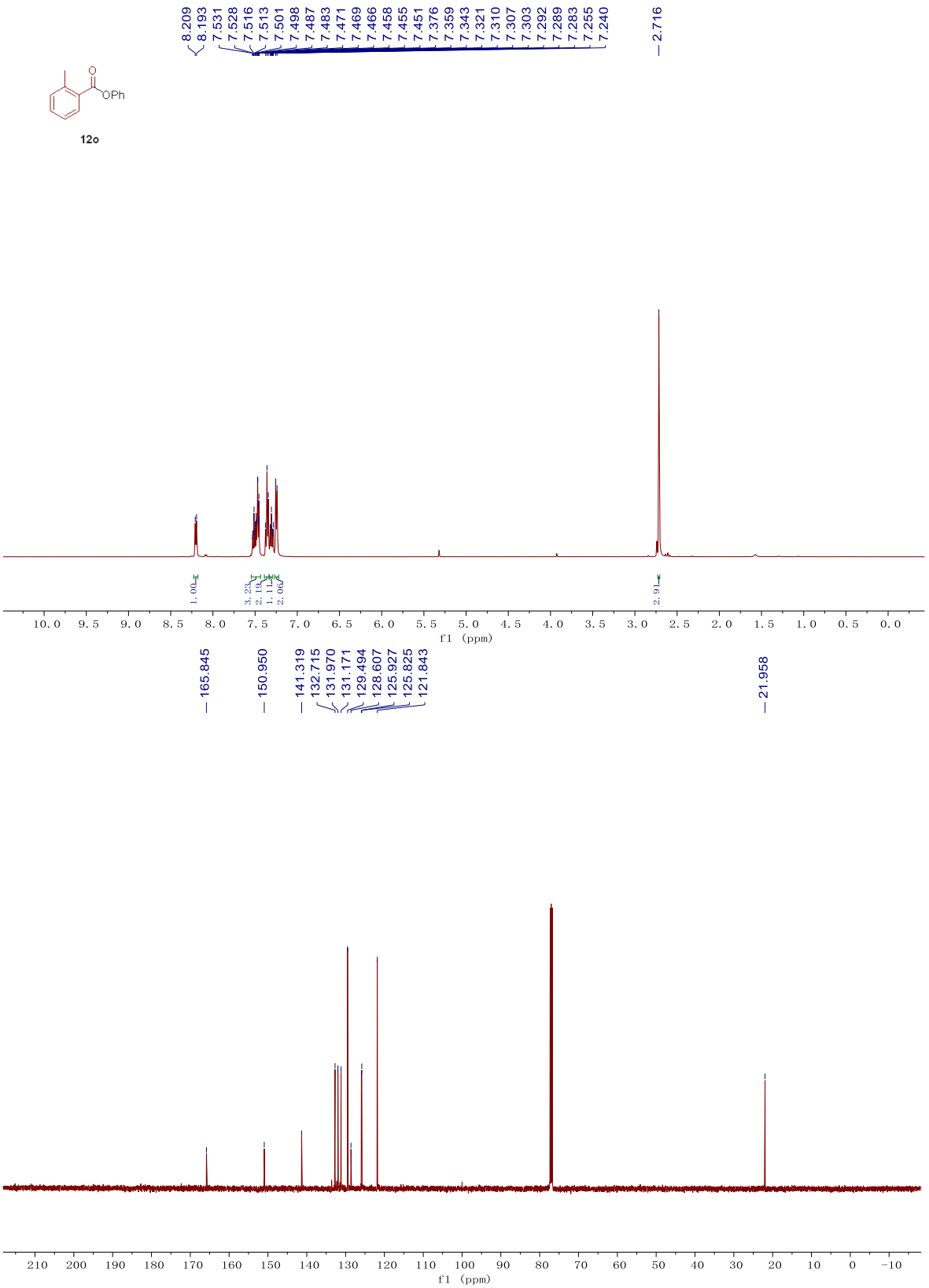
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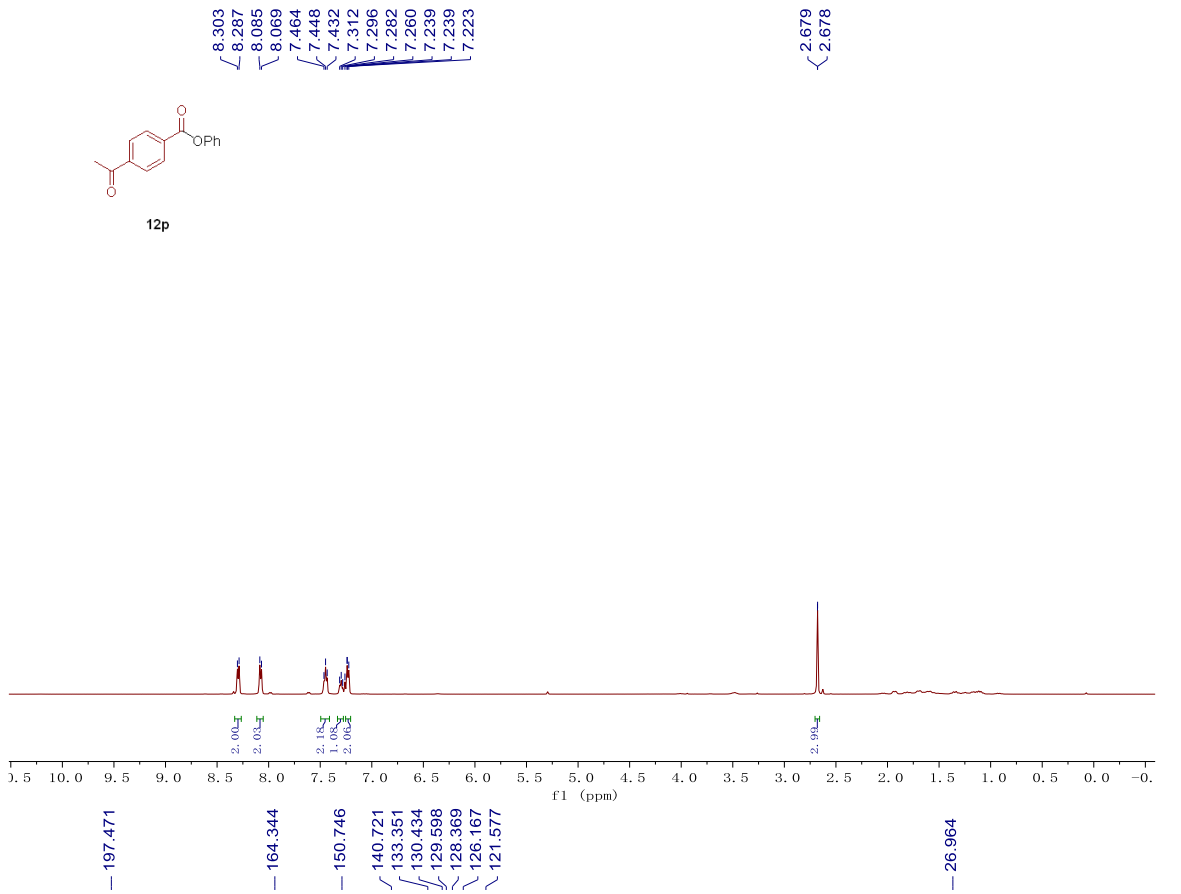
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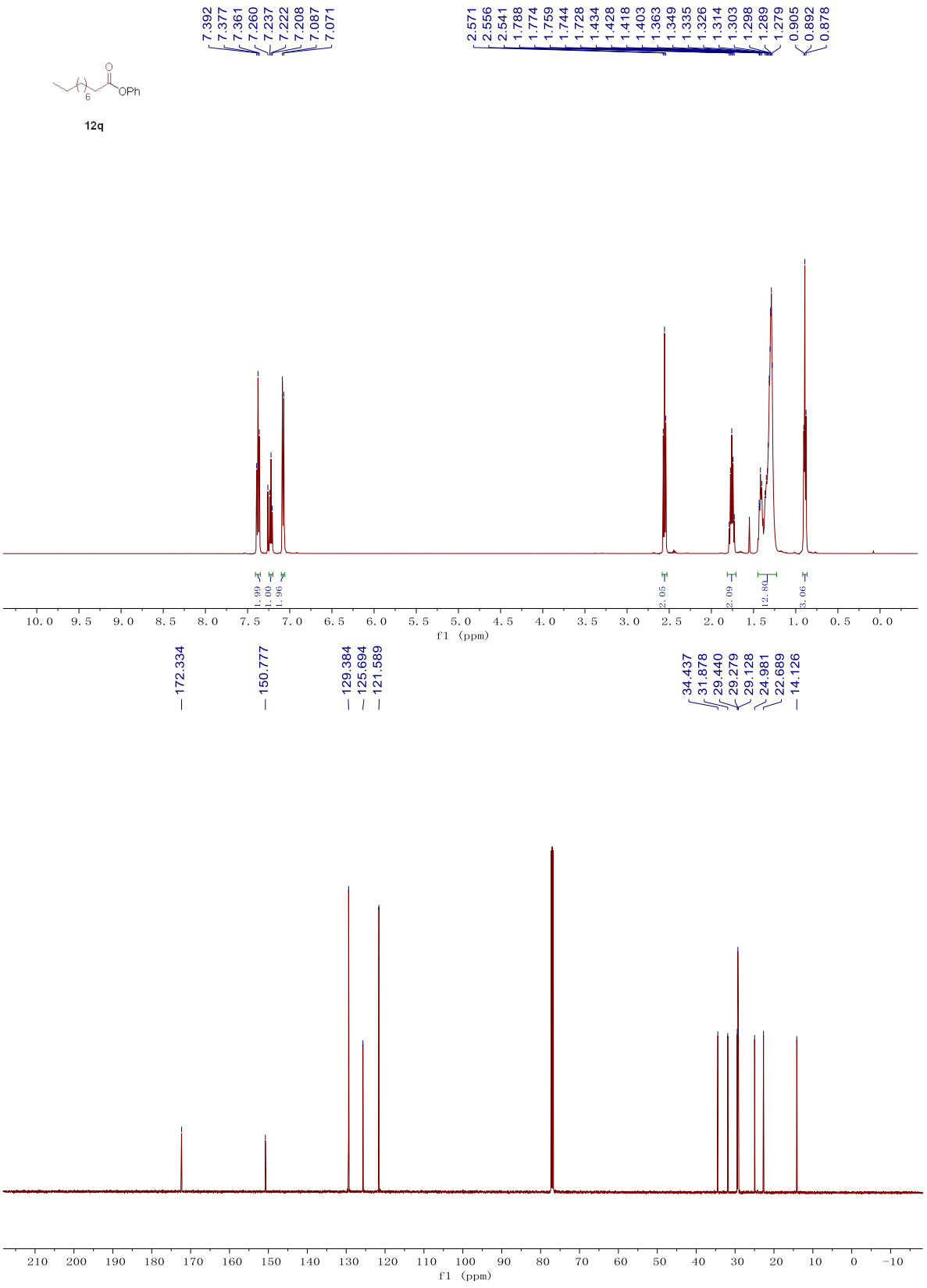
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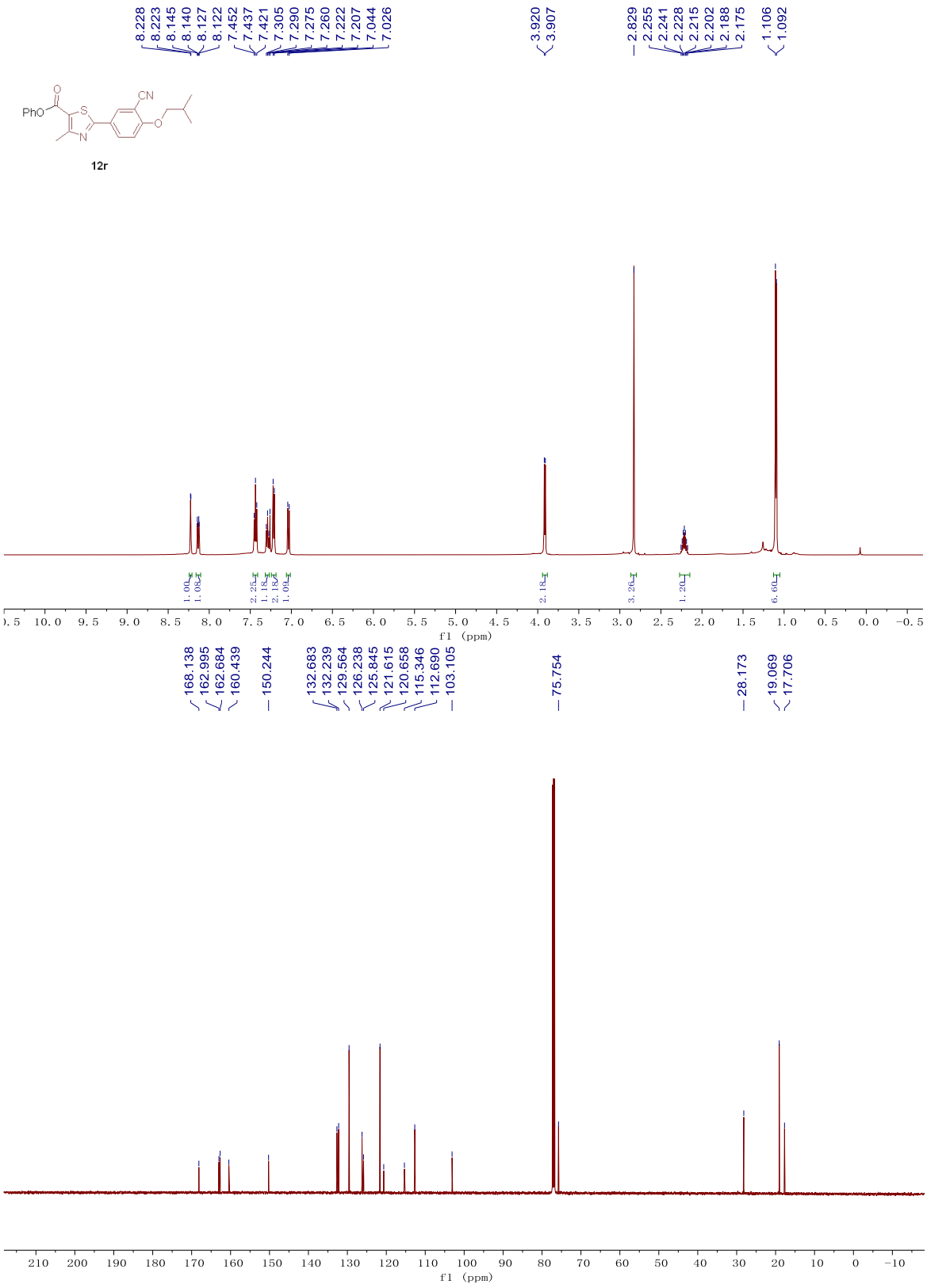
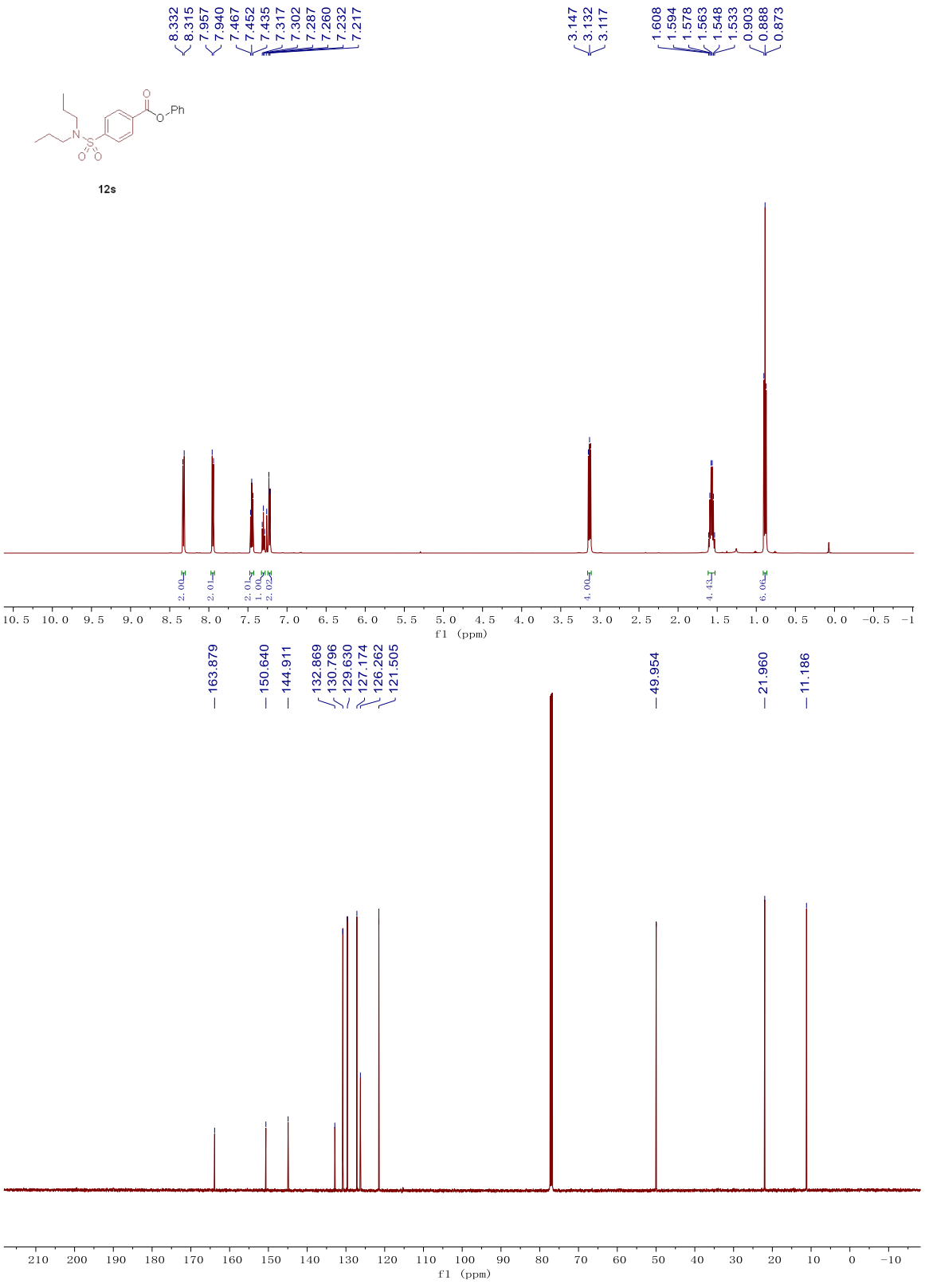
0.878
OPh
6
12q
1.99
1.00
1.96
2.05
2.09
12.80
3.06
f1 (ppm)
172.334
150.777
129.384
125.694
121.589
34.437
31.878
29.440
29.279
29.128
24.981
22.689
14.126
f1 (ppm)


8.228
8.223
8.145
8.140
8.127
8.122
7.452
7.437
7.421
7.305
7.290
7.275
7.260
7.222
7.207
7.044
7.026
3.920
3.907
2.829
2.255
2.241
2.228
2.215
2.202
2.188
2.175
1.106
1.092
PhO
O
S
N
CN
O
12r
1.00
1.08
2.25
1.18
2.18
1.09
2.18
3.26
1.20
6.60
f1 (ppm)
168.138
162.995
162.684
160.439
150.244
132.683
132.239
129.564
126.238
125.845
121.615
120.658
115.346
112.690
103.105
75.754
28.173
19.069
17.706
f1 (ppm)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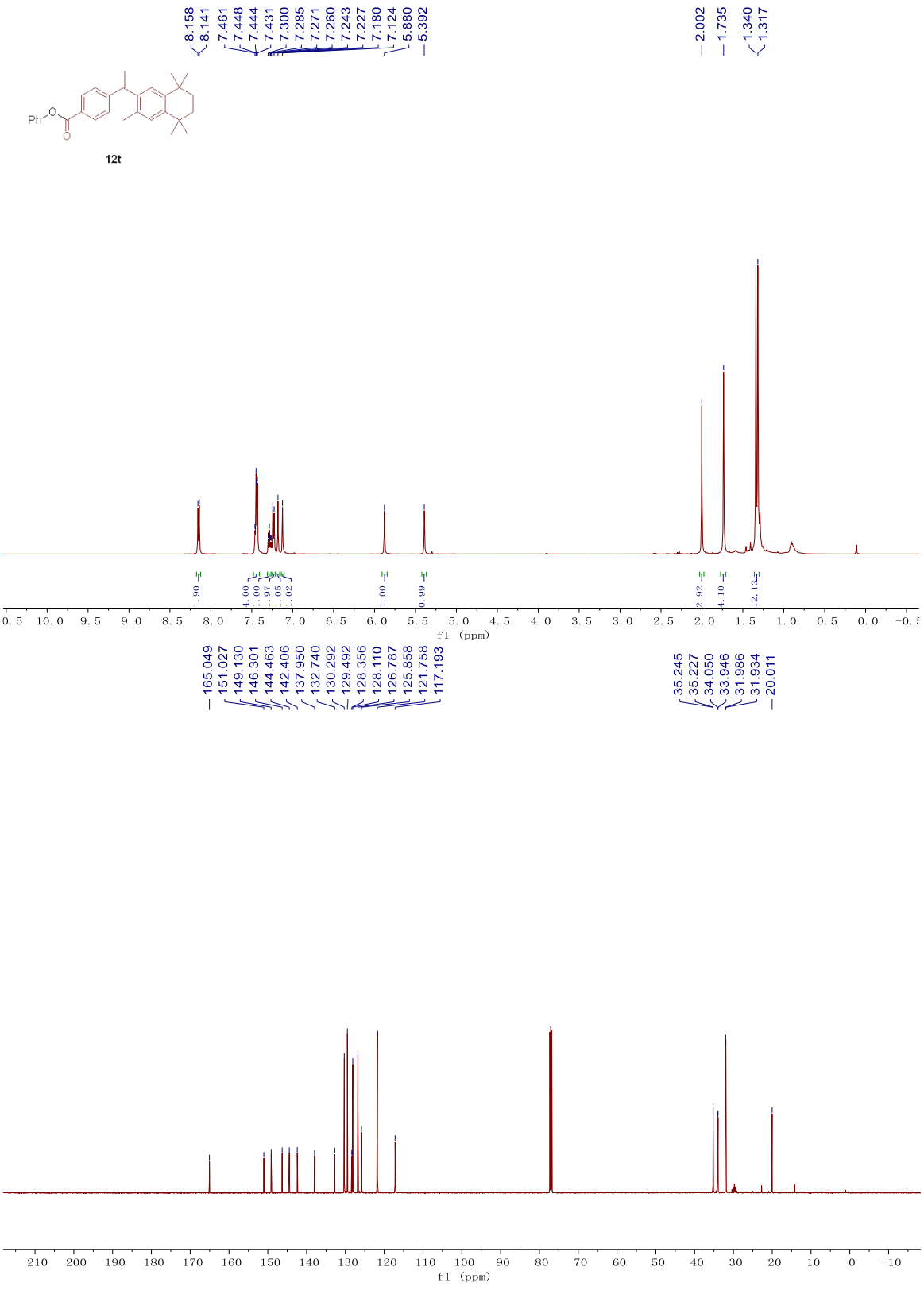
8.315
7.957
7.940
7.467
7.452
7.435
7.317
7.302
7.287
7.260
7.232
7.217
3.147
3.132
3.117
1.608
1.594
1.578
1.563
1.548
1.533
0.903
0.888
0.873
Ph
O
O
N
S
O
O
12s
2.00
2.01
2.01
1.00
2.02
4.00
4.43
6.06
f1 (ppm)
163.879
150.640
144.911
132.869
130.796
129.630
127.174
126.262
121.505
49.954
21.960
11.186
f1 (ppm)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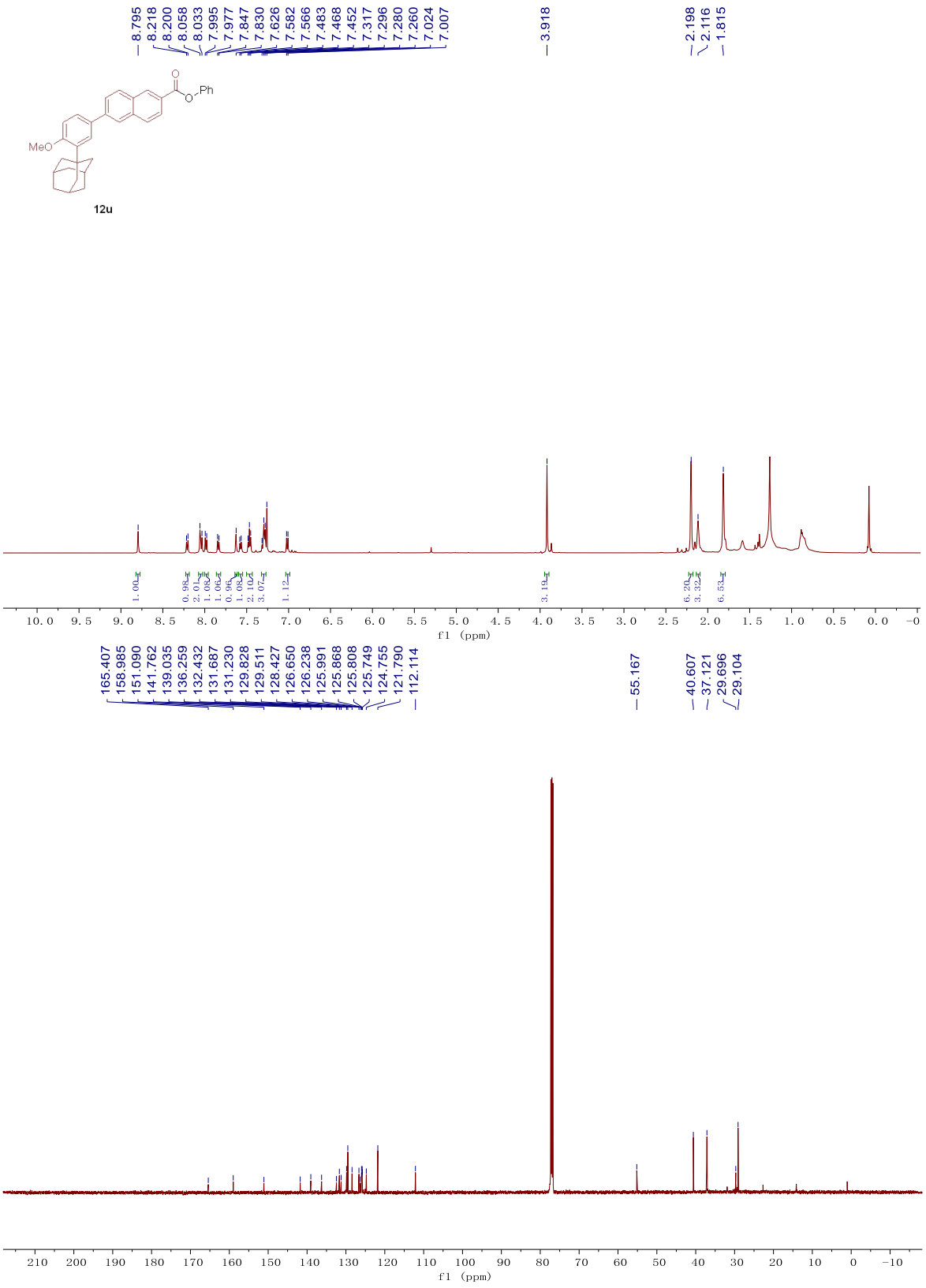
8.141
7.461
7.448
7.444
7.431
7.300
7.285
7.271
7.260
7.243
7.227
7.180
7.124
5.880
5.392
2.002
1.735
1.340
1.317
Ph
O
O
12t
1.90
4.00
1.00
1.97
1.05
1.02
1.00
0.99
2.92
4.10
12.13
f1 (ppm)
165.049
151.027
149.130
146.301
144.463
142.406
137.950
132.740
130.292
129.492
128.356
128.110
126.787
125.858
121.758
117.193
35.245
35.227
34.050
33.946
31.986
31.934
20.011
f1 (ppm)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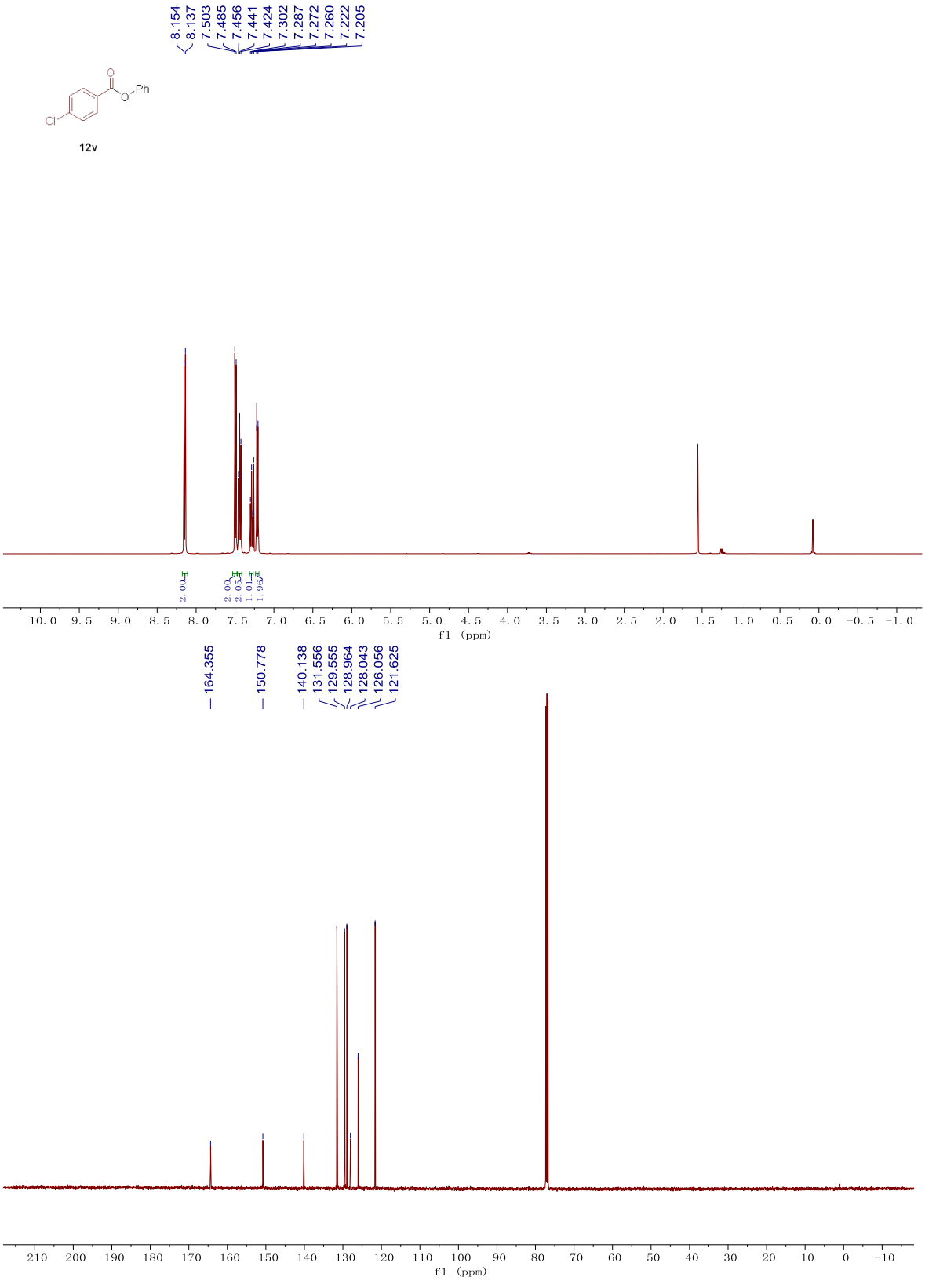
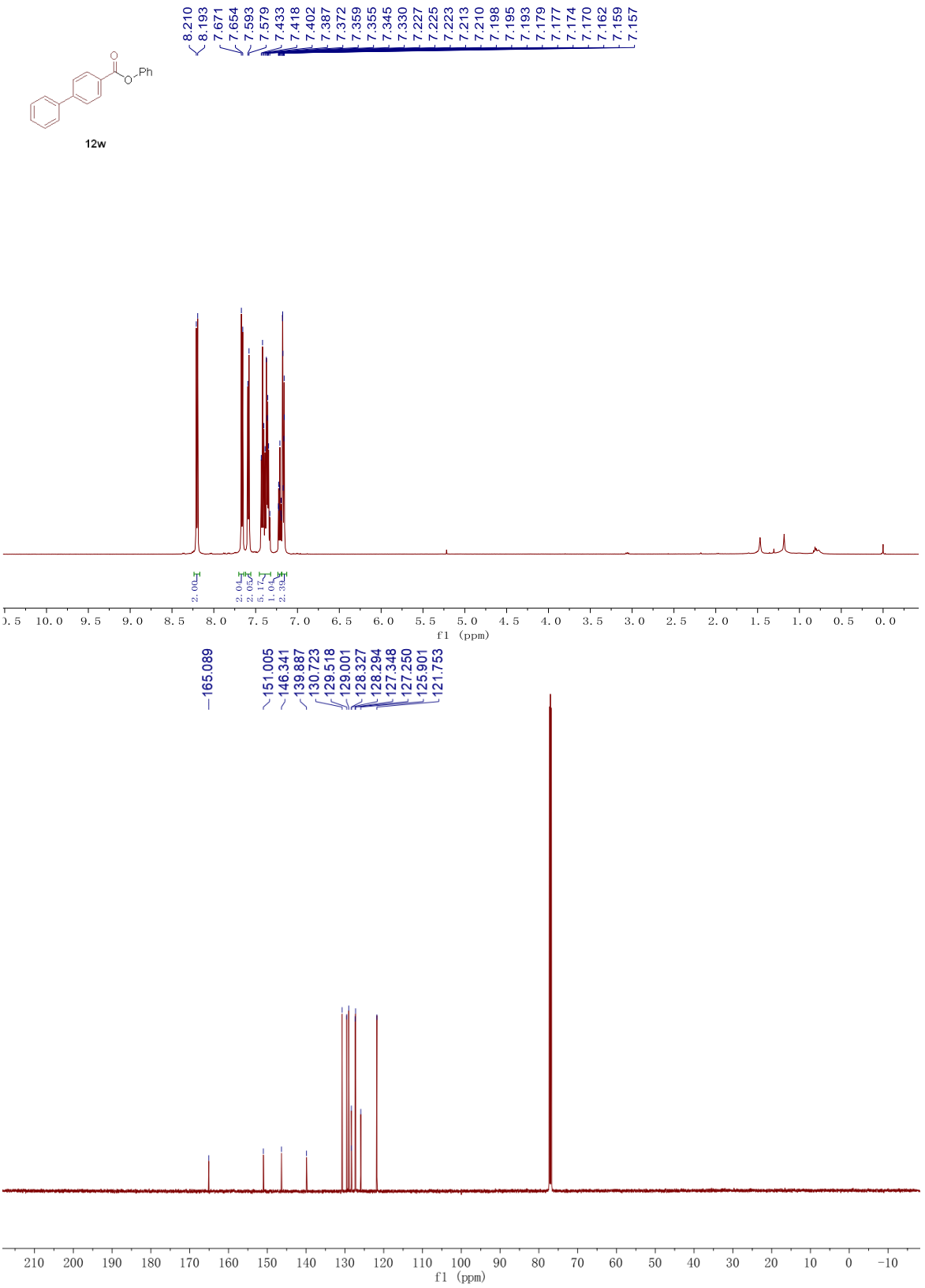
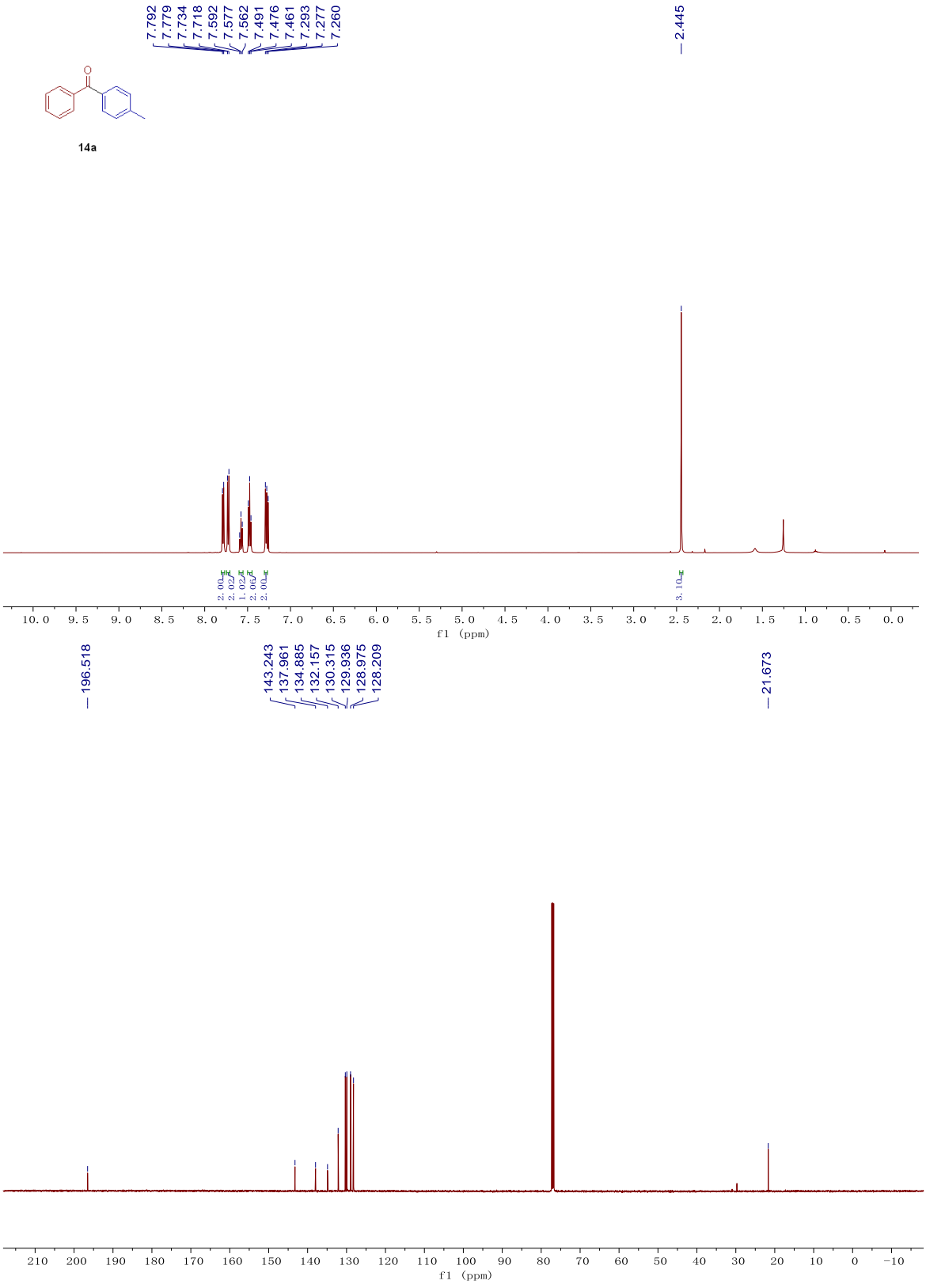
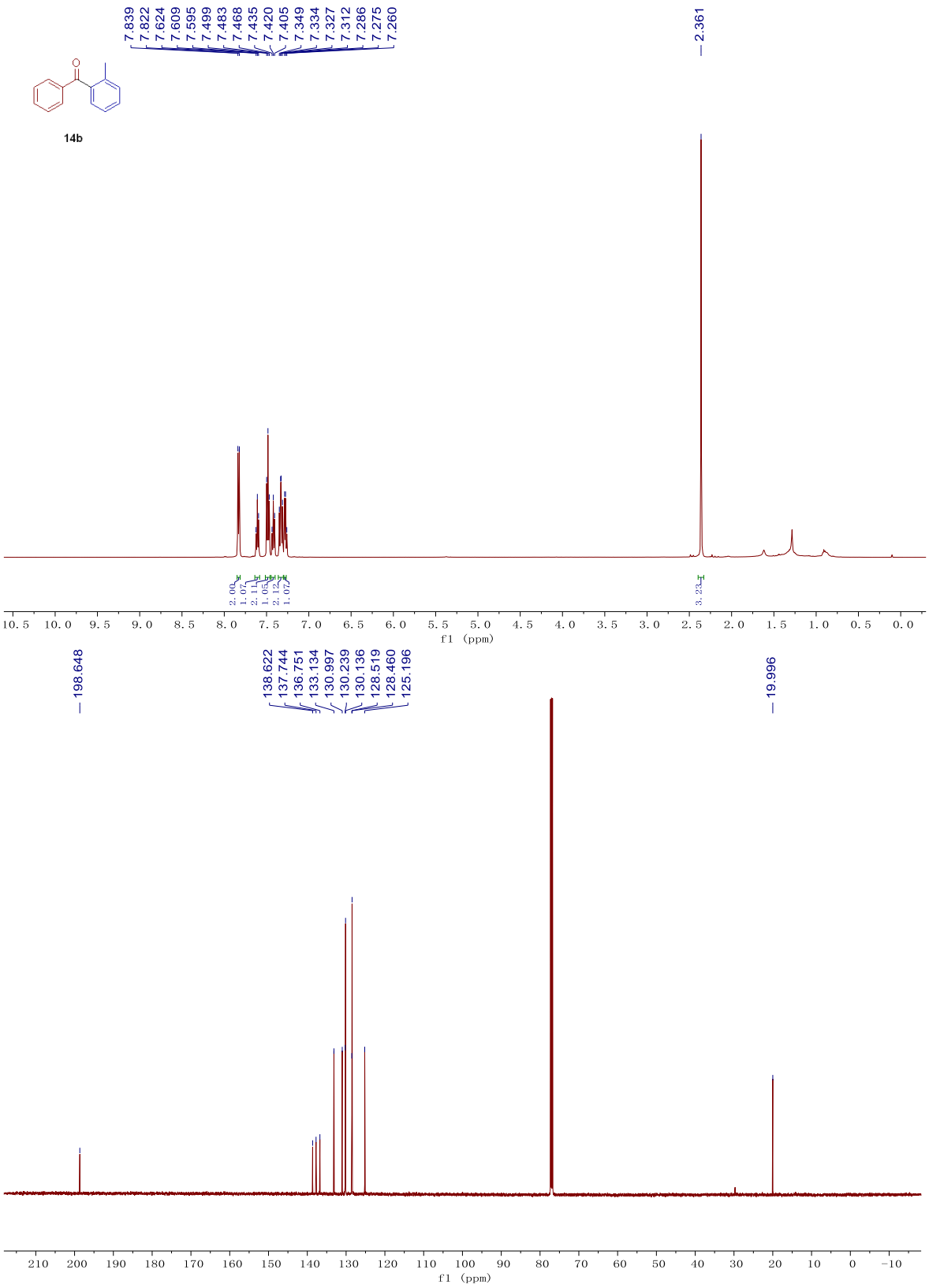
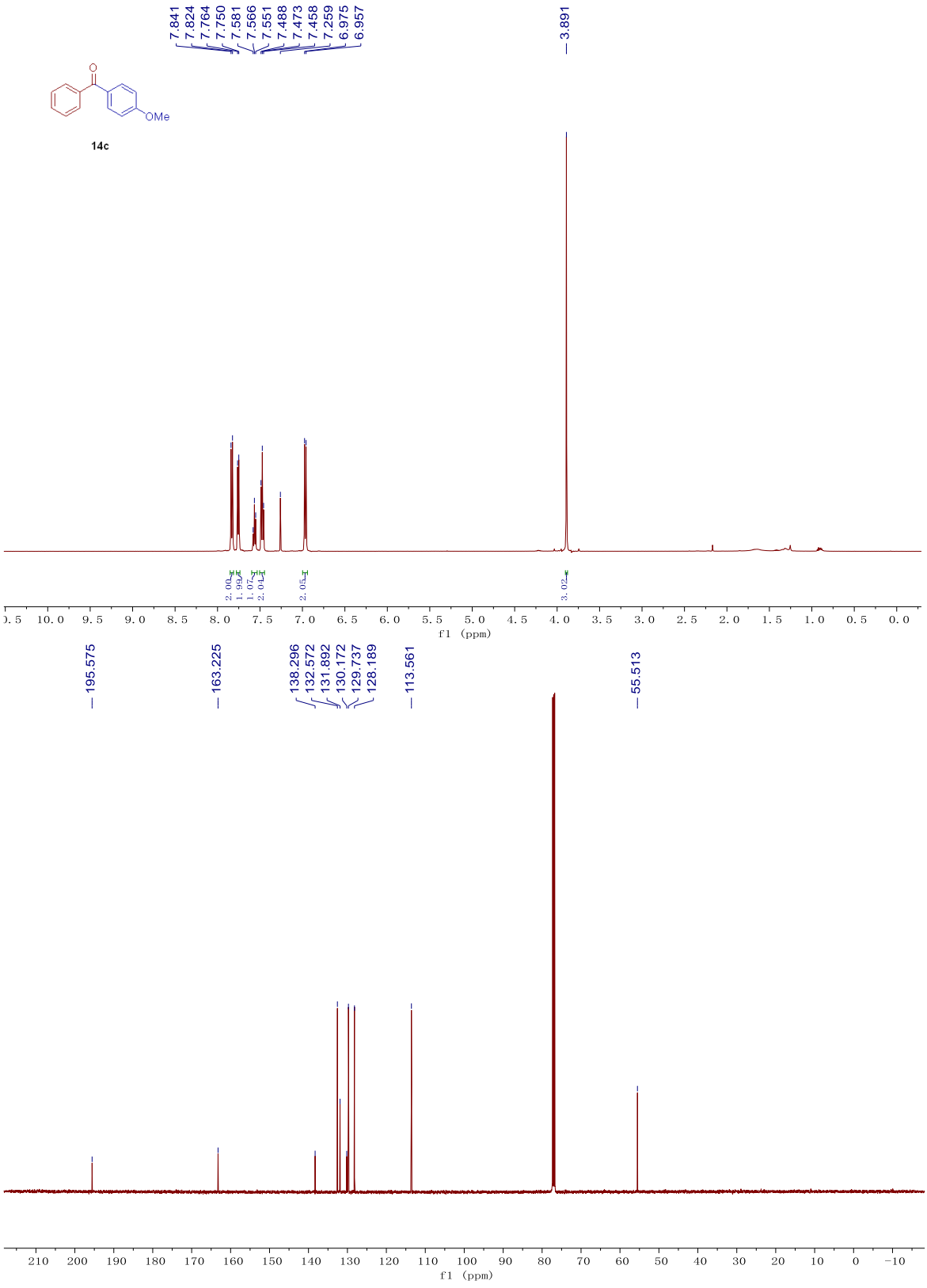
8.218
8.200
8.058
8.033
7.995
7.977
7.847
7.830
7.626
7.582
7.566
7.483
7.468
7.452
7.317
7.296
7.280
7.260
7.024
7.007
3.918
2.198
2.116
1.815
MeO
Ph
12u
1.00
0.98
2.01
1.04
1.06
0.96
1.08
2.10
3.07
1.12
3.19
6.20
3.32
6.53
f1 (ppm)
165.407
158.985
151.090
141.762
139.035
136.259
132.432
131.687
131.230
129.828
129.511
128.427
126.650
126.238
125.991
125.868
125.808
125.749
124.755
121.790
112.114
55.167
40.607
37.121
29.696
29.104
f1 (ppm)

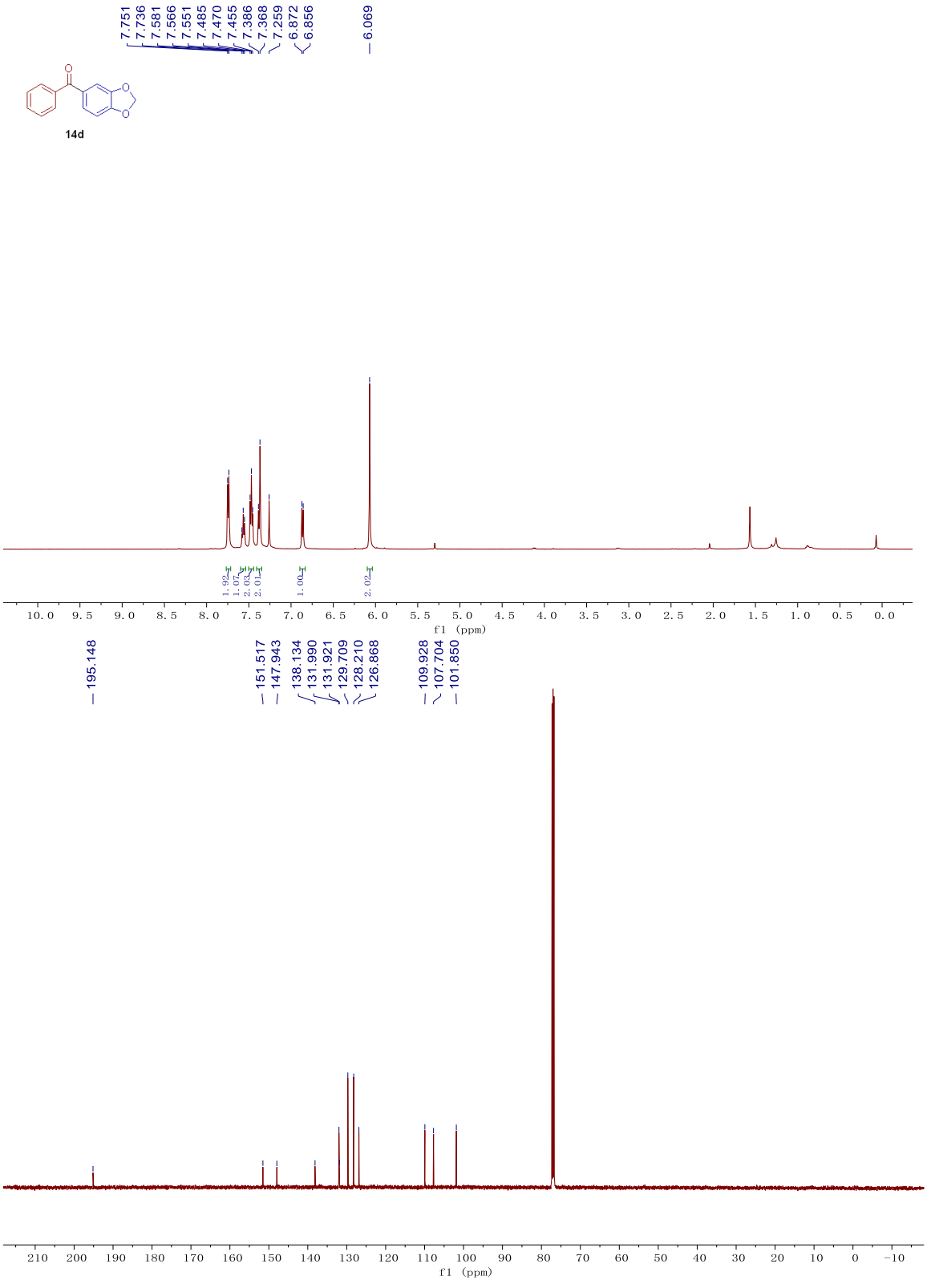

8.154
8.137
7.503
7.485
7.456
7.441
7.424
7.302
7.287
7.272
7.260
7.222
7.205
O
O
Ph
Cl
12v
2.00
2.00
2.05
1.01
1.90
f1 (ppm)
164.355
150.778
140.138
131.556
129.555
128.964
128.043
126.056
121.625
f1 (ppm)

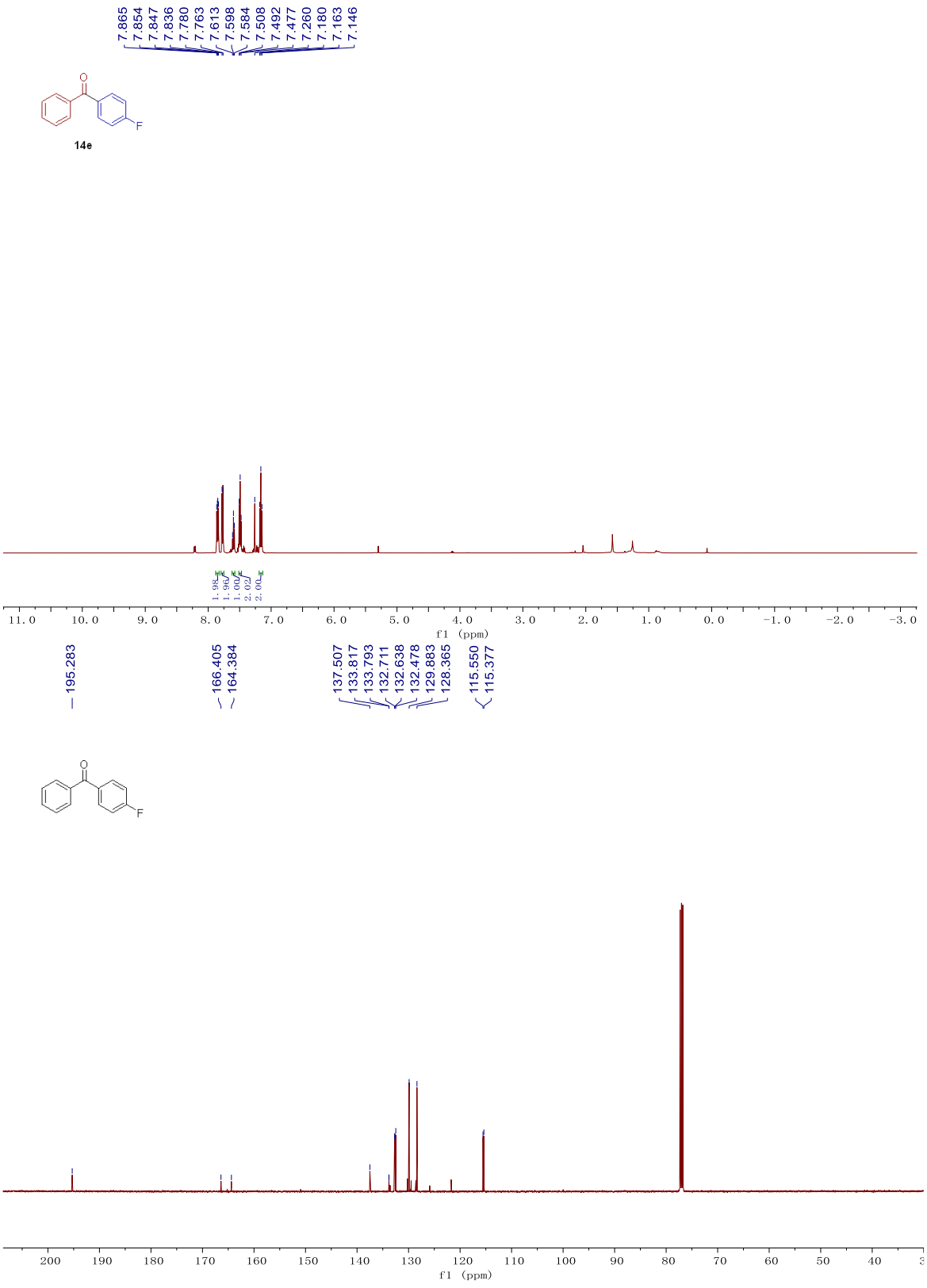

8.210
8.193
7.671
7.654
7.593
7.579
7.433
7.418
7.402
7.387
7.372
7.359
7.355
7.345
7.330
7.227
7.225
7.223
7.213
7.210
7.198
7.195
7.193
7.179
7.177
7.174
7.170
7.162
7.159
7.157
O
O
Ph
12w
2.00
2.04
2.05
5.17
1.04
2.39
f1 (ppm)
165.089
151.005
146.341
139.887
130.723
129.518
129.001
128.327
128.294
127.348
127.250
125.901
121.753
f1 (ppm)

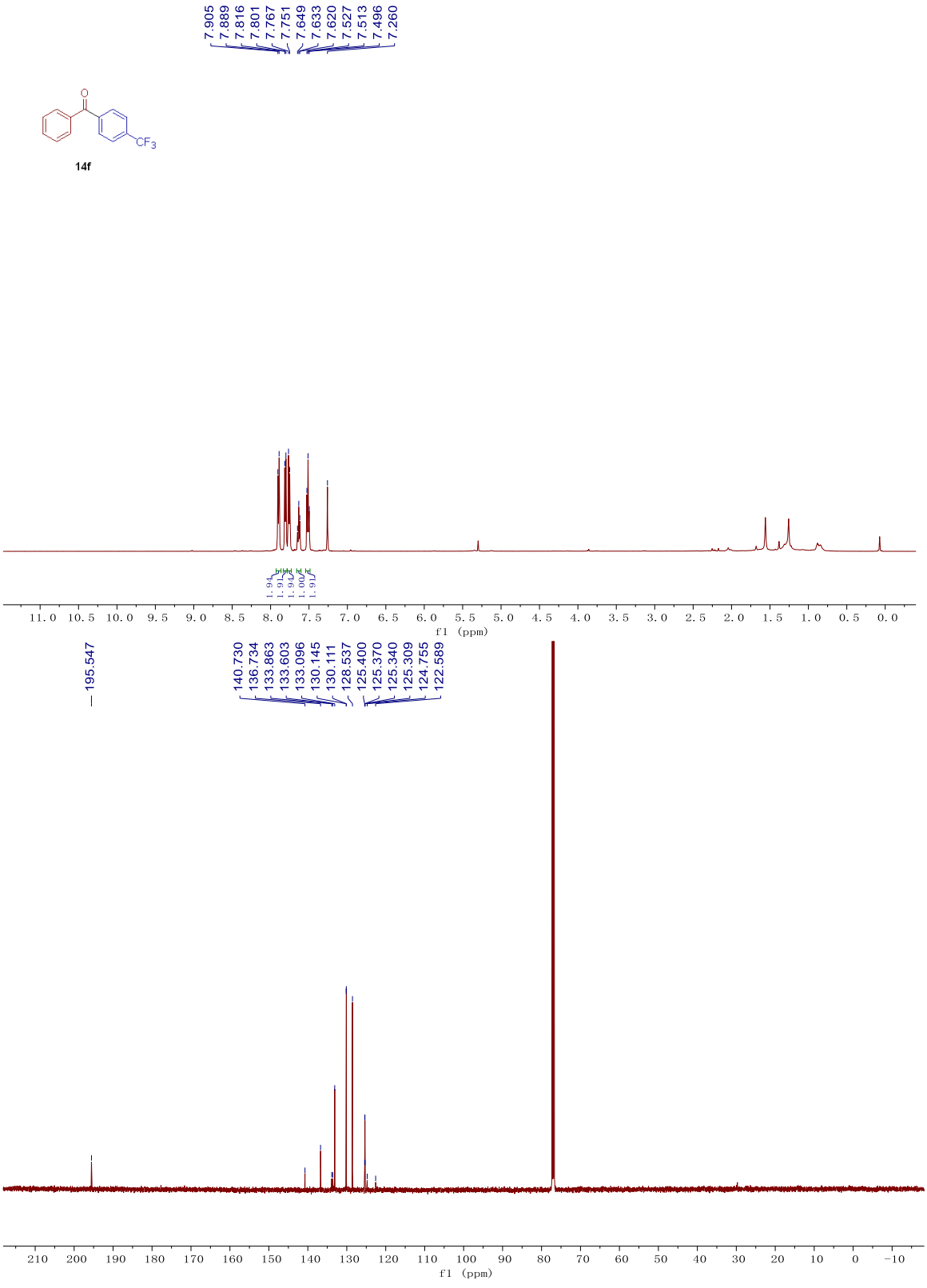

7.792
7.779
7.734
7.718
7.592
7.577
7.562
7.491
7.476
7.461
7.293
7.277
7.260
2.445
14a
2.00
2.02
1.02
2.06
2.00
3.10
f1 (ppm)
196.518
143.243
137.961
134.885
132.157
130.315
129.936
128.975
128.209
21.673
f1 (ppm)

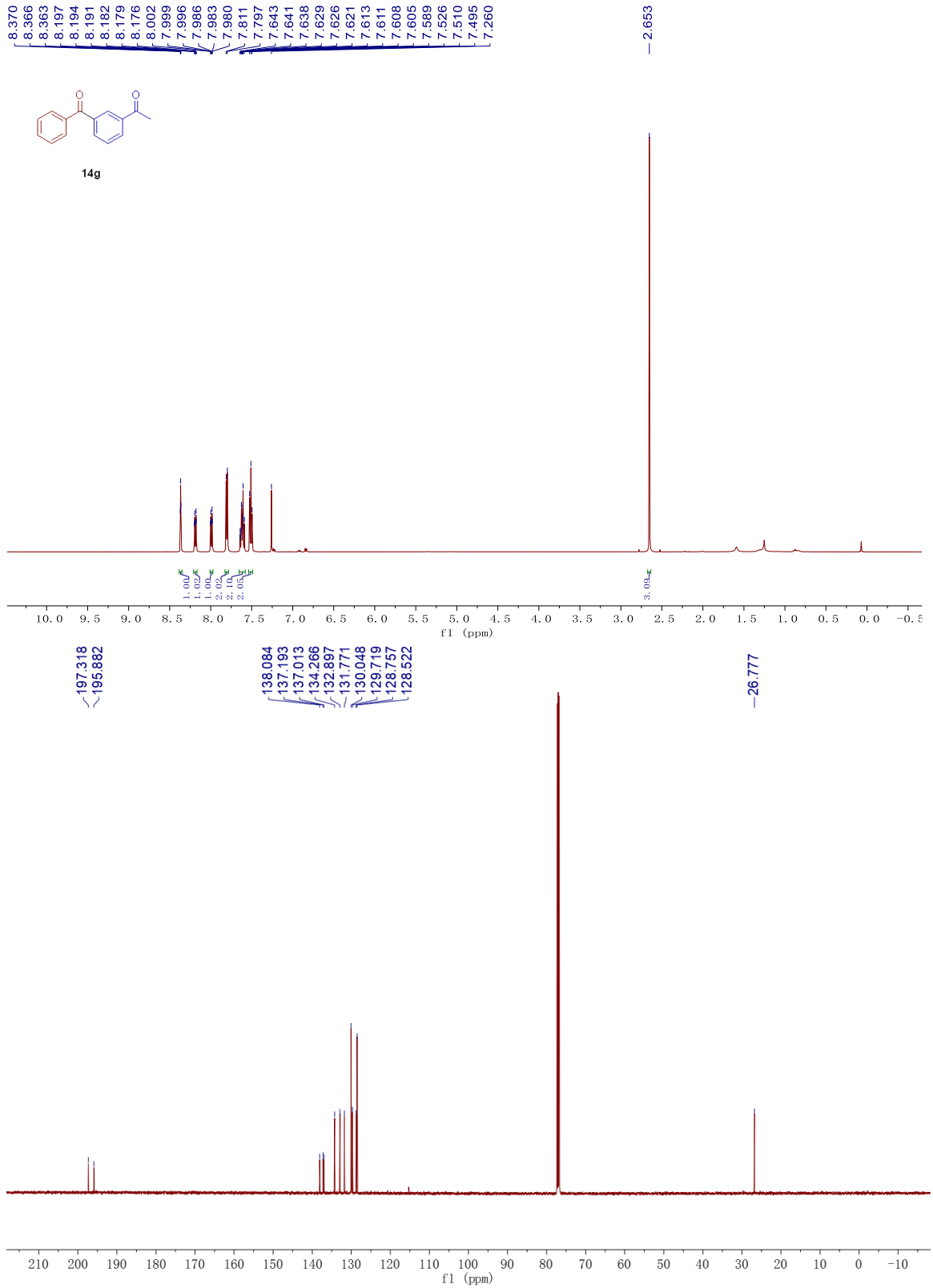

7.839
7.822
7.624
7.609
7.595
7.499
7.483
7.468
7.435
7.420
7.405
7.349
7.334
7.327
7.312
7.286
7.275
7.260
2.361
14b
2.00
1.07
2.11
1.05
2.12
1.07
3.23
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
198.648
138.622
137.744
136.751
133.134
130.997
130.239
130.136
128.519
128.460
125.196
19.996
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

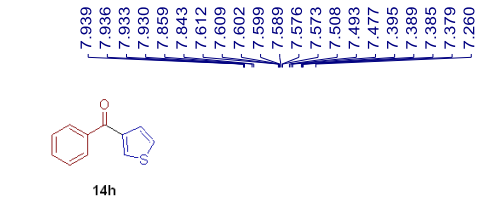

7.841
7.824
7.764
7.750
7.581
7.566
7.551
7.488
7.473
7.458
7.259
6.975
6.957
3.891
OMe
14c
2.00
1.99
1.07
2.04
2.05
3.02
f1 (ppm)
195.575
163.225
138.296
132.572
131.892
130.172
129.737
128.189
113.561
55.513
f1 (ppm)


7.751
7.736
7.581
7.566
7.551
7.485
7.470
7.455
7.386
7.368
7.259
6.872
6.856
6.069
14d
1.92
1.07
2.03
2.01
1.00
2.02
f1 (ppm)
195.148
151.517
147.943
138.134
131.990
131.921
129.709
128.210
126.868
109.928
107.704
101.850
f1 (ppm)

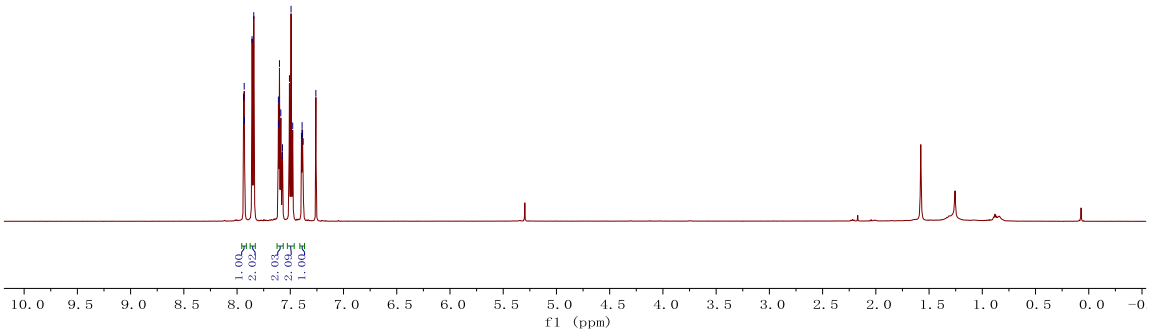

7.865
7.854
7.847
7.836
7.780
7.763
7.613
7.598
7.584
7.508
7.492
7.477
7.260
7.180
7.163
7.146
14e
1.98
1.96
1.00
2.02
2.00
f1 (ppm)
195.283
166.405
164.384
137.507
133.817
133.793
132.711
132.638
132.478
129.883
128.365
115.550
115.377
f1 (ppm)

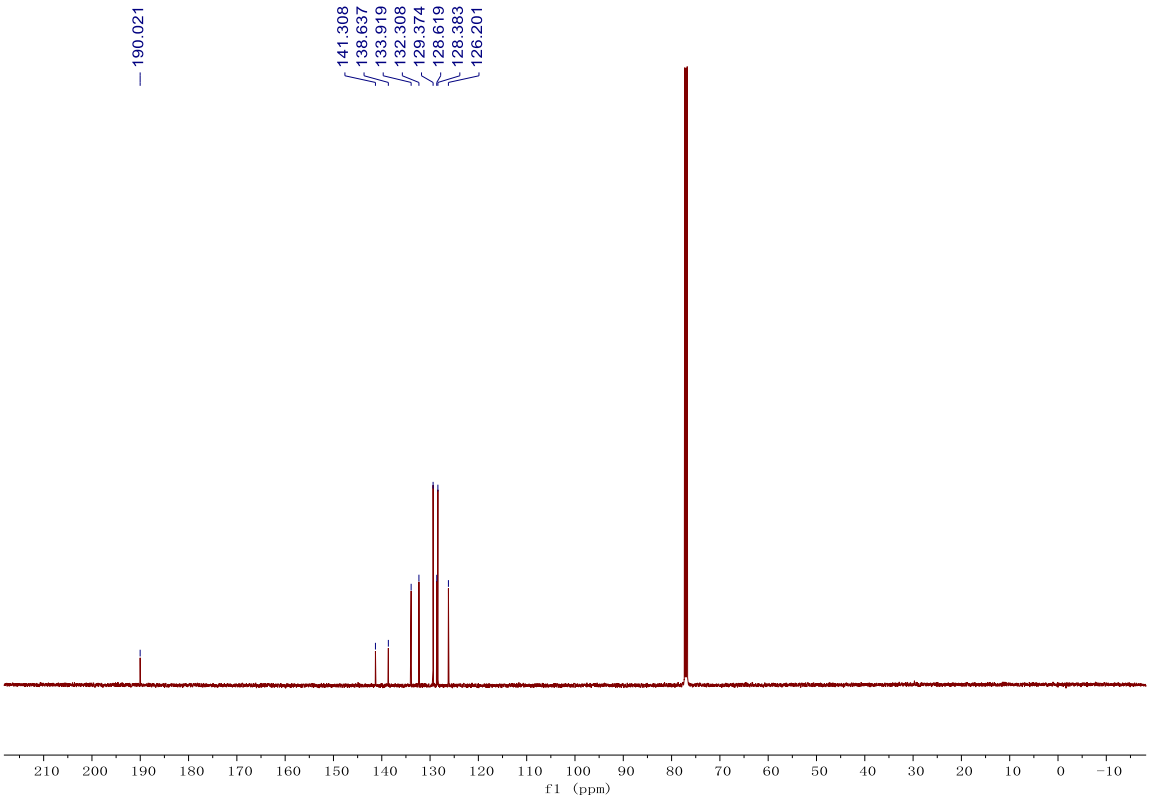

7.905
7.889
7.816
7.801
7.767
7.751
7.649
7.633
7.620
7.527
7.513
7.496
7.260
O
CF3
14f
1.91
1.91
1.91
1.00
1.91
f1 (ppm)
195.547
140.730
136.734
133.863
133.603
133.096
130.145
130.111
128.537
125.400
125.370
125.340
125.309
124.755
122.589
f1 (ppm)

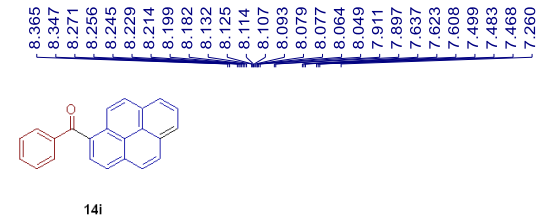

8.370
8.366
8.363
8.197
8.194
8.191
8.182
8.179
8.176
8.002
7.999
7.996
7.986
7.983
7.980
7.811
7.797
7.643
7.641
7.638
7.629
7.626
7.621
7.613
7.611
7.608
7.605
7.589
7.526
7.510
7.495
7.260
2.653
14g
1.00
1.02
1.00
2.02
2.10
2.05
3.09
f1 (ppm)
197.318
195.882
138.084
137.193
137.013
134.266
132.897
131.771
130.048
129.719
128.757
128.522
26.777
f1 (ppm)


7.939
7.936
7.933
7.930
7.859
7.843
7.612
7.609
7.602
7.599
7.589
7.576
7.573
7.508
7.493
7.477
7.395
7.389
7.385
7.379
7.260
O
S

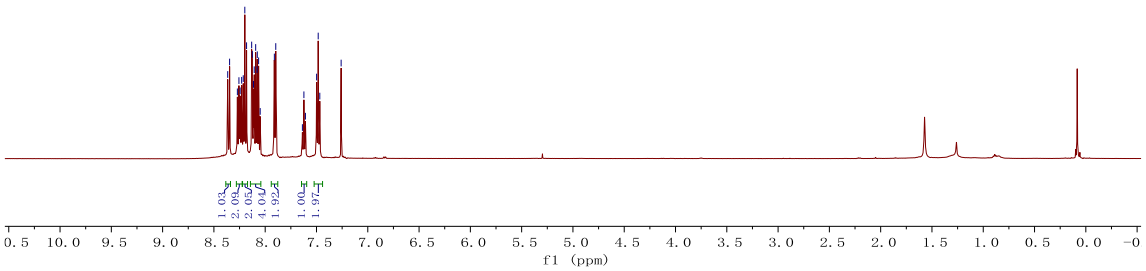
14h

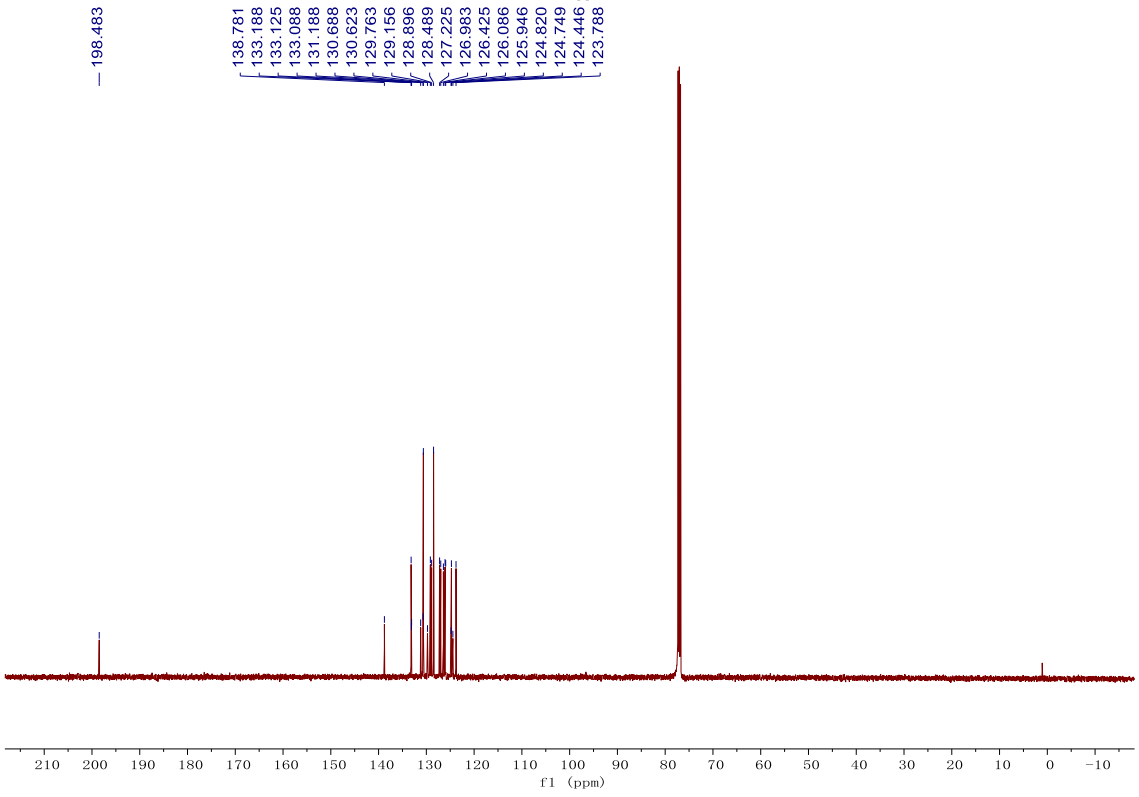

1.00
2.02
2.03
2.09
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

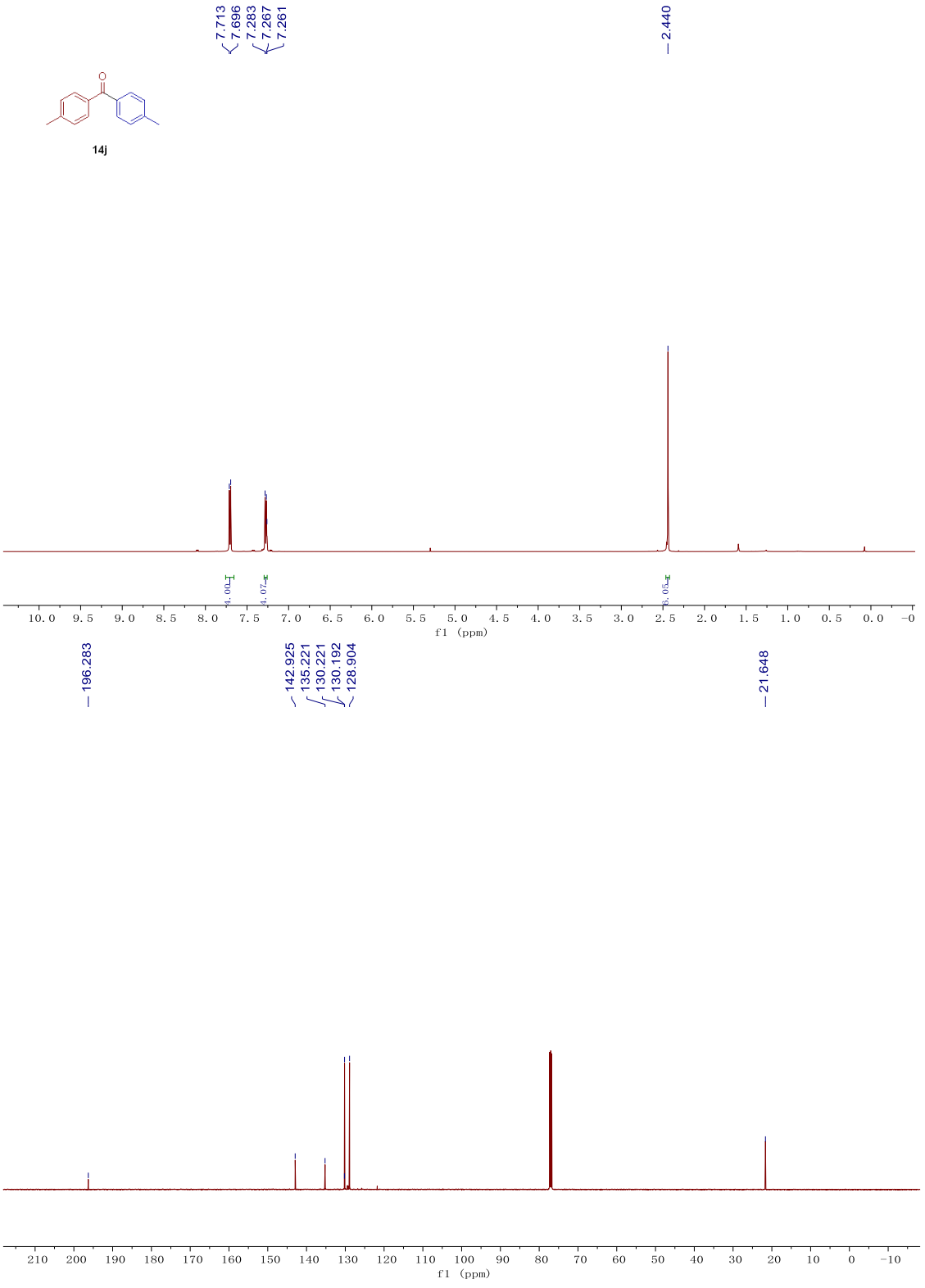

190.021
141.308
138.637
133.919
132.308
129.374
128.619
128.383
126.201
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

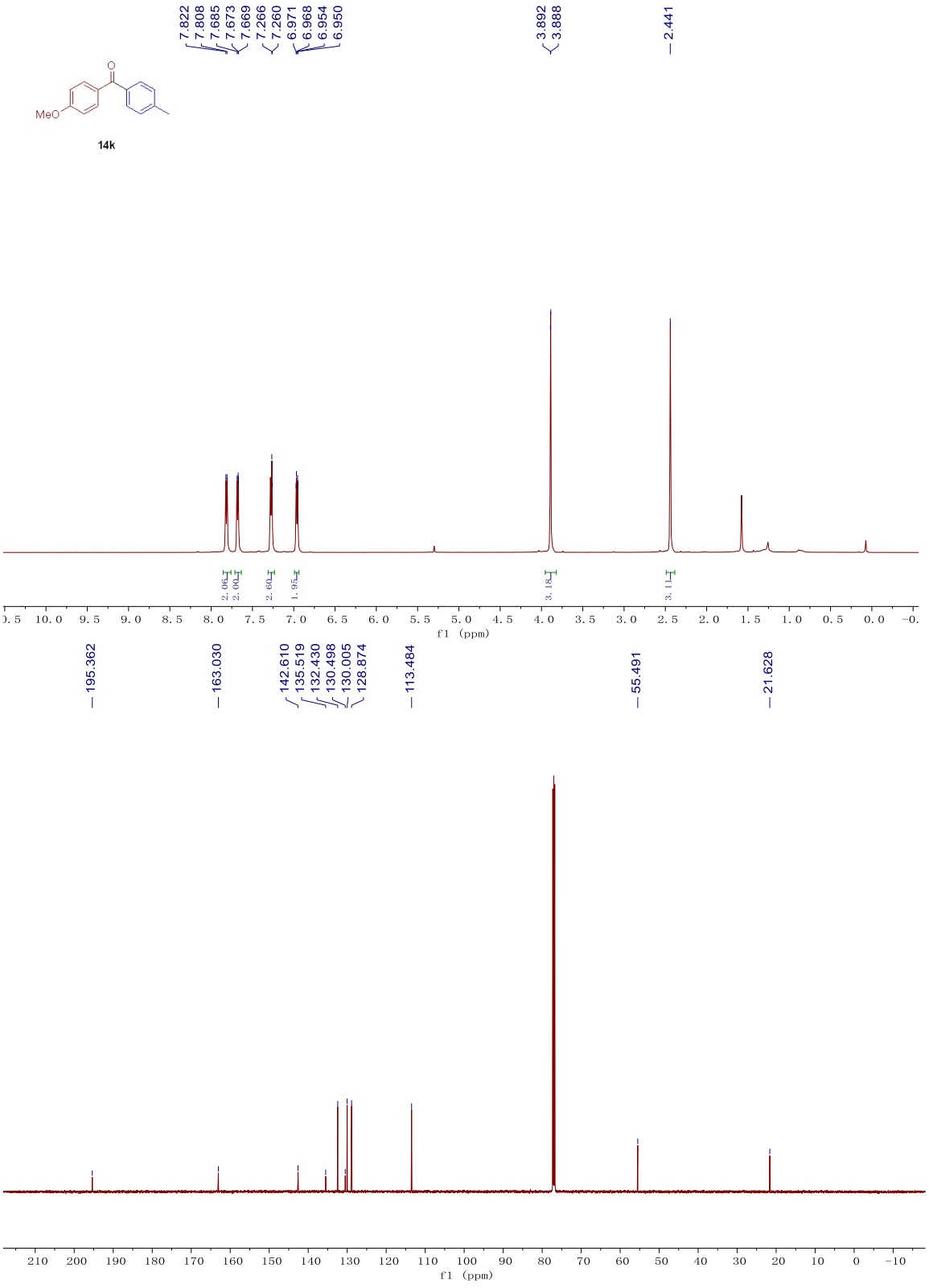

8.365
8.347
8.271
8.256
8.245
8.229
8.214
8.199
8.182
8.132
8.125
8.114
8.107
8.093
8.079
8.077
8.064
8.049
7.911
7.897
7.637
7.623
7.608
7.499
7.483
7.468
7.260
O

14i


1.03
2.09
2.05
4.04
1.92
1.00
1.97
f1 (ppm)


198.483
138.781
133.188
133.125
133.088
131.188
130.688
130.623
129.763
129.156
128.896
128.489
127.225
126.983
126.425
126.086
125.946
124.820
124.749
124.446
123.788
f1 (ppm)


7.713
7.696
7.283
7.267
7.261
2.440
14j
4.00
4.07
3.05
f1 (ppm)
196.283
142.925
135.221
130.221
130.192
128.904
21.648
f1 (ppm)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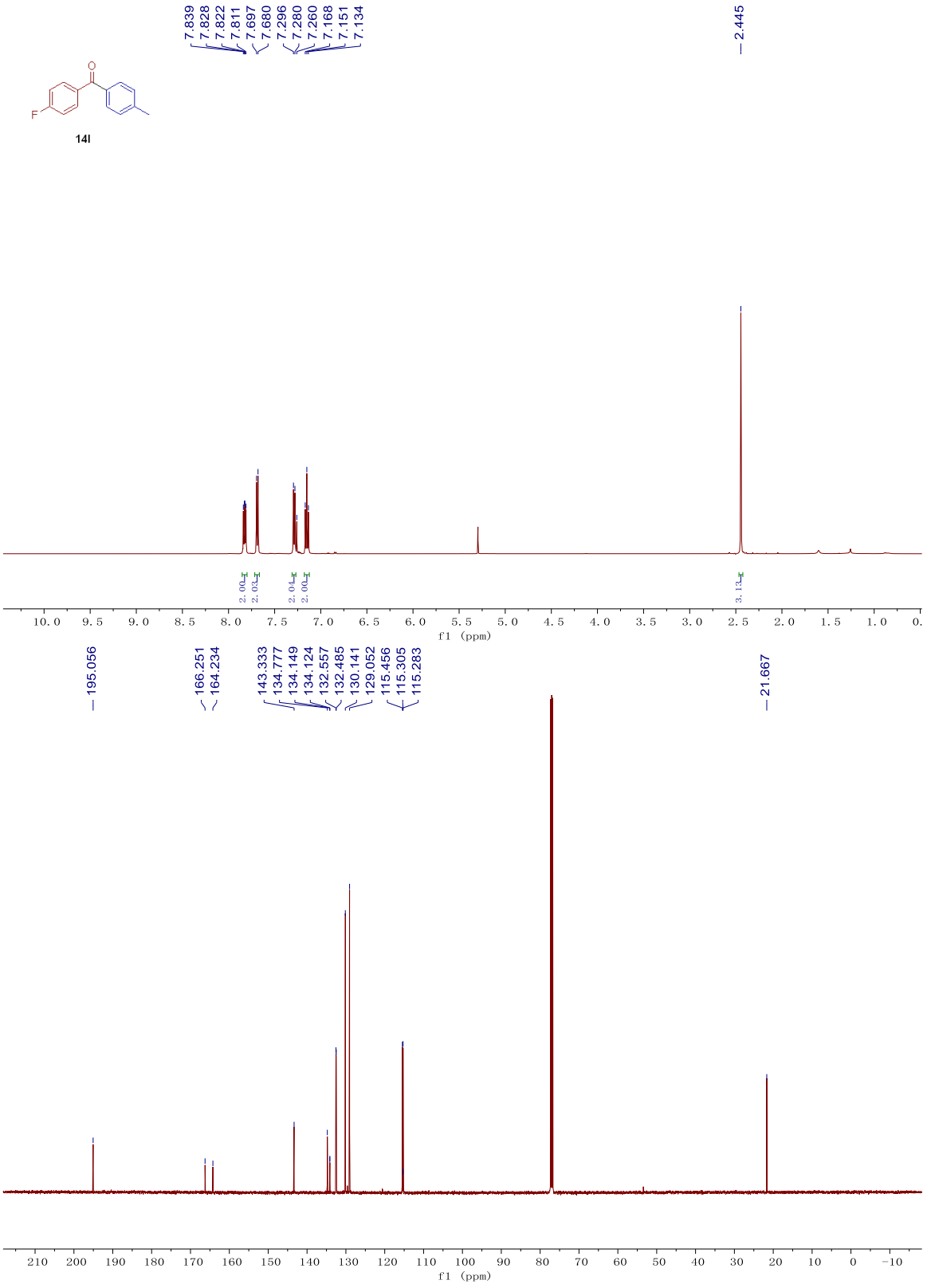
7.685
7.673
7.669
7.266
7.260
6.971
6.968
6.954
6.950
3.892
3.888
2.441
MeO
14k
2.06
2.00
2.60
1.95
3.18
3.11
f1 (ppm)
195.362
163.030
142.610
135.519
132.430
130.498
130.005
128.874
113.484
55.491
21.628
f1 (ppm)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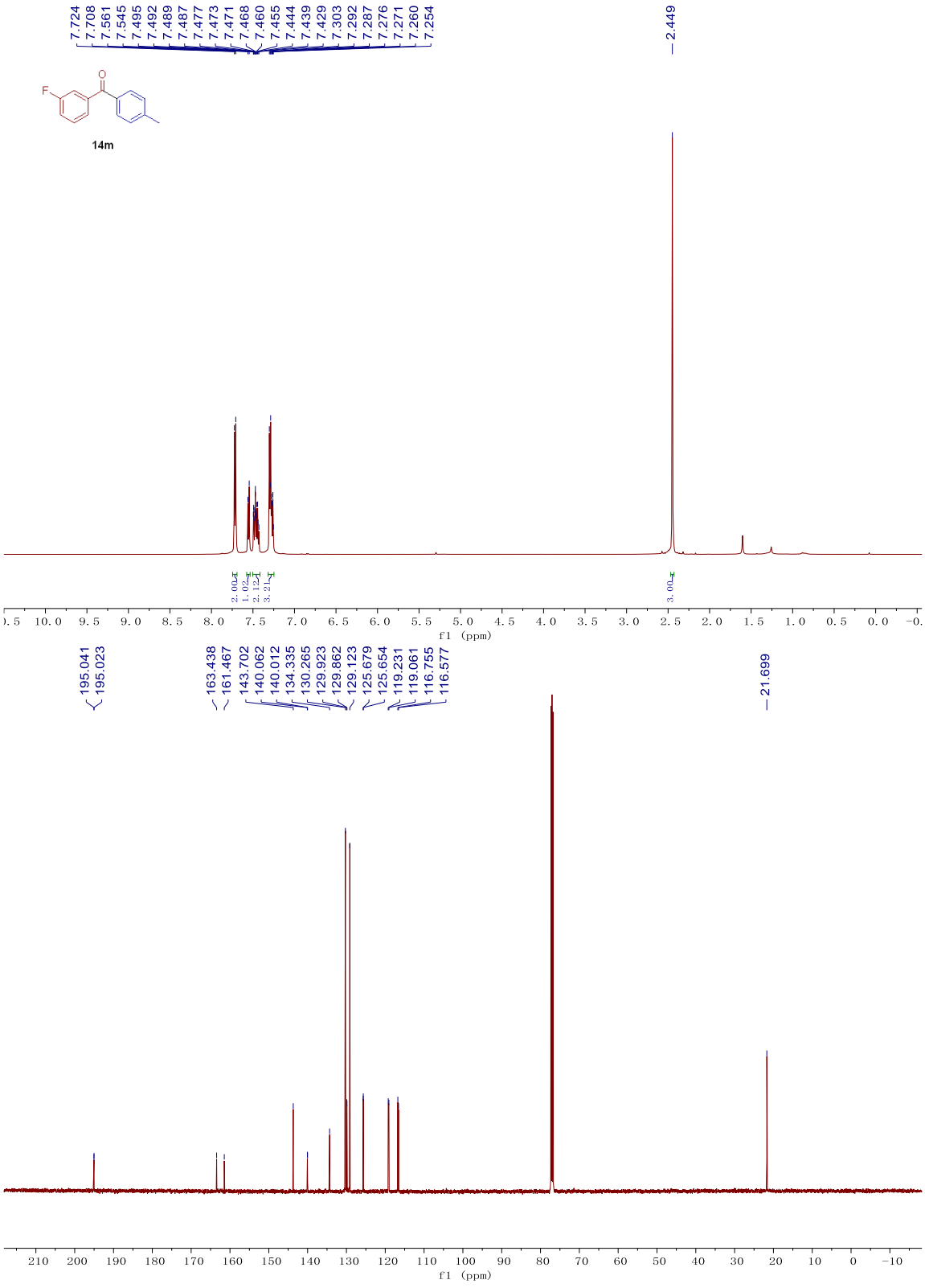
7.822
7.811
7.697
7.680
7.296
7.280
7.260
7.168
7.151
7.134
2.445
F
O
14l
2.00
2.03
2.04
2.00
3.13
f1 (ppm)
195.056
166.251
164.234
143.333
134.777
134.149
134.124
132.557
132.485
130.141
129.052
115.456
115.305
115.283
21.667
f1 (ppm)


7.724
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7.561
7.545
7.495
7.492
7.489
7.487
7.477
7.473
7.471
7.468
7.460
7.455
7.444
7.439
7.429
7.303
7.292
7.287
7.276
7.271
7.260
7.254
2.449
F
O
14m
2.00
1.02
2.12
3.21
3.00
f1 (ppm)
195.041
195.023
163.438
161.467
143.702
140.062
140.012
134.335
130.265
129.923
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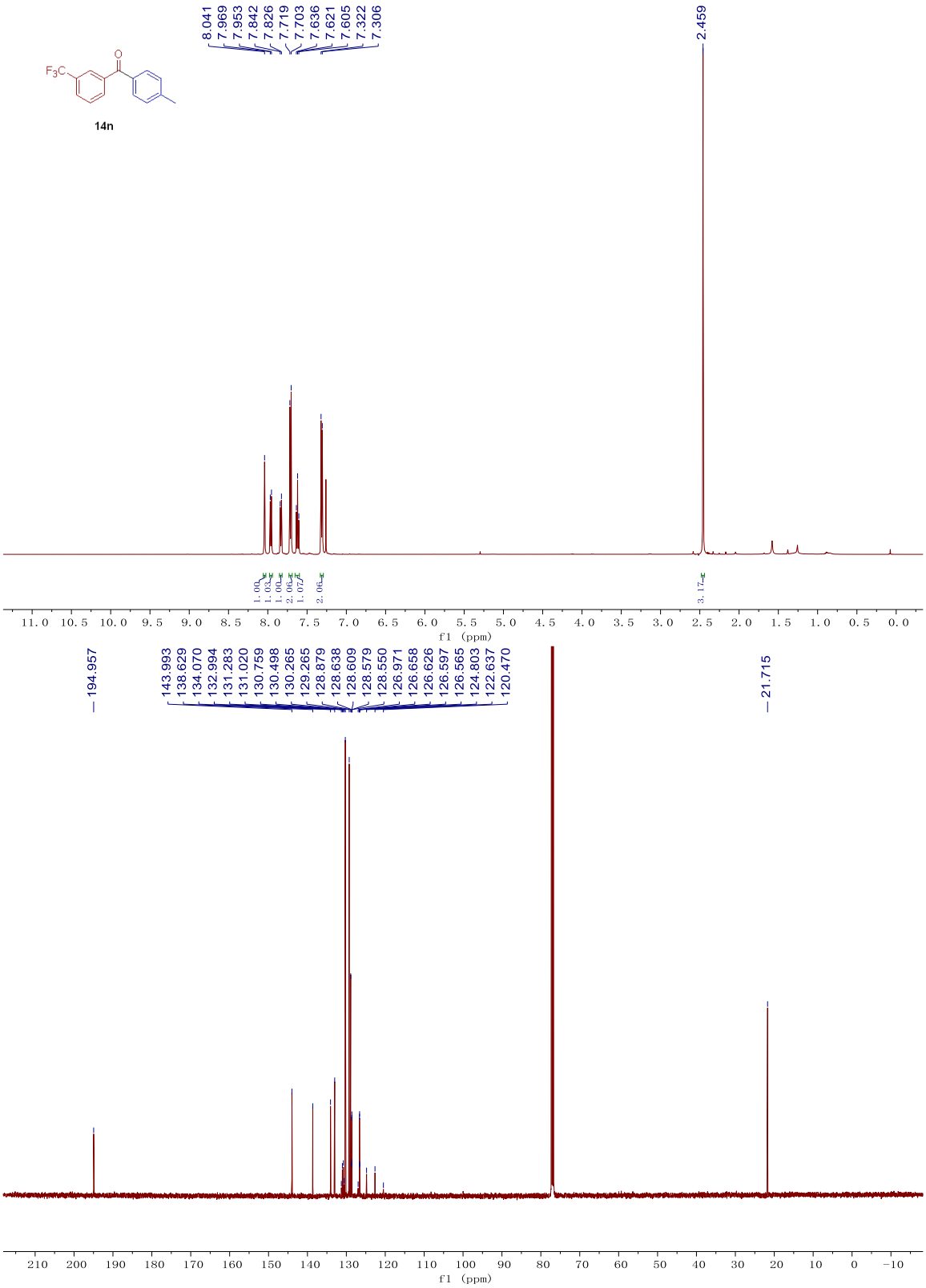
125.679
125.654
119.231
119.061
116.755
116.577
21.699
f1 (ppm)


8.041
7.969
7.953
7.842
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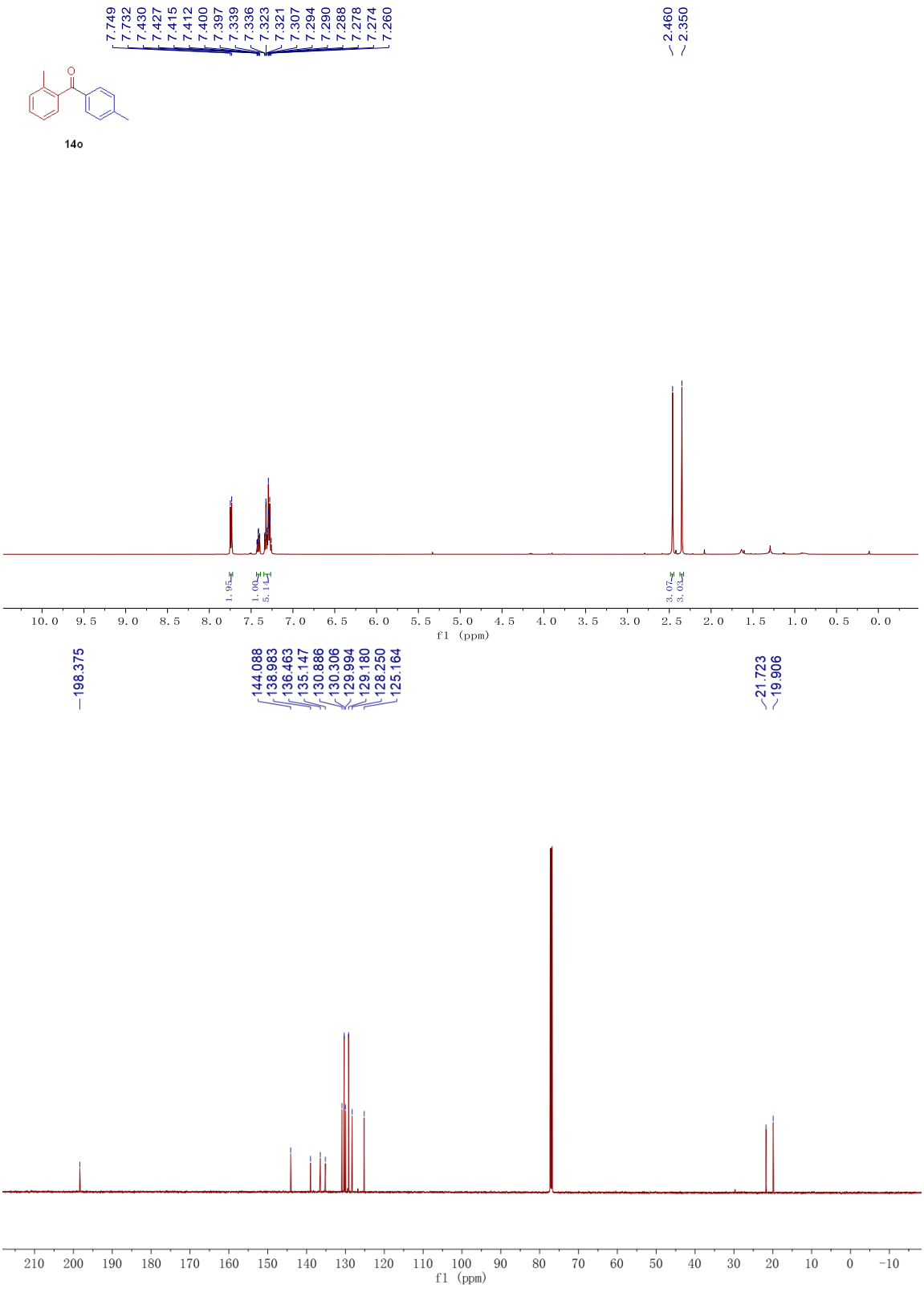
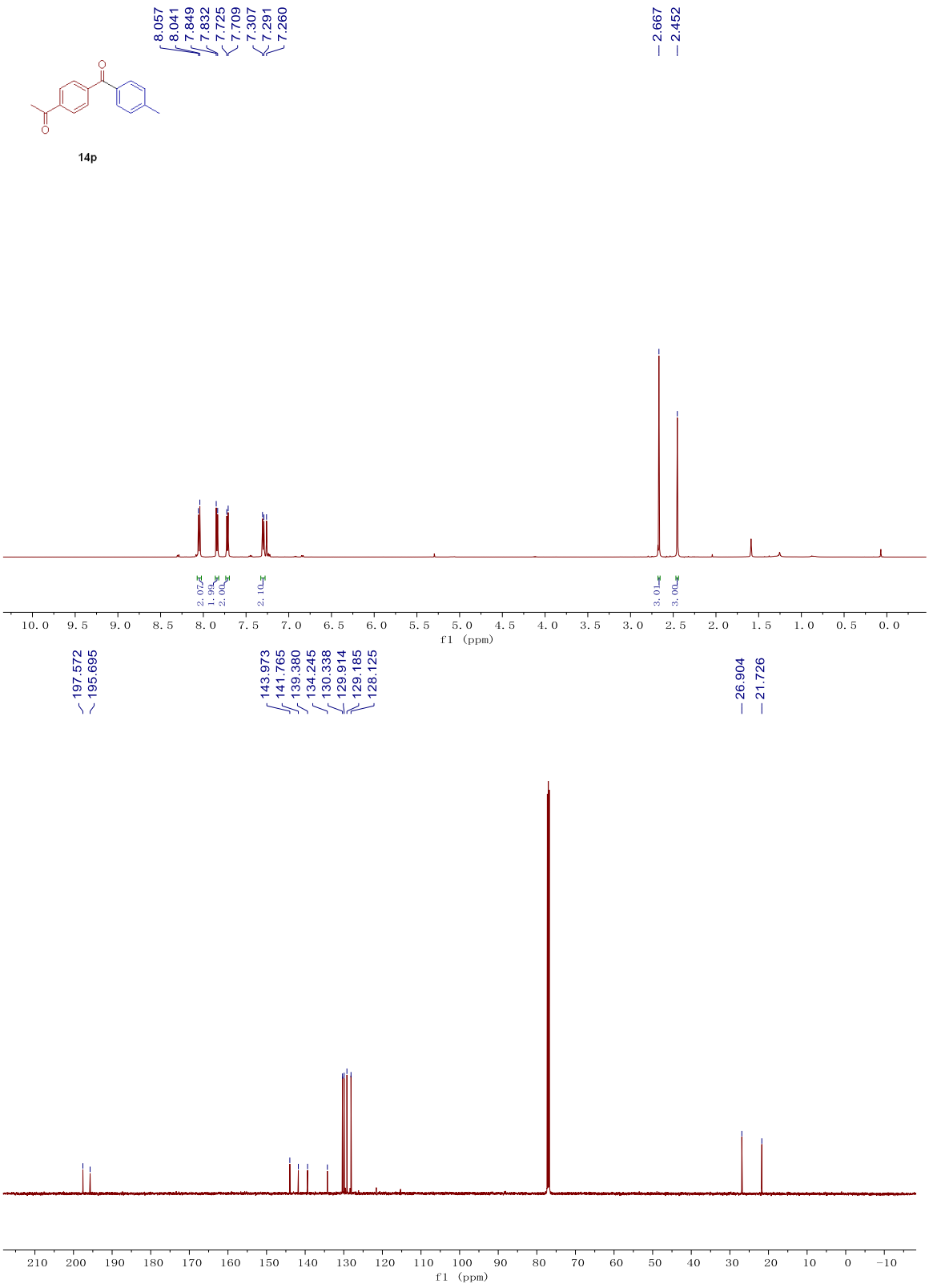
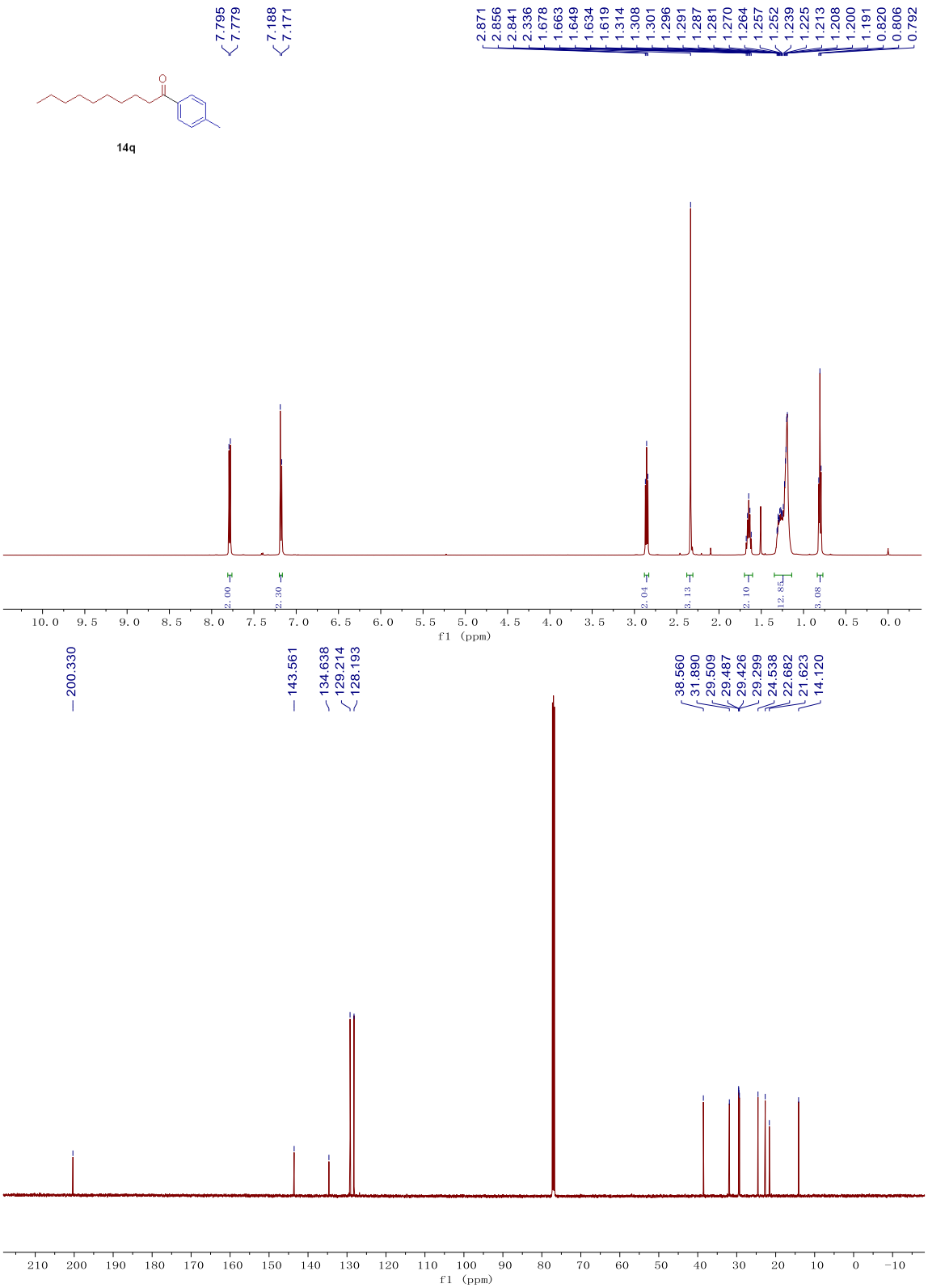
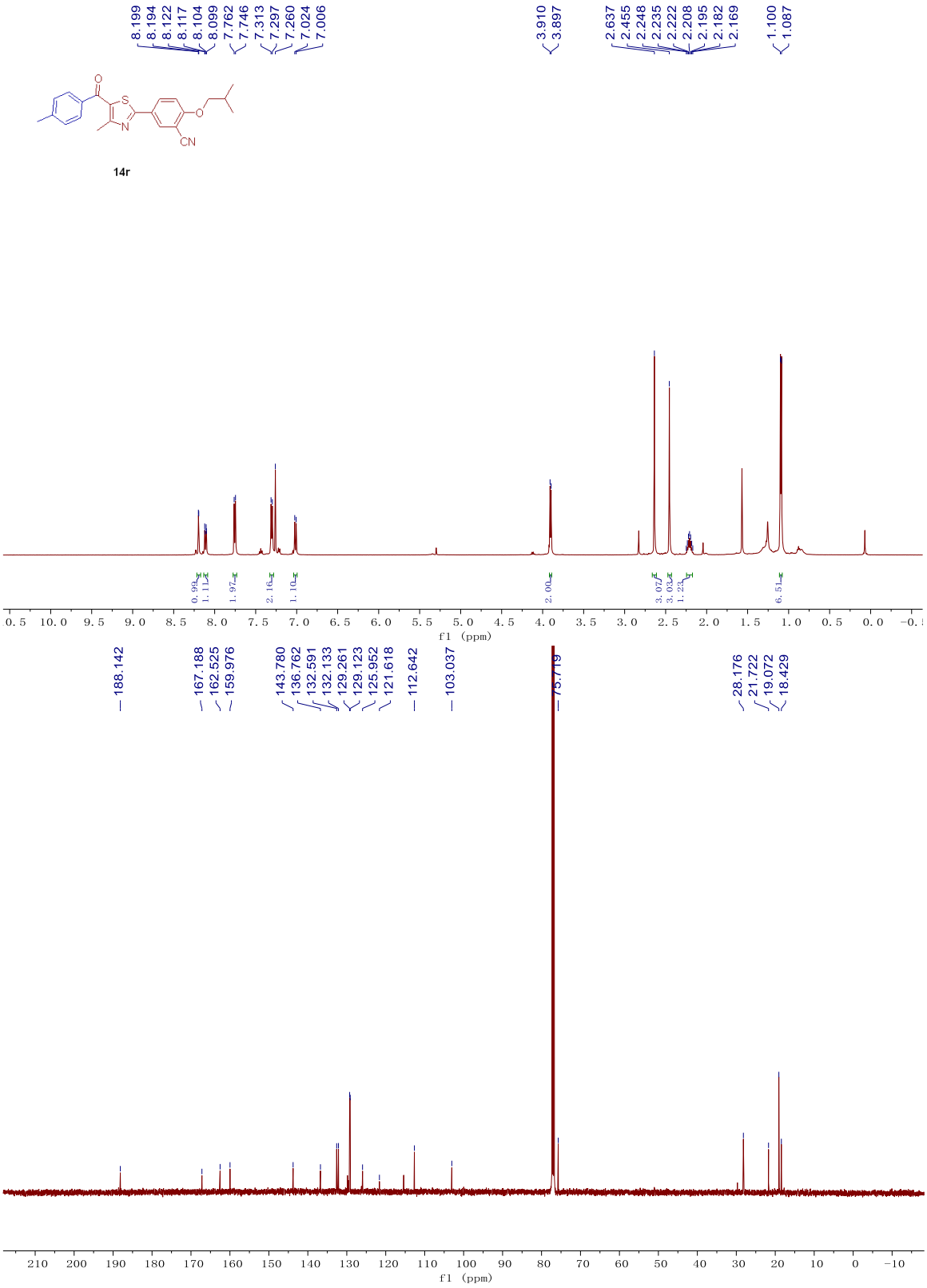
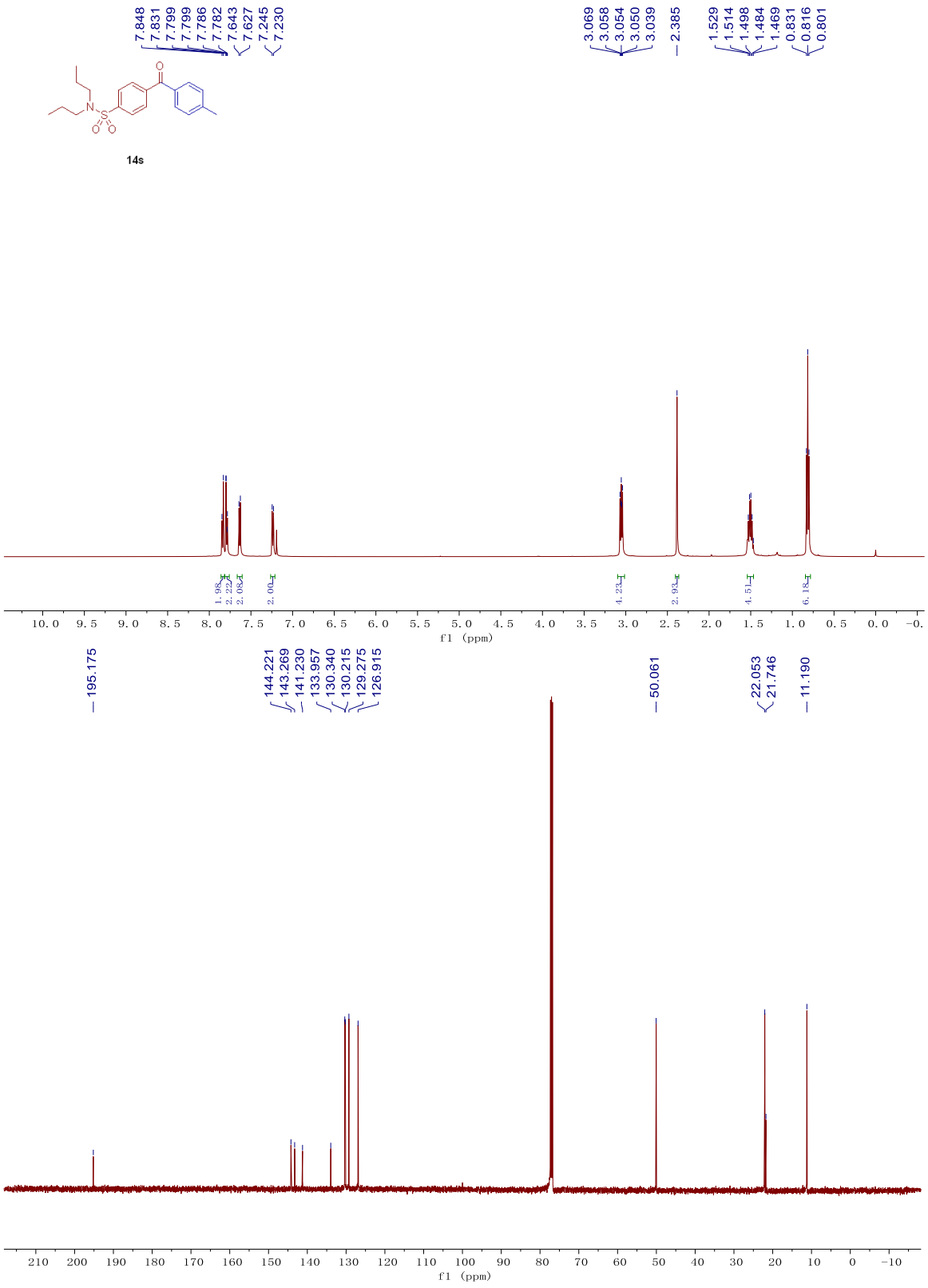
7.719
7.703
7.636
7.621
7.605
7.322
7.306
2.459
F3C
O
14n
1.00
1.02
1.00
2.00
1.07
2.06
3.17
f1 (ppm)
194.957
143.993
138.629
134.070
132.994
131.283
131.020
130.759
130.498
130.265
129.265
128.879
128.638
128.609
128.579
128.550
126.971
126.658
126.626
126.597
126.565
124.803
122.637
120.470
21.715
f1 (ppm)

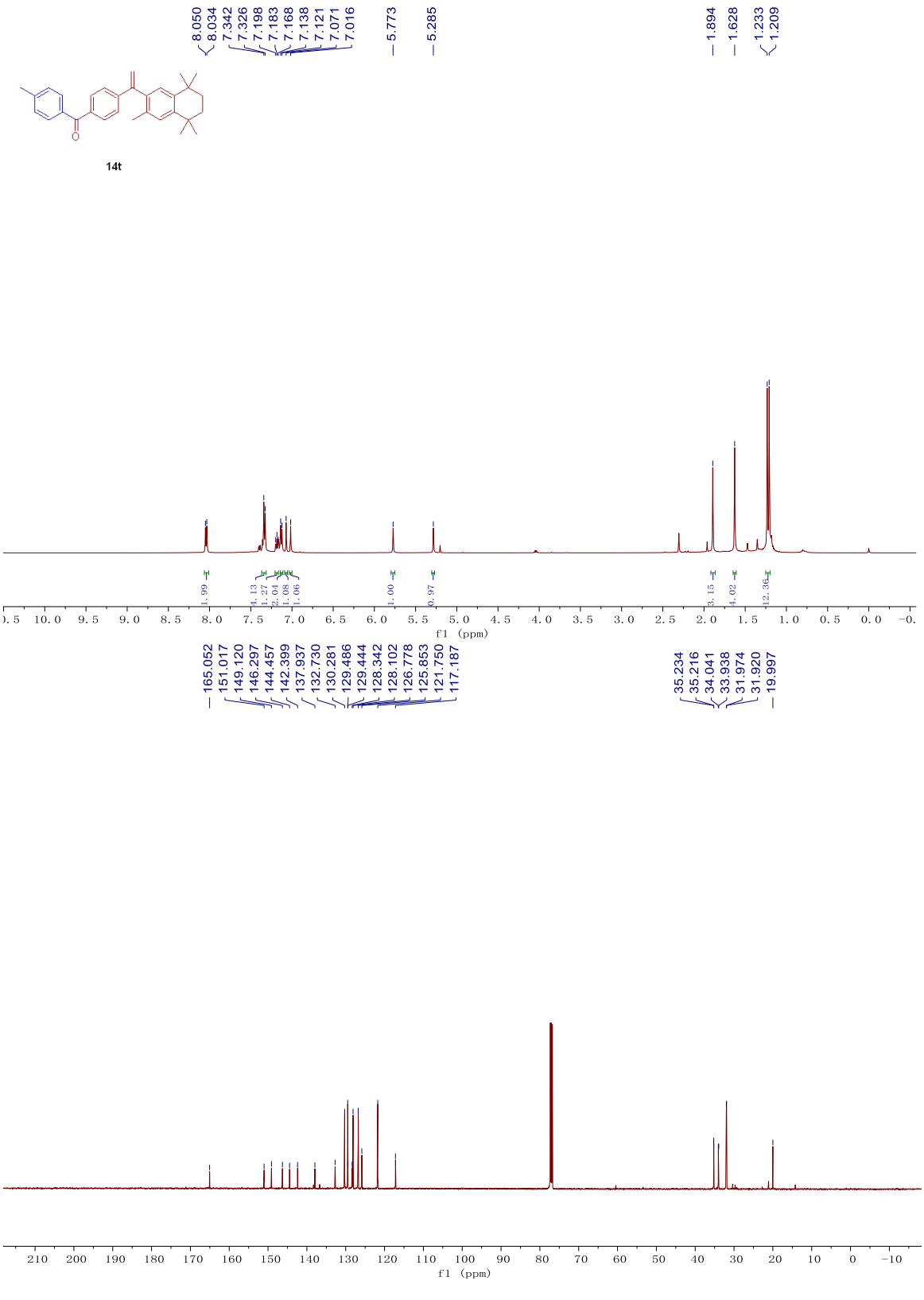

7.749
7.732
7.430
7.427
7.415
7.412
7.400
7.397
7.339
7.336
7.323
7.321
7.307
7.294
7.290
7.288
7.278
7.274
7.260
2.460
2.350
14o
1.95
1.00
5.14
3.07
3.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
198.375
144.088
138.983
136.463
135.147
130.886
130.306
129.994
129.180
128.250
125.164
21.723
19.906
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

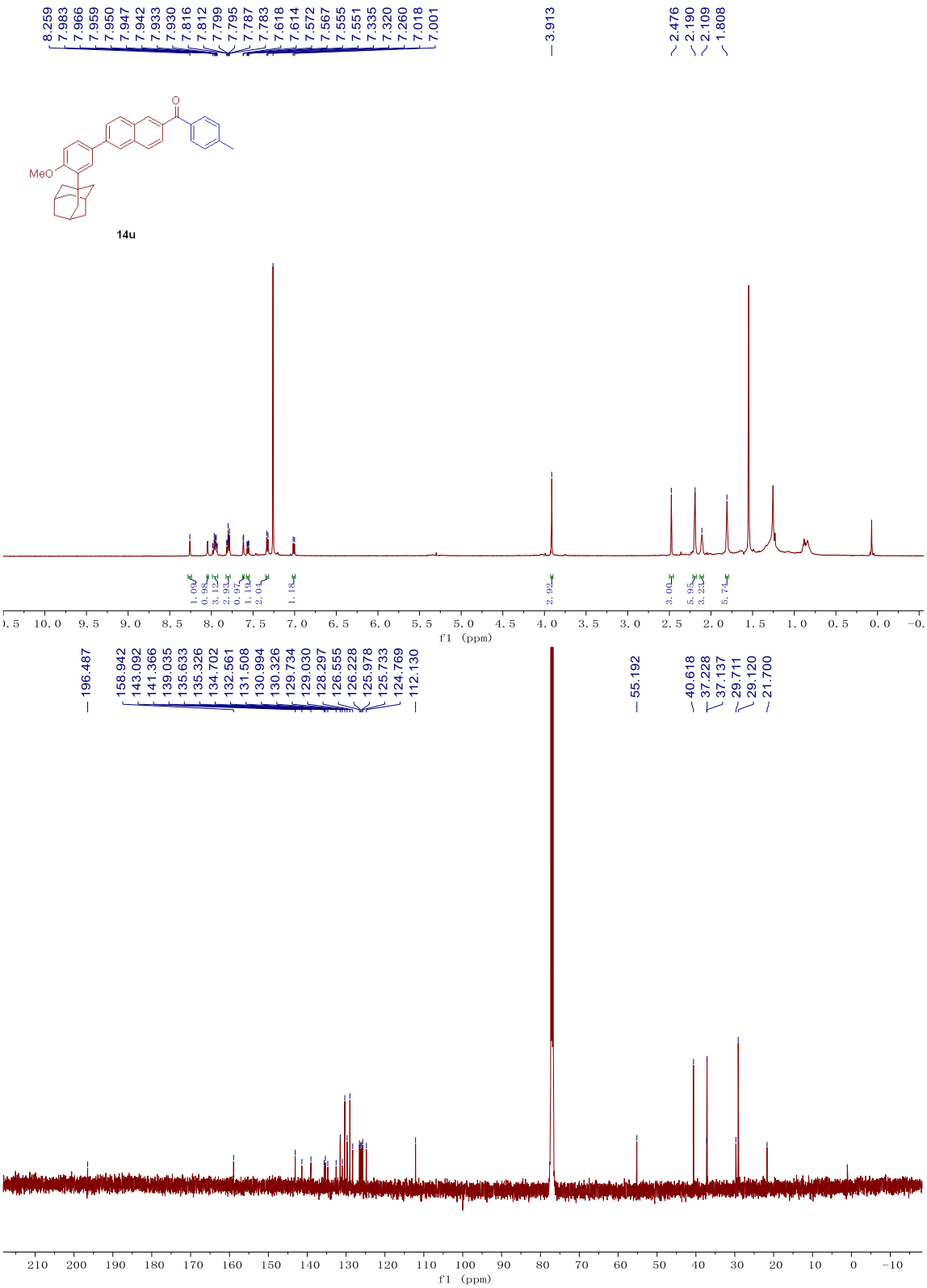

8.057
8.041
7.849
7.832
7.725
7.709
7.307
7.291
7.260
2.667
2.452
14p
2.07
1.99
2.00
2.10
3.01
3.00
f1 (ppm)
197.572
195.695
143.973
141.765
139.380
134.245
130.338
129.914
129.185
128.125
26.904
21.726
f1 (ppm)

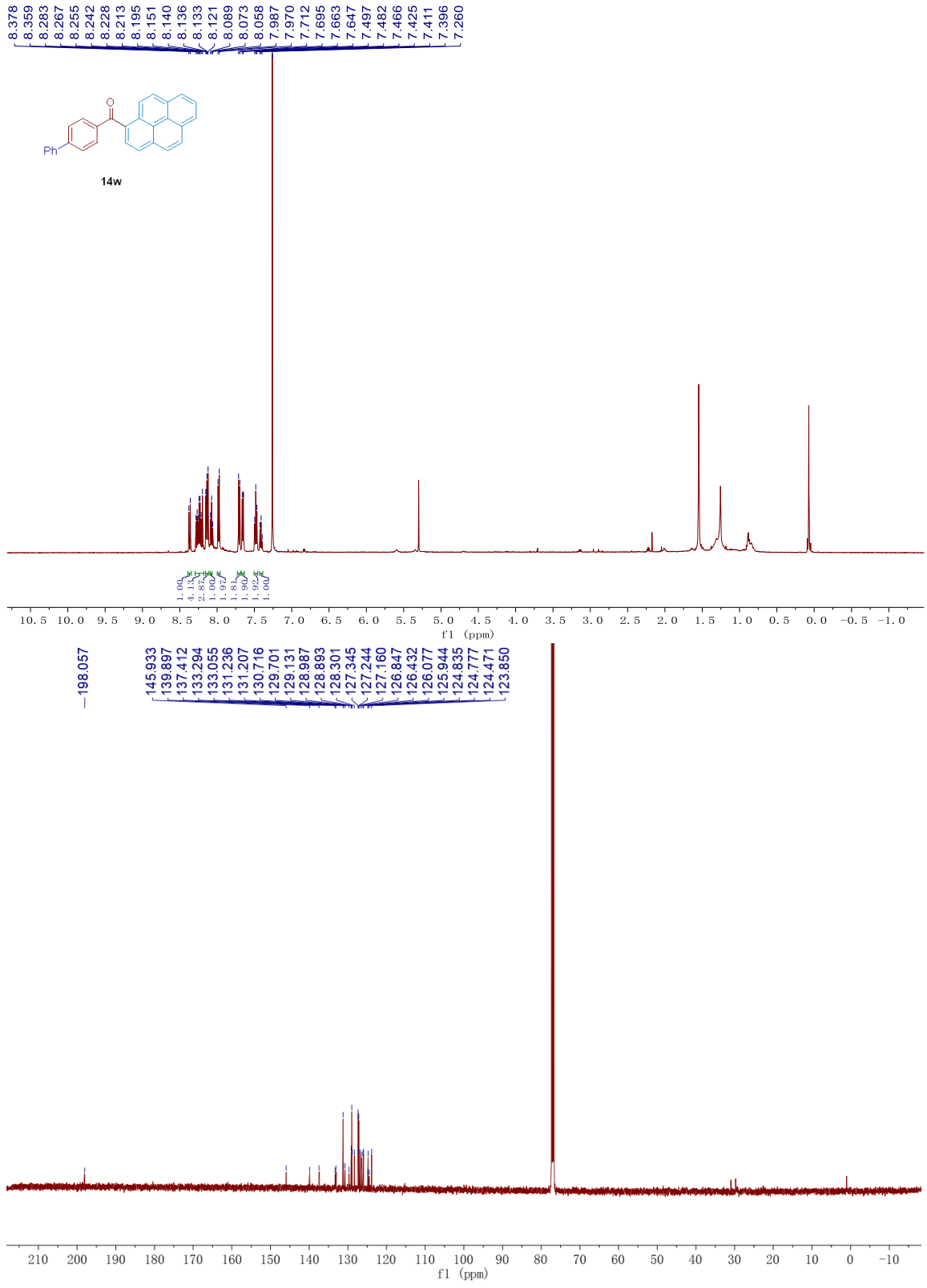

7.795
7.779
7.188
7.171
2.871
2.856
2.841
2.336
1.678
1.663
1.649
1.634
1.619
1.314
1.308
1.301
1.296
1.291
1.287
1.281
1.270
1.264
1.257
1.252
1.239
1.225
1.213
1.208
1.200
1.191
0.820
0.806
0.792
14q
2.00
2.30
2.04
3.13
2.10
12.85
3.08
f1 (ppm)
200.330
143.561
134.638
129.214
128.193
38.560
31.890
29.509
29.487
29.426
29.299
24.538
22.682
21.623
14.120
f1 (ppm)


8.199
8.194
8.122
8.117
8.104
8.099
7.762
7.746
7.313
7.297
7.260
7.024
7.006
3.910
3.897
2.637
2.455
2.248
2.235
2.222
2.208
2.195
2.182
2.169
1.100
1.087
O
S
N
O
CN
14r
0.99
1.11
1.97
2.16
1.10
2.00
3.07
3.02
1.23
6.51
f1 (ppm)
188.142
167.188
162.525
159.976
143.780
136.762
132.591
132.133
129.261
129.123
125.952
121.618
112.642
103.037
79.719
28.176
21.722
19.072
18.429
f1 (ppm)


7.848
7.831
7.799
7.799
7.786
7.782
7.643
7.627
7.245
7.230
3.069
3.058
3.054
3.050
3.039
2.385
1.529
1.514
1.498
1.484
1.469
0.831
0.816
0.801
14s
f1 (ppm)
195.175
144.221
143.269
141.230
133.957
130.340
130.215
129.275
126.915
50.061
22.053
21.746
11.190
f1 (ppm)


8.050
8.034
7.342
7.326
7.198
7.183
7.168
7.138
7.121
7.071
7.016
5.773
5.285
1.894
1.628
1.233
1.209
14t
f1 (ppm)
165.052
151.017
149.120
146.297
144.457
142.399
137.937
132.730
130.281
129.486
129.444
128.342
128.102
126.778
125.853
121.750
117.187
35.234
35.216
34.041
33.938
31.974
31.920
19.997
f1 (ppm)


8.259
7.983
7.966
7.959
7.950
7.947
7.942
7.933
7.930
7.816
7.812
7.799
7.795
7.787
7.783
7.618
7.614
7.572
7.567
7.555
7.551
7.335
7.320
7.260
7.018
7.001
3.913
2.476
2.190
2.109
1.808
MeO
O
14u
1.00
0.98
3.12
2.93
0.97
1.13
2.04
1.18
2.92
3.00
5.95
3.23
5.74
f1 (ppm)
196.487
158.942
143.092
141.366
139.035
135.633
135.326
134.702
132.561
131.508
130.994
130.326
129.734
129.030
128.297
126.555
126.228
125.978
125.733
124.769
112.130
55.192
40.618
37.228
37.137
29.711
29.120
21.700
f1 (ppm)


8.378
8.359
8.283
8.267
8.255
8.242
8.228
8.213
8.195
8.151
8.140
8.136
8.133
8.121
8.089
8.073
8.058
7.987
7.970
7.712
7.695
7.663
7.647
7.497
7.482
7.466
7.425
7.411
7.396
7.260
O
Ph
14w
1.00
4.13
2.87
1.00
1.97
1.81
1.90
1.92
1.00
f1 (ppm)
198.057
145.933
139.897
137.412
133.294
133.055
131.236
131.207
130.716
129.701
129.131
128.987
128.893
128.301
127.345
127.244
127.160
126.847
126.432
126.077
125.944
124.835
124.777
124.471
123.850
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 Li and 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.

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

IPr-IV				**SIPr-IV**			
66				68			
IPrIV SCF Done: -1287.32550879 A.U.				SIPrIV SCF Done: -1288.52862548 A.U.			
N	1.083488	0.011775	0.980144	N	-1.096758	0.020217	0.945352
C	2.454394	0.019288	0.542433	C	-2.450535	-0.094194	0.490430
N	-1.083488	-0.011591	0.980163	N	1.096589	-0.019685	0.945510
C	3.116703	-1.222713	0.378546	C	-3.236236	1.087025	0.427044
C	4.457045	-1.189010	-0.054636	C	-4.572539	0.965568	0.000551
H	5.001787	-2.134189	-0.203840	H	-5.206150	1.862850	-0.071284
C	5.102522	0.030594	-0.310780	C	-5.106254	-0.286583	-0.345724
H	6.150444	0.034894	-0.651006	H	-6.153786	-0.362326	-0.678903
C	4.418573	1.243899	-0.141619	C	-4.311279	-1.439489	-0.272763
H	4.932621	2.193488	-0.358504	H	-4.740122	-2.414416	-0.554853
C	3.077297	1.266108	0.290480	C	-2.967897	-1.369610	0.150073
C	2.382708	-2.547203	0.574846	C	-2.605714	2.446066	0.723728
H	1.461285	-2.337495	1.158797	H	-1.769286	2.269458	1.434736
C	1.934197	-3.100851	-0.794712	C	-1.979409	3.025260	-0.564133
H	1.303127	-2.349647	-1.322967	H	-1.261323	2.302428	-1.014646
H	1.342678	-4.032445	-0.669684	H	-1.440049	3.972868	-0.351260
H	2.813765	-3.329151	-1.433977	H	-2.768129	3.235578	-1.317798
C	3.205080	-3.579264	1.368283	C	-3.572234	3.445905	1.381157
H	4.101657	-3.914786	0.805061	H	-4.375498	3.763474	0.682801
H	2.594233	-4.483523	1.571964	H	-3.028171	4.364965	1.683409
H	3.550098	-3.168463	2.339997	H	-4.057576	3.017762	2.283064
C	2.311304	2.581340	0.408425	C	-2.104501	-2.628157	0.195072

H	1.357805	2.367860	0.936225	H	-1.112720	-2.344719	0.604974
C	1.941495	3.101268	-0.996542	C	-1.847874	-3.164578	-1.227074
H	2.852916	3.325700	-1.590889	H	-2.793903	-3.461111	-1.728092
H	1.333883	4.028134	-0.927513	H	-1.178496	-4.049973	-1.198951
H	1.346967	2.329567	-1.538662	H	-1.353924	-2.373695	-1.837122
C	3.070668	3.638234	1.232481	C	-2.702377	-3.705335	1.121401
H	3.341411	3.254358	2.238149	H	-2.870035	-3.312073	2.146172
H	2.445760	4.546183	1.365248	H	-2.021561	-4.579737	1.192975
H	4.007848	3.958127	0.729538	H	-3.678381	-4.076514	0.742652
C	-0.000004	0.000013	0.118410	C	-0.000025	0.000121	0.127803
C	0.684858	0.007931	2.318510	C	-0.754637	-0.148655	2.372498
H	1.411130	0.015191	3.136826	H	-1.342861	0.543749	3.008811
C	-0.684837	-0.007623	2.318521	C	0.754283	0.149440	2.372567
H	-1.411098	-0.014740	3.136850	H	1.342435	-0.542836	3.009082
C	-2.454395	-0.019211	0.542452	C	2.450430	0.094351	0.490740
C	-3.077211	-1.266073	0.290505	C	2.968121	1.369624	0.150278
C	-4.418483	-1.243953	-0.141610	C	4.311557	1.439150	-0.272434
H	-4.932468	-2.193580	-0.358480	H	4.740645	2.413953	-0.554589
C	-5.102508	-0.030695	-0.310796	C	5.106272	0.286050	-0.345200
H	-6.150422	-0.035069	-0.651045	H	6.153855	0.361510	-0.678284
C	-4.457116	1.188955	-0.054657	C	4.572230	-0.965941	0.001146
H	-5.001916	2.134094	-0.203894	H	5.205641	-1.863376	-0.070563
C	-3.116786	1.222747	0.378549	C	3.235867	-1.087044	0.427552
C	-2.311163	-2.581273	0.408491	C	2.104991	2.628366	0.195012
H	-1.357602	-2.367719	0.936150	H	1.113147	2.345232	0.604955
C	-3.070410	-3.638084	1.232758	C	2.703065	3.705620	1.121125
H	-3.340962	-3.254119	2.238444	H	2.870567	3.312562	2.145999
H	-2.445504	-4.546039	1.365483	H	2.022441	4.580192	1.192451
H	-4.007693	-3.957981	0.730009	H	3.679176	4.076498	0.742351
C	-1.941515	-3.101338	-0.996467	C	1.848524	3.164535	-1.227263
H	-2.853000	-3.325760	-1.590719	H	2.794634	3.460785	-1.728299
H	-1.333957	-4.028238	-0.927420	H	1.179298	4.050051	-1.199357
H	-1.346972	-2.329714	-1.538686	H	1.354461	2.373616	-1.837170
C	-2.382840	2.547270	0.574834	C	2.605002	-2.445907	0.724257
H	-1.461531	2.337624	1.158986	H	1.768409	-2.269040	1.435010
C	-1.934049	3.100745	-0.794707	C	1.978936	-3.025149	-0.563690
H	-1.303021	2.349410	-1.322827	H	1.261005	-2.302291	-1.014398
H	-1.342410	4.032262	-0.669669	H	1.439455	-3.972699	-0.350867
H	-2.813493	3.329119	-1.434114	H	2.767800	-3.235583	-1.317173
C	-3.205355	3.579425	1.367989	C	3.571152	-3.445846	1.382095
H	-4.101781	3.914954	0.804528	H	4.374567	-3.763651	0.684019
H	-2.594517	4.483672	1.571746	H	3.026829	-4.364770	1.684298
H	-3.550625	3.168715	2.339652	H	4.056302	-3.017685	2.284097
Pd	-0.000032	-0.000112	-1.812866	Pd	0.000203	-0.000199	-1.802314
				H	0.983023	1.191614	2.697301
				H	-0.983410	-1.190771	2.697383
Zero-point correction= 0.552882 (Hartree/Particle)				Zero-point correction= 0.575206 (Hartree/Particle)			
Thermal correction to Energy= 0.585580				Thermal correction to Energy= 0.608405			
Thermal correction to Enthalpy= 0.586525				Thermal correction to Enthalpy= 0.609349			
Thermal correction to Gibbs Free Energy= 0.487302				Thermal correction to Gibbs Free Energy= 0.510008			
Sum of electronic and zero-point Energies= -1286.772627				Sum of electronic and zero-point Energies= -1287.953419			
Sum of electronic and thermal Energies= -1286.739928				Sum of electronic and thermal Energies= -1287.920221			
Sum of electronic and thermal Enthalpies= -1286.738984				Sum of electronic and thermal Enthalpies= -1287.919277			
Sum of electronic and thermal Free Energies= -1286.838207				Sum of electronic and thermal Free Energies= -1288.018618			

IPr-V				**SIPr-V**			
91				93			
IPrV SCF Done: -1938.78588211 A.U.				SIPrV SCF Done: -1939.98738511 A.U.			
C	1.437257	-0.687490	-2.418657	C	1.507414	-0.800334	-2.374121
O	0.863006	-0.548199	-3.478805	O	0.962289	-0.666619	-3.449173
Pd	-0.222019	-0.696765	-0.451441	Pd	-0.239591	-0.656861	-0.444998
O	1.129324	-1.901939	-1.648262	O	1.106883	-1.954295	-1.560370

C	4.705118	1.835726	-1.174477
C	4.224918	1.857339	-2.495489
H	4.472414	0.963860	0.811282
C	4.116804	0.973565	-0.228614
C	3.165659	1.016143	-2.870782
C	2.574524	0.147926	-1.925127
C	3.054506	0.138804	-0.594887
H	2.770698	1.021114	-3.897578
H	2.564279	-0.491239	0.162406
H	5.534188	2.497236	-0.876351
H	4.675111	2.534586	-3.238403
N	-0.784289	1.535274	1.492001
N	-2.598415	0.825601	0.549228
C	-1.233865	0.629357	0.551985
C	-1.838172	2.270426	2.045230
C	-2.986284	1.819561	1.448333
C	0.591235	1.700596	1.890186
C	1.273909	2.863356	1.451147
C	2.569315	3.085817	1.959398
C	3.159722	2.174879	2.846611
C	2.489451	0.994370	3.203227
C	1.188818	0.723997	2.731389
C	0.662043	3.764047	0.378952
H	4.169096	2.371656	3.242390
C	0.454186	-0.570207	3.080166
C	-3.497887	0.015437	-0.229649
C	-3.953402	-1.203489	0.330957
C	-4.822441	-1.988668	-0.452244
C	-5.213127	-1.571181	-1.733833
C	-4.733205	-0.364405	-2.265233
C	-3.859098	0.456914	-1.525246
C	-3.456106	-1.692528	1.690279
H	-5.892032	-2.200511	-2.331181
C	-3.238640	1.710998	-2.134873
H	-1.668823	3.035874	2.808705
H	-4.034256	2.104234	1.581142
H	3.130705	3.977612	1.645338
H	2.987996	0.271359	3.865199
H	-0.434987	3.805047	0.553310
H	-0.049716	-0.881717	2.133656
H	-5.190157	-2.948530	-0.056944
H	-5.029974	-0.061791	-3.281244
H	-2.964222	-0.837078	2.198868
H	-2.830614	2.322363	-1.301585
C	-2.047345	1.309410	-3.032375
H	-2.392051	0.706290	-3.898472
H	-1.521983	2.207264	-3.419910
H	-1.314518	0.694387	-2.465015
C	-4.256758	2.583693	-2.891442
H	-3.778374	3.527360	-3.227206
H	-4.640177	2.075281	-3.801392
H	-5.128617	2.844144	-2.255481
C	-4.595995	-2.174141	2.607143
H	-5.091951	-3.083412	2.206530
H	-4.199201	-2.433927	3.611001
H	-5.373885	-1.392864	2.734649
C	-2.377802	-2.780628	1.499517
H	-1.948934	-3.087605	2.477303
H	-2.798953	-3.680651	1.003514
H	-1.549115	-2.389474	0.859546
C	-0.633658	-0.354811	4.152415
H	-1.197352	-1.296178	4.324109
H	-0.182426	-0.043411	5.119101

C	4.881578	1.573619	-1.128441
C	4.473789	1.532545	-2.473201
H	4.482277	0.868436	0.896882
C	4.185199	0.823989	-0.160332
C	3.377805	0.740527	-2.849602
C	2.679352	-0.015505	-1.881407
C	3.086442	0.038730	-0.528453
H	3.037217	0.699583	-3.895016
H	2.507594	-0.494705	0.241238
H	5.738155	2.198560	-0.829202
H	5.009245	2.122753	-3.233576
N	-0.759179	1.677497	1.333859
N	-2.594088	0.882874	0.437221
C	-1.243118	0.732820	0.479129
C	-1.812573	2.549771	1.907145
C	-3.109443	1.930618	1.340523
C	0.611357	1.826999	1.730409
C	1.336575	2.943038	1.234461
C	2.616915	3.190562	1.768313
C	3.166531	2.341316	2.738860
C	2.471612	1.192154	3.146659
C	1.183494	0.903983	2.651907
C	0.789525	3.760230	0.064521
H	4.163634	2.556139	3.155874
C	0.439949	-0.370743	3.050560
C	-3.475957	-0.014462	-0.250369
C	-3.903142	-1.194163	0.412552
C	-4.791442	-2.046339	-0.272835
C	-5.235491	-1.732675	-1.566449
C	-4.788812	-0.565932	-2.206253
C	-3.900323	0.317813	-1.562290
C	-3.346229	-1.580707	1.781005
H	-5.929060	-2.411852	-2.087653
C	-3.316632	1.529388	-2.282967
H	-1.666222	3.603838	1.585328
H	-3.751023	1.475387	2.127904
H	3.201071	4.049557	1.407087
H	2.941441	0.508107	3.868777
H	-0.316124	3.801899	0.160806
H	-0.055852	-0.721800	2.112762
H	-5.130307	-2.977604	0.208209
H	-5.126710	-0.345749	-3.230642
H	-2.817709	-0.695985	2.191474
H	-2.937023	2.224021	-1.502411
C	-2.098017	1.088411	-3.124130
H	-2.407708	0.384614	-3.924982
H	-1.603832	1.962097	-3.598729
H	-1.347874	0.564708	-2.489427
C	-4.348892	2.294111	-3.129874
H	-3.898563	3.221892	-3.540521
H	-4.694867	1.693715	-3.997947
H	-5.242989	2.575806	-2.534895
C	-4.441118	-1.971835	2.790356
H	-4.967131	-2.902654	2.489826
H	-3.996757	-2.155899	3.791296
H	-5.204663	-1.172528	2.892227
C	-2.284925	-2.689554	1.624133
H	-1.809136	-2.925928	2.599862
H	-2.731638	-3.620988	1.216772
H	-1.487852	-2.348276	0.918389
C	-0.655644	-0.111997	4.103117
H	-1.215991	-1.045810	4.320589
H	-0.216079	0.255866	5.055109

H	-1.365227	0.421574	3.851461
C	1.391964	-1.722953	3.468816
H	1.878389	-1.561446	4.455018
H	0.812554	-2.667007	3.543707
H	2.187119	-1.875675	2.709888
C	1.181982	5.210394	0.406950
H	2.250503	5.268684	0.109167
H	0.613951	5.832425	-0.315178
H	1.080913	5.670121	1.412396
C	0.883862	3.118578	-1.008992
H	0.395684	3.719782	-1.804607
H	1.968239	3.054114	-1.235332
H	0.474689	2.086953	-1.050554
C	2.124637	-2.731653	-1.137883
C	1.918985	-3.303012	0.129698
C	3.277900	-3.017518	-1.888296
C	2.892013	-4.166379	0.657359
H	1.002885	-3.041799	0.683675
C	4.247654	-3.874827	-1.341783
H	3.412992	-2.563727	-2.881337
C	4.061877	-4.450882	-0.071793
H	2.735374	-4.611580	1.652591
H	5.158531	-4.095077	-1.920539
H	4.827097	-5.121844	0.348077

Zero-point correction= 0.744647 (Hartree/Particle)
Thermal correction to Energy= 0.790363
Thermal correction to Enthalpy= 0.791307
Thermal correction to Gibbs Free Energy= 0.665182
Sum of electronic and zero-point Energies= -1938.041235
Sum of electronic and thermal Energies= -1937.995519
Sum of electronic and thermal Enthalpies= -1937.994575
Sum of electronic and thermal Free Energies= -1938.120700

H	-1.390829	0.640990	3.758249
C	1.369139	-1.509384	3.498705
H	1.842177	-1.310400	4.484488
H	0.786922	-2.449143	3.602296
H	2.174764	-1.693147	2.758228
C	1.299296	5.210206	0.020519
H	2.383259	5.256736	-0.217202
H	0.772947	5.776905	-0.775154
H	1.138344	5.736773	0.984599
C	1.095315	3.016675	-1.255398
H	0.670376	3.562846	-2.123791
H	2.191182	2.924150	-1.402509
H	0.670211	1.990787	-1.246339
C	2.047694	-2.810786	-0.991444
C	1.800109	-3.297302	0.303197
C	3.187589	-3.203895	-1.713228
C	2.718231	-4.183647	0.888199
H	0.896598	-2.953634	0.831567
C	4.101891	-4.084087	-1.110705
H	3.355558	-2.815315	-2.728579
C	3.874103	-4.575896	0.187615
H	2.529686	-4.561455	1.905464
H	5.002012	-4.389398	-1.667198
H	4.596029	-5.265262	0.652000
H	-3.731739	2.659246	0.778674
H	-1.767235	2.532839	3.016173

Zero-point correction= 0.766924 (Hartree/Particle)
Thermal correction to Energy= 0.813294
Thermal correction to Enthalpy= 0.814238
Thermal correction to Gibbs Free Energy= 0.686575
Sum of electronic and zero-point Energies= -1939.220461
Sum of electronic and thermal Energies= -1939.174091
Sum of electronic and thermal Enthalpies= -1939.173147
Sum of electronic and thermal Free Energies= -1939.300810

IPr-V-VI			
91			
IPrV-VI SCF Done: -1938.78773316 A.U.			
C	-1.794858	0.553234	-1.392911
O	-2.007850	-0.179154	-2.343756
Pd	0.259838	0.541676	-0.654281
O	-0.958713	1.893819	-1.764714
C	-4.572882	0.815900	1.914459
C	-4.692424	-0.172572	0.921674
H	-3.393324	2.500859	2.639192
C	-3.505142	1.732741	1.858077
C	-3.769964	-0.226414	-0.134972
C	-2.706999	0.701700	-0.206043
C	-2.569759	1.669372	0.816119
H	-3.847780	-0.991744	-0.920439
H	-1.733281	2.379501	0.799958
H	-5.301260	0.865180	2.739438
H	-5.509889	-0.909580	0.967438
N	2.255413	-1.007034	0.900652
C	3.979636	-0.759957	-1.410177
H	3.368481	-1.627321	-1.084592
C	3.996069	0.255722	-0.269465
C	3.130111	0.134190	0.846191
C	1.013656	-0.999993	0.307374
C	3.042025	1.106619	1.872711
C	2.004821	0.995634	2.987758
H	1.631189	-0.050518	2.996869

SIPr-V-VI			
93			
SIPrV-VI SCF Done: -1939.98853017 A.U.			
C	-1.527556	0.684967	-1.836491
O	-1.145563	0.318790	-2.935974
Pd	0.257651	0.741235	-0.316270
O	-1.050081	2.072669	-1.390127
C	-5.222625	-0.663849	-0.054274
C	-4.978084	-0.824717	-1.429084
H	-4.423008	0.045658	1.845683
C	-4.246926	-0.065268	0.764622
C	-3.765592	-0.385447	-1.983652
C	-2.786100	0.217494	-1.164333
C	-3.036019	0.371205	0.214602
H	-3.563295	-0.487023	-3.060722
H	-2.253592	0.809869	0.849543
H	-6.171666	-1.012904	0.382903
H	-5.737249	-1.293205	-2.075461
N	2.595654	-0.730798	0.672315
C	3.253079	-1.066851	-2.153598
H	2.656699	-1.722646	-1.488225
C	3.809971	0.075493	-1.307814
C	3.452269	0.241088	0.055591
C	1.243899	-0.741632	0.501374
C	3.909414	1.334636	0.835557
C	3.395508	1.536232	2.258708
H	3.072347	0.541163	2.634473

C	4.820174	1.397930	-0.322927	C	4.662754	1.040554	-1.880507
H	5.500917	1.533639	-1.177915	H	4.948988	0.947378	-2.940239
C	4.770485	2.370801	0.687262	C	5.136796	2.124151	-1.126686
H	5.420960	3.257788	0.624617	H	5.800433	2.868957	-1.594391
C	3.886896	2.229767	1.768791	C	4.758663	2.272852	0.217221
H	3.843397	3.012621	2.541842	H	5.122383	3.139775	0.790046
C	2.564644	-2.251805	1.448855	C	3.126741	-1.995638	1.218134
C	0.796913	1.901891	2.665000	C	2.137928	2.432941	2.230562
H	-0.009330	1.772683	3.416696	H	1.697201	2.538605	3.244505
H	1.095117	2.971862	2.647387	H	2.386345	3.444943	1.846263
H	0.382853	1.640728	1.662426	H	1.361085	1.994638	1.556669
C	2.587771	1.291139	4.381849	C	4.458029	2.084069	3.227193
H	1.822027	1.110258	5.164709	H	4.061455	2.105588	4.263713
H	3.466311	0.649546	4.601754	H	5.377822	1.462864	3.220509
H	2.908547	2.349874	4.479700	H	4.750372	3.124814	2.972516
C	3.278628	-0.160058	-2.647922	C	2.278630	-0.535559	-3.224405
H	3.843419	0.708367	-3.048387	H	2.797659	0.118851	-3.956703
H	3.189892	-0.918134	-3.454332	H	1.818981	-1.377237	-3.783924
H	2.252112	0.185632	-2.386233	H	1.456113	0.047890	-2.759087
C	5.385869	-1.289606	-1.748601	C	4.369676	-1.933118	-2.767415
H	5.884265	-1.721117	-0.855786	H	5.060062	-2.320409	-1.988706
H	5.322933	-2.080316	-2.525136	H	3.933886	-2.800661	-3.306620
H	6.043102	-0.488432	-2.148513	H	4.977912	-1.360467	-3.499480
C	1.485999	-3.058520	1.196881	C	1.839700	-2.735067	1.639776
H	1.299845	-4.111257	1.430172	H	1.791103	-3.780455	1.273744
H	3.517601	-2.444395	1.950254	H	3.696325	-2.538557	0.429912
N	0.552473	-2.281498	0.503785	N	0.778681	-1.910158	1.014859
C	-0.736317	-2.758868	0.063287	C	-0.594023	-2.326790	0.974494
C	-0.943656	-2.983977	-1.322999	C	-1.130327	-2.822232	-0.247908
C	-1.731061	-2.981973	1.051451	C	-1.363649	-2.240279	2.164264
C	-2.211470	-3.467898	-1.703882	C	-2.464143	-3.276801	-0.227653
C	-2.973974	-3.476148	0.610365	C	-2.682804	-2.732970	2.133275
C	-3.208259	-3.720508	-0.751176	C	-3.223709	-3.254396	0.950503
H	-2.426909	-3.639826	-2.767387	H	-2.926543	-3.644863	-1.153945
H	-3.778077	-3.658872	1.337192	H	-3.307111	-2.679891	3.037655
H	-4.190287	-4.099736	-1.076476	H	-4.263346	-3.617002	0.935679
C	0.155479	-2.696869	-2.347660	C	-0.305008	-2.821810	-1.538215
H	0.563039	-1.695047	-2.075982	H	0.189701	-1.826310	-1.585132
C	-1.468187	-2.648419	2.522718	C	-0.816638	-1.524575	3.401151
H	-0.439792	-2.995325	2.764295	H	0.285241	-1.655791	3.412369
C	1.308737	-3.721017	-2.260624	C	0.796938	-3.902673	-1.537244
H	2.119002	-3.444979	-2.968293	H	1.385093	-3.850148	-2.477479
H	1.757093	-3.775731	-1.248879	H	1.510496	-3.785195	-0.700267
H	0.953250	-4.738679	-2.530762	H	0.354996	-4.919466	-1.465539
C	-0.353085	-2.584993	-3.792025	C	-1.148610	-2.951676	-2.814732
H	0.475321	-2.251975	-4.451256	H	-0.505406	-2.787776	-3.702990
H	-0.710321	-3.561487	-4.186118	H	-1.603742	-3.961102	-2.913201
H	-1.168379	-1.840390	-3.866487	H	-1.949254	-2.190297	-2.849214
C	-2.418838	-3.361791	3.498212	C	-1.351699	-2.084342	4.730549
H	-2.097186	-3.177819	4.544114	H	-0.822975	-1.615488	5.586361
H	-3.457662	-2.978964	3.408533	H	-2.432714	-1.867552	4.863921
H	-2.440885	-4.459191	3.333385	H	-1.215477	-3.183713	4.798323
C	-1.502943	-1.121581	2.755918	C	-1.072981	-0.004952	3.289426
H	-0.833009	-0.574199	2.064234	H	-0.631224	0.405300	2.354404
H	-2.526772	-0.733557	2.591216	H	-2.163624	0.205197	3.276641
H	-1.202721	-0.877964	3.797007	H	-0.628882	0.535339	4.152218
C	-1.353111	3.180400	-1.487755	C	-1.915080	3.006735	-0.837236
C	-2.647244	3.616812	-1.836177	C	-3.101379	3.349403	-1.512056
C	-0.437312	4.066274	-0.883712	C	-1.568101	3.629308	0.374963
C	-3.023245	4.941361	-1.562113	C	-3.953679	4.313814	-0.951463
H	-3.344260	2.905008	-2.302870	H	-3.349631	2.847755	-2.458928
C	-0.823072	5.391625	-0.627037	C	-2.423218	4.602170	0.917774
H	0.561822	3.688168	-0.613662	H	-0.634115	3.329707	0.876557

C	-2.117750	5.834097	-0.958624
H	-4.038241	5.279913	-1.824987
H	-0.106361	6.083201	-0.155628
H	-2.420170	6.871586	-0.747586

Zero-point correction= 0.744056 (Hartree/Particle)
Thermal correction to Energy= 0.789187
Thermal correction to Enthalpy= 0.790131
Thermal correction to Gibbs Free Energy= 0.665925
Sum of electronic and zero-point Energies= -1938.043677
Sum of electronic and thermal Energies= -1937.998546
Sum of electronic and thermal Enthalpies= -1937.997602
Sum of electronic and thermal Free Energies= -1938.121808

C	-3.620625	4.943433	0.262107
H	-4.888593	4.576092	-1.471602
H	-2.152918	5.091760	1.866894
H	-4.293138	5.699779	0.695728
H	1.711024	-2.761959	2.744632
H	3.818087	-1.803031	2.064552

Zero-point correction= 0.766238 (Hartree/Particle)
Thermal correction to Energy= 0.811958
Thermal correction to Enthalpy= 0.812902
Thermal correction to Gibbs Free Energy= 0.687371
Sum of electronic and zero-point Energies= -1939.222293
Sum of electronic and thermal Energies= -1939.176572
Sum of electronic and thermal Enthalpies= -1939.175628
Sum of electronic and thermal Free Energies= -1939.301159

IPr-VI

91
IPrVI SCF Done: -1938.81230569 A.U.

Pd	-0.220097	-0.782434	-0.580312
N	-2.535485	0.814859	0.388331
C	-3.265798	1.010506	-2.434867
H	-2.527580	1.606500	-1.859316
C	-3.823836	-0.068215	-1.512456
C	-3.427410	-0.176248	-0.159391
C	-1.170482	0.679192	0.356634
C	-3.829154	-1.239863	0.689093
C	-3.242527	-1.410641	2.089495
H	-2.736081	-0.462992	2.368402
C	-4.719539	-1.043543	-1.997293
H	-5.055587	-0.993465	-3.044834
C	-5.168194	-2.086615	-1.174264
H	-5.863237	-2.840870	-1.576056
C	-4.715257	-2.192688	0.150196
H	-5.045715	-3.039468	0.771731
C	-2.925787	1.928053	1.130589
C	-2.161245	-2.513294	2.073086
H	-1.656013	-2.587413	3.059011
H	-2.600737	-3.503743	1.831444
H	-1.381207	-2.304006	1.307375
C	-4.312042	-1.684694	3.162535
H	-3.847237	-1.717784	4.170031
H	-5.092275	-0.895942	3.167254
H	-4.817240	-2.660483	3.002991
C	-2.492538	0.372324	-3.606456
H	-3.166981	-0.200471	-4.277920
H	-1.990009	1.156847	-4.207575
H	-1.707941	-0.313435	-3.227229
C	-4.370910	1.968499	-2.922019
H	-4.893285	2.453068	-2.070611
H	-3.939618	2.766540	-3.562060
H	-5.135184	1.432635	-3.524570
C	-1.772020	2.511739	1.585248
H	-1.605845	3.391383	2.212957
H	-3.978781	2.189437	1.270327
N	-0.711122	1.739284	1.104564
C	0.675542	1.964911	1.437433
C	1.375870	2.999645	0.769783
C	1.278396	1.127607	2.416507
C	2.719971	3.214431	1.139881
C	2.619733	1.393888	2.749211
C	3.332167	2.427993	2.122287
H	3.298125	4.003997	0.637220

SIPr-VI

93
SIPrVI SCF Done: -1940.01495850 A.U.

Pd	-0.199005	-0.892095	-0.242591
N	-2.558707	0.814219	0.119991
C	-2.835723	0.265232	-2.763019
H	-2.091104	0.918039	-2.263392
C	-3.574931	-0.526131	-1.688694
C	-3.400644	-0.268790	-0.305437
C	-1.205411	0.751884	0.199952
C	-4.044152	-1.039014	0.700074
C	-3.720120	-0.813728	2.174828
H	-3.376042	0.237973	2.284216
C	-4.451481	-1.570324	-2.049900
H	-4.607194	-1.796819	-3.116301
C	-5.113211	-2.331665	-1.077032
H	-5.789820	-3.145283	-1.383243
C	-4.903055	-2.074951	0.287079
H	-5.407704	-2.698766	1.040419
C	-3.074177	2.185699	0.299023
C	-2.539355	-1.719970	2.586869
H	-2.245782	-1.538439	3.641974
H	-2.809074	-2.791081	2.476745
H	-1.645598	-1.538839	1.949531
C	-4.926201	-1.006897	3.110410
H	-4.660397	-0.714507	4.147520
H	-5.794478	-0.395412	2.788671
H	-5.253872	-2.067116	3.148400
C	-2.030980	-0.668367	-3.688762
H	-2.695472	-1.314641	-4.300544
H	-1.400412	-0.071428	-4.377892
H	-1.357286	-1.320301	-3.096324
C	-3.805085	1.162982	-3.559207
H	-4.360758	1.857254	-2.893780
H	-3.252043	1.769213	-4.307190
H	-4.557591	0.555454	-4.106275
C	-1.864030	2.889509	0.935428
H	-1.690319	3.908019	0.539664
H	-3.980043	2.193198	0.938078
N	-0.752727	1.980130	0.576892
C	0.595587	2.256375	0.984953
C	1.411053	3.068253	0.149677
C	1.070117	1.726270	2.215541
C	2.736047	3.312151	0.561061
C	2.401952	2.006399	2.580956
C	3.231303	2.782418	1.759994
H	3.395321	3.920378	-0.076288

H	3.126998	0.765519	3.495140
H	4.385166	2.606877	2.390592
C	0.712591	3.872483	-0.293751
H	-0.174332	3.321252	-0.670837
C	0.514311	-0.037312	3.047415
H	-0.111886	-0.470212	2.237954
C	0.231668	5.206353	0.319924
H	-0.475875	5.050745	1.159022
H	1.092385	5.787506	0.714502
H	-0.278771	5.828125	-0.445287
C	1.628503	4.136822	-1.503713
H	1.052611	4.634351	-2.310720
H	2.475642	4.806140	-1.243218
H	2.038043	3.193873	-1.912301
C	-0.433279	0.438591	4.169113
H	-1.026584	-0.413872	4.562576
H	0.142774	0.874582	5.013000
H	-1.148383	1.206276	3.810793
C	1.423415	-1.175239	3.538182
H	2.116306	-1.517934	2.742404
H	2.025188	-0.882328	4.424935
H	0.804375	-2.045790	3.838492
C	0.875053	0.527540	-1.588753
O	0.377965	1.319460	-2.366636
O	0.526919	-2.489359	-1.390508
C	5.121753	-0.047816	-1.160271
C	4.590957	0.507257	-2.341563
H	4.671991	-0.860845	0.813461
C	4.268574	-0.404842	-0.102711
C	3.209287	0.707840	-2.465773
C	2.347597	0.342469	-1.404448
C	2.886142	-0.221328	-0.230255
H	2.773867	1.134110	-3.382658
H	2.201749	-0.512922	0.577004
H	6.207161	-0.214333	-1.071801
H	5.260926	0.779188	-3.172786
C	1.699712	-2.956038	-0.960923
C	1.921222	-3.298929	0.406819
C	2.786640	-3.117878	-1.865859
C	3.174572	-3.747230	0.847845
H	1.077828	-3.183717	1.107429
C	4.035936	-3.565600	-1.415180
H	2.623113	-2.842267	-2.918994
C	4.246402	-3.878644	-0.057316
H	3.317851	-3.997696	1.912658
H	4.867792	-3.658043	-2.132965
H	5.232166	-4.225687	0.290180
Zero-point correction=			0.744623 (Hartree/Particle)
Thermal correction to Energy=			0.790606
Thermal correction to Enthalpy=			0.791550
Thermal correction to Gibbs Free Energy=			0.664862
Sum of electronic and zero-point Energies=			-1938.067683
Sum of electronic and thermal Energies=			-1938.021700
Sum of electronic and thermal Enthalpies=			-1938.020756
Sum of electronic and thermal Free Energies=			-1938.147444

H	2.799812	1.600157	3.524228
H	4.274463	2.974391	2.056220
C	0.868455	3.704448	-1.127784
H	-0.039057	3.132917	-1.416249
C	0.193010	0.892336	3.148507
H	-0.781027	0.720321	2.646215
C	0.465711	5.173484	-0.860971
H	-0.240478	5.270079	-0.010245
H	1.360439	5.782297	-0.609556
H	-0.010256	5.622269	-1.758335
C	1.853479	3.630535	-2.308863
H	1.359377	3.981781	-3.238077
H	2.742320	4.276112	-2.144524
H	2.199484	2.594284	-2.478727
C	-0.090800	1.652627	4.460962
H	-0.789542	1.076845	5.104044
H	0.841579	1.817839	5.041391
H	-0.540750	2.648287	4.263958
C	0.801222	-0.497353	3.416670
H	0.924223	-1.062123	2.469585
H	1.796244	-0.428192	3.903687
H	0.142853	-1.092189	4.082359
C	0.950046	0.143291	-1.490691
O	0.491901	0.745799	-2.444005
O	0.514987	-2.757313	-0.555515
C	5.180232	-0.352022	-0.851660
C	4.676858	-0.079675	-2.138599
H	4.688599	-0.686778	1.245356
C	4.303823	-0.451686	0.242123
C	3.300067	0.096330	-2.331285
C	2.414847	-0.008856	-1.232390
C	2.925884	-0.294055	0.050502
H	2.885847	0.299837	-3.330726
H	2.226824	-0.387079	0.891963
H	6.261602	-0.502466	-0.705271
H	5.363569	-0.012742	-2.997397
C	1.751318	-3.140817	-0.231310
C	2.122458	-3.398538	1.119512
C	2.746052	-3.306138	-1.236515
C	3.433067	-3.777270	1.447558
H	1.346324	-3.294403	1.894472
C	4.054112	-3.675205	-0.897635
H	2.462681	-3.096804	-2.279418
C	4.412765	-3.909971	0.444933
H	3.695077	-3.969496	2.501714
H	4.812514	-3.769352	-1.692295
H	5.443435	-4.197764	0.705536
H	-1.944221	2.955943	2.045249
H	-3.343780	2.614352	-0.693127
Zero-point correction=			0.766556 (Hartree/Particle)
Thermal correction to Energy=			0.813237
Thermal correction to Enthalpy=			0.814181
Thermal correction to Gibbs Free Energy=			0.686049
Sum of electronic and zero-point Energies=			-1939.248403
Sum of electronic and thermal Energies=			-1939.201722
Sum of electronic and thermal Enthalpies=			-1939.200778
Sum of electronic and thermal Free Energies=			-1939.328910

IPr-VII			
97			
IPrVII SCF Done: -3402.63990626 A.U.			
Pd	0.008451	0.167219	-0.474090

SIPr-VII			
99			
SIPrVII SCF Done: -3403.84155121 A.U.			
Pd	0.025234	0.180188	-0.416759

N	2.291334	-1.589621	0.295597
C	2.601219	-1.798806	-2.602174
H	1.771368	-2.191611	-1.982466
C	3.428893	-0.840880	-1.752174
C	3.256150	-0.731039	-0.351001
C	0.944906	-1.330790	0.385500
C	3.968690	0.204841	0.447241
C	3.678942	0.376850	1.936527
H	2.606302	0.130362	2.070597
C	4.410122	-0.019494	-2.352570
H	4.585767	-0.096758	-3.437342
C	5.166819	0.879764	-1.584470
H	5.937965	1.502521	-2.067081
C	4.938438	0.995528	-0.202760
H	5.511530	1.730081	0.381762
C	2.618197	-2.779746	0.948426
C	3.859935	1.828552	2.415879
H	3.415739	1.945197	3.425363
H	4.932974	2.110124	2.493599
H	3.351043	2.542328	1.739772
C	4.528898	-0.579800	2.800809
H	4.279220	-0.448345	3.874666
H	4.356321	-1.644057	2.547556
H	5.612809	-0.369985	2.673148
C	1.925174	-1.076535	-3.782698
H	2.661495	-0.649424	-4.497404
H	1.275982	-1.782707	-4.337451
H	1.262533	-0.267297	-3.411164
C	3.457474	-2.993578	-3.069763
H	3.903164	-3.530091	-2.206005
H	2.838081	-3.716610	-3.640486
H	4.290940	-2.664021	-3.727195
C	1.457637	-3.260696	1.492200
H	1.256033	-4.140724	2.108150
H	3.639518	-3.169874	0.957720
N	0.447922	-2.360238	1.140435
C	-0.919875	-2.464523	1.589430
C	-1.736061	-3.472423	1.018341
C	-1.383657	-1.555478	2.585196
C	-3.047206	-3.609460	1.520689
C	-2.702545	-1.748137	3.046120
C	-3.519969	-2.768254	2.533384
H	-3.708942	-4.379307	1.096247
H	-3.105716	-1.078185	3.818069
H	-4.546414	-2.890074	2.914386
C	-1.245016	-4.384863	-0.104470
H	-0.339218	-3.917418	-0.543266
C	-0.525398	-0.396738	3.099633
H	-0.092668	0.118764	2.210447
C	-0.863149	-5.777659	0.442054
H	-0.081821	-5.721116	1.226934
H	-1.747489	-6.279277	0.890084
H	-0.479755	-6.426969	-0.373075
C	-2.276678	-4.514538	-1.242810
H	-1.822126	-5.044301	-2.104914
H	-3.167602	-5.098206	-0.926975
H	-2.613930	-3.521727	-1.596370
C	0.653384	-0.876662	3.974665
H	1.270836	-0.005932	4.277222
H	0.285428	-1.378471	4.895803
H	1.319433	-1.585848	3.444473
C	-1.327423	0.683916	3.839084
H	-2.181259	1.044140	3.228206

N	2.346207	-1.496765	0.258692
C	2.714014	-1.573947	-2.653808
H	1.929884	-2.073440	-2.050935
C	3.492763	-0.629382	-1.744083
C	3.264456	-0.571071	-0.344905
C	1.006398	-1.318552	0.393487
C	3.918238	0.377579	0.493687
C	3.571040	0.499493	1.975764
H	2.488148	0.278859	2.047633
C	4.455127	0.247985	-2.294062
H	4.663809	0.210072	-3.375585
C	5.147304	1.159177	-1.481236
H	5.904665	1.827388	-1.923246
C	4.868819	1.229194	-0.105281
H	5.390152	1.973554	0.513959
C	2.751107	-2.872498	0.617462
C	3.757134	1.923716	2.525546
H	3.285681	2.000177	3.526549
H	4.829726	2.192687	2.644564
H	3.270007	2.670728	1.868927
C	4.347681	-0.515565	2.840214
H	4.043979	-0.426085	3.904337
H	4.161838	-1.563180	2.531105
H	5.442907	-0.337126	2.779595
C	1.951811	-0.799792	-3.747683
H	2.638090	-0.249137	-4.427270
H	1.347517	-1.498673	-4.360154
H	1.237383	-0.085689	-3.288129
C	3.630558	-2.656779	-3.259220
H	4.163258	-3.227236	-2.469391
H	3.038367	-3.375554	-3.863321
H	4.403079	-2.212603	-3.923555
C	1.563153	-3.334764	1.472217
H	1.753252	-3.229892	2.564137
H	2.863554	-3.478819	-0.310401
N	0.500685	-2.385426	1.058790
C	-0.849961	-2.523395	1.530273
C	-1.639961	-3.575302	0.990738
C	-1.352999	-1.634976	2.532461
C	-2.932296	-3.775584	1.518321
C	-2.653333	-1.888314	3.016675
C	-3.430482	-2.951461	2.531787
H	-3.561099	-4.582623	1.111911
H	-3.073958	-1.232322	3.791121
H	-4.441326	-3.121462	2.935505
C	-1.147945	-4.475037	-0.142134
H	-0.227698	-4.013274	-0.557089
C	-0.564835	-0.422933	3.036434
H	-0.163513	0.108163	2.141783
C	-0.817828	-5.893568	0.373687
H	-0.095620	-5.882376	1.216946
H	-1.735698	-6.399455	0.742415
H	-0.390943	-6.519484	-0.438236
C	-2.162944	-4.552851	-1.301290
H	-1.713522	-5.087112	-2.163746
H	-3.078992	-5.107803	-1.006663
H	-2.460507	-3.544911	-1.645691
C	0.643313	-0.815002	3.911588
H	1.185486	0.098767	4.229796
H	0.317752	-1.364523	4.821201
H	1.369918	-1.450484	3.370173
C	-1.425201	0.615881	3.771726
H	-2.308761	0.913065	3.169039

H	-1.717560	0.328073	4.818150
H	-0.667769	1.556123	4.006446
C	-1.076777	-1.093365	-1.550470
O	-0.598704	-1.965223	-2.276785
O	-0.773757	1.811159	-1.572226
C	-5.357829	-0.473903	-1.687422
C	-4.623049	-0.660176	-2.874734
H	-5.265377	-0.354527	0.488054
C	-4.697386	-0.485303	-0.446547
C	-3.236730	-0.867737	-2.817793
C	-2.566218	-0.849142	-1.574212
C	-3.305384	-0.653403	-0.391606
H	-2.649715	-1.041268	-3.733024
H	-2.784717	-0.660593	0.576073
H	-6.448014	-0.320138	-1.732348
H	-5.138025	-0.649537	-3.849030
K	1.819651	2.587404	-1.845428
K	-0.826041	4.866302	1.349060
C	0.945694	2.708288	0.976398
O	1.276802	3.818195	0.366312
O	0.233066	2.695775	2.034163
O	1.378430	1.573787	0.431624
C	-1.748469	2.580972	-1.128811
C	-2.405777	2.369748	0.125862
C	-2.178361	3.709717	-1.899733
C	-3.446933	3.206486	0.555047
H	-2.051036	1.539341	0.753885
C	-3.205514	4.554151	-1.448917
H	-1.687992	3.888322	-2.870728
C	-3.859603	4.314502	-0.219173
H	-3.946144	2.987882	1.514878
H	-3.515799	5.407205	-2.076088
H	-4.687613	4.959781	0.113863

H	-1.780851	0.249969	4.760175
H	-0.817730	1.528959	3.916581
C	-0.976379	-1.125991	-1.521517
O	-0.450874	-2.001760	-2.209591
O	-0.825635	1.784267	-1.527693
C	-5.248183	-0.536842	-1.862917
C	-4.447233	-0.647729	-3.016078
H	-5.277772	-0.541420	0.317129
C	-4.657397	-0.616651	-0.589856
C	-3.064307	-0.851220	-2.894474
C	-2.464862	-0.900834	-1.616611
C	-3.268909	-0.777546	-0.466214
H	-2.426737	-0.963326	-3.785126
H	-2.802281	-0.831887	0.527390
H	-6.335460	-0.386607	-1.959454
H	-4.907422	-0.581771	-4.015290
K	1.726362	2.690593	-1.781222
K	-1.074833	4.849492	1.381685
C	0.812497	2.792555	1.031881
O	1.082562	3.908180	0.403403
O	0.115627	2.761507	2.099694
O	1.291309	1.671793	0.497264
C	-1.845067	2.501403	-1.097623
C	-2.511741	2.251860	0.144811
C	-2.319937	3.608895	-1.872903
C	-3.597928	3.036336	0.561278
H	-2.133544	1.431111	0.771706
C	-3.393055	4.401207	-1.435235
H	-1.824429	3.814168	-2.835957
C	-4.051688	4.126559	-0.215136
H	-4.101067	2.789310	1.512094
H	-3.735741	5.239858	-2.064953
H	-4.914368	4.730114	0.108040
H	3.717358	-2.881105	1.157374
H	1.265605	-4.379938	1.271489

Zero-point correction=	0.762524 (Hartree/Particle)
Thermal correction to Energy=	0.816436
Thermal correction to Enthalpy=	0.817381
Thermal correction to Gibbs Free Energy=	0.673477
Sum of electronic and zero-point Energies=	-3401.877382
Sum of electronic and thermal Energies=	-3401.823470
Sum of electronic and thermal Enthalpies=	-3401.822526
Sum of electronic and thermal Free Energies=	-3401.966429

Zero-point correction=	0.785088 (Hartree/Particle)
Thermal correction to Energy=	0.839464
Thermal correction to Enthalpy=	0.840408
Thermal correction to Gibbs Free Energy=	0.695759
Sum of electronic and zero-point Energies=	-3403.056464
Sum of electronic and thermal Energies=	-3403.002087
Sum of electronic and thermal Enthalpies=	-3403.001143
Sum of electronic and thermal Free Energies=	-3403.145792

IPr-VII-VIII			
97			
IPrVII-VIII SCF Done: -3402.61388020 A.U.			
Pd	-0.307811	-0.731940	0.062123
N	-2.327643	1.275480	0.707984
C	-2.262031	2.496298	-1.912662
H	-1.313162	2.335537	-1.354796
C	-3.151232	1.289551	-1.603081
C	-3.183058	0.703914	-0.307788
C	-0.991178	0.962912	0.787775
C	-3.946068	-0.447615	0.011431
C	-3.928227	-1.049073	1.413451
H	-2.925400	-0.847451	1.846600
C	-3.954784	0.691408	-2.593990
H	-3.954000	1.104408	-3.612764
C	-4.737851	-0.437789	-2.307350
H	-5.361496	-0.885091	-3.098861
C	-4.729725	-1.003679	-1.021946

SIPr-VII-VIII			
99			
SIPrVII-VIII SCF Done: -3403.81647798 A.U.			
Pd	-0.407548	-0.663062	0.125870
N	-2.270974	1.499391	0.401742
C	-1.556793	2.457348	-2.231176
H	-0.718336	2.188972	-1.551765
C	-2.648493	1.405693	-2.020447
C	-3.008246	0.963940	-0.711382
C	-0.985421	1.136854	0.649885
C	-4.022930	-0.005563	-0.492880
C	-4.401277	-0.471940	0.908320
H	-3.535323	-0.259127	1.569559
C	-3.332250	0.837557	-3.112571
H	-3.069225	1.142217	-4.135337
C	-4.343047	-0.118069	-2.919896
H	-4.871968	-0.540057	-3.790275
C	-4.685671	-0.529829	-1.623475

H	-5.342217	-1.893966	-0.814118	H	-5.480252	-1.278495	-1.480996
C	-2.668583	2.271687	1.623779	C	-2.785349	2.456909	1.403268
C	-4.100086	-2.577873	1.422335	C	-4.632642	-1.992353	0.991628
H	-3.892171	-2.970086	2.438076	H	-4.707904	-2.306266	2.052195
H	-5.133244	-2.887360	1.152068	H	-5.573243	-2.300948	0.485554
H	-3.380206	-3.061793	0.732895	H	-3.783636	-2.544975	0.543474
C	-4.998733	-0.376984	2.301941	C	-5.645155	0.295668	1.411102
H	-4.960662	-0.788860	3.332093	H	-5.877116	0.022864	2.462188
H	-4.856893	0.720239	2.371734	H	-5.511126	1.396241	1.359727
H	-6.017286	-0.559060	1.895920	H	-6.533611	0.047755	0.790931
C	-1.882743	2.631540	-3.396427	C	-0.975627	2.488407	-3.652607
H	-2.754641	2.917969	-4.023212	H	-1.707013	2.878809	-4.392706
H	-1.120784	3.429816	-3.511942	H	-0.091454	3.157919	-3.677238
H	-1.452459	1.688005	-3.783746	H	-0.648628	1.478885	-3.969186
C	-2.886019	3.816754	-1.408139	C	-2.053603	3.864412	-1.833228
H	-3.099629	3.796915	-0.322527	H	-2.400615	3.906047	-0.783157
H	-2.192509	4.663850	-1.594415	H	-1.241223	4.611892	-1.948183
H	-3.836925	4.028395	-1.941957	H	-2.901423	4.176274	-2.479305
C	-1.512971	2.615344	2.274679	C	-1.498936	2.876228	2.153357
H	-1.311570	3.360083	3.049678	H	-1.199519	3.925723	1.946250
H	-3.691801	2.643900	1.724093	H	-3.310683	3.304240	0.917110
N	-0.494560	1.821370	1.739928	N	-0.486119	1.934708	1.624056
C	0.914261	2.085612	1.920583	C	0.907900	2.076925	1.950720
C	1.468632	3.163450	1.182766	C	1.647327	3.101131	1.295838
C	1.679327	1.247658	2.769413	C	1.501990	1.214121	2.908148
C	2.849393	3.402908	1.330121	C	3.006522	3.250933	1.631436
C	3.061291	1.515375	2.853399	C	2.872524	1.395005	3.190806
C	3.638635	2.582525	2.147739	C	3.617635	2.405098	2.567585
H	3.317171	4.226190	0.768677	H	3.603551	4.029590	1.131180
H	3.694442	0.878440	3.488546	H	3.360288	0.729800	3.920842
H	4.720794	2.771881	2.231368	H	4.686054	2.529329	2.806365
C	0.619072	4.052511	0.274364	C	1.018833	4.031795	0.259751
H	-0.369657	3.566830	0.151076	H	-0.020443	3.690171	0.083394
C	1.018229	0.151341	3.593408	C	0.718231	0.114454	3.610817
H	0.161436	-0.247325	3.016274	H	-0.310252	0.100149	3.202338
C	0.372192	5.423061	0.939496	C	0.953579	5.482103	0.783971
H	-0.100404	5.312765	1.937179	H	0.436413	5.543836	1.764516
H	1.327107	5.973177	1.080063	H	1.972490	5.901759	0.922991
H	-0.294293	6.050226	0.310379	H	0.414973	6.135650	0.065546
C	1.207432	4.215413	-1.139562	C	1.736734	3.963897	-1.101222
H	0.510278	4.804083	-1.772402	H	1.234368	4.628919	-1.835078
H	2.177938	4.754282	-1.128555	H	2.795386	4.288139	-1.027357
H	1.370217	3.234492	-1.625200	H	1.731887	2.935020	-1.506706
C	0.468791	0.744433	4.909756	C	0.626949	0.367153	5.128590
H	-0.056071	-0.038978	5.495401	H	-0.000343	-0.412724	5.608755
H	1.289087	1.156852	5.536732	H	1.626778	0.343812	5.614227
H	-0.254286	1.564371	4.717279	H	0.173459	1.356957	5.347812
C	1.926789	-1.057106	3.865756	C	1.302027	-1.278437	3.300046
H	2.401512	-1.416402	2.930717	H	1.385705	-1.413272	2.200774
H	2.731941	-0.833076	4.599210	H	2.309757	-1.421795	3.747491
H	1.318019	-1.892656	4.265170	H	0.614801	-2.061735	3.680729
C	0.107319	-0.011072	-1.744290	C	0.425728	-0.212198	-1.623869
O	-0.689406	-0.187402	-2.685038	O	-0.189584	-0.463392	-2.677987
O	1.230137	-2.489905	-1.472990	O	1.138212	-2.810564	-0.764056
C	3.983142	1.689990	-2.581135	C	4.432271	1.344948	-1.930724
C	3.037693	1.531420	-3.615282	C	3.605274	1.286903	-3.070639
H	4.386459	1.439603	-0.452945	H	4.590581	0.946319	0.206386
C	3.653542	1.329750	-1.264741	C	3.945296	0.919580	-0.683499
C	1.774930	0.995503	-3.331777	C	2.303264	0.784826	-2.960920
C	1.433627	0.632769	-2.006811	C	1.800458	0.370562	-1.704318
C	2.380642	0.814918	-0.976913	C	2.630165	0.448454	-0.566555
H	1.028637	0.837586	-4.125678	H	1.648776	0.696851	-3.840651
H	2.105355	0.546758	0.052481	H	2.235650	0.121604	0.407188

H	4.983672	2.092153	-2.808113
H	3.297458	1.816380	-4.647658
K	-1.353409	-2.639079	-2.271394
K	1.231615	-4.515054	0.340963
C	-0.801400	-3.009037	1.436880
O	-1.032816	-3.095780	0.133000
O	-0.583016	-4.034925	2.138330
O	-0.702557	-1.782498	1.907237
C	2.500300	-2.264441	-1.218353
C	2.958693	-2.007688	0.120651
C	3.500995	-2.251002	-2.242980
C	4.307864	-1.749051	0.408564
H	2.193748	-1.911114	0.913963
C	4.843186	-1.984669	-1.944368
H	3.172006	-2.417219	-3.281321
C	5.266757	-1.735293	-0.620321
H	4.601726	-1.520932	1.447343
H	5.580598	-1.955350	-2.764410
H	6.323949	-1.518652	-0.401784

Zero-point correction= 0.761790 (Hartree/Particle)
Thermal correction to Energy= 0.815211
Thermal correction to Enthalpy= 0.816155
Thermal correction to Gibbs Free Energy= 0.674158
Sum of electronic and zero-point Energies= -3401.852091
Sum of electronic and thermal Energies= -3401.798669
Sum of electronic and thermal Enthalpies= -3401.797725
Sum of electronic and thermal Free Energies= -3401.939722

H	5.465410	1.717622	-2.019382
H	3.989261	1.619431	-4.048403
K	-1.373595	-2.679460	-2.131421
K	0.474018	-4.499959	1.141408
C	-1.496929	-2.614332	1.631943
O	-1.424910	-2.896447	0.334137
O	-1.537185	-3.528873	2.500811
O	-1.412836	-1.337849	1.931004
C	2.438119	-2.686622	-0.964063
C	3.367999	-2.621292	0.126843
C	2.997728	-2.586555	-2.278204
C	4.748130	-2.477798	-0.085319
H	2.968857	-2.625232	1.156119
C	4.374402	-2.426262	-2.478611
H	2.301241	-2.594862	-3.132986
C	5.268355	-2.375450	-1.388409
H	5.425551	-2.420301	0.783840
H	4.761952	-2.327240	-3.506733
H	6.349039	-2.245860	-1.554555
H	-1.586117	2.753941	3.252228
H	-3.503965	1.949047	2.078411

Zero-point correction= 0.784266 (Hartree/Particle)
Thermal correction to Energy= 0.838070
Thermal correction to Enthalpy= 0.839014
Thermal correction to Gibbs Free Energy= 0.697472
Sum of electronic and zero-point Energies= -3403.032212
Sum of electronic and thermal Energies= -3402.978408
Sum of electronic and thermal Enthalpies= -3402.977464
Sum of electronic and thermal Free Energies= -3403.119006

IPr-VIIIpost			
97			
IPrVIIImesKOPh SCF Done: -3402.63905587 A.U.			
Pd	-0.083711	0.299054	0.671308
N	1.780350	2.031562	-0.809486
C	1.276603	0.714643	-3.334886
H	1.504512	0.109350	-2.430210
C	0.436091	1.900977	-2.857607
C	0.688206	2.534237	-1.608974
C	1.658893	0.902197	-0.035981
C	-0.109557	3.585015	-1.091666
C	0.152437	4.175109	0.291318
H	0.701696	3.411855	0.880188
C	-0.632499	2.406536	-3.625288
H	-0.869079	1.944210	-4.594350
C	-1.409292	3.484319	-3.167191
H	-2.229064	3.872072	-3.793675
C	-1.156718	4.061305	-1.911153
H	-1.785422	4.892088	-1.555247
C	3.092539	2.506691	-0.813368
C	-1.140450	4.462778	1.073824
H	-0.893139	4.770500	2.108949
H	-1.744186	5.274262	0.614070
H	-1.763546	3.551312	1.165894
C	1.033327	5.438480	0.180285
H	1.258279	5.846460	1.187733
H	1.998173	5.222274	-0.323015
H	0.519501	6.231386	-0.404812
C	0.543606	-0.214937	-4.316049
H	0.394297	0.261880	-5.308402
H	1.151353	-1.128341	-4.482061
H	-0.438690	-0.527544	-3.912219

SIPr-VIIIpost			
99			
SIPrVIIImesKOPh SCF Done: -3403.84100268 A.U.			
Pd	0.002790	0.166405	0.636409
N	1.792313	2.131951	-0.566349
C	1.219649	1.159815	-3.237221
H	1.373670	0.399804	-2.441501
C	0.424818	2.301876	-2.599350
C	0.708452	2.752680	-1.274437
C	1.714233	0.891983	-0.016784
C	-0.047592	3.776014	-0.643481
C	0.200616	4.181287	0.806072
H	0.818190	3.386032	1.272533
C	-0.615995	2.948260	-3.297442
H	-0.866250	2.626047	-4.318509
C	-1.341477	4.001354	-2.712704
H	-2.136747	4.503793	-3.286975
C	-1.063896	4.405057	-1.397506
H	-1.652679	5.215287	-0.939465
C	3.112674	2.760574	-0.342743
C	-1.100949	4.239886	1.627754
H	-0.867994	4.422089	2.695610
H	-1.779936	5.049289	1.283994
H	-1.637976	3.272264	1.593123
C	0.959116	5.525027	0.875954
H	1.205922	5.782121	1.927183
H	1.904157	5.501278	0.293904
H	0.340832	6.349935	0.460915
C	0.484180	0.450527	-4.384780
H	0.375987	1.102151	-5.278359
H	1.064819	-0.440464	-4.700535
H	-0.516529	0.102014	-4.064391

C	2.619813	1.176520	-3.943609
H	3.218618	1.781287	-3.235605
H	3.232673	0.296607	-4.231591
H	2.446065	1.786502	-4.855389
C	3.823398	1.634281	-0.048835
H	4.886956	1.607836	0.205257
H	3.381652	3.410601	-1.357006
N	2.937017	0.652460	0.400807
C	3.347695	-0.595567	0.998023
C	3.918853	-1.566798	0.134157
C	3.135244	-0.816688	2.379877
C	4.333201	-2.782463	0.712138
C	3.557844	-2.057873	2.901417
C	4.159222	-3.024807	2.082549
H	4.778426	-3.560153	0.072157
H	3.411986	-2.265463	3.972603
H	4.484357	-3.984426	2.515299
C	4.082989	-1.331426	-1.367622
H	3.591735	-0.370960	-1.621636
C	2.496120	0.230603	3.284265
H	2.030950	1.005265	2.643871
C	5.571481	-1.189867	-1.745892
H	6.060879	-0.377485	-1.169746
H	6.128864	-2.128625	-1.541456
H	5.680513	-0.959616	-2.826661
C	3.383835	-2.416402	-2.209103
H	3.465125	-2.171997	-3.289202
H	3.838592	-3.417619	-2.058389
H	2.309593	-2.493668	-1.953539
C	3.567896	0.918540	4.155338
H	3.106030	1.710181	4.781275
H	4.064751	0.191155	4.833174
H	4.356547	1.389020	3.531079
C	1.354991	-0.356432	4.135797
H	0.620219	-0.885566	3.494714
H	1.726877	-1.064541	4.907345
H	0.808699	0.461762	4.644974
C	-0.498712	-0.958102	-0.806152
O	-1.238690	-0.587426	-1.730466
O	-5.073879	0.202581	0.457973
C	0.863387	-5.054249	-0.718965
C	0.081354	-4.588988	-1.795708
H	1.802021	-4.546855	1.184523
C	1.189169	-4.190816	0.342727
C	-0.368394	-3.261709	-1.812362
C	-0.027099	-2.383119	-0.756312
C	0.747173	-2.859295	0.322979
H	-0.992803	-2.875564	-2.632438
H	1.007353	-2.164224	1.137894
H	-0.180348	-5.270249	-2.621070
K	-3.058961	1.155480	-0.769111
K	-4.240133	-0.138564	2.833064
C	-1.508943	1.184473	2.604802
O	-1.887783	0.220621	1.718686
O	-2.295761	1.550409	3.504062
O	-0.307677	1.644853	2.383233
C	-5.080941	-1.015838	-0.048127
C	-3.927705	-1.878633	0.029450
C	-6.227257	-1.558449	-0.722086
C	-3.924655	-3.164115	-0.538692
H	-3.017338	-1.503964	0.528752
C	-6.210725	-2.845163	-1.276634
H	-7.124152	-0.920751	-0.790928

C	2.609916	1.635218	-3.713331
H	3.212852	2.068727	-2.892615
H	3.185204	0.784960	-4.135702
H	2.512116	2.409196	-4.503793
C	3.975291	1.557425	0.098995
H	4.674076	1.212054	-0.694750
H	3.033948	3.528012	0.456834
N	2.956291	0.520299	0.374383
C	3.317888	-0.815230	0.761152
C	3.779031	-1.702797	-0.248864
C	3.196937	-1.208893	2.118628
C	4.159699	-3.001573	0.140123
C	3.587252	-2.523080	2.453064
C	4.073215	-3.407379	1.479575
H	4.511334	-3.713691	-0.623156
H	3.502849	-2.857146	3.498902
H	4.372708	-4.428678	1.764297
C	3.851179	-1.293932	-1.718915
H	3.460299	-0.260689	-1.802583
C	2.649454	-0.273008	3.190431
H	2.236546	0.623240	2.686967
C	5.305940	-1.281863	-2.231698
H	5.958713	-0.644599	-1.598895
H	5.741590	-2.303519	-2.232139
H	5.350955	-0.898038	-3.272798
C	2.948373	-2.171517	-2.607218
H	2.989226	-1.823629	-3.660879
H	3.264357	-3.235419	-2.591393
H	1.894937	-2.133462	-2.270679
C	3.771962	0.188874	4.142765
H	3.374383	0.902476	4.894409
H	4.216054	-0.670132	4.690395
H	4.593894	0.691296	3.589839
C	1.476355	-0.911683	3.960046
H	0.702163	-1.286357	3.259170
H	1.809385	-1.756428	4.600571
H	0.989324	-0.154290	4.605708
C	-0.474796	-0.997300	-0.902920
O	-1.140533	-0.544999	-1.846802
O	-4.907359	0.441643	0.478208
C	0.351688	-5.235303	-0.775111
C	-0.437779	-4.695012	-1.810651
H	1.486552	-4.810608	1.040454
C	0.865070	-4.397101	0.231510
C	-0.706930	-3.320172	-1.841484
C	-0.185327	-2.470988	-0.836491
C	0.595446	-3.020592	0.202452
H	-1.326555	-2.871322	-2.632840
H	1.000111	-2.351926	0.979219
H	-0.846830	-5.354109	-2.593123
K	-2.838696	1.268439	-0.725279
K	-4.142483	-0.298366	2.794678
C	-1.330834	0.831169	2.710012
O	-1.730904	-0.074995	1.777398
O	-2.075004	1.116652	3.671938
O	-0.154682	1.347095	2.459602
C	-5.069484	-0.726516	-0.112270
C	-4.027563	-1.724241	-0.124640
C	-6.287181	-1.080306	-0.787132
C	-4.196948	-2.962405	-0.768621
H	-3.066238	-1.496481	0.368648
C	-6.440570	-2.319891	-1.421691
H	-7.099969	-0.335244	-0.789275

C -5.062767 -3.664261 -1.196335	C -5.401297 -3.276600 -1.423014
H -3.008429 -3.775621 -0.469759	H -3.363421 -3.685400 -0.760272
H -7.113299 -3.222929 -1.787803	H -7.392779 -2.550797 -1.930150
H -5.060340 -4.672301 -1.640051	H -5.532977 -4.247352 -1.926315
H 1.216842 -6.098004 -0.708013	H 0.564168 -6.316477 -0.753231
	H 3.481092 3.257858 -1.262121
	H 4.567252 1.763503 1.013170
Zero-point correction= 0.761633 (Hartree/Particle)	Zero-point correction= 0.784467 (Hartree/Particle)
Thermal correction to Energy= 0.816229	Thermal correction to Energy= 0.839449
Thermal correction to Enthalpy= 0.817173	Thermal correction to Enthalpy= 0.840393
Thermal correction to Gibbs Free Energy= 0.669276	Thermal correction to Gibbs Free Energy= 0.691776
Sum of electronic and zero-point Energies= -3401.877423	Sum of electronic and zero-point Energies= -3403.056536
Sum of electronic and thermal Energies= -3401.822827	Sum of electronic and thermal Energies= -3403.001554
Sum of electronic and thermal Enthalpies= -3401.821883	Sum of electronic and thermal Enthalpies= -3403.000610
Sum of electronic and thermal Free Energies= -3401.969780	Sum of electronic and thermal Free Energies= -3403.149227

IPr-VIII	**SIPr-VIII**
84	86
IPrVIII SCF Done: -2495.86298696 A.U.	SIPrVIII SCF Done: -2497.06653782 A.U.
Pd -0.040381 -0.844282 0.075092	Pd 0.014474 -0.843140 0.052910
N 2.245928 1.059930 0.527183	N 2.178882 1.102022 0.528882
C 2.344065 -0.374719 3.083618	C 2.303732 -0.414188 3.039722
H 1.589939 0.360060 2.736712	H 1.533815 0.313756 2.713073
C 3.267466 -0.703779 1.915760	C 3.240327 -0.678773 1.865458
C 3.190435 -0.020199 0.679446	C 3.146399 0.049738 0.653242
C 0.937309 0.861855 0.174325	C 0.882805 0.917097 0.194293
C 3.971613 -0.365529 -0.452132	C 3.976851 -0.216759 -0.466323
C 3.794389 0.317689 -1.807316	C 3.810785 0.531610 -1.786893
H 2.975591 1.060137 -1.713842	H 3.005544 1.283390 -1.646281
C 4.225467 -1.732899 2.020059	C 4.226753 -1.682570 1.944929
H 4.321176 -2.284894 2.968385	H 4.325349 -2.269160 2.872127
C 5.044971 -2.072850 0.933625	C 5.073182 -1.954084 0.859902
H 5.784519 -2.882954 1.037050	H 5.833316 -2.747474 0.941876
C 4.910843 -1.403565 -0.291856	C 4.943766 -1.232403 -0.336058
H 5.535814 -1.703163 -1.147883	H 5.595184 -1.473234 -1.191220
C 2.583740 2.413548 0.485482	C 2.512410 2.520507 0.758867
C 3.355252 -0.689031 -2.889969	C 3.337746 -0.418185 -2.906583
H 3.158455 -0.156118 -3.845075	H 3.119432 0.157981 -3.831634
H 4.149086 -1.440034 -3.090452	H 4.124935 -1.161828 -3.155278
H 2.433571 -1.228979 -2.588319	H 2.429120 -0.978158 -2.602689
C 5.061435 1.095936 -2.214991	C 5.090862 1.296751 -2.177591
H 4.898622 1.628994 -3.175488	H 4.927489 1.884808 -3.105481
H 5.343323 1.846671 -1.446943	H 5.412822 1.995336 -1.376224
H 5.927938 0.414514 -2.352517	H 5.934878 0.600862 -2.370135
C 1.549102 -1.616749 3.532045	C 1.535698 -1.687321 3.446124
H 2.208718 -2.400238 3.963049	H 2.212571 -2.467817 3.854973
H 0.802384 -1.330155 4.300089	H 0.779685 -1.443667 4.220125
H 0.998478 -2.053261 2.673044	H 1.000132 -2.110982 2.571437
C 3.124836 0.262370 4.250591	C 3.063948 0.201217 4.232122
H 3.656099 1.182114 3.927169	H 3.582140 1.139886 3.942433
H 2.435436 0.535102 5.077121	H 2.364711 0.434510 5.062647
H 3.884939 -0.437180 4.660645	H 3.835262 -0.495816 4.624975
C 1.458098 3.086467 0.086994	C 1.294804 3.236750 0.144157
H 1.274941 4.149022 -0.094006	H 1.503680 3.635787 -0.874574
H 3.592409 2.761799 0.725777	H 3.472870 2.784927 0.272362
N 0.461689 2.123170 -0.094357	N 0.302300 2.142053 0.052838
C -0.842149 2.365670 -0.658514	C -0.978958 2.351181 -0.557249
C -1.846334 2.944972 0.155032	C -2.034539 2.879855 0.234074
C -1.063845 1.981786 -2.010877	C -1.152230 2.045639 -1.938320
C -3.099469 3.196111 -0.443274	C -3.276788 3.113782 -0.390261
C -2.337530 2.248918 -2.551374	C -2.416469 2.298578 -2.510263
C -3.340971 2.860284 -1.781656	C -3.468157 2.830086 -1.749113

H	-3.902725	3.646645	0.159077
H	-2.546938	1.969162	-3.594276
H	-4.327695	3.062308	-2.228228
C	-1.594623	3.289425	1.620714
H	-0.705784	2.710215	1.946384
C	0.033815	1.331556	-2.853211
H	0.674528	0.742540	-2.166741
C	-1.284429	4.793416	1.783569
H	-0.410777	5.106516	1.176454
H	-2.150875	5.411043	1.463264
H	-1.065772	5.035707	2.844781
C	-2.762215	2.872009	2.535379
H	-2.475207	3.008894	3.597960
H	-3.670110	3.486634	2.355341
H	-3.024461	1.805689	2.394575
C	0.921745	2.409319	-3.510045
H	1.757279	1.934363	-4.065540
H	0.337633	3.028148	-4.224751
H	1.363492	3.088679	-2.751736
C	-0.496959	0.317796	-3.877634
H	-1.129219	-0.446013	-3.381819
H	-1.076758	0.798437	-4.695188
H	0.353341	-0.223043	-4.338101
C	-1.196113	-0.274059	1.566049
O	-0.911462	0.220898	2.651869
C	-5.276446	-1.504011	0.693981
C	-4.664792	-1.865400	1.911814
H	-5.047374	-0.394814	-1.176244
C	-4.567651	-0.711735	-0.235536
C	-3.359455	-1.426915	2.204368
C	-2.635947	-0.667119	1.260831
C	-3.246448	-0.317247	0.035998
H	-2.879727	-1.679465	3.163118
H	-2.675601	0.267127	-0.701471
H	-6.310679	-1.819798	0.479249
H	-5.217496	-2.474027	2.646317
K	-2.987195	-3.883739	-0.997812
C	-0.339180	-2.867433	-1.461762
O	-0.958252	-2.686432	-0.265636
O	-0.752016	-3.768925	-2.237774
O	0.609263	-2.009964	-1.695921

Zero-point correction= 0.669778 (Hartree/Particle)
Thermal correction to Energy= 0.715432
Thermal correction to Enthalpy= 0.716377
Thermal correction to Gibbs Free Energy= 0.589857
Sum of electronic and zero-point Energies= -2495.193209
Sum of electronic and thermal Energies= -2495.147555
Sum of electronic and thermal Enthalpies= -2495.146610
Sum of electronic and thermal Free Energies= -2495.273130

H	-4.111276	3.516750	0.204072
H	-2.577179	2.072700	-3.575965
H	-4.446746	3.019447	-2.218607
C	-1.840113	3.210699	1.711044
H	-0.908773	2.702470	2.036987
C	-0.031034	1.484211	-2.811516
H	0.798325	1.165720	-2.149711
C	-1.671718	4.734305	1.906700
H	-0.850453	5.148256	1.285114
H	-2.600538	5.272050	1.618726
H	-1.455628	4.974481	2.969131
C	-2.982516	2.676189	2.596330
H	-2.734572	2.828520	3.666953
H	-3.939213	3.205727	2.399111
H	-3.139759	1.591965	2.440715
C	0.522537	2.569013	-3.759384
H	1.380002	2.172165	-4.342578
H	-0.252948	2.907444	-4.479598
H	0.870196	3.463423	-3.200666
C	-0.468230	0.226096	-3.584736
H	-0.841738	-0.551533	-2.889437
H	-1.253255	0.454278	-4.336794
H	0.398238	-0.214017	-4.117065
C	-1.226950	-0.317400	1.491930
O	-0.991826	0.167736	2.593800
C	-5.193301	-1.776857	0.474797
C	-4.606285	-2.103502	1.714468
H	-4.965925	-0.648122	-1.383510
C	-4.502171	-0.937273	-0.426146
C	-3.341935	-1.586621	2.055124
C	-2.633630	-0.779023	1.139931
C	-3.220074	-0.460221	-0.104780
H	-2.880520	-1.815001	3.028790
H	-2.662168	0.167313	-0.816179
H	-6.196665	-2.156605	0.220706
H	-5.146617	-2.748239	2.427102
K	-2.711087	-4.062946	-1.037974
C	-0.074636	-2.973264	-1.365736
O	-0.786010	-2.750879	-0.229582
O	-0.385437	-3.943277	-2.105592
O	0.840210	-2.078842	-1.592477
H	2.611703	2.705012	1.852356
H	0.916449	4.067523	0.770675

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= 0.610515
Sum of electronic and zero-point Energies= -2496.374917
Sum of electronic and thermal Energies= -2496.328487
Sum of electronic and thermal Enthalpies= -2496.327543
Sum of electronic and thermal Free Energies= -2496.456023

IPr-IX+KOPh			
113			
IPrIX+KOPh SCF Done: -3810.65678807 A.U.			
Pd	-0.634768	0.127620	0.471635
K	3.822901	-2.350304	-1.676648
O	3.492724	-0.557454	0.578904
H	4.165776	-0.829508	1.235049
B	2.242423	-1.326693	0.727361
O	2.551006	-2.750442	0.859742
H	1.737097	-3.256452	1.041263
C	1.310641	-0.722870	1.948815

SIPr-IX+KOPh			
115			
SIPrIX+KOPh SCF Done: -3811.85730661 A.U.			
Pd	-0.639001	0.127200	0.432208
K	3.827404	-2.346152	-1.644599
O	3.530564	-0.469180	0.595610
H	4.199366	-0.747824	1.253306
B	2.281354	-1.241017	0.742114
O	2.594958	-2.662179	0.894042
H	1.785598	-3.168639	1.094033
C	1.330661	-0.627856	1.943016

C	0.799943	-1.545378	2.997246
C	1.126657	0.688109	2.113945
C	0.143157	-1.013057	4.112951
H	0.932667	-2.637748	2.932380
C	0.452489	1.231764	3.236659
H	1.603701	1.375738	1.397353
C	-0.041972	0.381420	4.232118
H	-0.238325	-1.685845	4.897766
H	0.324637	2.323231	3.310995
H	-0.571451	0.794502	5.105179
C	1.626183	-0.013498	-1.361699
O	2.403799	0.046611	-2.354719
O	1.555713	-1.191825	-0.674790
O	0.891384	0.956624	-0.948305
N	-2.179912	2.273221	-0.877233
N	-2.931711	0.351531	-1.553712
C	-2.050767	0.921982	-0.674811
C	-3.116967	2.538798	-1.876348
C	-3.588137	1.326838	-2.307766
C	-1.507042	3.266837	-0.069934
C	-0.400950	3.961177	-0.617535
C	0.237001	4.909521	0.209623
C	-0.201167	5.137369	1.520581
C	-1.294762	4.424696	2.036505
C	-1.977919	3.471755	1.256352
C	0.079769	3.725339	-2.046985
H	0.317178	5.876722	2.151869
C	-3.180181	2.704503	1.805345
C	-3.183585	-1.067930	-1.621632
C	-4.256188	-1.587648	-0.853378
C	-4.472111	-2.979620	-0.914447
C	-3.655578	-3.801469	-1.702095
C	-2.592119	-3.255594	-2.436374
C	-2.318750	-1.874610	-2.403494
C	-5.154899	-0.680122	-0.013543
H	-3.834258	-4.887802	-1.725055
C	-1.141686	-1.266297	-3.164359
H	-3.367321	3.559770	-2.176643
H	-4.320984	1.067857	-3.076509
H	1.098482	5.472234	-0.180435
H	-1.621745	4.609812	3.069663
H	-0.261287	2.712684	-2.344223
H	-3.098624	1.661091	1.439299
H	-5.282603	-3.427893	-0.321623
H	-1.943377	-3.921835	-3.023148
H	-4.556159	0.213850	0.263263
H	-0.757762	-0.424037	-2.550790
C	0.031145	-2.242030	-3.365232
H	-0.211987	-3.040758	-4.098250
H	0.909576	-1.680958	-3.742740
H	0.327590	-2.710827	-2.406126
C	-1.600286	-0.685024	-4.519959
H	-2.386442	0.086420	-4.394575
H	-0.745076	-0.213161	-5.047247
H	-2.010401	-1.486402	-5.171125
C	-5.623941	-1.330331	1.299438
H	-6.146219	-0.577208	1.924505
H	-6.339437	-2.160518	1.119102
H	-4.768290	-1.715719	1.884178
C	-6.372364	-0.205172	-0.838114
H	-7.002920	-1.070577	-1.133975
H	-7.000058	0.489587	-0.241434
H	-6.071166	0.322179	-1.764380

C	0.830356	-1.435254	3.007873
C	1.113617	0.782136	2.070094
C	0.153868	-0.890074	4.105709
H	0.987836	-2.525736	2.971799
C	0.420187	1.338546	3.173967
H	1.575596	1.463579	1.337544
C	-0.061803	0.502350	4.187916
H	-0.218379	-1.551173	4.904692
H	0.264410	2.427739	3.219606
H	-0.604296	0.926224	5.047789
C	1.648888	0.042786	-1.371168
O	2.463583	0.120809	-2.332099
O	1.600235	-1.125901	-0.663970
O	0.844077	0.976989	-1.013208
N	-2.120727	2.252518	-0.908860
N	-2.985946	0.310244	-1.488641
C	-2.072679	0.913669	-0.692072
C	-2.982934	2.579371	-2.069382
C	-3.825615	1.303041	-2.203946
C	-1.527335	3.235503	-0.042795
C	-0.425092	4.003116	-0.498834
C	0.112598	4.966730	0.380015
C	-0.414503	5.150007	1.664390
C	-1.500657	4.373398	2.096787
C	-2.085696	3.404895	1.258817
C	0.159220	3.827334	-1.897098
H	0.025547	5.902352	2.338323
C	-3.286944	2.583062	1.725985
C	-3.189581	-1.110745	-1.559573
C	-4.260059	-1.689919	-0.828060
C	-4.423511	-3.088472	-0.901557
C	-3.561168	-3.875583	-1.673153
C	-2.509320	-3.280566	-2.385564
C	-2.290993	-1.890652	-2.340696
C	-5.245100	-0.839389	-0.027446
H	-3.696532	-4.967907	-1.706114
C	-1.128213	-1.244360	-3.094641
H	-3.582322	3.489187	-1.873641
H	-3.997004	0.993125	-3.252542
H	0.966930	5.578382	0.051652
H	-1.900286	4.524190	3.110026
H	-0.153921	2.825950	-2.256078
H	-3.152560	1.552396	1.341340
H	-5.234455	-3.567966	-0.333216
H	-1.827684	-3.917217	-2.967757
H	-4.754795	0.136590	0.177441
H	-0.746729	-0.417176	-2.461737
C	0.056876	-2.194288	-3.342153
H	-0.183495	-2.975338	-4.094960
H	0.920903	-1.608640	-3.716057
H	0.374312	-2.687756	-2.402227
C	-1.604159	-0.625093	-4.426434
H	-2.404561	0.125272	-4.270535
H	-0.762013	-0.119040	-4.942977
H	-2.007334	-1.408429	-5.103258
C	-5.617123	-1.443725	1.338790
H	-6.253927	-0.731278	1.903398
H	-6.196387	-2.384850	1.231172
H	-4.715033	-1.643244	1.946058
C	-6.522585	-0.587798	-0.862913
H	-7.072355	-1.540401	-1.019122
H	-7.203920	0.117825	-0.342201
H	-6.296146	-0.175901	-1.867620

C	1.615776	3.718321	-2.159998
H	1.920284	3.354205	-3.162563
H	2.052431	4.730228	-2.019799
H	2.028889	3.023292	-1.404170
C	-0.528874	4.769215	-3.008723
H	-0.203105	5.795029	-2.732702
H	-0.204998	4.576358	-4.053238
H	-1.637405	4.759099	-2.990033
C	-3.201460	2.598682	3.336571
H	-3.396425	3.577339	3.826195
H	-4.005631	1.902266	3.647124
H	-2.247177	2.187644	3.719264
C	-4.507255	3.294732	1.278899
H	-5.366046	2.689668	1.638853
H	-4.646938	4.336909	1.637801
H	-4.549490	3.306902	0.171307
C	-1.778968	-2.406774	1.401437
C	-0.950203	-2.974464	0.410902
C	-2.448578	-3.254745	2.311829
C	-0.797022	-4.366386	0.326899
C	-2.294280	-4.646229	2.227974
C	-1.467868	-5.206589	1.234481
H	-0.406540	-2.310521	-0.280072
H	-3.071650	-2.796715	3.095321
H	-0.155733	-4.796159	-0.459463
H	-2.815017	-5.301045	2.944967
H	-1.345649	-6.299813	1.170867
C	-1.930834	-0.906026	1.556880
O	-2.733184	-0.440196	2.353333
O	5.948943	-0.926252	-1.524263
K	4.410275	1.238174	-1.151108
C	6.568685	-0.593253	-0.424312
C	7.274212	0.659797	-0.299975
C	6.532500	-1.400210	0.771966
C	7.819866	1.092171	0.921115
H	7.406582	1.265119	-1.215742
C	7.080014	-0.954078	1.983028
H	6.052021	-2.392481	0.715607
C	7.716041	0.302196	2.081649
H	8.347186	2.061147	0.963321
H	7.012967	-1.602463	2.873740
H	8.141576	0.644287	3.037579

Zero-point correction= 0.884869 (Hartree/Particle)
Thermal correction to Energy= 0.948076
Thermal correction to Enthalpy= 0.949020
Thermal correction to Gibbs Free Energy= 0.784389
Sum of electronic and zero-point Energies= -3809.771919
Sum of electronic and thermal Energies= -3809.708712
Sum of electronic and thermal Enthalpies= -3809.707768
Sum of electronic and thermal Free Energies= -3809.872399

C	1.699950	3.814994	-1.895344
H	2.077500	3.515691	-2.895078
H	2.128657	4.811471	-1.654851
H	2.054310	3.070154	-1.156605
C	-0.378751	4.916261	-2.851598
H	-0.043080	5.924291	-2.526114
H	-0.011201	4.752505	-3.886838
H	-1.487768	4.936957	-2.878803
C	-3.385852	2.437067	3.250874
H	-3.645391	3.394782	3.751460
H	-4.176063	1.701671	3.501659
H	-2.436797	2.053369	3.672946
C	-4.604218	3.142746	1.146764
H	-5.460693	2.496432	1.433424
H	-4.801899	4.166338	1.530561
H	-4.583344	3.202109	0.040372
C	-1.701616	-2.436823	1.386475
C	-0.845841	-2.985974	0.408814
C	-2.351864	-3.298262	2.298247
C	-0.642654	-4.372546	0.341537
C	-2.149552	-4.684439	2.229810
C	-1.292849	-5.226025	1.251648
H	-0.321690	-2.310621	-0.285666
H	-3.000355	-2.854758	3.069224
H	0.021547	-4.787986	-0.433480
H	-2.655991	-5.349665	2.947461
H	-1.131777	-6.314899	1.201283
C	-1.900419	-0.940663	1.528706
O	-2.715540	-0.494525	2.323897
O	5.986076	-0.985118	-1.516383
K	4.525842	1.231420	-1.179520
C	6.628309	-0.645578	-0.430838
C	7.388407	0.578469	-0.350976
C	6.565937	-1.413056	0.789723
C	7.965806	1.022039	0.851402
H	7.536702	1.150112	-1.285695
C	7.146112	-0.956313	1.981485
H	6.038824	-2.382714	0.768303
C	7.839556	0.271931	2.035937
H	8.535707	1.967486	0.859583
H	7.058865	-1.573835	2.892148
H	8.290370	0.622616	2.977058
H	-4.811080	1.397297	-1.699243
H	-2.350976	2.758206	-2.966985

Zero-point correction= 0.907290 (Hartree/Particle)
Thermal correction to Energy= 0.971016
Thermal correction to Enthalpy= 0.971960
Thermal correction to Gibbs Free Energy= 0.806504
Sum of electronic and zero-point Energies= -3810.950016
Sum of electronic and thermal Energies= -3810.886291
Sum of electronic and thermal Enthalpies= -3810.885347
Sum of electronic and thermal Free Energies= -3811.050803

IPr-IX			
100			
IPrIX SCF Done: -2903.88813871 A.U.			
Pd	-0.152886	0.297567	0.525626
K	1.956024	4.985017	-1.086102
O	0.803105	4.441073	1.160725
H	0.742958	4.694510	2.097245
B	1.413166	3.091556	1.066777
O	2.871865	3.232726	1.150945

SIPr-IX			
102			
SIPrIX SCF Done: -2905.08833367 A.U.			
Pd	0.143274	-0.313182	0.469109
K	-1.678310	-5.108385	-1.086801
O	-0.449434	-4.518139	1.108840
H	-0.318233	-4.773930	2.037382
B	-1.147903	-3.210574	1.064607
O	-2.588628	-3.443157	1.214739

H	3.297700	2.356210	1.094592	H	-3.071704	-2.596016	1.165463
C	0.770382	2.074568	2.194044	C	-0.514642	-2.161407	2.167636
C	1.585676	1.456642	3.188217	C	-1.315985	-1.603470	3.208427
C	-0.644781	1.913132	2.344396	C	0.892816	-1.904981	2.244754
C	1.040276	0.720456	4.246312	C	-0.764973	-0.836633	4.241825
H	2.679224	1.573206	3.118962	H	-2.401077	-1.795034	3.197196
C	-1.200156	1.166025	3.414865	C	1.453386	-1.122802	3.285951
H	-1.322525	2.464012	1.671810	H	1.569128	-2.398411	1.527690
C	-0.359002	0.567780	4.360170	C	0.624417	-0.587904	4.279521
H	1.704768	0.253570	4.991419	H	-1.417757	-0.419049	5.025460
H	-2.294228	1.062173	3.487088	H	2.538439	-0.934280	3.293223
H	-0.783821	-0.019671	5.189770	H	1.051890	0.023870	5.090030
C	-0.078808	2.788773	-1.013978	C	0.210935	-2.781680	-1.094745
O	-0.182291	3.694919	-1.873800	O	0.335794	-3.678053	-1.960815
O	1.146838	2.637257	-0.388854	O	-0.984607	-2.723040	-0.398967
O	-0.994422	1.945491	-0.695503	O	1.068893	-1.863454	-0.827799
N	-2.286025	-1.157062	-0.935037	N	2.186629	1.179563	-0.990140
N	-0.364909	-1.828651	-1.690408	N	0.200103	1.894544	-1.617357
C	-0.934573	-1.009272	-0.753177	C	0.854264	1.066745	-0.767329
C	-2.555309	-2.056474	-1.964994	C	2.464601	1.986963	-2.201509
C	-1.344084	-2.476884	-2.447934	C	1.145444	2.750445	-2.376893
C	-3.261913	-0.482170	-0.107787	C	3.203470	0.665828	-0.111474
C	-3.885192	0.688936	-0.605787	C	3.999708	-0.432663	-0.524972
C	-4.769638	1.358142	0.264829	C	4.987660	-0.895653	0.369238
C	-5.012274	0.880251	1.560035	C	5.169609	-0.297203	1.622211
C	-4.386575	-0.290264	2.016521	C	4.367867	0.788084	2.009252
C	-3.492995	-1.002065	1.193119	C	3.370870	1.297585	1.155673
C	-3.660448	1.178653	-2.033948	C	3.838628	-1.078627	-1.897854
H	-5.699534	1.427498	2.225140	H	5.942063	-0.680722	2.308078
C	-2.837836	-2.302402	1.654998	C	2.521078	2.500888	1.563839
C	1.057607	-1.997698	-1.862972	C	-1.226590	1.969697	-1.761865
C	1.671046	-3.133356	-1.278407	C	-1.924234	3.046648	-1.154653
C	3.061381	-3.280391	-1.462948	C	-3.323058	3.101742	-1.323596
C	3.793718	-2.336711	-2.193768	C	-3.996912	2.126151	-2.067577
C	3.157646	-1.214274	-2.745897	C	-3.287174	1.064821	-2.649170
C	1.774550	-1.006504	-2.583140	C	-1.891493	0.952000	-2.503436
C	0.862854	-4.184417	-0.518564	C	-1.192714	4.145807	-0.386288
H	4.880392	-2.465375	-2.318361	H	-5.091101	2.180759	-2.180599
C	1.075943	0.233378	-3.139421	C	-1.124182	-0.228070	-3.100283
H	-3.576886	-2.313809	-2.256411	H	3.342695	2.642600	-2.046229
H	-1.086156	-3.163045	-3.258837	H	0.825955	2.851360	-3.431780
H	-5.266239	2.278103	-0.077218	H	5.618585	-1.749137	0.077684
H	-4.590796	-0.654259	3.034078	H	4.519852	1.244753	2.998093
H	-2.656332	0.821927	-2.345389	H	2.819716	-0.826013	-2.256508
H	-1.823974	-2.345133	1.207148	H	1.491364	2.320768	1.196198
H	3.577611	-4.143331	-1.016766	H	-3.892190	3.918646	-0.854885
H	3.754820	-0.469910	-3.291967	H	-3.836787	0.293226	-3.207552
H	-0.078157	-3.701925	-0.178671	H	-0.198701	3.742002	-0.095945
H	0.298775	0.528137	-2.402864	H	-0.320253	-0.494152	-2.382737
C	2.008920	1.446295	-3.297705	C	-1.978739	-1.494866	-3.281761
H	2.740002	1.308423	-4.123503	H	-2.726822	-1.385420	-4.096544
H	1.397082	2.343422	-3.520595	H	-1.314320	-2.346303	-3.531549
H	2.557683	1.650264	-2.356363	H	-2.505056	-1.757837	-2.342181
C	0.359784	-0.078502	-4.471837	C	-0.445147	0.158215	-4.431594
H	-0.382082	-0.895049	-4.362423	H	0.244615	1.017069	-4.310448
H	-0.180557	0.819899	-4.836183	H	0.145555	-0.694425	-4.826441
H	1.092391	-0.383476	-5.249715	H	-1.202165	0.441180	-5.194160
C	1.577272	-4.708780	0.739578	C	-1.898933	4.561080	0.916653
H	0.899200	-5.381799	1.303645	H	-1.275062	5.297069	1.465096
H	2.486860	-5.294204	0.488064	H	-2.879683	5.043725	0.720539
H	1.862124	-3.878675	1.411881	H	-2.054213	3.690795	1.579982
C	0.493868	-5.355807	-1.456538	C	-0.986565	5.378632	-1.297682
H	1.411126	-5.871523	-1.812865	H	-1.965453	5.844452	-1.540788

H	-0.134537	-6.101130	-0.925211	H	-0.360326	6.144591	-0.793328
H	-0.065147	-5.014957	-2.350738	H	-0.505147	5.115789	-2.261747
C	-3.648853	2.710954	-2.166200	C	3.909688	-2.615714	-1.854637
H	-3.365071	2.994255	-3.200628	H	3.640241	-3.033105	-2.846437
H	-4.649993	3.151933	-1.969218	H	4.930335	-2.978967	-1.606385
H	-2.899619	3.154233	-1.484482	H	3.183159	-3.014268	-1.122278
C	-4.724858	0.566028	-2.973591	C	4.891718	-0.511821	-2.877796
H	-5.740877	0.916952	-2.692074	H	5.916156	-0.797570	-2.555488
H	-4.538662	0.868679	-4.025723	H	4.734197	-0.912848	-3.901565
H	-4.738115	-0.542104	-2.934964	H	4.867353	0.596390	-2.932902
C	-2.624825	-2.384815	3.172795	C	2.383246	2.680246	3.081763
H	-3.583549	-2.450497	3.731188	H	3.340013	2.979258	3.561841
H	-2.032983	-3.289612	3.417158	H	1.637755	3.471997	3.295733
H	-2.051772	-1.510363	3.535312	H	2.016000	1.749256	3.554506
C	-3.644678	-3.515995	1.141534	C	3.044649	3.797127	0.908333
H	-3.146822	-4.465851	1.429996	H	2.384302	4.654594	1.157872
H	-4.668432	-3.518478	1.573428	H	4.069057	4.035568	1.266220
H	-3.745042	-3.508571	0.037001	H	3.090497	3.718070	-0.196166
C	2.354338	-0.959958	1.344892	C	-2.450269	0.707118	1.355652
C	2.925244	-0.098367	0.385599	C	-2.962248	-0.185578	0.391272
C	3.196619	-1.656796	2.238958	C	-3.336075	1.321447	2.268446
C	4.317844	0.052019	0.306873	C	-4.339032	-0.449399	0.328237
C	4.588476	-1.495885	2.169487	C	-4.711093	1.050302	2.211700
C	5.153216	-0.643621	1.200739	C	-5.217094	0.165264	1.239860
H	2.257557	0.463792	-0.287006	H	-2.263184	-0.681702	-0.300763
H	2.733131	-2.306447	2.997558	H	-2.918331	1.996467	3.031339
H	4.751320	0.712313	-0.461325	H	-4.726108	-1.135786	-0.441789
H	5.240422	-2.034575	2.875891	H	-5.395427	1.526971	2.931898
H	6.246812	-0.520806	1.144830	H	-6.297601	-0.046053	1.195367
C	0.851289	-1.125733	1.467128	C	-0.964372	0.990219	1.470807
O	0.377661	-2.025151	2.148824	O	-0.557853	1.891532	2.192324
				H	2.673422	1.312996	-3.060904
				H	1.185527	3.763604	-1.921338
Zero-point correction=			0.794190 (Hartree/Particle)	Zero-point correction=			0.816713 (Hartree/Particle)
Thermal correction to Energy=			0.848110	Thermal correction to Energy=			0.871054
Thermal correction to Enthalpy=			0.849054	Thermal correction to Enthalpy=			0.871998
Thermal correction to Gibbs Free Energy=			0.707709	Thermal correction to Gibbs Free Energy=			0.730719
Sum of electronic and zero-point Energies=			-2903.093948	Sum of electronic and zero-point Energies=			-2904.271620
Sum of electronic and thermal Energies=			-2903.040028	Sum of electronic and thermal Energies=			-2904.217280
Sum of electronic and thermal Enthalpies=			-2903.039084	Sum of electronic and thermal Enthalpies=			-2904.216336
Sum of electronic and thermal Free Energies=			-2903.180429	Sum of electronic and thermal Free Energies=			-2904.357614

IPr-IX-X			**SIPr-IX-X**			
100			102			
IPrIX-X SCF Done: -2903.87014116 A.U.			SIPrIX-XFlllall SCF Done: -2905.07180674 A.U.			
Pd	0.194526	-0.322354	0.314165	Pd	0.227466	0.310989	-0.245163
K	2.742811	-3.804757	-3.084346	K	3.305273	3.581643	2.902262
O	2.325983	-3.741394	-0.542851	O	2.638593	3.616169	0.421537
H	2.430046	-4.131148	0.344529	H	2.732890	3.963825	-0.484435
B	1.068053	-3.031545	-0.600309	B	1.343511	2.985084	0.547312
O	-0.050252	-3.818653	-0.319498	O	0.266472	3.818154	0.249980
H	-0.879065	-3.299928	-0.344864	H	-0.589904	3.350649	0.319950
C	1.416449	-1.883554	1.199594	C	1.583504	1.704387	-1.165114
C	0.990141	-2.731320	2.259120	C	1.256634	2.549398	-2.263177
C	2.740900	-1.357468	1.302325	C	2.860043	1.065172	-1.220216
C	1.824962	-3.050257	3.344871	C	2.142292	2.764955	-3.333609
H	-0.016912	-3.176446	2.208632	H	0.290379	3.078453	-2.253465
C	3.580858	-1.668819	2.383274	C	3.748958	1.269685	-2.287214
H	3.115275	-0.682332	0.515088	H	3.163182	0.387642	-0.405185
C	3.127233	-2.519219	3.410211	C	3.396456	2.125022	-3.348511
H	1.457285	-3.710966	4.147720	H	1.850996	3.428558	-4.164910
H	4.591863	-1.231476	2.432035	H	4.718526	0.744940	-2.296466

H	3.783227	-2.761286	4.262446	H	4.091595	2.285855	-4.188831
C	1.843063	-1.152061	-2.106564	C	1.956491	1.066329	2.090131
O	2.587874	-1.288247	-3.109028	O	2.771536	1.118651	3.044292
O	0.999998	-2.243806	-1.815812	O	1.272418	2.256893	1.799232
O	1.738998	-0.132914	-1.364079	O	1.659043	0.045581	1.401670
N	0.400865	2.649877	0.303205	N	0.189371	-2.613390	-0.262577
N	-1.583079	2.151113	-0.413703	N	-1.822075	-1.946839	0.317423
C	-0.407643	1.582882	0.000002	C	-0.565138	-1.525723	0.023251
C	-0.265786	3.857766	0.108505	C	-0.627294	-3.839610	-0.368688
C	-1.517054	3.546865	-0.357456	C	-1.904073	-3.426409	0.376659
C	1.799374	2.491510	0.643400	C	1.592596	-2.562897	-0.580403
C	2.753223	2.601936	-0.401592	C	2.524155	-2.740289	0.479962
C	4.101090	2.375421	-0.061322	C	3.893000	-2.653153	0.162690
C	4.470577	2.045063	1.251015	C	4.316877	-2.408466	-1.152623
C	3.499845	1.930769	2.256358	C	3.377952	-2.245742	-2.180041
C	2.136232	2.144310	1.974289	C	1.994922	-2.313262	-1.917393
C	2.348406	2.976817	-1.826176	C	2.065924	-3.067170	1.899976
H	5.530275	1.860124	1.490223	H	5.393561	-2.336807	-1.376654
C	1.071372	2.033854	3.060302	C	0.981613	-2.149373	-3.046264
C	-2.650421	1.391897	-1.012375	C	-2.808687	-1.123565	0.951987
C	-3.850966	1.203818	-0.286859	C	-4.010724	-0.844058	0.249924
C	-4.882277	0.480397	-0.921478	C	-4.983455	-0.053301	0.893534
C	-4.707802	-0.045788	-2.207892	C	-4.768626	0.444933	2.185123
C	-3.488848	0.121577	-2.884933	C	-3.569729	0.164164	2.857827
C	-2.424179	0.838720	-2.303784	C	-2.561391	-0.620877	2.262174
C	-4.027940	1.756925	1.125205	C	-4.265462	-1.399186	-1.149221
H	-5.524101	-0.613037	-2.682796	H	-5.538523	1.065790	2.670431
C	-1.087330	1.008470	-3.026623	C	-1.269152	-0.913909	3.023463
H	0.208242	4.820162	0.318769	H	-0.111863	-4.707954	0.082807
H	-2.354232	4.180062	-0.663163	H	-2.830543	-3.797375	-0.101230
H	4.871153	2.440751	-0.844229	H	4.639957	-2.770442	0.962076
H	3.799962	1.647539	3.275821	H	3.720366	-2.040029	-3.205632
H	1.293940	2.656933	-1.960695	H	1.040859	-2.656018	2.010693
H	0.105027	1.801272	2.570293	H	-0.013618	-1.963331	-2.593607
H	-5.828668	0.309447	-0.386938	H	-5.919245	0.186993	0.365877
H	-3.357204	-0.323294	-3.882284	H	-3.408389	0.568015	3.869096
H	-3.012798	1.948912	1.532310	H	-3.291281	-1.766108	-1.535779
H	-0.293565	1.026769	-2.252016	H	-0.495791	-1.203993	2.284775
C	-0.731397	-0.173366	-3.942369	C	-0.705258	0.325438	3.739383
H	-1.382994	-0.229412	-4.841360	H	-1.335641	0.639224	4.599199
H	0.316137	-0.069541	-4.290925	H	0.309849	0.107727	4.129037
H	-0.796589	-1.132723	-3.389424	H	-0.611823	1.179049	3.038819
C	-1.029828	2.354539	-3.779169	C	-1.454314	-2.093257	4.000888
H	-1.193026	3.211231	-3.093295	H	-1.814743	-3.005808	3.481969
H	-0.034237	2.487532	-4.252162	H	-0.491618	-2.339762	4.496557
H	-1.802636	2.399796	-4.576533	H	-2.196288	-1.845389	4.790237
C	-4.709883	0.755311	2.075905	C	-4.765857	-0.329692	-2.137649
H	-4.678470	1.141406	3.115189	H	-4.851998	-0.764238	-3.155048
H	-5.777711	0.596151	1.813886	H	-5.768338	0.057226	-1.855929
H	-4.197094	-0.225177	2.064912	H	-4.064082	0.522829	-2.194083
C	-4.802942	3.092451	1.095876	C	-5.254604	-2.584629	-1.083977
H	-5.827230	2.942152	0.692198	H	-6.254699	-2.241845	-0.741825
H	-4.896883	3.513656	2.118816	H	-5.379485	-3.051533	-2.083749
H	-4.303330	3.850962	0.460058	H	-4.920694	-3.369741	-0.373729
C	3.173422	2.269729	-2.915917	C	2.929355	-2.431337	3.002939
H	2.745336	2.502359	-3.914241	H	2.466742	-2.623478	3.994618
H	4.226502	2.625193	-2.930516	H	3.948107	-2.875234	3.035842
H	3.160132	1.170963	-2.783589	H	3.014398	-1.335814	2.869585
C	2.416402	4.509411	-2.018740	C	1.996052	-4.599371	2.098001
H	3.462773	4.866518	-1.908860	H	3.010885	-5.046071	2.026610
H	2.062609	4.792863	-3.032697	H	1.581962	-4.850392	3.097741
H	1.799850	5.056994	-1.278441	H	1.367838	-5.098042	1.331743
C	1.322969	0.878453	4.041944	C	1.267827	-0.926560	-3.934630

H 2.219422 1.047617 4.676327	H 2.221876 -1.027180 -4.494499
H 0.449197 0.765467 4.714452	H 0.451110 -0.799182 -4.673536
H 1.453702 -0.077139 3.497408	H 1.317580 -0.003408 -3.327967
C 0.919085 3.386951 3.787554	C 0.904972 -3.445367 -3.883160
H 0.110986 3.333948 4.547436	H 0.121076 -3.361671 -4.665434
H 1.861449 3.669429 4.304761	H 1.873215 -3.646420 -4.390555
H 0.668484 4.203363 3.077394	H 0.674350 -4.331907 -3.254848
C -2.210912 -1.726152 1.237867	C -2.032276 1.885511 -1.238392
C -2.589157 -1.977037 -0.098806	C -2.414222 2.188424 0.086641
C -2.739494 -2.531485 2.270742	C -2.468014 2.718105 -2.292445
C -3.492074 -3.011634 -0.396698	C -3.232869 3.299190 0.351654
C -3.611115 -3.588913 1.966349	C -3.252718 3.849941 -2.020777
C -3.994013 -3.828556 0.632762	C -3.642335 4.140044 -0.699313
H -2.190920 -1.334990 -0.899467	H -2.089329 1.524962 0.902758
H -2.448403 -2.311402 3.309489	H -2.177019 2.457893 -3.322062
H -3.800753 -3.175644 -1.441048	H -3.549737 3.502882 1.386542
H -4.000199 -4.229429 2.774157	H -3.569221 4.509544 -2.844841
H -4.686355 -4.652394 0.397011	H -4.268688 5.021833 -0.490011
C -1.269211 -0.593724 1.607672	C -1.189083 0.667494 -1.569881
O -1.457337 0.023606 2.650751	O -1.427692 0.037697 -2.596514
	H -0.819699 -4.062978 -1.442317
	H -1.900305 -3.753347 1.441047
Zero-point correction= 0.791512 (Hartree/Particle)	Zero-point correction= 0.814035 (Hartree/Particle)
Thermal correction to Energy= 0.845654	Thermal correction to Energy= 0.868626
Thermal correction to Enthalpy= 0.846598	Thermal correction to Enthalpy= 0.869571
Thermal correction to Gibbs Free Energy= 0.703731	Thermal correction to Gibbs Free Energy= 0.726354
Sum of electronic and zero-point Energies= -2903.078629	Sum of electronic and zero-point Energies= -2904.257771
Sum of electronic and thermal Energies= -2903.024487	Sum of electronic and thermal Energies= -2904.203180
Sum of electronic and thermal Enthalpies= -2903.023543	Sum of electronic and thermal Enthalpies= -2904.202236
Sum of electronic and thermal Free Energies= -2903.166410	Sum of electronic and thermal Free Energies= -2904.345453

IPr-X	**SIPr-X**
100	102
IPrX SCF Done: -2903.89620157 A.U.	SIPrX SCF Done: -2905.09727979 A.U.
Pd -0.170564 -0.496751 -0.357985	Pd -0.147314 0.490921 0.304023
K -4.008351 -1.408466 1.326537	K -3.881202 1.521441 -1.324689
O -1.920546 -3.340986 1.906662	O -1.741719 3.431925 -1.953332
H -1.848224 -4.099650 1.289668	H -1.657249 4.197296 -1.346891
B -0.638867 -2.861237 2.169790	B -0.470078 2.915303 -2.190625
O 0.437019 -3.693710 2.016995	O 0.627443 3.715955 -2.031080
H 1.279997 -3.202118 1.955066	H 1.453710 3.199712 -1.938072
C -1.090767 -2.280790 -0.913209	C -0.987769 2.311360 0.866268
C -0.558105 -3.594293 -0.920689	C -0.407369 3.603900 0.889162
C -2.460092 -2.162920 -1.287570	C -2.357504 2.240814 1.248503
C -1.355435 -4.725981 -1.191209	C -1.159227 4.760271 1.184695
H 0.501958 -3.752239 -0.668264	H 0.655428 3.727369 0.631253
C -3.264110 -3.283939 -1.584239	C -3.117167 3.385283 1.571071
H -2.912472 -1.157048 -1.374593	H -2.845158 1.251543 1.330352
C -2.719304 -4.580739 -1.511407	C -2.524676 4.661618 1.514941
H -0.903479 -5.731901 -1.158410	H -0.669395 5.748675 1.164504
H -4.315605 -3.144682 -1.895392	H -4.170340 3.279331 1.889376
H -3.340115 -5.463552 -1.734377	H -3.109611 5.563325 1.758454
C -1.614391 -0.723752 2.484418	C -1.498740 0.801452 -2.492043
O -2.431865 -0.681513 3.420764	O -2.313550 0.778320 -3.429693
O -0.485806 -1.559507 2.616831	O -0.347931 1.601366 -2.616340
O -1.720337 -0.121931 1.361814	O -1.628043 0.200070 -1.368287
N -0.562561 2.446702 -0.734104	N -0.694362 -2.385141 0.712435
N 1.469157 2.221460 -0.028720	N 1.417663 -2.217875 0.143797
C 0.325684 1.503798 -0.265502	C 0.264381 -1.519890 0.288047
C 0.024804 3.708315 -0.819555	C -0.208445 -3.776935 0.843053
C 1.309673 3.569792 -0.364769	C 1.311024 -3.610295 0.645434
C -1.946423 2.129172 -0.999813	C -2.049735 -1.989828 0.982798

C	-2.898354	2.386485	0.020103	C	-3.044580	-2.219673	-0.006196
C	-4.235313	2.014700	-0.237650	C	-4.360106	-1.788126	0.268702
C	-4.593296	1.398530	-1.448382	C	-4.672259	-1.146312	1.478579
C	-3.623921	1.153346	-2.435185	C	-3.674960	-0.943186	2.446302
C	-2.275312	1.514454	-2.234891	C	-2.346598	-1.363473	2.225296
C	-2.507839	3.091961	1.316612	C	-2.730027	-2.982145	-1.289932
H	-5.644149	1.119799	-1.633777	H	-5.706497	-0.820831	1.680113
C	-1.224524	1.312450	-3.322807	C	-1.289273	-1.213367	3.316304
C	2.625393	1.669582	0.633352	C	2.548753	-1.734928	-0.593489
C	3.796642	1.429809	-0.125068	C	3.776712	-1.509301	0.080659
C	4.913871	0.906168	0.558443	C	4.874293	-1.054633	-0.679016
C	4.853564	0.625671	1.928522	C	4.751258	-0.816125	-2.052329
C	3.668587	0.848149	2.648470	C	3.522588	-1.027737	-2.697943
C	2.520215	1.370131	2.021471	C	2.395706	-1.494431	-1.993165
C	3.868319	1.740245	-1.618884	C	3.930355	-1.764748	1.577943
H	5.735104	0.210073	2.441991	H	5.616580	-0.449328	-2.627052
C	1.213458	1.582085	2.790432	C	1.060131	-1.724894	-2.705838
H	-0.518334	4.580706	-1.192576	H	-0.471547	-4.188371	1.837840
H	2.112589	4.300200	-0.234251	H	1.743948	-4.325839	-0.082153
H	-5.007260	2.222513	0.520227	H	-5.154662	-1.976410	-0.471656
H	-3.916331	0.670330	-3.379294	H	-3.930692	-0.448853	3.395616
H	-1.427539	2.898562	1.480288	H	-1.630896	-2.935497	-1.432870
H	-0.237357	1.206867	-2.829924	H	-0.292296	-1.237289	2.834203
H	5.839197	0.699837	0.000130	H	5.835702	-0.865364	-0.178012
H	3.634113	0.600145	3.718920	H	3.440183	-0.822149	-3.774793
H	2.826005	1.794324	-1.997599	H	2.909124	-1.781847	2.013937
H	0.397417	1.227770	2.123945	H	0.269082	-1.321772	-2.037789
C	1.115203	0.758402	4.083980	C	0.926631	-0.976456	-4.041718
H	1.806461	1.131450	4.870490	H	1.584767	-1.403888	-4.828932
H	0.084327	0.821672	4.488196	H	-0.118289	-1.047062	-4.406802
H	1.321325	-0.313824	3.900460	H	1.155294	0.100665	-3.927562
C	0.960952	3.077688	3.086793	C	0.780802	-3.229840	-2.910433
H	0.930256	3.691527	2.164773	H	0.756175	-3.786947	-1.953720
H	-0.011695	3.204389	3.606933	H	-0.200447	-3.376323	-3.408603
H	1.757033	3.487788	3.744392	H	1.562720	-3.692807	-3.549388
C	4.583337	0.642063	-2.427440	C	4.698976	-0.647052	2.306751
H	4.488703	0.852161	-3.512368	H	4.662820	-0.816440	3.402494
H	5.668123	0.594981	-2.192658	H	5.769446	-0.620208	2.011234
H	4.138040	-0.352044	-2.237743	H	4.254349	0.344389	2.102763
C	4.546888	3.108399	-1.853672	C	4.613096	-3.130859	1.819747
H	5.597537	3.088581	-1.492874	H	5.654960	-3.114123	1.433970
H	4.561204	3.358921	-2.935199	H	4.656115	-3.365973	2.904259
H	4.029615	3.931128	-1.320056	H	4.089332	-3.962164	1.304681
C	-3.250581	2.581760	2.562786	C	-3.370867	-2.389428	-2.556469
H	-2.860135	3.096465	3.465547	H	-3.058809	-2.976824	-3.445535
H	-4.338879	2.804873	2.519187	H	-4.481107	-2.438249	-2.520650
H	-3.105070	1.494596	2.712696	H	-3.059524	-1.340616	-2.723749
C	-2.706691	4.618355	1.167995	C	-3.145505	-4.464351	-1.128181
H	-3.782646	4.858166	1.028301	H	-4.251241	-4.551269	-1.059980
H	-2.352460	5.148603	2.076845	H	-2.810362	-5.065514	-1.999637
H	-2.159050	5.030874	0.297831	H	-2.727291	-4.922054	-0.208101
C	-1.420828	0.027300	-4.140868	C	-1.357227	0.125356	4.068096
H	-2.330547	0.063288	-4.778675	H	-2.287104	0.229230	4.668058
H	-0.547932	-0.121817	-4.806831	H	-0.497275	0.202009	4.762711
H	-1.482214	-0.856458	-3.475482	H	-1.287781	0.975401	3.362207
C	-1.173410	2.562815	-4.228707	C	-1.383134	-2.407768	4.292609
H	-0.375614	2.455204	-4.993131	H	-0.575087	-2.353724	5.052051
H	-2.140125	2.711260	-4.756658	H	-2.357677	-2.409038	4.826995
H	-0.964065	3.482782	-3.643488	H	-1.295564	-3.381222	3.765609
C	2.348832	-1.841646	-0.907832	C	2.389970	1.762006	0.888332
C	2.608843	-1.779940	0.477750	C	2.690496	1.699108	-0.489369
C	3.056486	-2.768037	-1.702694	C	3.068552	2.695528	1.700316
C	3.575394	-2.615529	1.058649	C	3.669392	2.540435	-1.042322

C	3.993136	-3.635339	-1.114079
C	4.259952	-3.557453	0.265085
H	2.051926	-1.048575	1.084710
H	2.850907	-2.797551	-2.784193
H	3.803601	-2.521796	2.132915
H	4.524049	-4.373978	-1.736064
H	5.005674	-4.227191	0.722394
C	1.325075	-0.926458	-1.561704
O	1.493442	-0.547828	-2.716855

Zero-point correction= 0.793013 (Hartree/Particle)
Thermal correction to Energy= 0.847669
Thermal correction to Enthalpy= 0.848613
Thermal correction to Gibbs Free Energy= 0.704890
Sum of electronic and zero-point Energies= -2903.103189
Sum of electronic and thermal Energies= -2903.048533
Sum of electronic and thermal Enthalpies= -2903.047588
Sum of electronic and thermal Free Energies= -2903.191312

C	4.014591	3.569955	1.137791
C	4.322885	3.490628	-0.232369
H	2.161951	0.964737	-1.116579
H	2.832821	2.725647	2.775569
H	3.931101	2.444147	-2.108768
H	4.520799	4.314147	1.773610
H	5.076749	4.164496	-0.669761
C	1.354267	0.846294	1.519883
O	1.526948	0.428390	2.661981
H	-0.670455	-4.425785	0.068805
H	1.866441	-3.710998	1.601146

Zero-point correction= 0.815603 (Hartree/Particle)
Thermal correction to Energy= 0.870805
Thermal correction to Enthalpy= 0.871749
Thermal correction to Gibbs Free Energy= 0.727190
Sum of electronic and zero-point Energies= -2904.281677
Sum of electronic and thermal Energies= -2904.226475
Sum of electronic and thermal Enthalpies= -2904.225531
Sum of electronic and thermal Free Energies= -2904.370090

IPr-XI

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IPrXI SCF Done: -1863.61012560 A.U.

Pd	-0.519637	0.778847	0.259356
C	-1.285223	2.627588	0.640755
C	-0.700792	3.862328	1.003983
C	-2.692556	2.599473	0.450925
C	-1.481379	5.025304	1.151500
H	0.386981	3.926322	1.174645
C	-3.478524	3.759365	0.592637
H	-3.202189	1.651765	0.189792
C	-2.872182	4.979523	0.943709
H	-0.999498	5.976821	1.433563
H	-4.569329	3.706534	0.435756
H	-3.482457	5.889903	1.060871
N	-1.325846	-2.039249	-0.329844
N	0.833676	-2.030151	-0.403786
C	-0.242277	-1.207143	-0.195005
C	-0.943413	-3.350597	-0.607788
C	0.427859	-3.345613	-0.651199
C	-2.670313	-1.517928	-0.273659
C	-3.205437	-0.930277	-1.448993
C	-4.497263	-0.372956	-1.361209
C	-5.211073	-0.394414	-0.154313
C	-4.646137	-0.966963	0.995794
C	-3.360019	-1.541782	0.964845
C	-2.397017	-0.821922	-2.739953
H	-6.214518	0.056828	-0.103950
C	-2.695880	-2.066431	2.234304
C	2.195983	-1.556002	-0.451150
C	3.045823	-1.834961	0.646588
C	4.374074	-1.369480	0.569992
C	4.816335	-0.635133	-0.536862
C	3.942165	-0.347556	-1.595676
C	2.609601	-0.801957	-1.584873
C	2.560695	-2.620501	1.863529
H	5.850133	-0.257481	-0.566937
C	1.643104	-0.488724	-2.729996
H	-1.672519	-4.153650	-0.751033
H	1.146719	-4.145658	-0.848894
H	-4.941458	0.103641	-2.248794
H	-5.207344	-0.950320	1.942204

SIPr-XI

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SIPrXI SCF Done: -1864.81241305 A.U.

Pd	0.530344	0.750600	-0.291108
C	1.336840	2.585880	-0.675342
C	0.772245	3.834552	-1.022666
C	2.745783	2.528913	-0.507241
C	1.573631	4.982523	-1.176060
H	-0.316434	3.922383	-1.175814
C	3.552847	3.673362	-0.655208
H	3.240496	1.571012	-0.257704
C	2.966304	4.907476	-0.990236
H	1.106645	5.945105	-1.445304
H	4.644557	3.597054	-0.515177
H	3.592977	5.806085	-1.111863
N	1.308779	-2.022719	0.283930
N	-0.882277	-2.010505	0.304757
C	0.214055	-1.233024	0.147293
C	0.985511	-3.403717	0.694105
C	-0.536083	-3.450409	0.443068
C	2.640269	-1.481534	0.282192
C	3.150347	-0.895213	1.471914
C	4.453972	-0.359834	1.432319
C	5.214216	-0.399209	0.255230
C	4.682612	-0.967231	-0.913315
C	3.388662	-1.522944	-0.925328
C	2.305363	-0.769438	2.736416
H	6.226520	0.034645	0.241712
C	2.765380	-2.051362	-2.213266
C	-2.224375	-1.505151	0.395522
C	-3.130371	-1.750479	-0.668772
C	-4.448941	-1.270161	-0.537925
C	-4.842067	-0.544072	0.591508
C	-3.923438	-0.284617	1.618682
C	-2.600277	-0.761398	1.554588
C	-2.716981	-2.518929	-1.921950
H	-5.868727	-0.152998	0.665396
C	-1.603105	-0.479577	2.682003
H	1.256953	-3.556396	1.764166
H	-1.111947	-3.915161	1.267853
H	4.871215	0.114886	2.334247
H	5.279595	-0.963803	-1.837836

H	-1.476195	-1.428672	-2.616229
H	-1.844593	-2.710627	1.925971
H	5.064581	-1.566812	1.403790
H	4.304035	0.258520	-2.437391
H	1.450405	-2.583277	1.858694
H	0.697738	-0.154611	-2.249051
C	2.106217	0.655267	-3.644732
H	2.986821	0.366101	-4.257874
H	1.291931	0.922397	-4.349433
H	2.370272	1.563291	-3.069771
C	1.325103	-1.737639	-3.582817
H	0.902446	-2.567609	-2.984297
H	0.582993	-1.484687	-4.369471
H	2.242045	-2.111606	-4.086290
C	3.024938	-2.005138	3.197305
H	2.560275	-2.548797	4.046145
H	4.125518	-2.080481	3.327183
H	2.723575	-0.942165	3.265648
C	2.997951	-4.098874	1.764267
H	4.106106	-4.178102	1.770420
H	2.609140	-4.683710	2.624332
H	2.637679	-4.581104	0.832883
C	-1.953632	0.638239	-2.969486
H	-1.310402	0.717726	-3.870844
H	-2.826451	1.311106	-3.102492
H	-1.370082	1.023336	-2.099101
C	-3.151787	-1.387387	-3.958112
H	-4.063295	-0.797172	-4.190711
H	-2.503494	-1.359166	-4.858877
H	-3.463503	-2.438941	-3.789895
C	-2.110164	-0.885777	3.041078
H	-2.916265	-0.192563	3.361659
H	-1.581503	-1.251835	3.945392
H	-1.387303	-0.299176	2.431691
C	-3.639640	-2.929326	3.092581
H	-3.082689	-3.374014	3.943097
H	-4.465316	-2.327522	3.527611
H	-4.093008	-3.754728	2.504925
C	2.242853	1.803851	0.735655
C	2.115409	2.497258	-0.484495
C	3.482222	1.809875	1.413573
C	3.209192	3.195242	-1.017662
C	4.578902	2.496752	0.872991
C	4.444300	3.192544	-0.342722
H	1.135388	2.478278	-0.990836
H	3.564921	1.259697	2.362840
H	3.098671	3.749006	-1.963577
H	5.545912	2.488960	1.400846
H	5.303939	3.738237	-0.764102
C	1.092007	1.050285	1.356733
O	1.166692	0.565548	2.474084

H	1.356358	-1.315137	2.562344
H	1.916498	-2.707651	-1.922635
H	-5.171630	-1.448637	-1.348853
H	-4.245935	0.314225	2.481223
H	-1.606181	-2.531467	-1.946622
H	-0.667604	-0.134429	2.188770
C	-2.036038	0.639680	3.641383
H	-2.904850	0.339599	4.265945
H	-1.204174	0.880512	4.334954
H	-2.305445	1.566408	3.100030
C	-1.272643	-1.749928	3.495174
H	-0.851631	-2.558194	2.868498
H	-0.526091	-1.521360	4.284833
H	-2.184039	-2.147115	3.990488
C	-3.177417	-1.836804	-3.224786
H	-2.776451	-2.385844	-4.102375
H	-4.283857	-1.833254	-3.320864
H	-2.807303	-0.794802	-3.273071
C	-3.235309	-3.973778	-1.857393
H	-4.345906	-3.989286	-1.885567
H	-2.866362	-4.566953	-2.720805
H	-2.927153	-4.488973	-0.924156
C	1.931634	0.705603	2.990924
H	1.268491	0.795620	3.876663
H	2.832524	1.329833	3.166894
H	1.394441	1.137960	2.114257
C	2.984312	-1.408697	3.962740
H	3.920441	-0.877994	4.236687
H	2.310408	-1.366147	4.844180
H	3.242492	-2.471850	3.775714
C	2.173318	-0.877956	-3.026019
H	2.972278	-0.165748	-3.321653
H	1.673148	-1.246901	-3.945455
H	1.426189	-0.308549	-2.428244
C	3.739380	-2.892520	-3.058119
H	3.205691	-3.348709	-3.917558
H	4.557711	-2.272362	-3.481292
H	4.203199	-3.707919	-2.464501
C	-2.211826	1.860015	-0.687190
C	-2.035836	2.537435	0.536011
C	-3.467277	1.904256	-1.333060
C	-3.097191	3.258098	1.102948
C	-4.531683	2.614070	-0.758655
C	-4.348434	3.294160	0.459576
H	-1.045164	2.488316	1.018755
H	-3.588179	1.363228	-2.283311
H	-2.948503	3.799602	2.050739
H	-5.511798	2.635308	-1.261296
H	-5.182752	3.857533	0.907714
C	-1.096945	1.084684	-1.344767
O	-1.205538	0.622595	-2.468868
H	1.549743	-4.141146	0.087917
H	-0.780162	-3.992666	-0.494694

Zero-point correction=	0.739629 (Hartree/Particle)
Thermal correction to Energy=	0.784814
Thermal correction to Enthalpy=	0.785758
Thermal correction to Gibbs Free Energy=	0.660731
Sum of electronic and zero-point Energies=	-1862.870497
Sum of electronic and thermal Energies=	-1862.825312
Sum of electronic and thermal Enthalpies=	-1862.824367
Sum of electronic and thermal Free Energies=	-1862.949394

Zero-point correction=	0.762122 (Hartree/Particle)
Thermal correction to Energy=	0.807762
Thermal correction to Enthalpy=	0.808706
Thermal correction to Gibbs Free Energy=	0.683917
Sum of electronic and zero-point Energies=	-1864.050291
Sum of electronic and thermal Energies=	-1864.004651
Sum of electronic and thermal Enthalpies=	-1864.003707
Sum of electronic and thermal Free Energies=	-1864.128497

IPr-XI-XII				**SIPr-XI-XII**			
90				92			
IPrXI-XII SCF Done: -1863.60227353 A.U.				SIPrXI-XII SCF Done: -1864.80269255 A.U.			
Pd	0.326903	0.797086	0.150754	Pd	-0.330496	0.771187	-0.176693
C	0.205315	2.905505	0.162997	C	-0.276143	2.880236	-0.120472
C	-0.281842	3.542148	1.328548	C	0.216771	3.557765	-1.260445
C	1.212268	3.545852	-0.597818	C	-1.313582	3.474958	0.635973
C	0.276378	4.759835	1.760404	C	-0.364216	4.771872	-1.672294
H	-1.103331	3.087123	1.903166	H	1.059173	3.137658	-1.831363
C	1.778835	4.753371	-0.160255	C	-1.901016	4.679474	0.218726
H	1.524258	3.091972	-1.553063	H	-1.634112	2.987926	1.571668
C	1.312902	5.360534	1.023288	C	-1.428060	5.328459	-0.939695
H	-0.103708	5.244640	2.674655	H	0.020360	5.288766	-2.566869
H	2.576161	5.234606	-0.750166	H	-2.721476	5.125216	0.804751
H	1.745919	6.316528	1.359700	H	-1.878087	6.282168	-1.259812
N	1.755916	-1.860685	0.089862	N	-1.733902	-1.845450	-0.205365
N	-0.371373	-2.236246	0.076390	N	0.423845	-2.221819	-0.226190
C	0.543540	-1.210963	0.089305	C	-0.515053	-1.245224	-0.189274
C	1.605718	-3.247233	0.087411	C	-1.666139	-3.319543	-0.144794
C	0.255279	-3.485784	0.079799	C	-0.156749	-3.583395	-0.336576
C	3.002933	-1.147651	-0.020500	C	-2.951803	-1.117723	0.015890
C	3.654149	-0.726016	1.163784	C	-3.685718	-0.659119	-1.108253
C	4.856792	-0.006198	1.018010	C	-4.867339	0.069066	-0.868668
C	5.372879	0.283046	-0.254483	C	-5.298482	0.329042	0.441593
C	4.689436	-0.127278	-1.409264	C	-4.547959	-0.122653	1.537225
C	3.482828	-0.849583	-1.320394	C	-3.356998	-0.851810	1.349605
C	3.020624	-0.944759	2.535375	C	-3.139916	-0.850861	-2.520284
H	6.312545	0.850519	-0.347512	H	-6.223756	0.902949	0.609791
C	2.683757	-1.204237	-2.572122	C	-2.513717	-1.280024	2.547289
C	-1.797567	-2.032884	0.010190	C	1.836230	-1.983171	-0.118976
C	-2.368539	-1.625362	-1.225021	C	2.381863	-1.629653	1.148236
C	-3.765160	-1.437990	-1.247479	C	3.776337	-1.436642	1.218058
C	-4.546628	-1.662359	-0.105684	C	4.591387	-1.601329	0.089899
C	-3.950387	-2.056012	1.100526	C	4.027762	-1.927904	-1.150999
C	-2.556137	-2.234872	1.190260	C	2.636950	-2.106532	-1.285002
C	-1.503581	-1.396094	-2.467231	C	1.490351	-1.437454	2.379186
H	-5.635015	-1.502385	-0.151196	H	5.677783	-1.442567	0.174083
C	-1.870178	-2.538020	2.523913	C	1.993631	-2.311353	-2.658238
H	2.464426	-3.925109	0.080241	H	-2.294008	-3.775192	-0.938259
H	-0.316139	-4.418989	0.065541	H	0.276147	-4.257058	0.430007
H	5.389091	0.346990	1.914549	H	-5.452358	0.452871	-1.718799
H	5.091626	0.132524	-2.400959	H	-4.884400	0.107879	2.560654
H	2.245411	-1.733142	2.424745	H	-2.409882	-1.688102	-2.477796
H	1.875753	-1.904656	-2.274818	H	-1.642634	-1.846797	2.162314
H	-4.251277	-1.096974	-2.171744	H	4.236183	-1.139045	2.170468
H	-4.577488	-2.200699	1.992582	H	4.678686	-2.016422	-2.033418
H	-0.620645	-0.812241	-2.128938	H	0.616501	-0.840357	2.038890
H	-0.968410	-3.151322	2.309776	H	1.083567	-2.931431	-2.519138
C	-1.376667	-1.225920	3.175209	C	1.520069	-0.957134	-3.231955
H	-2.237458	-0.566682	3.416831	H	2.387313	-0.285380	-3.405429
H	-0.827609	-1.434193	4.117647	H	0.996075	-1.098621	-4.200766
H	-0.701116	-0.664553	2.496044	H	0.826134	-0.444544	-2.531926
C	-2.744066	-3.344227	3.499609	C	2.891605	-3.054610	-3.662003
H	-3.148994	-4.263412	3.027759	H	3.278520	-4.006331	-3.242255
H	-2.149829	-3.644319	4.387413	H	2.323091	-3.289028	-4.585842
H	-3.602614	-2.747438	3.874258	H	3.763584	-2.439431	-3.969719
C	-2.192423	-0.559477	-3.554712	C	2.155095	-0.634782	3.507192
H	-1.460577	-0.313001	-4.350263	H	1.402143	-0.397819	4.285651
H	-3.033161	-1.108031	-4.032160	H	2.975960	-1.203374	3.995646
H	-2.568018	0.399388	-3.150319	H	2.555010	0.328025	3.137826
C	-0.992746	-2.725992	-3.065591	C	0.963181	-2.777062	2.935748
H	-1.840877	-3.348638	-3.422614	H	1.801257	-3.422983	3.274271
H	-0.329519	-2.522657	-3.932831	H	0.297198	-2.595409	3.805383

H	-0.411449	-3.325884	-2.338120
C	2.299191	0.344282	2.984136
H	1.769801	0.190671	3.947631
H	3.016385	1.183073	3.103977
H	1.540478	0.664775	2.227284
C	4.026712	-1.428617	3.595860
H	4.785985	-0.652299	3.828059
H	3.503054	-1.664023	4.545728
H	4.564868	-2.339781	3.261798
C	1.997959	0.060215	-3.133261
H	2.750250	0.797952	-3.485506
H	1.340765	-0.196613	-3.990284
H	1.369582	0.553080	-2.361115
C	3.534682	-1.917563	-3.639234
H	2.897809	-2.227159	-4.494100
H	4.327136	-1.254352	-4.046221
H	4.028504	-2.823748	-3.230609
C	-2.428402	1.833302	-0.501547
C	-2.756842	1.330143	0.772992
C	-3.457101	2.311265	-1.342539
C	-4.089037	1.310945	1.208393
C	-4.791221	2.292260	-0.907261
C	-5.110091	1.795484	0.370706
H	-1.942389	0.923986	1.397215
H	-3.183233	2.698761	-2.336316
H	-4.334590	0.900046	2.200256
H	-5.589533	2.669233	-1.566821
H	-6.157926	1.780515	0.711484
C	-1.007268	1.840964	-1.016032
O	-0.763998	1.998015	-2.211601

H	0.378828	-3.347493	2.189339
C	-2.359243	0.409582	-2.950519
H	-1.883717	0.269010	-3.943837
H	-3.027881	1.294225	-2.999114
H	-1.549342	0.653650	-2.217595
C	-4.221143	-1.222913	-3.550574
H	-4.934667	-0.388926	-3.720117
H	-3.756766	-1.454117	-4.531949
H	-4.806831	-2.108335	-3.226890
C	-1.942235	-0.054577	3.287909
H	-2.751147	0.561616	3.734966
H	-1.270049	-0.377419	4.110685
H	-1.349539	0.589932	2.607002
C	-3.290431	-2.216226	3.493781
H	-2.633089	-2.570191	4.315852
H	-4.155663	-1.698814	3.960243
H	-3.682967	-3.105641	2.957166
C	2.379013	1.872603	0.596851
C	2.765297	1.431339	-0.683688
C	3.365197	2.339491	1.493581
C	4.112628	1.455532	-1.069176
C	4.714388	2.364435	1.108706
C	5.091395	1.924256	-0.174273
H	1.983926	1.037155	-1.354049
H	3.046750	2.681018	2.490864
H	4.402504	1.089043	-2.066314
H	5.479393	2.730658	1.812330
H	6.151547	1.941785	-0.474320
C	0.942746	1.818029	1.062372
O	0.657283	1.932320	2.253634
H	0.069890	-4.021697	-1.333093
H	-2.045912	-3.678008	0.838521

Zero-point correction=	0.739026 (Hartree/Particle)
Thermal correction to Energy=	0.783426
Thermal correction to Enthalpy=	0.784370
Thermal correction to Gibbs Free Energy=	0.662200
Sum of electronic and zero-point Energies=	-1862.863247
Sum of electronic and thermal Energies=	-1862.818848
Sum of electronic and thermal Enthalpies=	-1862.817903
Sum of electronic and thermal Free Energies=	-1862.940073

Zero-point correction=	0.761380 (Hartree/Particle)
Thermal correction to Energy=	0.806405
Thermal correction to Enthalpy=	0.807349
Thermal correction to Gibbs Free Energy=	0.684058
Sum of electronic and zero-point Energies=	-1864.041313
Sum of electronic and thermal Energies=	-1863.996288
Sum of electronic and thermal Enthalpies=	-1863.995343
Sum of electronic and thermal Free Energies=	-1864.118635

IPr-XII			
90			
IPrXII SCF Done: -1863.63323391 A.U.			
Pd	0.214095	0.601693	0.511521
C	-0.156194	2.455575	1.578798
C	-0.491288	2.133325	2.938923
C	1.240028	2.479946	1.208052
C	0.510258	1.895638	3.881454
H	-1.548416	2.126540	3.244047
C	2.238699	2.217469	2.186982
H	1.525747	2.912590	0.236814
C	1.878340	1.934449	3.506059
H	0.234180	1.678241	4.925355
H	3.297069	2.243371	1.884499
H	2.656787	1.736878	4.260196
N	1.787761	-1.304092	-1.218825
N	-0.217806	-2.071618	-0.988374
C	0.588898	-1.028490	-0.601961
C	1.730884	-2.478657	-1.968627
C	0.457437	-2.969102	-1.820170
C	2.914045	-0.418006	-1.072935

SIPr-XII			
92			
SIPrXII SCF Done: -1864.83644498 A.U.			
Pd	0.210992	-0.619047	-0.477526
C	-0.174441	-2.532045	-1.442528
C	-0.495977	-2.298464	-2.824019
C	1.218317	-2.537766	-1.057264
C	0.515142	-2.123503	-3.769234
H	-1.550285	-2.308665	-3.138643
C	2.227041	-2.338632	-2.040938
H	1.496253	-2.911498	-0.059516
C	1.879931	-2.139604	-3.378437
H	0.250094	-1.974861	-4.827939
H	3.281609	-2.345382	-1.724651
H	2.665957	-1.992363	-4.136227
N	1.812595	1.348480	1.083431
N	-0.248051	2.063212	0.907766
C	0.595110	1.061850	0.551971
C	1.797344	2.534398	1.965085
C	0.438075	3.172837	1.607448
C	2.889426	0.402299	1.027739

C	3.824457	-0.655735	-0.013854	C	3.865431	0.557998	0.010729
C	4.856797	0.284503	0.173532	C	4.875653	-0.418724	-0.085176
C	4.966252	1.410850	-0.657175	C	4.909404	-1.507131	0.801092
C	4.047855	1.617017	-1.697166	C	3.934737	-1.636616	1.801912
C	2.998340	0.705387	-1.930509	C	2.903116	-0.685633	1.938451
C	3.633048	-1.825291	0.948983	C	3.749895	1.688511	-1.008273
H	5.775269	2.139405	-0.488184	H	5.703210	-2.265582	0.708183
C	1.984792	0.955573	-3.044669	C	1.849951	-0.835204	3.034554
C	-1.588325	-2.206388	-0.567426	C	-1.586306	2.194305	0.412500
C	-2.609731	-1.736524	-1.432113	C	-2.657896	1.827697	1.269926
C	-3.942797	-1.931231	-1.022279	C	-3.970003	2.032012	0.803874
C	-4.238982	-2.551334	0.201272	C	-4.204797	2.568213	-0.472417
C	-3.206590	-2.951846	1.060830	C	-3.131819	2.873390	-1.321143
C	-1.853729	-2.785351	0.697267	C	-1.797753	2.694029	-0.897787
C	-2.274381	-0.945153	-2.694129	C	-2.376506	1.128679	2.597430
H	-5.289363	-2.699110	0.499270	H	-5.239284	2.726394	-0.817449
C	-0.737047	-3.155768	1.670491	C	-0.641163	2.978516	-1.853504
H	2.590683	-2.852864	-2.532507	H	2.662786	3.197424	1.760618
H	-0.028402	-3.862438	-2.224155	H	-0.140895	3.505249	2.493135
H	5.576276	0.142453	0.994676	H	5.640477	-0.337717	-0.872950
H	4.139955	2.509217	-2.336377	H	3.970216	-2.498792	2.486587
H	2.965154	-2.561067	0.452144	H	3.142020	2.491459	-0.537268
H	1.267109	0.108708	-3.044717	H	1.065891	-0.068968	2.859231
H	-4.763632	-1.574368	-1.661617	H	-4.823575	1.752378	1.438804
H	-3.451947	-3.402422	2.035478	H	-3.330875	3.259475	-2.333654
H	-1.260319	-1.254556	-3.028468	H	-1.394790	1.499716	2.966426
H	0.229161	-3.062856	1.131778	H	0.307651	2.851506	-1.291280
C	-0.699820	-2.143195	2.835012	C	-0.617745	1.932611	-2.987587
H	-1.653456	-2.149139	3.404833	H	-1.555470	1.956827	-3.582549
H	0.124808	-2.382826	3.537845	H	0.233386	2.116369	-3.675471
H	-0.528248	-1.113131	2.447615	H	-0.495327	0.910288	-2.562723
C	-0.850260	-4.607643	2.173226	C	-0.671061	4.420160	-2.397188
H	-0.878001	-5.328873	1.330142	H	-0.681577	5.164742	-1.573755
H	0.017546	-4.861829	2.817215	H	0.220772	4.615161	-3.029184
H	-1.766334	-4.763634	2.781458	H	-1.567369	4.604269	-3.026608
C	-2.205968	0.559036	-2.345324	C	-2.223073	-0.390133	2.353902
H	-1.933670	1.160602	-3.237226	H	-1.966126	-0.918865	3.295423
H	-3.182082	0.921863	-1.959899	H	-3.164158	-0.822395	1.953843
H	-1.446936	0.752959	-1.555802	H	-1.422537	-0.602628	1.610432
C	-3.243880	-1.208754	-3.859675	C	-3.424127	1.417126	3.685647
H	-4.257654	-0.806273	-3.650502	H	-4.405026	0.956584	3.441842
H	-2.881988	-0.703372	-4.778802	H	-3.099350	0.983582	4.654145
H	-3.344558	-2.292708	-4.076782	H	-3.584343	2.506281	3.829016
C	2.908237	-1.344715	2.224864	C	2.965840	1.201416	-2.246184
H	2.685446	-2.199620	2.897627	H	2.783800	2.036773	-2.955065
H	3.533162	-0.616237	2.782999	H	3.530266	0.408224	-2.779708
H	1.954466	-0.832784	1.968819	H	1.987688	0.761362	-1.951220
C	4.948400	-2.553116	1.280647	C	5.105623	2.300608	-1.401354
H	5.641124	-1.909521	1.863303	H	5.730113	1.583943	-1.975665
H	4.745017	-3.451899	1.899602	H	4.953788	3.187287	-2.051763
H	5.479891	-2.877582	0.361954	H	5.686755	2.618148	-0.510645
C	1.167835	2.234486	-2.778567	C	1.138142	-2.199922	2.988113
H	1.815971	3.135201	-2.739422	H	1.841073	-3.041114	3.165349
H	0.417825	2.394072	-3.580826	H	0.356830	-2.251877	3.774764
H	0.623468	2.164548	-1.815005	H	0.639437	-2.367913	2.012995
C	2.669333	0.984639	-4.426585	C	2.473621	-0.566885	4.421422
H	1.914034	1.099480	-5.232236	H	1.698400	-0.604812	5.215767
H	3.377012	1.836559	-4.511642	H	3.244014	-1.329106	4.665854
H	3.241016	0.052432	-4.617733	H	2.966690	0.427315	4.463506
C	-2.588485	2.459203	0.596913	C	-2.616018	-2.467383	-0.485823
C	-2.990982	1.216480	1.139339	C	-3.010946	-1.259684	-1.107271
C	-3.555521	3.271266	-0.037896	C	-3.590068	-3.236858	0.190527
C	-4.331370	0.807139	1.062980	C	-4.350801	-0.843633	-1.065577

C -4.895317 2.863797 -0.110376	C -4.929137 -2.822780 0.228024
C -5.287942 1.629618 0.442742	C -5.314005 -1.623897 -0.402795
H -2.237914 0.537571 1.572524	H -2.254486 -0.608915 -1.574901
H -3.221310 4.219741 -0.485440	H -3.261890 -4.156606 0.698375
H -4.620036 -0.171202 1.474030	H -4.633850 0.108190 -1.537936
H -5.639557 3.508686 -0.604691	H -5.678685 -3.434180 0.755703
H -6.339530 1.305672 0.382268	H -6.364897 -1.293806 -0.369880
C -1.150930 2.928328 0.547251	C -1.180757 -2.934806 -0.393408
O -0.797406 3.713884 -0.343642	O -0.837419 -3.660384 0.551141
	H 0.541640 4.043067 0.918988
	H 1.851491 2.217283 3.031681
Zero-point correction= 0.740239 (Hartree/Particle)	Zero-point correction= 0.762563 (Hartree/Particle)
Thermal correction to Energy= 0.785315	Thermal correction to Energy= 0.808162
Thermal correction to Enthalpy= 0.786259	Thermal correction to Enthalpy= 0.809106
Thermal correction to Gibbs Free Energy= 0.660072	Thermal correction to Gibbs Free Energy= 0.682191
Sum of electronic and zero-point Energies= -1862.892995	Sum of electronic and zero-point Energies= -1864.073882
Sum of electronic and thermal Energies= -1862.847919	Sum of electronic and thermal Energies= -1864.028283
Sum of electronic and thermal Enthalpies= -1862.846975	Sum of electronic and thermal Enthalpies= -1864.027339
Sum of electronic and thermal Free Energies= -1862.973162	Sum of electronic and thermal Free Energies= -1864.154254

IMes-IV	**IPR*-IV**
48	122
IMesIV SCF Done: -1051.60758570 A.U.	ItPrIV SCF Done: -2820.25288244 A.U.
Pd -0.001719 0.004242 -1.694153	Pd 0.672727 0.052479 -1.950569
N -1.083961 0.011423 1.083132	N -0.079377 -1.092025 0.828087
N 1.085746 -0.007376 1.080844	N -0.011202 1.063214 0.785769
C -0.000019 0.002665 0.223182	C 0.025932 -0.037211 -0.051292
C -0.682723 0.006913 2.421170	C -0.181460 -0.667092 2.159387
C 0.687359 -0.004663 2.419719	C -0.146598 0.699694 2.130369
C -2.453754 0.009993 0.644696	C -0.113233 -2.464570 0.408382
C -3.115875 -1.228461 0.497045	C 1.108477 -3.136818 0.163219
C -4.464006 -1.205726 0.091601	C 1.047049 -4.498558 -0.186539
C -5.140600 0.002893 -0.170316	C -0.191496 -5.153387 -0.304750
C -4.434359 1.215369 -0.022644	C -1.390917 -4.448383 -0.122805
C -3.086878 1.245582 0.380743	C -1.369590 -3.082520 0.220287
C 2.454713 -0.009620 0.639767	C 2.420730 -2.355505 0.249999
C 3.119213 1.227000 0.487387	C 2.775235 -1.968297 1.682466
C 4.464686 1.200501 0.073331	C 3.532555 -0.801351 1.914829
C 5.137035 -0.010102 -0.190249	C 3.866224 -0.404143 3.219015
C 4.426657 -1.220351 -0.043383	C 3.448658 -1.176640 4.318951
C 3.081896 -1.246868 0.368972	C 2.710099 -2.352305 4.098801
H -1.407756 0.011737 3.240993	C 2.378146 -2.745573 2.789460
H 1.414137 -0.010508 3.237984	C 3.558560 -3.035846 -0.505525
H -4.998494 -2.162809 -0.030089	C 3.520093 -3.031427 -1.917666
H -4.947054 2.168747 -0.234693	C 4.533256 -3.650565 -2.664150
H 4.999598 2.156211 -0.056512	C 5.605618 -4.285492 -2.008754
H 4.933062 -2.174712 -0.265866	C 5.651731 -4.295259 -0.604224
C 6.593073 -0.019685 -0.600596	C 4.633361 -3.674110 0.143078
H 6.910992 0.958753 -1.013850	H -0.220047 -6.222474 -0.568488
H 7.249752 -0.240346 0.269940	C -2.633433 -2.227137 0.238536
H 6.796556 -0.798302 -1.364562	C -3.818611 -2.931920 0.889335
C -6.579112 0.004233 -0.638843	C -4.743908 -3.688477 0.140661
H -7.099849 -0.938191 -0.374396	C -5.804042 -4.356658 0.777957
H -7.151163 0.848537 -0.201463	C -5.958577 -4.271369 2.172983
H -6.634706 0.113272 -1.744456	C -5.044126 -3.514604 2.928115
C 2.371662 2.519007 0.708856	C -3.982777 -2.852692 2.288802
H 1.514839 2.582190 0.001778	C -2.936542 -1.635288 -1.147691
H 1.942354 2.577626 1.731610	C -4.076717 -0.816118 -1.308183

H	3.025168	3.399609	0.555176
C	2.294748	-2.530227	0.464504
H	2.934661	-3.416378	0.287060
H	1.806774	-2.641122	1.455887
H	1.476247	-2.520337	-0.290669
C	-2.365518	-2.518357	0.721349
H	-1.936792	-2.574615	1.744510
H	-3.016888	-3.400689	0.568518
H	-1.508144	-2.580752	0.014949
C	-2.305332	2.531986	0.481229
H	-2.948595	3.415828	0.304409
H	-1.820063	2.642855	1.473989
H	-1.485231	2.527433	-0.272164

C	-4.342073	-0.172162	-2.525311
C	-3.471405	-0.345329	-3.616642
C	-2.344620	-1.170589	-3.478411
C	-2.076885	-1.809733	-2.251846
C	0.023975	2.421480	0.313514
C	-1.208938	3.054430	0.030058
C	-1.187396	4.410617	-0.347455
C	0.030419	5.101154	-0.461681
C	1.245885	4.432893	-0.248822
C	1.265630	3.074908	0.123776
C	-2.504775	2.247615	0.122950
C	-2.990257	2.114413	1.566126
C	-2.774458	3.130070	2.519893
C	-3.210260	2.973813	3.848346
C	-3.874710	1.799478	4.243617
C	-4.108317	0.785511	3.296727
C	-3.669165	0.946677	1.973702
C	-3.566042	2.739388	-0.863355
C	-3.223590	2.808768	-2.233431
C	-4.163329	3.220477	-3.188226
C	-5.473641	3.552219	-2.792823
C	-5.826604	3.474305	-1.435538
C	-4.875949	3.076076	-0.475425
H	0.032046	6.165053	-0.746857
C	2.572224	2.284502	0.184827
C	3.686393	3.065407	0.872349
C	4.661657	3.783940	0.151457
C	5.643596	4.532501	0.825268
C	5.665746	4.570349	2.230273
C	4.696696	3.856086	2.959276
C	3.715726	3.112906	2.283263
C	2.928968	1.673277	-1.182189
C	4.088384	0.905200	-1.337486
C	4.300729	0.112740	-2.497939
C	3.350127	0.089521	-3.520002
C	2.180813	0.909386	-3.439526
C	1.975381	1.718315	-2.263816
H	-0.240699	-1.373306	2.991682
H	-0.226448	1.444415	2.927184
H	1.984150	-5.042141	-0.379872
H	-2.359791	-4.951886	-0.261460
H	2.229313	-1.401039	-0.304997
H	3.867361	-0.206848	1.051892
H	4.453766	0.514941	3.371724
H	3.704168	-0.865723	5.344498
H	2.387914	-2.969994	4.952740
H	1.790800	-3.662865	2.622763
H	2.688709	-2.514373	-2.424517
H	4.492483	-3.627747	-3.765111
H	6.405311	-4.768070	-2.593116
H	6.488584	-4.786975	-0.082615
H	4.676975	-3.676784	1.243509
H	-2.408757	-1.351714	0.884578
H	-4.637679	-3.735543	-0.954854
H	-6.518934	-4.942964	0.178688
H	-6.793541	-4.789418	2.670851
H	-5.160221	-3.437148	4.021140
H	-3.265846	-2.257655	2.879064
H	-4.774775	-0.685313	-0.466159
H	-5.218848	0.487889	-2.613407
H	-3.670260	0.172692	-4.567932
H	-1.654502	-1.316306	-4.324495
H	-1.187568	-2.450821	-2.159376

	H -2.138016 4.918444 -0.571074 H 2.202466 4.960633 -0.384684 H -2.254956 1.218097 -0.224100 H -2.243120 4.047463 2.221500 H -3.025932 3.776542 4.580346 H -4.211252 1.675714 5.285239 H -4.632206 -0.140156 3.584108 H -3.856229 0.151443 1.238562 H -2.208006 2.515186 -2.545858 H -3.878080 3.263897 -4.251466 H -6.216578 3.868199 -3.542380 H -6.849567 3.729271 -1.115273 H -5.158860 3.018905 0.586984 H 2.363666 1.406659 0.836025 H 4.655080 3.738648 -0.949048 H 6.399907 5.086743 0.246584 H 6.438408 5.152172 2.757550 H 4.707309 3.876875 4.060979 H 2.954011 2.554347 2.852405 H 4.839825 0.891512 -0.531339 H 5.204719 -0.510575 -2.570030 H 3.510808 -0.538469 -4.411155 H 1.588630 1.102067 -4.350552 H 1.251159 2.550230 -2.292508
Zero-point correction= 0.385694 (Hartree/Particle) Thermal correction to Energy= 0.411540 Thermal correction to Enthalpy= 0.412484 Thermal correction to Gibbs Free Energy= 0.326199 Sum of electronic and zero-point Energies= -1051.221891 Sum of electronic and thermal Energies= -1051.196046 Sum of electronic and thermal Enthalpies= -1051.195101 Sum of electronic and thermal Free Energies= -1051.281387	Zero-point correction= 0.966437 (Hartree/Particle) Thermal correction to Energy= 1.024295 Thermal correction to Enthalpy= 1.025240 Thermal correction to Gibbs Free Energy= 0.869666 Sum of electronic and zero-point Energies= -2819.286445 Sum of electronic and thermal Energies= -2819.228587 Sum of electronic and thermal Enthalpies= -2819.227643 Sum of electronic and thermal Free Energies= -2819.383216

IMes-V	**IPR*-V**
73	147
IMesV SCF Done: -1703.09171886 A.U.	ItPrV SCF Done: -3471.70129056 A.U.
C -0.198226 1.086562 1.290449	C -0.645678 3.490860 -1.687756
O -1.153934 1.334115 1.999372	O -1.686977 3.621125 -2.293739
Pd -0.392297 0.518539 -0.597098	Pd 0.184062 0.796418 -1.006769
O 0.505501 2.081953 -1.538995	O 0.358477 2.587529 -2.217265
C 3.878708 1.810830 2.489745	C 0.475827 5.785888 1.764411
C 2.811981 2.447532 3.156904	C -0.838462 5.830012 1.265843
H 4.444107 0.429676 0.897062	H 2.459717 4.914688 1.546404
C 3.619807 0.918127 1.436788	C 1.432291 4.953110 1.152248
C 1.489276 2.193072 2.770869	C -1.190609 5.064089 0.146481
C 1.226801 1.303579 1.700621	C -0.233439 4.220349 -0.466010
C 2.298919 0.671364 1.038204	C 1.080456 4.159983 0.053948
H 0.641273 2.677819 3.278450	H -2.209288 5.097514 -0.262751
H 2.085351 -0.009952 0.203403	H 1.817776 3.486187 -0.402374
H 4.917624 2.022014 2.789912	H 0.756433 6.396310 2.637478
H 3.017175 3.148512 3.981789	H -1.595369 6.468338 1.747535
C 1.836439 2.089902 -1.635362	C 1.405054 3.101144 -2.984310
C 2.566746 1.021141 -2.238132	C 2.645104 2.446788 -2.911897
C 2.585658 3.179364 -1.105645	C 1.213370 4.227585 -3.803426
C 3.968552 1.023655 -2.263102	C 3.711514 2.928549 -3.687337
H 1.997226 0.176845 -2.658780	H 2.762307 1.585917 -2.234591
C 3.986998 3.174709 -1.139109	C 2.297106 4.702219 -4.562338
H 2.027764 4.001808 -0.632147	H 0.227475 4.712415 -3.851742
C 4.694211 2.097166 -1.708954	C 3.545688 4.055991 -4.512550
H 4.504012 0.176948 -2.725760	H 4.684366 2.416250 -3.630738
H 4.540694 4.020033 -0.697916	H 2.156532 5.584922 -5.205983
H 5.795444 2.097363 -1.727793	H 4.387472 4.431694 -5.114426

N	-2.590257	-1.480698	0.114801
N	-0.618024	-2.381197	0.154215
C	-1.260938	-1.182825	-0.058211
C	-2.771333	-2.831271	0.419437
C	-1.523749	-3.401008	0.445298
C	-3.649682	-0.512889	-0.018227
C	-4.021401	-0.079874	-1.311310
C	-5.047241	0.880493	-1.406400
C	-5.688257	1.402796	-0.266228
C	-5.288210	0.933584	1.001827
C	-4.268428	-0.023076	1.155626
C	0.814789	-2.505421	0.079752
C	1.558784	-2.491701	1.279288
C	2.964085	-2.497844	1.175752
C	3.616436	-2.475717	-0.071665
C	2.830905	-2.504915	-1.243303
C	1.426793	-2.530697	-1.196282
H	-3.766858	-3.258475	0.574098
H	-1.198681	-4.428958	0.632687
H	-5.350524	1.233123	-2.406226
H	-5.777496	1.334211	1.905118
H	3.562910	-2.451945	2.099599
H	3.328608	-2.483099	-2.226783
C	5.118385	-2.353230	-0.175548
H	5.609197	-2.400669	0.816559
H	5.551571	-3.151558	-0.814445
H	5.387878	-1.381519	-0.644614
C	-6.751627	2.470206	-0.393482
H	-7.259229	2.430712	-1.378415
H	-7.522891	2.378193	0.398356
H	-6.301840	3.482716	-0.295299
C	0.861652	-2.354443	2.610809
H	0.278229	-1.408189	2.643253
H	0.141863	-3.178906	2.796669
H	1.588235	-2.333165	3.445287
C	0.595968	-2.510584	-2.456481
H	1.197764	-2.791691	-3.342073
H	-0.276486	-3.192209	-2.387725
H	0.186265	-1.490502	-2.634743
C	-3.324344	-0.593365	-2.549414
H	-3.034823	-1.659563	-2.454983
H	-3.964390	-0.479847	-3.446189
H	-2.387068	-0.021095	-2.731992
C	-3.821895	-0.490140	2.519981
H	-4.378014	0.033384	3.321394
H	-3.971406	-1.581999	2.657934
H	-2.741775	-0.278564	2.657741

N	-0.391604	-1.999010	0.018380
N	-0.189853	-0.559826	1.612523
C	-0.136177	-0.657652	0.236009
C	-0.585418	-2.701510	1.210726
C	-0.470644	-1.785701	2.222486
C	-0.458919	-2.571753	-1.293486
C	0.751752	-2.945459	-1.922859
C	0.679623	-3.507057	-3.209702
C	-0.564368	-3.691801	-3.837593
C	-1.748138	-3.290119	-3.202588
C	-1.716400	-2.705088	-1.920527
C	2.077968	-2.734733	-1.190457
C	2.370256	-3.913661	-0.264209
C	2.559382	-3.706408	1.117567
C	2.829817	-4.778030	1.985155
C	2.907026	-6.086802	1.479560
C	2.706627	-6.311581	0.104380
C	2.437545	-5.235318	-0.757215
C	3.207483	-2.340833	-2.141570
C	3.006316	-1.205772	-2.961496
C	4.014760	-0.756421	-3.824870
C	5.250722	-1.430161	-3.879368
C	5.463209	-2.552492	-3.061965
C	4.446663	-3.005410	-2.197166
H	-0.607920	-4.136687	-4.844203
C	-2.982402	-2.150407	-1.263549
C	-4.028083	-3.249441	-1.082291
C	-4.954356	-3.584423	-2.093564
C	-5.867287	-4.636846	-1.910865
C	-5.872853	-5.370169	-0.710607
C	-4.959465	-5.040702	0.306275
C	-4.045579	-3.989962	0.118521
C	-3.484629	-0.879081	-1.961391
C	-4.799586	-0.410814	-1.742296
C	-5.242781	0.791435	-2.319701
C	-4.374660	1.550722	-3.123307
C	-3.058461	1.107009	-3.330922
C	-2.616833	-0.095656	-2.753163
C	0.026639	0.682211	2.297291
C	-1.065792	1.576270	2.431639
C	-0.842619	2.771430	3.134885
C	0.408896	3.033269	3.720495
C	1.477174	2.139600	3.560055
C	1.316270	0.963992	2.797893
C	-2.403055	1.173696	1.812792
C	-3.119499	0.086094	2.617850
C	-2.863723	-0.146042	3.983778
C	-3.532968	-1.175637	4.672104
C	-4.467608	-1.983763	4.002350
C	-4.740867	-1.747439	2.641309
C	-4.073870	-0.718931	1.959418
C	-3.343436	2.320900	1.468103
C	-3.535129	2.653764	0.113694
C	-4.411396	3.689057	-0.252614
C	-5.100790	4.411584	0.736037
C	-4.926289	4.076459	2.093126
C	-4.063055	3.029191	2.455243
H	0.555524	3.961862	4.293276
C	2.490980	0.053717	2.442094
C	3.292394	-0.361259	3.676882
C	4.442896	0.337522	4.094270
C	5.132596	-0.050710	5.256611
C	4.687245	-1.149834	6.011364

	C 3.546046 -1.860830 5.596233 C 2.855586 -1.467012 4.438551 C 3.379327 0.603147 1.318910 C 4.120793 -0.306635 0.534159 C 4.987383 0.142946 -0.473861 C 5.145296 1.520419 -0.703030 C 4.416901 2.437915 0.072054 C 3.540025 1.979807 1.070863 H -0.770650 -3.779057 1.221400 H -0.587459 -1.881550 3.305308 H 1.611586 -3.778261 -3.729694 H -2.714472 -3.407680 -3.714997 H 1.939811 -1.839742 -0.545498 H 2.473565 -2.689147 1.526830 H 2.979008 -4.581492 3.058930 H 3.117680 -6.931824 2.154168 H 2.755946 -7.335371 -0.299792 H 2.269681 -5.420014 -1.830042 H 2.041705 -0.669761 -2.901484 H 3.835555 0.130274 -4.452660 H 6.044903 -1.079061 -4.557413 H 6.428074 -3.083666 -3.091863 H 4.625411 -3.879960 -1.553463 H -2.699345 -1.827923 -0.238737 H -4.976464 -2.994115 -3.023315 H -6.585013 -4.881638 -2.710208 H -6.592142 -6.191910 -0.565983 H -4.961349 -5.600597 1.255296 H -3.340745 -3.721781 0.922137 H -5.492795 -1.002134 -1.123298 H -6.270332 1.139756 -2.130182 H -4.715400 2.496393 -3.573151 H -2.355466 1.713843 -3.918586 H -1.575624 -0.418218 -2.908033 H -1.654134 3.507507 3.222008 H 2.456076 2.355056 4.015954 H -2.147748 0.713398 0.833801 H -2.119802 0.475026 4.508164 H -3.319601 -1.346836 5.739732 H -4.987034 -2.793292 4.539544 H -5.469761 -2.373672 2.103354 H -4.293908 -0.523081 0.897878 H -2.992811 2.094644 -0.665179 H -4.536804 3.927693 -1.319545 H -5.784869 5.227602 0.452531 H -5.479078 4.625438 2.872531 H -3.959109 2.739653 3.513808 H 2.051203 -0.879116 2.040872 H 4.809483 1.182752 3.490098 H 6.031122 0.504936 5.569554 H 5.232084 -1.457739 6.917866 H 3.194052 -2.729085 6.176263 H 1.961454 -2.023994 4.110448 H 4.026468 -1.388535 0.712796 H 5.529931 -0.589893 -1.090439 H 5.826199 1.876364 -1.491531 H 4.516508 3.519620 -0.112719 H 2.960621 2.701972 1.660867
Zero-point correction= 0.576155 (Hartree/Particle) Thermal correction to Energy= 0.615540 Thermal correction to Enthalpy= 0.616484 Thermal correction to Gibbs Free Energy= 0.501471 Sum of electronic and zero-point Energies= -1702.515564 Sum of electronic and thermal Energies= -1702.476179 Sum of electronic and thermal Enthalpies= -1702.475235	Zero-point correction= 1.159636 (Hartree/Particle) Thermal correction to Energy= 1.231169 Thermal correction to Enthalpy= 1.232113 Thermal correction to Gibbs Free Energy= 1.046704 Sum of electronic and zero-point Energies= -3470.541655 Sum of electronic and thermal Energies= -3470.470122 Sum of electronic and thermal Enthalpies= -3470.469177

Sum of electronic and thermal Free Energies= -1702.590248	Sum of electronic and thermal Free Energies= -3470.654586

IMes-V-VI			**IPR*-V-VI**		
73			147		
IMesV-VI SCF Done: -1703.07008902 A.U.			ItPrV-VI SCF Done: -3471.70220796 A.U.		
C	-1.370568	0.637911 -1.353703	C	0.261588	-2.982335 1.187028
O	-1.656488	0.113734 -2.415918	O	1.034595	-2.930616 2.126455
Pd	0.611184	0.279576 -0.708165	Pd	0.630830	-1.406906 -0.291215
O	-0.367879	1.991814 -1.538405	O	0.971842	-3.510971 -0.204706
C	-4.301138	1.251557 1.765759	C	-3.927887	-3.825018 1.844354
C	-4.690299	0.933579 0.452649	C	-3.093321	-3.335932 2.863497
H	-2.623323	1.620939 3.107746	H	-4.043537	-4.401323 -0.255043
C	-2.934687	1.372649 2.080842	C	-3.399892	-4.028100 0.556901
C	-3.718390	0.731534 -0.539336	C	-1.740174	-3.080086 2.603728
C	-2.348770	0.856632 -0.228044	C	-1.204669	-3.274177 1.309547
C	-1.963879	1.177520 1.088715	C	-2.057483	-3.733948 0.281529
H	-3.997767	0.465790 -1.569983	H	-1.071227	-2.716329 3.394456
H	-0.889050	1.255238 1.320532	H	-1.676839	-3.883249 -0.732742
H	-5.063728	1.406030 2.546027	H	-4.990862	-4.029517 2.045500
H	-5.758019	0.832920 0.201539	H	-3.495414	-3.153620 3.872566
C	-0.596625	3.162160 -0.862980	C	0.535354	-4.493706 -1.052990
C	-1.792100	3.877074 -1.092056	C	0.390476	-5.815732 -0.582692
C	0.366085	3.672570 0.033738	C	0.269145	-4.186074 -2.404624
C	-2.019437	5.088134 -0.420670	C	-0.046957	-6.816751 -1.463958
H	-2.533586	3.459236 -1.789021	H	0.603563	-6.029204 0.475324
C	0.134127	4.891598 0.691000	C	-0.157809	-5.199160 -3.278262
H	1.286872	3.090329 0.201783	H	0.372000	-3.141353 -2.738238
C	-1.060687	5.602578 0.472591	C	-0.324922	-6.516429 -2.811842
H	-2.958899	5.636474 -0.596735	H	-0.173367	-7.846258 -1.092432
H	0.892302	5.286269 1.386806	H	-0.374527	-4.950242 -4.329282
H	-1.244473	6.553553 0.996630	H	-0.668876	-7.307525 -3.495961
N	0.195805	-2.522075 0.410387	N	0.218491	1.226448 1.212173
N	2.263867	-1.886181 0.500829	N	0.432367	1.490909 -0.923974
C	1.015802	-1.462317 0.099764	C	0.334992	0.508596 0.040335
C	0.913829	-3.571880 0.987307	C	0.264146	2.603748 0.983467
C	2.223780	-3.170618 1.045110	C	0.395658	2.773536 -0.366255
C	-1.234987	-2.506082 0.247952	C	-0.196818	0.629836 2.456488
C	-1.790910	-2.787376 -1.019135	C	0.753428	0.003384 3.297942
C	-3.193339	-2.754486 -1.129420	C	0.277323	-0.579280 4.487121
C	-4.022811	-2.458056 -0.029956	C	-1.091592	-0.548154 4.807323
C	-3.422410	-2.177979 1.212702	C	-2.016741	0.058150 3.943574
C	-2.025896	-2.184409 1.374219	C	-1.578459	0.678023 2.757629
C	3.428551	-1.047634 0.397493	C	2.211446	-0.058540 2.843373
C	3.705584	-0.144338 1.450857	C	2.773684	1.325639 2.514607
C	4.838206	0.678678 1.321879	C	3.576385	1.482765 1.368554
C	5.673668	0.622601 0.185220	C	4.093004	2.739932 1.016356
C	5.345280	-0.276966 -0.848193	C	3.816948	3.864419 1.816208
C	4.220595	-1.121918 -0.768718	C	3.030206	3.715533 2.972246
H	0.425139	-4.501462 1.294885	C	2.510816	2.455075 3.317275
H	3.123605	-3.672793 1.413571	C	3.162800	-0.818227 3.765165
H	-3.649519	-2.949115 -2.114024	C	3.723464	-2.039135 3.336681
H	-4.055643	-1.902934 2.071248	C	4.626025	-2.738531 4.156368
H	5.072001	1.391755 2.130201	C	4.978745	-2.230496 5.418456
H	5.976242	-0.316754 -1.751472	C	4.426774	-1.011921 5.854034
C	6.863238	1.547671 0.055991	C	3.531609	-0.309979 5.030183
H	7.286630	1.812939 1.046001	H	-1.443328	-1.031708 5.732461
H	7.670591	1.096090 -0.555649	C	-2.529131	1.435244 1.834830
H	6.568885	2.498462 -0.440474	C	-2.765687	2.875548 2.296672
C	-5.523780	-2.408521 -0.200428	C	-3.006053	3.216900 3.643603
H	-5.930958	-3.399166 -0.496721	C	-3.256630	4.550777 4.012927

H	-6.033058	-2.093896	0.731785
H	-5.806820	-1.690279	-0.999097
C	2.768151	-0.043345	2.629345
H	1.779949	0.338862	2.287513
H	2.579007	-1.034409	3.092633
H	3.161450	0.639580	3.406904
C	3.820430	-2.036692	-1.900538
H	4.554502	-2.004597	-2.728389
H	3.718088	-3.089980	-1.564000
H	2.826852	-1.733052	-2.298010
C	-0.911875	-3.038873	-2.217776
H	-0.013526	-3.635331	-1.959311
H	-1.467112	-3.561009	-3.021188
H	-0.563324	-2.063977	-2.622288
C	-1.375435	-1.818459	2.686585
H	-2.125452	-1.461613	3.418218
H	-0.832234	-2.677992	3.135245
H	-0.628659	-1.010178	2.536154

C	-3.266758	5.566011	3.040096
C	-3.019495	5.236909	1.695184
C	-2.767990	3.905127	1.330486
C	-3.807992	0.675982	1.473562
C	-5.094412	1.176105	1.753871
C	-6.235869	0.546373	1.223377
C	-6.099966	-0.574734	0.386576
C	-4.818300	-1.090571	0.118777
C	-3.683830	-0.486292	0.679626
C	0.452268	1.229782	-2.336873
C	-0.775971	0.981509	-2.998461
C	-0.744891	0.813813	-4.396231
C	0.464759	0.888986	-5.104098
C	1.673284	1.092195	-4.421114
C	1.689403	1.250270	-3.022196
C	-2.093038	0.871867	-2.226795
C	-2.864229	2.189840	-2.122948
C	-2.320700	3.413881	-2.565293
C	-3.023795	4.621510	-2.392552
C	-4.287769	4.623515	-1.779408
C	-4.839493	3.408262	-1.334475
C	-4.135433	2.206807	-1.501326
C	-2.894807	-0.324885	-2.746768
C	-2.413765	-1.618743	-2.449395
C	-3.077384	-2.758159	-2.927640
C	-4.243034	-2.622466	-3.705359
C	-4.724779	-1.338584	-4.011665
C	-4.049686	-0.196455	-3.542345
H	0.467149	0.768695	-6.198861
C	3.000976	1.322840	-2.245057
C	3.959476	2.345478	-2.850971
C	4.938841	1.987379	-3.800706
C	5.767054	2.965304	-4.378900
C	5.631609	4.315570	-4.011281
C	4.663804	4.682033	-3.058377
C	3.835767	3.703140	-2.484909
C	3.612163	-0.065672	-2.016121
C	4.856454	-0.165217	-1.353141
C	5.398340	-1.415059	-1.016247
C	4.710510	-2.596636	-1.351150
C	3.488035	-2.514366	-2.032851
C	2.936978	-1.258021	-2.354596
H	0.180024	3.325733	1.798266
H	0.448160	3.674028	-0.983518
H	0.989670	-1.090449	5.150701
H	-3.094589	0.036996	4.168891
H	2.178059	-0.624782	1.883730
H	3.776286	0.600529	0.740205
H	4.705907	2.847224	0.106686
H	4.215293	4.853220	1.538395
H	2.808973	4.589735	3.605705
H	1.860636	2.352703	4.201407
H	3.428370	-2.447507	2.358682
H	5.053390	-3.691551	3.805254
H	5.684722	-2.780024	6.061643
H	4.700676	-0.601088	6.839176
H	3.118030	0.651608	5.372354
H	-2.018037	1.533630	0.857444
H	-2.989103	2.433862	4.416618
H	-3.442056	4.797630	5.070645
H	-3.461599	6.610688	3.330775
H	-3.021083	6.017886	0.918150
H	-2.565537	3.656104	0.278170

	H -5.201156 2.090931 2.356725 H -7.235488 0.954261 1.444032 H -6.989375 -1.042844 -0.064110 H -4.691423 -1.948260 -0.557017 H -2.682284 -0.897975 0.465270 H -1.687939 0.611613 -4.926874 H 2.625233 1.117984 -4.972933 H -1.825305 0.600720 -1.182097 H -1.336172 3.423433 -3.058413 H -2.578276 5.565320 -2.745770 H -4.837738 5.567594 -1.640870 H -5.819994 3.391016 -0.833781 H -4.575900 1.267333 -1.139112 H -1.501623 -1.714580 -1.824728 H -2.678543 -3.759320 -2.698600 H -4.769498 -3.516321 -4.076295 H -5.632662 -1.220762 -4.624781 H -4.433669 0.805463 -3.788521 H 2.751530 1.695758 -1.229096 H 5.062327 0.927193 -4.073587 H 6.528135 2.668522 -5.118216 H 6.284207 5.080654 -4.460859 H 4.556930 5.736195 -2.756301 H 3.082670 3.987733 -1.731288 H 5.406913 0.754667 -1.099271 H 6.362292 -1.465948 -0.485657 H 5.129285 -3.579072 -1.082935 H 2.939975 -3.429955 -2.301262 H 1.984199 -1.207188 -2.904341
Zero-point correction= 0.575278 (Hartree/Particle) Thermal correction to Energy= 0.614158 Thermal correction to Enthalpy= 0.615102 Thermal correction to Gibbs Free Energy= 0.500652 Sum of electronic and zero-point Energies= -1702.494811 Sum of electronic and thermal Energies= -1702.455931 Sum of electronic and thermal Enthalpies= -1702.454987 Sum of electronic and thermal Free Energies= -1702.569437	Zero-point correction= 1.158471 (Hartree/Particle) Thermal correction to Energy= 1.229129 Thermal correction to Enthalpy= 1.230073 Thermal correction to Gibbs Free Energy= 1.049237 Sum of electronic and zero-point Energies= -3470.543737 Sum of electronic and thermal Energies= -3470.473079 Sum of electronic and thermal Enthalpies= -3470.472135 Sum of electronic and thermal Free Energies= -3470.652971

IMes-VI	**IPR*-VI**
73 IMesVI SCF Done: -1703.09435142 A.U. Pd 0.597104 0.640575 0.046438 C -0.606004 0.062554 -1.417193 O -0.158411 -0.327463 -2.481752 O 0.249368 2.629547 0.026864 C -4.808293 0.788030 -0.797837 C -4.321519 0.434985 -2.073283 H -4.300708 1.148173 1.291756 C -3.931029 0.859503 0.296944 C -2.956678 0.179937 -2.257041 C -2.067144 0.266873 -1.159822 C -2.567092 0.594118 0.117005 H -2.549493 -0.079770 -3.246111 H -1.864040 0.657074 0.960374 H -5.877759 1.015823 -0.661789 H -5.011983 0.373173 -2.929597 C -0.943779 3.180830 0.260653 C -1.433986 3.361304 1.585643 C -1.776462 3.595224 -0.817357 C -2.704736 3.910126 1.815071 H -0.788285 3.043012 2.420339 C -3.047976 4.133741 -0.578143	147 ItPrVI SCF Done: -3471.72755018 A.U. Pd -0.424001 -0.359807 -1.526632 C 0.255066 -2.186781 -1.192333 O 1.421493 -2.430785 -1.423875 O -1.393723 -0.684525 -3.278262 C -2.586296 -5.250602 -0.159103 C -1.224545 -5.568109 -0.338324 H -4.085224 -3.655644 -0.157930 C -3.026377 -3.922300 -0.292325 C -0.304134 -4.562606 -0.663054 C -0.745893 -3.226667 -0.802155 C -2.104082 -2.916395 -0.606822 H 0.764277 -4.785054 -0.806341 H -2.431428 -1.874365 -0.714996 H -3.307279 -6.047650 0.084173 H -0.881380 -6.609040 -0.226300 C -2.200281 -1.730346 -3.496832 C -3.603388 -1.633492 -3.292950 C -1.673120 -2.984239 -3.912645 C -4.436039 -2.749000 -3.470795 H -4.010841 -0.670717 -2.954425 C -2.511180 -4.094636 -4.083297

H	-1.403806	3.441356	-1.841924
C	-3.526806	4.293471	0.737277
H	-3.062883	4.036163	2.850900
H	-3.682576	4.423209	-1.432066
H	-4.527715	4.714927	0.920472
N	2.578097	-1.574538	0.302341
N	0.586637	-2.405894	0.496008
C	1.251324	-1.216560	0.300307
C	2.740563	-2.945230	0.499731
C	1.480200	-3.471357	0.622249
C	3.636491	-0.620435	0.089909
C	4.205681	0.017981	1.212869
C	5.218021	0.968065	0.977965
C	5.646240	1.287412	-0.326435
C	5.036089	0.632327	-1.417111
C	4.019743	-0.323635	-1.238165
C	-0.846593	-2.522517	0.551601
C	-1.532313	-3.027423	-0.578768
C	-2.937357	-3.072463	-0.519862
C	-3.651218	-2.642514	0.615503
C	-2.922943	-2.173521	1.727110
C	-1.518010	-2.100128	1.721096
H	3.730346	-3.410556	0.535945
H	1.134563	-4.494867	0.795881
H	5.675737	1.481649	1.839563
H	5.352198	0.883163	-2.443295
H	-3.492293	-3.438180	-1.399163
H	-3.467458	-1.830957	2.622348
C	-5.160406	-2.625262	0.614789
H	-5.583413	-3.458839	0.018111
H	-5.576492	-2.682137	1.640806
H	-5.519986	-1.675762	0.160238
C	6.704135	2.341957	-0.561785
H	7.313764	2.525313	0.345595
H	7.388389	2.056808	-1.387315
H	6.235023	3.308804	-0.847761
C	-0.780681	-3.475560	-1.808970
H	-0.092887	-2.681498	-2.165288
H	-0.165206	-4.378496	-1.608448
H	-1.478629	-3.718014	-2.633285
C	-0.758196	-1.529929	2.893716
H	-1.386316	-1.497846	3.805049
H	0.159863	-2.112188	3.115839
H	-0.423472	-0.492703	2.665052
C	3.695524	-0.284434	2.602386
H	3.752834	-1.368294	2.837727
H	4.266161	0.268685	3.372930
H	2.624549	0.002283	2.693917
C	3.317074	-0.980047	-2.401440
H	3.797707	-0.716857	-3.363225
H	3.313305	-2.086636	-2.305703
H	2.252181	-0.660655	-2.445032

H	-0.582950	-3.062171	-4.051224
C	-3.898706	-3.990267	-3.859743
H	-5.519077	-2.651045	-3.286476
H	-2.074764	-5.062160	-4.381706
H	-4.551805	-4.867912	-3.985435
N	0.632869	1.813749	0.113645
N	0.529795	0.089745	1.414451
C	0.349638	0.468542	0.105532
C	0.935317	2.274778	1.396514
C	0.868019	1.184674	2.219973
C	0.586635	2.600745	-1.089327
C	-0.643075	3.200455	-1.455967
C	-0.671501	3.978273	-2.626566
C	0.492831	4.146675	-3.396648
C	1.688816	3.509229	-3.033327
C	1.751163	2.701023	-1.880531
C	-1.867218	2.980473	-0.568612
C	-1.789727	3.818224	0.706118
C	-2.311694	3.298391	1.909175
C	-2.178192	4.000301	3.116638
C	-1.532540	5.250359	3.134295
C	-1.034041	5.792566	1.936632
C	-1.160345	5.079326	0.730606
C	-3.189593	3.061432	-1.329236
C	-3.432461	2.118295	-2.355494
C	-4.646252	2.132119	-3.059891
C	-5.636217	3.084486	-2.749036
C	-5.399252	4.024261	-1.732423
C	-4.180977	4.013333	-1.026496
H	0.459516	4.766833	-4.306101
C	2.985535	1.868565	-1.547117
C	4.248572	2.728293	-1.556612
C	5.108482	2.797797	-2.671055
C	6.235123	3.639495	-2.651811
C	6.519715	4.418232	-1.516509
C	5.667909	4.353595	-0.398283
C	4.541150	3.516090	-0.422192
C	3.078717	0.590209	-2.393474
C	4.144184	-0.307193	-2.155310
C	4.252426	-1.506235	-2.875875
C	3.283702	-1.838445	-3.840635
C	2.215316	-0.961716	-4.078435
C	2.116334	0.246045	-3.364037
C	0.266444	-1.250993	1.866810
C	1.318799	-2.205295	1.848041
C	1.002350	-3.521386	2.224502
C	-0.307322	-3.868921	2.595756
C	-1.321575	-2.904746	2.623503
C	-1.052630	-1.569329	2.264686
C	2.731721	-1.788758	1.417998
C	3.301798	-0.697122	2.324592
C	3.044067	-0.677965	3.711959
C	3.566558	0.342604	4.526193
C	4.355133	1.361416	3.962129
C	4.632327	1.340884	2.582891
C	4.113382	0.315916	1.775939
C	3.705195	-2.967153	1.290654
C	3.886561	-3.594836	0.039505
C	4.753720	-4.693192	-0.091792
C	5.452097	-5.185756	1.024450
C	5.279954	-4.565203	2.274352
C	4.417571	-3.462991	2.404141
H	-0.540965	-4.912379	2.855655

	C	-2.108690	-0.466709	2.382630
	C	-2.231065	0.050579	3.827152
	C	-3.357550	0.811267	4.213357
	C	-3.442672	1.377396	5.496212
	C	-2.399908	1.196259	6.422523
	C	-1.278758	0.434340	6.053584
	C	-1.198203	-0.136248	4.770915
	C	-3.453869	-0.802589	1.742511
	C	-3.790559	-0.236919	0.495006
	C	-5.017960	-0.519613	-0.126146
	C	-5.932342	-1.388771	0.492754
	C	-5.617872	-1.949167	1.744706
	C	-4.394994	-1.648997	2.368317
	H	1.137750	3.329639	1.601312
	H	1.041011	1.083646	3.293433
	H	-1.620390	4.442118	-2.935975
	H	2.588371	3.615708	-3.658943
	H	-1.801745	1.923380	-0.225985
	H	-2.817451	2.320011	1.898462
	H	-2.564140	3.554842	4.046658
	H	-1.417774	5.800541	4.081756
	H	-0.534038	6.774453	1.940211
	H	-0.743876	5.495371	-0.200337
	H	-2.668207	1.361823	-2.611229
	H	-4.817270	1.391511	-3.857614
	H	-6.589844	3.092805	-3.300576
	H	-6.167723	4.772820	-1.481311
	H	-4.001196	4.744731	-0.223269
	H	2.865637	1.522846	-0.498933
	H	4.899336	2.171968	-3.553072
	H	6.899174	3.682166	-3.529958
	H	7.406023	5.072135	-1.500637
	H	5.884344	4.957564	0.497637
	H	3.869786	3.463868	0.451519
	H	4.914986	-0.048679	-1.410800
	H	5.091245	-2.189796	-2.670279
	H	3.355004	-2.788553	-4.393078
	H	1.425640	-1.217639	-4.801063
	H	1.272057	0.918886	-3.572303
	H	1.790771	-4.287472	2.200361
	H	-2.341726	-3.195368	2.907818
	H	2.627915	-1.350245	0.400741
	H	2.401540	-1.458850	4.150887
	H	3.350039	0.345823	5.606573
	H	4.757383	2.166821	4.596845
	H	5.254372	2.127097	2.126557
	H	4.333050	0.301897	0.697320
	H	3.333126	-3.217396	-0.831043
	H	4.884201	-5.165396	-1.078987
	H	6.132293	-6.046267	0.920886
	H	5.826821	-4.936274	3.156061
	H	4.305518	-2.977276	3.385583
	H	-1.720618	0.397002	1.803176
	H	-4.181533	0.959704	3.498266
	H	-4.332740	1.965148	5.772532
	H	-2.465641	1.639345	7.428750
	H	-0.458860	0.273722	6.771880
	H	-0.319070	-0.742879	4.503749
	H	-3.071053	0.418835	-0.019161
	H	-5.252070	-0.047811	-1.092452
	H	-6.893821	-1.619130	0.007592
	H	-6.335525	-2.618132	2.245935
	H	-4.181277	-2.052118	3.370863

Zero-point correction= 0.576459 (Hartree/Particle)	Zero-point correction= 1.158714 (Hartree/Particle)
Thermal correction to Energy= 0.615698	Thermal correction to Energy= 1.230250
Thermal correction to Enthalpy= 0.616642	Thermal correction to Enthalpy= 1.231194
Thermal correction to Gibbs Free Energy= 0.501907	Thermal correction to Gibbs Free Energy= 1.047971
Sum of electronic and zero-point Energies= -1702.517892	Sum of electronic and zero-point Energies= -3470.568836
Sum of electronic and thermal Energies= -1702.478653	Sum of electronic and thermal Energies= -3470.497301
Sum of electronic and thermal Enthalpies= -1702.477709	Sum of electronic and thermal Enthalpies= -3470.496356
Sum of electronic and thermal Free Energies= -1702.592445	Sum of electronic and thermal Free Energies= -3470.679579

IMes-VII			**IPR*-VII**		
79			153		
IMesVII SCF Done: -3166.92207010 A.U.			ItPrVII SCF Done: -4935.54674951 A.U.		
Pd	-0.260380	-0.098434	0.345463	Pd	-1.027516	-0.881913	-0.783592
C	0.742619	-0.877227	1.873217	C	0.341681	-2.017839	-1.652099
O	0.197310	-1.516226	2.775675	O	0.743385	-1.734332	-2.780759
O	0.049445	1.811389	1.225177	O	-2.457419	-2.335020	-1.435878
C	4.924349	0.156191	2.331506	C	1.385075	-5.790243	0.175839
C	4.125129	-0.113286	3.461037	C	1.717657	-5.537882	-1.171404
H	4.983035	0.280412	0.154942	H	0.500219	-4.981851	1.996256
C	4.366337	0.076860	1.044310	C	0.734221	-4.805041	0.935450
C	2.775979	-0.458460	3.299796	C	1.386054	-4.309683	-1.759170
C	2.203486	-0.516882	2.007383	C	0.721260	-3.317842	-1.001186
C	3.011438	-0.251786	0.885477	C	0.412350	-3.574204	0.347977
H	2.135088	-0.683547	4.166437	H	1.622626	-4.091878	-2.812459
H	2.571699	-0.326407	-0.118664	H	-0.065235	-2.775714	0.932922
H	5.984225	0.430254	2.458968	H	1.650818	-6.755005	0.636207
H	4.560841	-0.050992	4.471465	H	2.233793	-6.310603	-1.763984
K	-2.620581	2.042491	0.942107	K	-4.147134	-0.541918	-2.573716
K	0.180683	4.446830	-2.030591	K	-5.692846	-1.730581	1.750536
C	-1.217571	2.015616	-1.665599	C	-3.775422	-0.202759	0.293278
O	-1.837128	3.103236	-1.288239	O	-4.986152	-0.244578	-0.196552
O	-0.291853	2.025411	-2.546512	O	-3.491484	-0.671933	1.442601
O	-1.577369	0.878835	-1.071619	O	-2.828151	0.358470	-0.453095
C	0.957751	2.693339	0.857217	C	-3.068646	-3.229883	-0.674862
C	1.860967	2.489180	-0.234632	C	-2.799672	-3.418448	0.718628
C	1.054624	3.945562	1.547896	C	-4.099527	-4.047340	-1.243885
C	2.821919	3.453314	-0.576917	C	-3.515816	-4.355141	1.478521
H	1.753474	1.566259	-0.821678	H	-2.068488	-2.757134	1.201244
C	2.003490	4.912350	1.180185	C	-4.827826	-4.963284	-0.467691
H	0.368958	4.122035	2.392748	H	-4.304067	-3.945601	-2.323492
C	2.906242	4.680750	0.117753	C	-4.548755	-5.132483	0.905612
H	3.518515	3.241274	-1.406605	H	-3.263820	-4.474928	2.546962
H	2.053565	5.859588	1.743697	H	-5.614204	-5.570726	-0.947283
H	3.670914	5.428303	-0.145488	H	-5.097427	-5.876007	1.505482
N	0.015551	-2.816528	-0.959980	N	0.978512	1.439985	-0.946640
N	-2.045351	-2.391592	-0.440490	N	0.397531	0.968012	1.092650
C	-0.774795	-1.867127	-0.367100	C	0.268088	0.518868	-0.206637
C	-0.736698	-3.909862	-1.393967	C	1.464131	2.470260	-0.134453
C	-2.038868	-3.642128	-1.062915	C	1.120196	2.162940	1.150379
C	1.423782	-2.641160	-1.201818	C	1.430779	1.283234	-2.308307
C	2.342389	-3.305310	-0.355466	C	0.518412	1.451121	-3.375388
C	3.711686	-3.111416	-0.603418	C	1.010786	1.379408	-4.689748
C	4.166605	-2.277309	-1.646516	C	2.360488	1.087199	-4.935080
C	3.214287	-1.631109	-2.457062	C	3.232783	0.859448	-3.865263
C	1.824938	-1.792954	-2.260702	C	2.794594	0.968552	-2.528509
C	-3.238158	-1.691304	-0.033958	C	-0.960684	1.655627	-3.073462
C	-3.974668	-0.992256	-1.020116	C	-1.293649	3.050975	-2.558555
C	-5.104260	-0.264936	-0.592013	C	-2.308839	3.201696	-1.587265
C	-5.496785	-0.224056	0.763300	C	-2.680363	4.482471	-1.143773
C	-4.738649	-0.950719	1.707444	C	-2.027467	5.625920	-1.641899
C	-3.605777	-1.705087	1.331560	C	-1.002093	5.479213	-2.593424
H	-0.274611	-4.761699	-1.901664	C	-0.641526	4.199157	-3.052700

H	-2.959221	-4.214957	-1.211733
H	4.445644	-3.599239	0.058669
H	3.555372	-0.971426	-3.272239
H	-5.684195	0.298482	-1.341915
H	-5.043145	-0.946379	2.767793
C	-6.731686	0.544214	1.184942
H	-6.885351	1.449144	0.561297
H	-7.644107	-0.082074	1.074087
H	-6.681046	0.857603	2.248006
C	5.649939	-2.075830	-1.858736
H	6.134194	-1.709174	-0.928429
H	6.152061	-3.029941	-2.128134
H	5.857684	-1.343860	-2.664568
C	-3.517398	-0.977483	-2.455128
H	-2.534464	-0.456341	-2.490525
H	-3.388031	-2.001458	-2.863084
H	-4.231595	-0.430359	-3.100005
C	-2.802931	-2.487509	2.336993
H	-3.308270	-2.515386	3.322040
H	-2.648047	-3.532793	1.995164
H	-1.785914	-2.052648	2.474950
C	1.854655	-4.136108	0.807270
H	1.201731	-4.971283	0.476483
H	2.702147	-4.565420	1.375378
H	1.251592	-3.516588	1.504443
C	0.824481	-1.057666	-3.115297
H	1.249710	-0.828857	-4.112607
H	-0.107232	-1.641716	-3.256765
H	0.512589	-0.084679	-2.660685

C	-1.855197	1.167023	-4.210716
C	-1.724045	-0.182722	-4.630817
C	-2.553443	-0.701108	-5.639512
C	-3.538260	0.112758	-6.239386
C	-3.674640	1.450794	-5.826415
C	-2.835228	1.976114	-4.821919
H	2.728270	1.011255	-5.970355
C	3.780257	0.735460	-1.378541
C	4.680844	1.958366	-1.145900
C	5.582472	2.412256	-2.133850
C	6.416202	3.517088	-1.898067
C	6.370975	4.190683	-0.663132
C	5.486799	3.742893	0.331732
C	4.651091	2.639023	0.088223
C	4.575383	-0.574053	-1.516707
C	5.843476	-0.706472	-0.909651
C	6.530909	-1.931754	-0.934673
C	5.968922	-3.045259	-1.582129
C	4.708955	-2.923025	-2.192066
C	4.013521	-1.701885	-2.155970
C	-0.054333	0.163775	2.206854
C	0.772358	-0.922476	2.613936
C	0.233419	-1.826050	3.546325
C	-1.047057	-1.619361	4.086654
C	-1.785177	-0.478059	3.756194
C	-1.302288	0.447970	2.812336
C	2.217110	-1.012488	2.106324
C	3.127891	0.065561	2.735685
C	2.692220	0.976577	3.718323
C	3.573977	1.934599	4.252529
C	4.913309	1.980988	3.831101
C	5.364628	1.057980	2.869471
C	4.480331	0.113870	2.328435
C	2.929882	-2.356058	2.260898
C	3.411701	-3.027116	1.121291
C	4.150133	-4.215320	1.239333
C	4.413677	-4.758208	2.507061
C	3.963030	-4.082459	3.656890
C	3.245468	-2.881722	3.534483
H	-1.464825	-2.356169	4.791064
C	-2.016738	1.754073	2.450359
C	-1.198425	2.961818	2.924684
C	-1.144524	4.124723	2.129390
C	-0.361619	5.224073	2.514093
C	0.378639	5.181652	3.710284
C	0.313292	4.035718	4.523567
C	-0.472278	2.936073	4.134005
C	-3.457739	1.913198	2.935426
C	-4.493945	2.098411	1.997228
C	-5.830847	2.225242	2.408674
C	-6.156787	2.186379	3.777520
C	-5.126512	2.053912	4.727193
C	-3.789808	1.934099	4.307918
H	2.034333	3.304025	-0.550639
H	1.334362	2.674872	2.090078
H	0.315085	1.520186	-5.530359
H	4.271206	0.554809	-4.062578
H	-1.184126	0.947796	-2.233518
H	-2.778056	2.293024	-1.166134
H	-3.480351	4.585213	-0.392143
H	-2.314014	6.628515	-1.285835
H	-0.479813	6.367548	-2.983892
H	0.159931	4.086219	-3.800760

	H -0.958418 -0.817234 -4.151807 H -2.432656 -1.750133 -5.954905 H -4.189124 -0.293591 -7.030116 H -4.435428 2.097400 -6.292877 H -2.945211 3.023978 -4.502238 H 3.187777 0.610514 -0.447033 H 5.647988 1.886981 -3.097709 H 7.111502 3.851759 -2.684537 H 7.026809 5.056425 -0.478444 H 5.445176 4.243577 1.312206 H 3.971633 2.291553 0.877760 H 6.295810 0.163362 -0.408868 H 7.514504 -2.013956 -0.445403 H 6.508708 -4.005184 -1.605301 H 4.245805 -3.790970 -2.686299 H 3.017137 -1.635928 -2.619181 H 0.814813 -2.709521 3.842990 H -2.781526 -0.323449 4.190317 H 2.185581 -0.807197 1.012381 H 1.647725 0.953907 4.061983 H 3.202854 2.648769 5.004716 H 5.603832 2.729449 4.251147 H 6.408274 1.087727 2.519159 H 4.839388 -0.602188 1.572586 H 3.207803 -2.618902 0.121126 H 4.508161 -4.712887 0.325896 H 4.984699 -5.695491 2.604003 H 4.191269 -4.482528 4.657993 H 2.955298 -2.324240 4.439204 H -2.049489 1.773865 1.339843 H -1.684424 4.145806 1.171189 H -0.314243 6.111412 1.862724 H 1.005129 6.037557 4.007676 H 0.883351 3.993359 5.465677 H -0.496155 2.029370 4.759623 H -4.252227 2.112081 0.924403 H -6.619877 2.349724 1.649603 H -7.204455 2.286628 4.105062 H -5.362858 2.057371 5.803677 H -2.991019 1.862199 5.062637
Zero-point correction= 0.594429 (Hartree/Particle) Thermal correction to Energy= 0.641401 Thermal correction to Enthalpy= 0.642345 Thermal correction to Gibbs Free Energy= 0.511453 Sum of electronic and zero-point Energies= -3166.327641 Sum of electronic and thermal Energies= -3166.280669 Sum of electronic and thermal Enthalpies= -3166.279725 Sum of electronic and thermal Free Energies= -3166.410617	Zero-point correction= 1.176599 (Hartree/Particle) Thermal correction to Energy= 1.255806 Thermal correction to Enthalpy= 1.256750 Thermal correction to Gibbs Free Energy= 1.056733 Sum of electronic and zero-point Energies= -4934.370151 Sum of electronic and thermal Energies= -4934.290944 Sum of electronic and thermal Enthalpies= -4934.290000 Sum of electronic and thermal Free Energies= -4934.490016

IMes-VII-VIII	**IPR*-VII-VIII**
79 IMesVII-VIIIFFlllall SCF Done: -3166.89620348 A.U. Pd 0.485520 -0.087984 -0.416212 C 0.168477 -0.240925 1.546225 O 1.094097 -0.475676 2.343468 O -0.367658 -2.705258 0.420519 C -3.899713 -0.299586 2.999493 C -2.824444 -0.555323 3.875641 H -4.481645 0.196914 0.958658 C -3.649667 0.010317 1.653443 C -1.508148 -0.510329 3.399544 C -1.246982 -0.197524 2.043895	153 ItPrVII-VIII SCF Done: -4935.53022151 A.U. Pd -1.279367 -0.788230 -0.377259 C -0.034410 -1.923351 -1.411228 O 0.007739 -1.795183 -2.649052 O -2.494633 -3.054563 -1.248658 C 2.203070 -5.097810 0.456153 C 2.001204 -5.091160 -0.937841 H 1.830340 -4.058511 2.338954 C 1.674927 -4.065750 1.249557 C 1.297999 -4.041569 -1.540256 C 0.762737 -2.998799 -0.748124

C	-2.330356	0.065561	1.178927	C	0.940425	-3.034185	0.649177
H	-0.652033	-0.725391	4.057777	H	1.118633	-4.022723	-2.625237
H	-2.124329	0.315827	0.127594	H	0.492381	-2.236555	1.255715
H	-4.936317	-0.353471	3.369367	H	2.771129	-5.917000	0.924600
H	-3.021222	-0.802413	4.931528	H	2.392543	-5.915051	-1.554500
K	2.212761	-2.370280	0.917154	K	-2.472189	-1.219344	-3.318366
K	-0.135343	-3.925864	-2.007690	K	-4.785260	-2.596254	-0.053160
C	1.137538	-1.528812	-2.608585	C	-3.897722	0.014407	-0.062077
O	1.633589	-1.998912	-1.474671	O	-3.668542	-0.551315	-1.238189
O	0.992588	-2.261847	-3.624956	O	-5.045475	0.046333	0.450685
O	0.709760	-0.278312	-2.556693	O	-2.817526	0.462055	0.558007
C	-1.673930	-2.807512	0.330493	C	-2.030660	-4.293423	-1.207873
C	-2.391699	-2.294304	-0.807434	C	-1.652409	-4.916482	0.023303
C	-2.464631	-3.429875	1.350700	C	-1.871247	-5.074922	-2.395773
C	-3.787649	-2.409580	-0.914079	C	-1.145577	-6.221549	0.059035
H	-1.825030	-1.720440	-1.564442	H	-1.716141	-4.306608	0.936802
C	-3.856693	-3.523537	1.238170	C	-1.372641	-6.386374	-2.348999
H	-1.940819	-3.799206	2.246842	H	-2.146826	-4.616767	-3.361285
C	-4.536351	-3.024281	0.105508	C	-1.002332	-6.974673	-1.124435
H	-4.296783	-1.984562	-1.795713	H	-0.835761	-6.653670	1.025297
H	-4.432666	-3.987232	2.057024	H	-1.262404	-6.957198	-3.286864
H	-5.632154	-3.102200	0.030114	H	-0.599016	-7.998711	-1.092839
N	2.075952	2.366870	-0.049535	N	0.309568	1.680770	-0.621937
N	0.037708	2.951323	-0.506002	N	0.631922	0.838288	1.364149
C	0.820806	1.850013	-0.272304	C	0.065745	0.554496	0.139612
C	2.076812	3.758212	-0.148782	C	0.983525	2.653631	0.124588
C	0.788816	4.127925	-0.438462	C	1.178608	2.131039	1.369149
C	3.206227	1.534112	0.279966	C	0.028459	1.746265	-2.046255
C	3.919596	0.907322	-0.770369	C	-1.213214	2.250305	-2.520327
C	4.945124	0.011592	-0.406614	C	-1.430410	2.240823	-3.916496
C	5.270910	-0.244676	0.943039	C	-0.459468	1.750501	-4.805080
C	4.555259	0.434581	1.951909	C	0.775050	1.297977	-4.318461
C	3.516067	1.335780	1.644325	C	1.044174	1.309337	-2.937659
C	-1.385597	2.892106	-0.719979	C	-2.273544	2.790418	-1.558096
C	-2.231588	3.130189	0.386672	C	-1.727256	3.913758	-0.682578
C	-3.618749	3.014762	0.184215	C	-2.093585	3.968396	0.677511
C	-4.155373	2.646934	-1.065483	C	-1.612300	5.000429	1.500772
C	-3.271712	2.431690	-2.142250	C	-0.752127	5.984388	0.979711
C	-1.874315	2.556405	-2.003661	C	-0.383144	5.937619	-0.376697
H	2.989146	4.346637	-0.012540	C	-0.871300	4.909386	-1.201419
H	0.334486	5.108229	-0.611100	C	-3.569044	3.200092	-2.272801
H	5.502881	-0.502677	-1.206778	C	-4.569983	2.232774	-2.516231
H	4.802522	0.252974	3.011252	C	-5.737130	2.570410	-3.222979
H	-4.294328	3.175031	1.039982	C	-5.928462	3.878703	-3.701830
H	-3.679740	2.157832	-3.129449	C	-4.942689	4.850237	-3.457263
C	-5.643214	2.436168	-1.233709	C	-3.776823	4.513558	-2.746788
H	-6.230138	3.048014	-0.519058	H	-0.657530	1.752549	-5.889237
H	-5.981181	2.682016	-2.261067	C	2.445024	1.002162	-2.412412
H	-5.908948	1.371110	-1.050269	C	3.135623	2.301327	-1.980444
C	6.397835	-1.193081	1.295183	C	2.800104	3.549544	-2.544977
H	6.455450	-2.045337	0.586251	C	3.393501	4.733530	-2.071183
H	7.380862	-0.674715	1.251717	C	4.336366	4.683854	-1.030153
H	6.290835	-1.599497	2.321976	C	4.704239	3.439369	-0.486020
C	-1.652624	3.418408	1.750453	C	4.115410	2.260500	-0.967405
H	-0.993886	2.582481	2.071019	C	3.306018	0.156982	-3.357289
H	-1.035057	4.341368	1.758642	C	4.454445	0.676844	-3.987732
H	-2.450724	3.525772	2.509613	C	5.237183	-0.130656	-4.833883
C	-0.940973	2.315082	-3.161265	C	4.883801	-1.470965	-5.060199
H	-1.479500	2.383988	-4.126484	C	3.732995	-1.994518	-4.441781
H	-0.108208	3.048485	-3.171851	C	2.950388	-1.188594	-3.600794
H	-0.469481	1.306705	-3.095674	C	0.874388	-0.102234	2.435894
C	3.566067	1.171727	-2.209675	C	2.204155	-0.576908	2.614980
H	3.494840	2.261348	-2.411269	C	2.454145	-1.485995	3.659059

H	4.319114	0.736807	-2.894291
H	2.571791	0.731589	-2.457692
C	2.754861	2.067634	2.721594
H	2.971962	1.646329	3.721475
H	3.018536	3.147493	2.734919
H	1.662321	1.993824	2.554847

C	1.430726	-1.897149	4.521473
C	0.135991	-1.399374	4.345356
C	-0.176379	-0.510042	3.294680
C	3.379170	-0.096553	1.758040
C	4.273033	0.896235	2.520147
C	3.815417	1.573077	3.671279
C	4.612176	2.541832	4.307751
C	5.891159	2.844265	3.812212
C	6.365927	2.165671	2.675202
C	5.564670	1.204981	2.036934
C	4.147710	-1.262893	1.131910
C	3.806842	-1.698277	-0.163549
C	4.474449	-2.772625	-0.770655
C	5.492100	-3.446375	-0.076045
C	5.842886	-3.027322	1.219753
C	5.182399	-1.939487	1.814962
H	1.647096	-2.600223	5.340925
C	-1.595707	0.039275	3.195437
C	-1.731519	1.113679	4.280218
C	-2.162513	0.818207	5.590656
C	-2.178739	1.813416	6.582748
C	-1.757170	3.121014	6.282154
C	-1.328235	3.426082	4.978176
C	-1.320670	2.431148	3.986192
C	-2.688705	-1.032129	3.218368
C	-4.030162	-0.637473	3.421928
C	-5.065654	-1.583229	3.475252
C	-4.785409	-2.954223	3.308606
C	-3.462877	-3.356342	3.037110
C	-2.430503	-2.399793	2.976651
H	1.256939	3.624834	-0.291905
H	1.679080	2.542722	2.249140
H	-2.382067	2.635454	-4.302202
H	1.556343	0.944653	-5.007674
H	-2.516184	1.949667	-0.867687
H	-2.740752	3.174246	1.085710
H	-1.909802	5.031080	2.560419
H	-0.370338	6.787633	1.629942
H	0.294350	6.700281	-0.793168
H	-0.559263	4.856744	-2.257433
H	-4.432035	1.205741	-2.140445
H	-6.510679	1.802352	-3.386395
H	-6.846155	4.143647	-4.251224
H	-5.083050	5.883208	-3.814698
H	-3.022542	5.290851	-2.552583
H	2.310795	0.400019	-1.487270
H	2.041685	3.600989	-3.341109
H	3.107110	5.701101	-2.513402
H	4.787204	5.611765	-0.644146
H	5.437327	3.384128	0.333022
H	4.405796	1.286515	-0.543817
H	4.745794	1.723112	-3.809463
H	6.133147	0.293769	-5.314663
H	5.500911	-2.105102	-5.716576
H	3.439245	-3.043099	-4.611926
H	2.036687	-1.600545	-3.145897
H	3.474168	-1.870683	3.797015
H	-0.666752	-1.701725	5.034015
H	2.955627	0.481026	0.909014
H	2.824287	1.332817	4.086496
H	4.229013	3.056387	5.203374
H	6.519118	3.597733	4.313330
H	7.371152	2.384044	2.280139

	H 5.952086 0.676215 1.152463 H 2.992096 -1.196590 -0.704786 H 4.187785 -3.077025 -1.787422 H 6.016235 -4.293759 -0.545538 H 6.647156 -3.542922 1.768798 H 5.495403 -1.592123 2.812554 H -1.739108 0.545450 2.218998 H -2.503656 -0.201167 5.831601 H -2.524309 1.565248 7.599220 H -1.767939 3.900424 7.060585 H -0.997248 4.447525 4.729604 H -0.992109 2.675573 2.963741 H -4.263482 0.430441 3.537722 H -6.100054 -1.243606 3.640528 H -5.590487 -3.703660 3.390434 H -3.226494 -4.420766 2.875810 H -1.406858 -2.733654 2.752870
Zero-point correction= 0.593060 (Hartree/Particle) Thermal correction to Energy= 0.639881 Thermal correction to Enthalpy= 0.640826 Thermal correction to Gibbs Free Energy= 0.509690 Sum of electronic and zero-point Energies= -3166.303143 Sum of electronic and thermal Energies= -3166.256322 Sum of electronic and thermal Enthalpies= -3166.255378 Sum of electronic and thermal Free Energies= -3166.386514	Zero-point correction= 1.175523 (Hartree/Particle) Thermal correction to Energy= 1.254457 Thermal correction to Enthalpy= 1.255401 Thermal correction to Gibbs Free Energy= 1.056897 Sum of electronic and zero-point Energies= -4934.354699 Sum of electronic and thermal Energies= -4934.275765 Sum of electronic and thermal Enthalpies= -4934.274820 Sum of electronic and thermal Free Energies= -4934.473325

IMes-VIIIpost	**IPR*-VIIIpost**
79 IMesVIIImesKOPh SCF Done: -3166.92528343 A.U. Pd 0.146257 0.489582 0.708969 N 0.267358 3.234105 -0.564413 C -0.865009 2.703630 -3.145811 H -0.326200 1.749643 -2.961983 C -1.737032 3.029932 -1.957821 C -1.166882 3.302409 -0.689226 C 0.921660 2.116075 -0.109751 C -1.948606 3.577903 0.458543 H -1.084891 2.889355 2.315883 C -3.144086 3.016481 -2.052366 H -3.608083 2.805414 -3.030644 C -3.968019 3.259072 -0.930014 C -3.352213 3.538382 0.307878 H -3.981509 3.738597 1.191020 C 1.174541 4.213325 -0.978767 C 2.428889 3.691260 -0.788340 H 3.423925 4.110361 -0.965809 H 0.842661 5.185239 -1.356385 N 2.251277 2.411003 -0.262200 C 3.282503 1.435966 -0.008332 C 3.793999 0.713997 -1.113403 C 3.663126 1.166842 1.324483 C 4.735025 -0.295293 -0.852683 C 4.607910 0.139937 1.527782 C 5.153339 -0.597546 0.459668 H 5.120573 -0.892304 -1.694897 H 4.916237 -0.095302 2.559919 C 3.290385 0.986340 -2.510947 H 3.574892 2.000193 -2.865297 C 3.039158 1.905642 2.483661 H 2.914290 2.985665 2.263661 C 0.393841 -0.509063 -0.989785 O -0.279117 -0.305128 -2.011661	

O -3.744253 -2.295617 0.551122 C 3.338895 -3.673726 -1.001171 C 2.790367 -3.207528 -2.212749 H 3.353686 -3.475107 1.168437 C 2.924807 -3.113489 0.220859 C 1.823236 -2.193193 -2.197926 C 1.418110 -1.613311 -0.973887 C 1.977295 -2.079426 0.235505 H 1.360329 -1.826720 -3.127052 H 1.648627 -1.625547 1.183803 H 3.111453 -3.649850 -3.169450 K -2.737934 -0.216644 -0.483113 K -2.501768 -2.759769 2.738225 C -0.941754 -0.173907 2.932373 O -0.785413 -0.983678 1.850561 O -1.564859 -0.577874 3.935011 O -0.405981 1.010499 2.765765 C -3.179306 -3.202291 -0.223563 C -1.746191 -3.304483 -0.349504 C -3.946577 -4.137324 -0.998224 C -1.140488 -4.253240 -1.191344 H -1.111943 -2.606093 0.223228 C -3.327665 -5.081122 -1.828638 H -5.044973 -4.083231 -0.917824 C -1.920931 -5.152429 -1.939023 H -0.039488 -4.274831 -1.262589 H -3.954230 -5.780478 -2.409036 H -1.447255 -5.895814 -2.599254 H 4.089836 -4.480285 -1.011566 C 6.156429 -1.702269 0.697029 H 6.263068 -1.941134 1.773919 H 5.851138 -2.628699 0.166521 H 7.160551 -1.421927 0.311381 C -5.475415 3.261712 -1.061891 H -5.850637 4.289072 -1.263091 H -5.817686 2.620351 -1.899462 H -5.969354 2.912328 -0.132298 H 3.651444 1.802877 3.400446 H 2.020779 1.510674 2.703219 H 3.689512 0.244455 -3.228492 H 2.181606 0.933613 -2.549295 H -0.103288 3.488471 -3.332215 H -1.470168 2.583531 -4.065176 H -0.358404 4.398902 1.694952 C -1.316393 3.850625 1.797424 H -1.995119 4.438907 2.445407	
Zero-point correction= 0.593720 (Hartree/Particle) Thermal correction to Energy= 0.641282 Thermal correction to Enthalpy= 0.642226 Thermal correction to Gibbs Free Energy= 0.508653 Sum of electronic and zero-point Energies= -3166.331563 Sum of electronic and thermal Energies= -3166.284001 Sum of electronic and thermal Enthalpies= -3166.283057 Sum of electronic and thermal Free Energies= -3166.416630	

IMes-VIII	**IPR*-VIII**
66 IMesVIII SCF Done: -2260.14652078 A.U. Pd -0.283921 0.524417 -0.120018 C 0.497357 0.334275 1.676510 O -0.000359 -0.048984 2.731627 C 4.465210 2.125197 1.647965	140 ItPrVIII SCF Done: -4028.77978331 A.U. Pd -0.136438 -0.892677 -1.276170 C 1.748759 -1.379397 -1.094203 O 2.718995 -0.626754 -1.110068 C 2.106323 -5.676166 -1.491902

C	3.548950	2.432000	2.674720
H	4.821156	0.934738	-0.151885
C	4.103039	1.204661	0.640261
C	2.284899	1.812994	2.701836
C	1.906153	0.921433	1.675497
C	2.822398	0.625524	0.642291
H	1.568160	2.022315	3.511667
H	2.516341	-0.055981	-0.165394
H	5.466387	2.587038	1.644026
H	3.830451	3.142508	3.469301
K	2.293611	4.006668	-0.753023
C	0.119715	2.431958	-1.784682
O	0.387317	2.473409	-0.455374
O	0.576749	3.334543	-2.533389
O	-0.561803	1.384240	-2.152815
N	-0.272025	-2.481662	-0.314940
N	-2.286576	-1.723588	-0.064400
C	-0.980215	-1.318004	-0.136416
C	-1.121087	-3.590028	-0.356358
C	-2.395478	-3.108996	-0.196626
C	1.157541	-2.508351	-0.471601
C	1.952469	-2.867860	0.643156
C	3.349453	-2.832975	0.485036
C	3.951308	-2.451240	-0.732557
C	3.119778	-2.108799	-1.816314
C	1.712107	-2.124379	-1.714755
C	-3.391008	-0.811341	0.100115
C	-3.930568	-0.186486	-1.046233
C	-5.002043	0.707333	-0.847060
C	-5.514439	0.984604	0.435356
C	-4.932161	0.343101	1.548828
C	-3.861013	-0.558195	1.409120
H	-0.741051	-4.605198	-0.505400
H	-3.365726	-3.614290	-0.172339
H	3.987784	-3.092228	1.345915
H	3.575464	-1.807435	-2.774211
H	-5.441147	1.208606	-1.725653
H	-5.316902	0.556887	2.560107
C	-6.636077	1.982252	0.623221
H	-7.256486	2.081222	-0.290456
H	-7.301473	1.698460	1.464457
H	-6.229103	2.991171	0.855354
C	5.457895	-2.381895	-0.844324
H	5.866499	-1.605677	-0.161232
H	5.931644	-3.343885	-0.555124
H	5.786172	-2.135558	-1.873814
C	-3.338660	-0.413623	-2.415253
H	-2.430031	0.218239	-2.540235
H	-3.029125	-1.468256	-2.566088
H	-4.058079	-0.142209	-3.212572
C	-3.191569	-1.199492	2.599844
H	-3.726397	-0.958450	3.539114
H	-3.147853	-2.305255	2.502071
H	-2.141683	-0.840535	2.691546
C	1.309701	-3.222148	1.962444
H	0.630349	-4.095312	1.867560
H	2.072510	-3.462384	2.727966
H	0.694822	-2.377283	2.338731
C	0.838386	-1.688221	-2.865028
H	1.380398	-1.760305	-3.828296
H	-0.085529	-2.297889	-2.933620
H	0.506935	-0.631634	-2.732224

C	2.684101	-4.821197	-2.453877
H	1.010404	-5.785323	0.396037
C	1.445906	-5.125568	-0.372060
C	2.608710	-3.424780	-2.297913
C	1.920514	-2.877787	-1.193827
C	1.339093	-3.731725	-0.233488
H	3.050545	-2.739683	-3.038438
H	0.799987	-3.287830	0.615267
H	2.188240	-6.769848	-1.604268
H	3.207947	-5.247694	-3.325143
K	-1.135876	-4.658109	-2.953862
C	-1.865620	-1.888638	-2.889213
O	-0.574666	-2.277166	-2.776341
O	-2.682070	-2.605510	-3.521988
O	-2.138582	-0.793814	-2.235997
N	0.502137	0.413007	1.410613
N	-0.419995	1.773411	-0.007394
C	0.002332	0.474445	0.128078
C	0.370671	1.650478	2.058478
C	-0.194352	2.509094	1.159157
C	0.911897	-0.793455	2.086631
C	2.290663	-1.021708	2.352343
C	2.633511	-2.158584	3.109837
C	1.647393	-3.009126	3.631402
C	0.296019	-2.762006	3.363840
C	-0.096372	-1.678431	2.548822
C	3.372795	-0.059501	1.844544
C	3.365115	1.269511	2.593096
C	3.610542	2.460713	1.879865
C	3.584642	3.704737	2.529471
C	3.316362	3.775934	3.908972
C	3.086531	2.592246	4.633604
C	3.113065	1.347348	3.979093
C	4.761221	-0.712509	1.817610
C	5.094888	-1.577558	0.750927
C	6.333275	-2.238483	0.726695
C	7.262788	-2.047149	1.765328
C	6.943875	-1.181400	2.825048
C	5.703318	-0.518263	2.849472
H	1.938027	-3.866607	4.258390
C	-1.575408	-1.475371	2.224359
C	-2.390820	-1.360864	3.523227
C	-3.520482	-2.156476	3.794649
C	-4.239654	-1.992986	4.994234
C	-3.839753	-1.032841	5.937360
C	-2.712720	-0.231115	5.673025
C	-1.998232	-0.394954	4.477639
C	-2.161021	-2.497913	1.241346
C	-3.154641	-2.063668	0.336697
C	-3.812049	-2.960307	-0.518002
C	-3.500572	-4.331414	-0.468810
C	-2.501745	-4.781784	0.415862
C	-1.834384	-3.870560	1.255470
C	-0.965763	2.316154	-1.228064
C	-2.374262	2.408254	-1.365937
C	-2.881097	3.015707	-2.526441
C	-2.012706	3.497219	-3.521552
C	-0.627656	3.339872	-3.388670
C	-0.077416	2.726478	-2.244397
C	-3.284410	1.823199	-0.284023
C	-3.264475	2.648240	0.999715
C	-3.147714	4.053443	0.970519
C	-3.104149	4.794486	2.165112

	C	-3.181015	4.137827	3.406600
	C	-3.320626	2.738351	3.443929
	C	-3.368258	2.003587	2.249069
	C	-4.705961	1.527775	-0.778110
	C	-4.900132	0.465757	-1.692385
	C	-6.187665	0.167126	-2.165635
	C	-7.298007	0.922057	-1.742138
	C	-7.108601	1.982402	-0.840235
	C	-5.820060	2.283058	-0.359743
	H	-2.426518	3.976017	-4.422912
	C	1.426734	2.469618	-2.153580
	C	2.170736	3.803988	-2.101139
	C	2.677450	4.433504	-3.256904
	C	3.293031	5.694894	-3.175388
	C	3.409432	6.348939	-1.936216
	C	2.904973	5.730545	-0.777718
	C	2.293228	4.469073	-0.861400
	C	1.918740	1.464677	-3.201377
	C	3.304919	1.274343	-3.386255
	C	3.788440	0.244220	-4.206767
	C	2.889705	-0.626592	-4.851776
	C	1.508752	-0.453288	-4.668447
	C	1.026948	0.587887	-3.853910
	H	0.701470	1.806414	3.087801
	H	-0.486833	3.558030	1.251204
	H	3.696742	-2.361910	3.303971
	H	-0.482550	-3.397995	3.811552
	H	3.109576	0.167503	0.790905
	H	3.802792	2.410697	0.795689
	H	3.767722	4.622816	1.949249
	H	3.287696	4.751904	4.418956
	H	2.879893	2.638276	5.714992
	H	2.908866	0.422518	4.542731
	H	4.376912	-1.710434	-0.072531
	H	6.574885	-2.905214	-0.116743
	H	8.235328	-2.564626	1.744629
	H	7.666845	-1.014245	3.639761
	H	5.469016	0.163438	3.681536
	H	-1.671775	-0.490591	1.722388
	H	-3.845341	-2.907307	3.058652
	H	-5.121904	-2.623648	5.188200
	H	-4.403495	-0.906038	6.875065
	H	-2.389614	0.527741	6.403782
	H	-1.121530	0.239218	4.269211
	H	-3.423503	-0.998850	0.291128
	H	-4.552267	-2.577114	-1.234576
	H	-4.042686	-5.042635	-1.114769
	H	-2.247438	-5.853829	0.471895
	H	-1.057493	-4.248155	1.934294
	H	-3.971347	3.088768	-2.655153
	H	0.050308	3.674135	-4.188748
	H	-2.830587	0.838109	-0.037909
	H	-3.066035	4.565431	-0.001742
	H	-3.004861	5.891226	2.125079
	H	-3.137298	4.716165	4.343275
	H	-3.386181	2.205736	4.405320
	H	-3.479676	0.908294	2.291611
	H	-4.021360	-0.111391	-2.037005
	H	-6.319245	-0.663572	-2.878137
	H	-8.307734	0.685202	-2.114772
	H	-7.969354	2.581340	-0.501166
	H	-5.684606	3.109966	0.354474
	H	1.626765	1.957087	-1.188376

	H 2.603034 3.917649 -4.227276 H 3.687056 6.169462 -4.088447 H 3.892927 7.336708 -1.872879 H 2.986503 6.236314 0.198229 H 1.899342 3.986552 0.048748 H 4.015555 1.926675 -2.855217 H 4.875141 0.110683 -4.330177 H 3.268289 -1.440671 -5.491331 H 0.787693 -1.144189 -5.130514 H -0.058510 0.695828 -3.713720
Zero-point correction= 0.502041 (Hartree/Particle) Thermal correction to Energy= 0.540627 Thermal correction to Enthalpy= 0.541571 Thermal correction to Gibbs Free Energy= 0.428213 Sum of electronic and zero-point Energies= -2259.644480 Sum of electronic and thermal Energies= -2259.605894 Sum of electronic and thermal Enthalpies= -2259.604950 Sum of electronic and thermal Free Energies= -2259.718308	Zero-point correction= 1.083601 (Hartree/Particle) Thermal correction to Energy= 1.154753 Thermal correction to Enthalpy= 1.155697 Thermal correction to Gibbs Free Energy= 0.971619 Sum of electronic and zero-point Energies= -4027.696182 Sum of electronic and thermal Energies= -4027.625030 Sum of electronic and thermal Enthalpies= -4027.624086 Sum of electronic and thermal Free Energies= -4027.808165

IMes-IX	**IPR*-IX**
82	156
IMesIX SCF Done: -2668.16980899 A.U.	ItPrIX SCF Done: -4436.81252989 A.U.
Pd -0.388342 0.034751 0.210651 K 0.230840 4.778677 -2.214273 O -1.049115 4.245900 -0.040531 H -1.397707 4.591114 0.798185 B -0.000033 3.240296 0.249870 O 1.277596 3.939856 0.439675 H 1.990204 3.294670 0.607813 C -0.434819 2.277696 1.515422 C 0.370679 2.184167 2.690517 C -1.714692 1.635852 1.572886 C -0.051665 1.491355 3.830515 H 1.351651 2.685855 2.697016 C -2.142297 0.929621 2.726175 H -2.420383 1.767798 0.736288 C -1.310053 0.850464 3.848134 H 0.604073 1.435771 4.714500 H -3.128777 0.440438 2.719737 H -1.631853 0.289873 4.740040 C -0.899888 2.038246 -1.847851 O -1.132708 2.671758 -2.900929 O 0.180091 2.452657 -1.076070 O -1.530429 0.999729 -1.429904 C 2.255724 -0.101666 1.492475 C 2.643192 0.777543 0.458338 C 3.180629 -0.429733 2.507978 C 3.930353 1.336996 0.453378 C 4.467301 0.127986 2.500454 C 4.842393 1.021211 1.477679 H 1.918405 1.028716 -0.334687 H 2.856981 -1.121602 3.300954 H 4.225704 2.017134 -0.361605 H 5.182617 -0.125664 3.299411 H 5.848900 1.470176 1.479383 C 0.856036 -0.681957 1.571383 O 0.565095 -1.474128 2.460800 N -1.669228 -2.450540 -0.808881 N 0.473237 -2.608755 -1.112859 C -0.493773 -1.771684 -0.620399 C -1.442273 -3.688431 -1.410425 C -0.089202 -3.788909 -1.607136	Pd -0.621894 -0.770049 0.884049 K -1.025305 -2.301504 4.963697 O -2.630737 -3.763116 3.654174 H -3.495556 -3.361526 3.400853 B -1.771316 -3.587264 2.481391 O -0.388424 -3.773020 2.920056 H 0.204146 -3.860981 2.150302 C -2.209936 -4.454803 1.186496 C -2.100203 -5.863888 1.299342 C -2.708508 -3.944896 -0.034779 C -2.448948 -6.723960 0.244253 H -1.721164 -6.289887 2.243845 C -3.073100 -4.797505 -1.094384 H -2.803923 -2.857562 -0.186922 C -2.937340 -6.189583 -0.963154 H -2.342211 -7.815370 0.360931 H -3.453148 -4.362812 -2.032211 H -3.214577 -6.857191 -1.795322 C -3.077976 -1.427604 1.765712 O -4.112591 -1.749862 2.359039 O -1.843219 -1.995440 2.147597 O -2.912380 -0.585560 0.807583 C 1.461268 -0.823645 3.014802 C 0.693385 0.159027 3.672834 C 2.558654 -1.408826 3.689972 C 1.009342 0.556360 4.985496 C 2.867236 -1.024342 5.003430 C 2.092590 -0.041961 5.656757 H -0.151629 0.619396 3.138417 H 3.156602 -2.166848 3.161852 H 0.409818 1.347354 5.463571 H 3.722463 -1.486064 5.522564 H 2.345776 0.266545 6.684091 C 1.132171 -1.301235 1.608834 O 1.865911 -2.107873 1.056763 N -0.394106 0.667699 -1.700826 N 1.066243 1.510984 -0.341265 C 0.118360 0.515837 -0.433566 C 0.217052 1.726960 -2.375323 C 1.124943 2.270297 -1.514998

C	-2.964034	-1.919696	-0.452363
C	-3.735534	-1.295486	-1.456491
C	-4.967761	-0.732869	-1.066243
C	-5.423246	-0.783948	0.264234
C	-4.622448	-1.435428	1.226637
C	-3.383347	-2.012610	0.895954
C	1.872099	-2.272960	-1.168304
C	2.756805	-2.878558	-0.244817
C	4.111628	-2.504442	-0.301741
C	4.587822	-1.567433	-1.239767
C	3.670639	-1.000798	-2.146077
C	2.302426	-1.332406	-2.132110
H	-2.264441	-4.371976	-1.642837
H	0.524419	-4.574517	-2.058022
H	-5.579898	-0.225117	-1.829591
H	-4.972789	-1.495424	2.271049
H	4.813724	-2.948024	0.422997
H	4.026508	-0.263425	-2.884708
C	6.038136	-1.147339	-1.233126
H	6.714104	-2.005542	-1.039833
H	6.338072	-0.676858	-2.191049
H	6.211801	-0.404243	-0.423813
C	-6.738058	-0.155949	0.670248
H	-7.257357	0.308582	-0.191409
H	-7.423370	-0.907645	1.117561
H	-6.581994	0.633274	1.436755
C	2.254613	-3.858498	0.788204
H	1.469455	-3.395237	1.421415
H	1.805051	-4.760098	0.321121
H	3.076716	-4.191864	1.450377
C	1.328566	-0.665981	-3.072044
H	1.849563	-0.220190	-3.941143
H	0.555940	-1.368685	-3.444408
H	0.777930	0.143903	-2.548060
C	-3.223862	-1.159779	-2.868037
H	-2.757684	-2.094046	-3.242716
H	-4.035598	-0.870218	-3.563261
H	-2.451980	-0.357886	-2.875905
C	-2.510122	-2.665286	1.937174
H	-3.065586	-2.828694	2.880993
H	-2.118542	-3.644105	1.588960
H	-1.620014	-2.037969	2.163147

C	-1.276915	-0.282726	-2.335899
C	-2.676635	-0.043507	-2.371215
C	-3.472405	-0.995719	-3.033381
C	-2.898099	-2.126365	-3.638475
C	-1.514531	-2.333775	-3.593256
C	-0.674066	-1.413133	-2.935527
C	-3.288900	1.197362	-1.700122
C	-2.740188	2.495440	-2.285046
C	-2.369755	3.556672	-1.433656
C	-1.801217	4.733643	-1.949142
C	-1.623886	4.877802	-3.337160
C	-2.026026	3.843229	-4.201733
C	-2.574358	2.659203	-3.677493
C	-4.824563	1.167684	-1.669390
C	-5.476023	0.395813	-0.680001
C	-6.877338	0.310607	-0.649337
C	-7.654345	0.993901	-1.602359
C	-7.015176	1.768834	-2.584812
C	-5.611381	1.856463	-2.616383
H	-3.543875	-2.852879	-4.156186
C	0.842197	-1.626025	-2.905116
C	1.374130	-1.712501	-4.340563
C	1.593663	-2.947112	-4.985581
C	2.034855	-2.989366	-6.319631
C	2.269633	-1.797483	-7.027700
C	2.057247	-0.560838	-6.391512
C	1.611151	-0.522318	-5.060357
C	1.305067	-2.786861	-2.019541
C	2.689987	-3.047415	-1.909386
C	3.165189	-4.099866	-1.113792
C	2.259452	-4.915936	-0.410868
C	0.882734	-4.659693	-0.504190
C	0.413123	-3.596211	-1.296501
C	1.816735	1.817671	0.846246
C	3.106793	1.246245	1.016227
C	3.798974	1.550375	2.201695
C	3.257664	2.440641	3.142393
C	2.009897	3.034688	2.921694
C	1.247196	2.713030	1.781048
C	3.740546	0.407560	-0.101986
C	4.019219	1.280313	-1.331032
C	4.396790	2.635074	-1.204572
C	4.631751	3.425506	-2.343572
C	4.496709	2.870234	-3.628506
C	4.139434	1.516610	-3.763847
C	3.906315	0.731211	-2.623651
C	5.003782	-0.347480	0.330897
C	4.909208	-1.690658	0.752682
C	6.052931	-2.392560	1.171033
C	7.310358	-1.764376	1.178769
C	7.415374	-0.427284	0.755842
C	6.272979	0.272002	0.330051
H	3.821519	2.675435	4.058241
C	-0.136030	3.331162	1.547019
C	-0.070687	4.831579	1.242440
C	-1.179618	5.667103	1.494909
C	-1.173891	7.012401	1.087122
C	-0.059216	7.545413	0.416074
C	1.052550	6.722087	0.163203
C	1.046895	5.379367	0.575790
C	-1.136849	2.936685	2.634749
C	-2.139658	1.993425	2.332127
C	-3.016511	1.512389	3.321826

	C -2.909801 1.992191 4.638594 C -1.946880 2.974178 4.946186 C -1.073139 3.445471 3.951934 H -0.079018 2.015175 -3.386097 H 1.808381 3.114561 -1.627000 H -4.561030 -0.844812 -3.067873 H -1.068583 -3.218595 -4.071717 H -2.957038 1.144890 -0.643306 H -2.515651 3.451563 -0.346217 H -1.489238 5.535108 -1.261812 H -1.175610 5.798301 -3.743565 H -1.900226 3.952504 -5.291102 H -2.849283 1.831890 -4.352108 H -4.865011 -0.144054 0.060082 H -7.362295 -0.298075 0.130663 H -8.753964 0.926501 -1.576923 H -7.611294 2.316120 -3.332966 H -5.129092 2.478890 -3.385103 H 1.297217 -0.712372 -2.471341 H 1.432683 -3.882495 -4.426756 H 2.202430 -3.962861 -6.807669 H 2.620787 -1.831663 -8.071211 H 2.242452 0.380153 -6.934616 H 1.453889 0.446338 -4.559253 H 3.408487 -2.429723 -2.472683 H 4.249714 -4.278861 -1.041607 H 2.628428 -5.749111 0.208610 H 0.150635 -5.283318 0.032135 H -0.666768 -3.406043 -1.337962 H 4.782887 1.092533 2.378232 H 1.611183 3.749151 3.654515 H 2.994353 -0.360059 -0.401305 H 4.480217 3.082551 -0.200880 H 4.918329 4.482874 -2.225529 H 4.673237 3.489817 -4.521952 H 4.029889 1.063849 -4.761536 H 3.616165 -0.323901 -2.741307 H 3.926982 -2.184930 0.747839 H 5.956096 -3.443970 1.487126 H 8.207200 -2.315553 1.503998 H 8.396370 0.074386 0.746659 H 6.373632 1.312062 -0.016895 H -0.530410 2.879970 0.613277 H -2.063408 5.253600 2.004490 H -2.052331 7.645548 1.289246 H -0.056032 8.598328 0.092989 H 1.932994 7.128055 -0.360085 H 1.923852 4.743726 0.374724 H -2.229649 1.590589 1.313588 H -3.772204 0.757946 3.051898 H -3.595114 1.624670 5.419634 H -1.881435 3.383414 5.967413 H -0.345591 4.233294 4.200850
Zero-point correction= 0.625073 (Hartree/Particle) Thermal correction to Energy= 0.671665 Thermal correction to Enthalpy= 0.672609 Thermal correction to Gibbs Free Energy= 0.544736 Sum of electronic and zero-point Energies= -2667.544736 Sum of electronic and thermal Energies= -2667.498144 Sum of electronic and thermal Enthalpies= -2667.497200 Sum of electronic and thermal Free Energies= -2667.625073	Zero-point correction= 1.208106 (Hartree/Particle) Thermal correction to Energy= 1.286718 Thermal correction to Enthalpy= 1.287662 Thermal correction to Gibbs Free Energy= 1.091408 Sum of electronic and zero-point Energies= -4435.604423 Sum of electronic and thermal Energies= -4435.525812 Sum of electronic and thermal Enthalpies= -4435.524868 Sum of electronic and thermal Free Energies= -4435.721122

IMes-IX-X				**IPR*-IX-X**			
82				156			
IMesIX-X SCF Done: -2668.14911189 A.U.				ItPrIX-X SCF Done: -4436.79286399 A.U.			
Pd	0.232522	-0.008911	-0.204537	Pd	0.075012	-1.185776	1.002780
K	1.983432	4.280164	2.691737	K	4.634759	-4.082543	0.663069
O	1.959625	3.667988	0.192398	O	2.638729	-3.987652	2.584720
H	2.197291	3.856484	-0.734045	H	2.160054	-4.450333	3.296656
B	0.740293	2.892714	0.215475	B	1.713355	-3.577853	1.568715
O	-0.350505	3.513992	-0.396588	O	0.930481	-4.612340	1.032343
H	-1.152694	2.955473	-0.365208	H	0.232058	-4.276212	0.435650
C	1.437360	1.427627	-1.229124	C	0.381817	-2.422310	2.777937
C	1.113311	2.008353	-2.486949	C	-0.547605	-3.372810	3.286708
C	2.793356	1.016278	-1.051056	C	1.029452	-1.592826	3.744723
C	2.072145	2.183385	-3.499647	C	-0.790786	-3.520792	4.663265
H	0.082160	2.356900	-2.659769	H	-1.068076	-4.040951	2.581871
C	3.755506	1.177926	-2.060734	C	0.779442	-1.720308	5.119950
H	3.098222	0.553578	-0.097503	H	1.748389	-0.830393	3.403403
C	3.400642	1.766687	-3.290072	C	-0.124741	-2.693004	5.586379
H	1.781476	2.639056	-4.461007	H	-1.509830	-4.278089	5.017747
H	4.789106	0.832880	-1.890510	H	1.289091	-1.052463	5.833459
H	4.154977	1.895983	-4.083727	H	-0.320532	-2.795646	6.666093
C	1.367038	1.431372	2.165796	C	3.049099	-1.556231	0.875047
O	1.936394	1.821375	3.211089	O	4.298312	-1.549479	0.761242
O	0.507349	2.365486	1.544113	O	2.408668	-2.767529	0.589419
O	1.447051	0.288503	1.623599	O	2.291649	-0.572171	1.141012
N	0.643956	-2.890273	0.400977	C	-2.065290	-3.103080	0.177514
N	-1.477754	-2.517377	0.621877	C	-1.310516	-3.561013	-0.919940
C	-0.292674	-1.887391	0.343601	C	-3.117551	-3.904535	0.674378
C	0.057373	-4.115868	0.712666	C	-1.600577	-4.794670	-1.524688
C	-1.286112	-3.882663	0.856791	C	-3.387275	-5.151956	0.091235
C	2.058001	-2.655079	0.219007	C	-2.633449	-5.598736	-1.011912
C	2.852002	-2.443899	1.369902	H	-0.520157	-2.912195	-1.321301
C	4.204770	-2.114345	1.171753	H	-3.710979	-3.529538	1.522525
C	4.759970	-1.995823	-0.118785	H	-1.016811	-5.117984	-2.400888
C	3.937081	-2.248475	-1.232215	H	-4.196247	-5.781645	0.494808
C	2.575249	-2.579563	-1.093315	H	-2.857327	-6.573390	-1.473706
C	-2.733530	-1.829090	0.763745	C	-1.805206	-1.753752	0.810389
C	-3.701097	-1.934258	-0.263692	O	-2.779129	-1.108451	1.205444
C	-4.909096	-1.234948	-0.089657	N	-0.462632	0.540979	-1.545065
C	-5.162479	-0.456172	1.057157	N	-0.070490	1.715477	0.240255
C	-4.171394	-0.385197	2.054968	C	-0.184908	0.417414	-0.207172
C	-2.941359	-1.060141	1.931384	C	-0.521891	1.889034	-1.926052
H	0.650034	-5.031297	0.802814	C	-0.306355	2.622888	-0.796334
H	-2.117408	-4.547294	1.110960	C	-0.715206	-0.547649	-2.457080
H	4.836533	-1.922197	2.054771	C	-2.053980	-0.785265	-2.865206
H	4.356537	-2.160289	-2.247610	C	-2.289895	-1.800051	-3.813019
H	-5.669491	-1.285567	-0.886073	C	-1.227116	-2.524253	-4.367456
H	-4.351788	0.227417	2.953931	C	0.085771	-2.289981	-3.935942
C	-2.261183	0.771939	-1.563602	C	0.368623	-1.328837	-2.944091
C	-2.584564	1.386831	-0.335069	C	-3.205277	0.074072	-2.325868
C	-3.113591	0.959500	-2.673072	C	-3.265292	1.422109	-3.050240
C	-3.729640	2.190101	-0.219315	C	-3.613190	2.577209	-2.322798
C	-4.258730	1.762496	-2.558942	C	-3.629634	3.837689	-2.937082
C	-4.565704	2.386183	-1.333816	C	-3.303535	3.963345	-4.300349
H	-1.929956	1.192474	0.533359	C	-2.969695	2.815137	-5.040357
H	-2.850931	0.458429	-3.617981	C	-2.949898	1.552612	-4.418955
H	-3.976431	2.652099	0.749358	C	-4.550196	-0.661182	-2.346319
H	-4.915925	1.911002	-3.431134	C	-4.905723	-1.478685	-1.252666
H	-5.460963	3.022970	-1.247336	C	-6.097329	-2.221251	-1.270970
C	-1.026073	-0.103117	-1.717016	C	-6.959785	-2.153064	-2.379457
O	-0.896984	-0.785039	-2.732030	C	-6.623975	-1.325709	-3.465349
C	6.194964	-1.553317	-0.297778	C	-5.429919	-0.583283	-3.447445
H	6.579585	-1.796368	-1.308751	H	-1.425036	-3.293971	-5.129863

H	6.281154	-0.451739	-0.166189
H	6.867644	-2.020858	0.451027
C	1.692050	-2.784713	-2.296275
H	1.001262	-3.642473	-2.159890
H	1.047853	-1.895414	-2.471436
H	2.293591	-2.959298	-3.209316
C	2.244889	-2.503127	2.749223
H	3.023402	-2.429294	3.532994
H	1.553657	-1.642899	2.872215
H	1.668918	-3.437486	2.915082
C	-1.860066	-0.931201	2.977376
H	-1.418523	-1.916389	3.235120
H	-1.018919	-0.310504	2.597418
H	-2.248434	-0.465859	3.903877
C	-3.424613	-2.729497	-1.516319
H	-4.316399	-2.762933	-2.171558
H	-2.590466	-2.275545	-2.092746
H	-3.124517	-3.773177	-1.287634
C	-6.457710	0.311552	1.180121
H	-6.507491	1.107061	0.405020
H	-7.338196	-0.347123	1.025543
H	-6.560965	0.796446	2.171404

C	1.783978	-1.175640	-2.375013
C	2.481521	0.121217	-2.778898
C	2.132258	0.832094	-3.944310
C	2.877970	1.955347	-4.347662
C	3.990098	2.372859	-3.595354
C	4.335479	1.679739	-2.419941
C	3.578237	0.571490	-2.008802
C	2.659719	-2.416027	-2.631697
C	3.885662	-2.356409	-3.324902
C	4.673888	-3.510007	-3.508862
C	4.240794	-4.754348	-3.018150
C	3.009080	-4.830719	-2.333363
C	2.240121	-3.673444	-2.136481
C	0.422131	2.064707	1.559246
C	1.746641	2.556218	1.682954
C	2.250476	2.783532	2.977969
C	1.458125	2.548012	4.109003
C	0.127787	2.131746	3.961000
C	-0.421602	1.897858	2.685448
C	2.558254	2.963168	0.454799
C	2.083453	4.321385	-0.074928
C	1.554461	5.313129	0.776312
C	1.083539	6.532697	0.254483
C	1.141835	6.781402	-1.127460
C	1.684910	5.803862	-1.982810
C	2.150430	4.587850	-1.460141
C	4.076242	2.912677	0.661108
C	4.661091	1.687521	1.049032
C	6.053757	1.555289	1.137570
C	6.890648	2.653106	0.858332
C	6.315750	3.883620	0.498341
C	4.916951	4.012776	0.398956
H	1.872785	2.713669	5.115931
C	-1.894430	1.543195	2.509982
C	-2.704339	2.640144	1.815009
C	-2.222352	3.945517	1.591975
C	-3.036552	4.921091	0.986005
C	-4.355801	4.611877	0.616019
C	-4.848305	3.310217	0.835274
C	-4.026090	2.332313	1.415822
C	-2.551161	1.100603	3.817840
C	-3.279011	1.999744	4.625531
C	-3.843339	1.577685	5.842003
C	-3.689573	0.245769	6.265637
C	-2.961213	-0.655045	5.467786
C	-2.392983	-0.231068	4.255755
H	-0.730679	2.193488	-2.953329
H	-0.315053	3.700655	-0.632650
H	-3.325471	-2.014509	-4.114955
H	0.912826	-2.884465	-4.349661
H	-2.975465	0.287705	-1.259690
H	-3.833791	2.493128	-1.249102
H	-3.880491	4.724804	-2.334164
H	-3.304233	4.953293	-4.783753
H	-2.712614	2.901734	-6.108391
H	-2.656608	0.662874	-4.998516
H	-4.248525	-1.520489	-0.371348
H	-6.351400	-2.855919	-0.406855
H	-7.895542	-2.734606	-2.393859
H	-7.298630	-1.251741	-4.333516
H	-5.182303	0.070290	-4.298417
H	1.654054	-1.139136	-1.269024
H	1.274125	0.495278	-4.548088

	H 2.591453 2.501176 -5.260981 H 4.579366 3.247026 -3.914518 H 5.185304 2.011390 -1.803545 H 3.862096 0.032086 -1.091101 H 4.238252 -1.392815 -3.721210 H 5.627936 -3.432432 -4.054654 H 4.845703 -5.661034 -3.183734 H 2.640645 -5.795159 -1.945804 H 1.304328 -3.746150 -1.569841 H 3.282986 3.148237 3.085161 H -0.506559 1.980511 4.845861 H 2.350507 2.216448 -0.343885 H 1.490750 5.121410 1.858654 H 0.663730 7.290427 0.935530 H 0.764363 7.731660 -1.537620 H 1.732990 5.984078 -3.068837 H 2.547362 3.813480 -2.133446 H 4.013482 0.823744 1.257116 H 6.477359 0.577184 1.414970 H 7.986083 2.551041 0.923272 H 6.958260 4.753337 0.285278 H 4.480063 4.976908 0.097928 H -1.955256 0.656966 1.843673 H -1.195462 4.206519 1.892767 H -2.632709 5.931340 0.811142 H -4.999706 5.377952 0.155353 H -5.876166 3.051353 0.535106 H -4.405303 1.311098 1.580012 H -3.408035 3.041529 4.291746 H -4.409450 2.293511 6.459863 H -4.137175 -0.089400 7.215247 H -2.827157 -1.700575 5.784789 H -1.814880 -0.937225 3.641880
Zero-point correction= 0.623479 (Hartree/Particle) Thermal correction to Energy= 0.670630 Thermal correction to Enthalpy= 0.671575 Thermal correction to Gibbs Free Energy= 0.541967 Sum of electronic and zero-point Energies= -2667.525633 Sum of electronic and thermal Energies= -2667.478482 Sum of electronic and thermal Enthalpies= -2667.477537 Sum of electronic and thermal Free Energies= -2667.607145	Zero-point correction= 1.206692 (Hartree/Particle) Thermal correction to Energy= 1.285991 Thermal correction to Enthalpy= 1.286935 Thermal correction to Gibbs Free Energy= 1.087687 Sum of electronic and zero-point Energies= -4435.586172 Sum of electronic and thermal Energies= -4435.506873 Sum of electronic and thermal Enthalpies= -4435.505929 Sum of electronic and thermal Free Energies= -4435.705177

IMes-X	**IPR*-X**
82 IMesX SCF Done: -2668.18220794 A.U. Pd 0.134646 0.225027 -0.306137 K 3.857807 1.652192 0.786242 O 1.362200 2.919369 2.095449 H 0.947768 3.567116 1.484581 B 0.421295 2.038794 2.600318 O -0.894332 2.413117 2.754204 H -1.427792 1.643469 3.028385 C 0.690068 2.137039 -0.860062 C 0.061392 3.375101 -0.562722 C 1.914970 2.216197 -1.579848 C 0.653841 4.613979 -0.888022 H -0.919767 3.377386 -0.058742 C 2.511625 3.449730 -1.924189 H 2.411254 1.279594 -1.899212 C 1.892524 4.659852 -1.556873 H 0.136588 5.553288 -0.627590 H 3.453777 3.466587 -2.501409	156 ItPrX SCF Done: -4436.80807985 A.U. Pd 0.079667 1.585682 -0.410202 K -4.150487 3.074930 -0.179359 O -1.844193 4.705074 -2.200984 H -1.312353 5.458008 -1.874179 B -1.018980 3.814659 -2.867083 O 0.161225 4.226728 -3.425559 H 0.739828 3.469483 -3.655996 C 0.006207 3.634570 -0.045132 C 0.871438 4.684568 -0.435349 C -1.034796 3.981216 0.858349 C 0.679083 6.010202 0.007767 H 1.704758 4.479248 -1.126061 C -1.227894 5.293910 1.323651 H -1.697204 3.184854 1.241008 C -0.374693 6.325674 0.886066 H 1.364990 6.803921 -0.333653 H -2.032980 5.512150 2.047669

H	2.350526	5.626648	-1.820998	H	-0.516523	7.358863	1.241847
C	2.010935	0.334452	2.355293	C	-2.504784	2.104641	-2.174192
O	3.071213	0.286846	2.999803	O	-3.665976	2.292384	-2.581408
O	0.840936	0.781118	3.008181	O	-1.442382	2.495244	-3.004791
O	1.868111	0.070090	1.113616	O	-2.171722	1.605573	-1.041806
C	-2.591489	1.036512	-1.287400	C	2.584260	1.996436	-1.780335
C	-2.800485	1.541419	0.009969	C	1.926805	1.559033	-2.952014
C	-3.621558	1.152586	-2.247573	C	3.758946	2.769705	-1.896802
C	-4.009790	2.168367	0.346134	C	2.444529	1.875564	-4.217493
C	-4.834889	1.770056	-1.912202	C	4.260667	3.111966	-3.163899
C	-5.028960	2.287203	-0.615498	C	3.608347	2.663894	-4.326062
H	-1.986894	1.430471	0.745551	H	1.013136	0.951260	-2.856158
H	-3.438865	0.747229	-3.255198	H	4.260746	3.108851	-0.977504
H	-4.158234	2.562288	1.364158	H	1.939135	1.499211	-5.120941
H	-5.635333	1.858172	-2.664856	H	5.167814	3.731518	-3.245504
H	-5.979091	2.780840	-0.354650	H	4.006674	2.925999	-5.319063
C	-1.284838	0.376300	-1.674998	C	2.034170	1.684628	-0.401999
O	-1.145330	-0.066298	-2.817666	O	2.801325	1.548671	0.554249
N	-1.235337	-2.589911	0.119379	N	0.807138	-1.526721	-0.225384
N	0.882487	-2.725986	-0.292319	N	-0.414709	-0.747625	1.385502
C	-0.128967	-1.809907	-0.101328	C	0.128477	-0.396134	0.168702
C	-0.924932	-3.952121	0.084400	C	0.668477	-2.562666	0.710480
C	0.418014	-4.036617	-0.177516	C	-0.091973	-2.065873	1.732526
C	-2.542152	-2.051709	0.396639	C	1.364892	-1.622704	-1.552413
C	-3.522661	-2.064666	-0.621619	C	2.762711	-1.541635	-1.757261
C	-4.776294	-1.497982	-0.322163	C	3.228358	-1.528914	-3.087000
C	-5.060723	-0.933833	0.935242	C	2.339082	-1.636371	-4.165842
C	-4.053385	-0.950218	1.920925	C	0.963724	-1.796474	-3.938196
C	-2.783530	-1.503650	1.677442	C	0.456393	-1.796409	-2.626345
C	2.255865	-2.354251	-0.524042	C	3.718046	-1.609991	-0.565244
C	3.157529	-2.401005	0.561384	C	3.761061	-3.032698	0.012443
C	4.475487	-1.951519	0.341056	C	4.275293	-3.223003	1.311902
C	4.883956	-1.438491	-0.906428	C	4.325451	-4.501641	1.886478
C	3.945559	-1.404172	-1.961292	C	3.865790	-5.620333	1.166227
C	2.625417	-1.872272	-1.802746	C	3.372856	-5.445915	-0.137337
H	-1.682706	-4.723293	0.253479	C	3.326659	-4.162337	-0.711472
H	1.082931	-4.898215	-0.291199	C	5.132910	-1.117807	-0.877432
H	-5.544535	-1.469464	-1.111768	C	5.503572	0.207315	-0.573824
H	-4.258130	-0.504456	2.908866	C	6.787743	0.679171	-0.895765
H	5.186596	-1.971331	1.183991	C	7.719745	-0.166140	-1.522024
H	4.253499	-1.018074	-2.947760	C	7.362557	-1.495171	-1.814997
C	6.307540	-0.968791	-1.127676	C	6.080587	-1.968216	-1.489155
H	6.810775	-0.707254	-0.173414	H	2.726161	-1.611151	-5.196415
H	6.920341	-1.764287	-1.605581	C	-1.003192	-2.121636	-2.316901
H	6.353049	-0.087733	-1.802455	C	-1.118036	-3.542445	-1.754121
C	-6.417788	-0.333269	1.216808	C	-0.182136	-4.548309	-2.070404
H	-6.823922	0.170817	0.316616	C	-0.259825	-5.818146	-1.471242
H	-7.147608	-1.116189	1.519982	C	-1.279566	-6.103869	-0.547592
H	-6.372173	0.414528	2.033982	C	-2.237185	-5.118041	-0.247727
C	2.717689	-2.863852	1.928437	C	-2.158293	-3.855232	-0.853751
H	1.657108	-2.602848	2.112961	C	-1.975752	-1.796675	-3.448532
H	2.813873	-3.966042	2.038814	C	-2.891396	-2.728145	-3.973342
H	3.323208	-2.375586	2.715535	C	-3.837791	-2.327878	-4.936450
C	1.641065	-1.847697	-2.944270	C	-3.883796	-0.994312	-5.377664
H	2.156549	-1.704126	-3.913792	C	-2.963574	-0.059614	-4.864746
H	1.059404	-2.791667	-2.992074	C	-2.013655	-0.465829	-3.917724
H	0.886772	-1.037309	-2.828528	C	-1.225932	0.176718	2.144908
C	-3.216907	-2.594373	-2.001320	C	-2.635036	0.105856	2.036968
H	-2.740925	-3.596026	-1.973120	C	-3.401125	1.047509	2.759364
H	-4.137467	-2.666652	-2.612253	C	-2.781516	2.026996	3.548007
H	-2.509786	-1.915162	-2.525535	C	-1.382051	2.061888	3.662101
C	-1.697427	-1.474518	2.723737	C	-0.581028	1.131967	2.975842
H	-2.098334	-1.188040	3.716062	C	-3.296063	-1.045373	1.279712

H	-1.198605	-2.461217	2.826605	C	-3.624479	-2.222498	2.216458
H	-0.895014	-0.756264	2.448483	C	-3.038670	-2.350464	3.494118
				C	-3.281208	-3.483792	4.290569
				C	-4.125139	-4.507589	3.829626
				C	-4.729410	-4.383559	2.565370
				C	-4.481273	-3.253573	1.769463
				C	-4.479337	-0.629524	0.408336
				C	-4.309031	-0.519800	-0.986553
				C	-5.368260	-0.125472	-1.822482
				C	-6.622657	0.178548	-1.265262
				C	-6.815535	0.058321	0.126542
				C	-5.756649	-0.357002	0.954135
				H	-3.394148	2.756574	4.102016
				C	0.930442	1.060947	3.188593
				C	1.280168	-0.221983	3.941195
				C	0.419124	-0.761646	4.921655
				C	0.736859	-1.962855	5.578955
				C	1.931513	-2.636762	5.271402
				C	2.804371	-2.095557	4.310520
				C	2.480161	-0.901202	3.647188
				C	1.491273	2.328138	3.833667
				C	1.731148	2.433970	5.218833
				C	2.173676	3.648033	5.776674
				C	2.379077	4.770960	4.956011
				C	2.150487	4.669120	3.570995
				C	1.717306	3.455930	3.014812
				H	1.102134	-3.553284	0.553344
				H	-0.410914	-2.518085	2.675002
				H	4.306862	-1.423764	-3.271283
				H	0.266259	-1.925351	-4.779570
				H	3.301271	-0.947733	0.224282
				H	4.642928	-2.347708	1.870533
				H	4.721929	-4.629794	2.906537
				H	3.896979	-6.623591	1.619721
				H	3.014856	-6.312958	-0.714465
				H	2.924119	-4.035288	-1.727517
				H	4.770391	0.864824	-0.081030
				H	7.060182	1.718717	-0.651726
				H	8.726056	0.205238	-1.773953
				H	8.089224	-2.170375	-2.294848
				H	5.809203	-3.013933	-1.705942
				H	-1.299838	-1.436569	-1.490495
				H	0.632550	-4.327417	-2.776790
				H	0.489394	-6.585543	-1.723145
				H	-1.329741	-7.091775	-0.062951
				H	-3.039500	-5.320317	0.478341
				H	-2.915512	-3.092228	-0.619326
				H	-2.875428	-3.769358	-3.616410
				H	-4.551197	-3.066433	-5.336165
				H	-4.637316	-0.681516	-6.118027
				H	-2.995278	0.996299	-5.172963
				H	-1.294218	0.265186	-3.520374
				H	-4.498903	0.991581	2.717858
				H	-0.893111	2.819225	4.291700
				H	-2.525819	-1.429474	0.578554
				H	-2.378185	-1.557467	3.876916
				H	-2.804579	-3.561260	5.280805
				H	-4.317566	-5.394327	4.453958
				H	-5.400935	-5.174011	2.193305
				H	-4.961726	-3.166693	0.782349
				H	-3.324276	-0.712556	-1.430887
				H	-5.188410	-0.038694	-2.903868
				H	-7.455178	0.494289	-1.914149

	H -7.804465 0.264776 0.567467 H -5.932805 -0.510733 2.030999 H 1.411256 0.994888 2.189568 H -0.518840 -0.236896 5.164487 H 0.048203 -2.372648 6.335440 H 2.184305 -3.580701 5.779758 H 3.741335 -2.618408 4.069848 H 3.151668 -0.485747 2.877849 H 1.573627 1.558139 5.867895 H 2.359914 3.714319 6.860919 H 2.721771 5.722053 5.394611 H 2.305102 5.536811 2.910072 H 1.538198 3.381102 1.933585
Zero-point correction= 0.624819 (Hartree/Particle) Thermal correction to Energy= 0.672590 Thermal correction to Enthalpy= 0.673534 Thermal correction to Gibbs Free Energy= 0.542387 Sum of electronic and zero-point Energies= -2667.557389 Sum of electronic and thermal Energies= -2667.509618 Sum of electronic and thermal Enthalpies= -2667.508674 Sum of electronic and thermal Free Energies= -2667.639821	Zero-point correction= 1.206874 (Hartree/Particle) Thermal correction to Energy= 1.287136 Thermal correction to Enthalpy= 1.288081 Thermal correction to Gibbs Free Energy= 1.085296 Sum of electronic and zero-point Energies= -4435.601206 Sum of electronic and thermal Energies= -4435.520943 Sum of electronic and thermal Enthalpies= -4435.519999 Sum of electronic and thermal Free Energies= -4435.722784

IMes-XI	**IPR*-XI**
72 IMesXI SCF Done: -1627.89204196 A.U. Pd 0.567013 0.451477 -0.166030 C 1.343887 2.332497 -0.244856 C 0.764850 3.609910 -0.426006 C 2.744632 2.278131 -0.012130 C 1.542654 4.782166 -0.364602 H -0.318600 3.699217 -0.613588 C 3.527876 3.446904 0.056042 H 3.251911 1.302947 0.121408 C 2.926701 4.706204 -0.121563 H 1.064022 5.765801 -0.508252 H 4.612610 3.372027 0.244738 H 3.534566 5.624495 -0.073824 C -2.176262 1.594661 -0.322794 C -1.996790 1.987186 1.018473 C -3.423098 1.810585 -0.951108 C -3.053731 2.571889 1.731223 C -4.474919 2.408774 -0.242564 C -4.295722 2.782452 1.102212 H -1.004798 1.830090 1.475260 H -3.542328 1.493404 -1.998067 H -2.906310 2.876078 2.779645 H -5.444804 2.576218 -0.737117 H -5.124634 3.247456 1.660150 C -1.082195 0.929553 -1.123756 O -1.227365 0.643371 -2.300472 N 1.327309 -2.418144 0.189414 N -0.832477 -2.389675 0.172521 C 0.256719 -1.565646 0.069904 C 0.922063 -3.740289 0.365929 C -0.450983 -3.722344 0.353997 C 2.671486 -1.897768 0.169657 C 3.269235 -1.536361 1.399035 C 4.544915 -0.942056 1.355665 C 5.205539 -0.692444 0.135871 C 4.566281 -1.061651 -1.066207 C 3.293446 -1.660342 -1.079486 C -2.192123 -1.916395 0.129652	146 ItPrXI SCF Done: -3396.52017244 A.U. Pd -0.720063 0.698401 -1.461601 C -1.809682 1.550814 -2.957208 C -2.626243 0.833171 -3.862630 C -1.970500 2.959951 -2.898878 C -3.618397 1.481983 -4.621978 H -2.508640 -0.257299 -3.960609 C -2.965417 3.613097 -3.651540 H -1.323736 3.558970 -2.234383 C -3.799960 2.872967 -4.510593 H -4.256374 0.895582 -5.304912 H -3.087492 4.706267 -3.569609 H -4.577191 3.381698 -5.104224 C 0.882831 -0.758291 -3.472613 C -0.095566 -1.763903 -3.343189 C 2.046273 -1.010097 -4.233386 C 0.083961 -3.006008 -3.966672 C 2.235470 -2.261546 -4.835483 C 1.252902 -3.261311 -4.707036 H -0.988754 -1.551440 -2.732590 H 2.800365 -0.216319 -4.325444 H -0.687614 -3.784118 -3.865499 H 3.156313 -2.457470 -5.407283 H 1.399417 -4.243749 -5.184603 C 0.735003 0.579981 -2.798722 O 1.512313 1.498115 -2.999168 N 0.052851 0.890493 1.455684 N 0.410858 -1.145203 0.845793 C 0.036484 0.074539 0.345259 C 0.412381 0.199239 2.611099 C 0.646234 -1.093271 2.226336 C -0.259324 2.294186 1.355322 C -1.610916 2.695851 1.443548 C -1.896026 4.070062 1.338189 C -0.861788 4.997822 1.134003 C 0.470470 4.570308 1.007866 C 0.794337 3.205032 1.110117 C -2.693897 1.631537 1.627117

C	-2.898772	-1.985984	-1.091112
C	-4.222878	-1.508750	-1.100785
C	-4.829163	-0.968506	0.051137
C	-4.074512	-0.894316	1.238230
C	-2.749382	-1.360614	1.303368
H	1.636789	-4.561389	0.479033
H	-1.187904	-4.525115	0.455750
H	5.023540	-0.641681	2.302139
H	5.063665	-0.853324	-2.027738
H	-4.789890	-1.541399	-2.045794
H	-4.519917	-0.434252	2.134946
C	-6.258189	-0.479613	0.016642
H	-6.536095	-0.103797	-0.988908
H	-6.965393	-1.300218	0.269806
H	-6.421464	0.338987	0.745865
C	6.538574	0.019019	0.103913
H	7.058380	-0.030439	1.081433
H	7.210796	-0.405037	-0.670054
H	6.394859	1.093644	-0.144032
C	-2.218306	-2.476627	-2.344785
H	-1.432340	-1.749436	-2.643725
H	-1.724440	-3.459648	-2.197592
H	-2.935753	-2.568507	-3.182846
C	-1.919219	-1.223128	2.555179
H	-2.526576	-0.856140	3.404571
H	-1.448553	-2.186013	2.846009
H	-1.089106	-0.503331	2.381292
C	2.518475	-1.724166	2.695940
H	2.197981	-2.777224	2.841019
H	3.132690	-1.423543	3.566324
H	1.592361	-1.108055	2.694787
C	2.567052	-1.962342	-2.367161
H	3.243075	-1.889278	-3.240515
H	2.108241	-2.972541	-2.356911
H	1.737091	-1.233735	-2.506497

C	-2.663165	1.017864	3.026230
C	-3.035329	-0.330595	3.210620
C	-2.973754	-0.929235	4.478602
C	-2.544518	-0.181869	5.590445
C	-2.188645	1.168007	5.422936
C	-2.248376	1.762390	4.149617
C	-4.071950	2.107057	1.170017
C	-4.279846	2.318882	-0.211311
C	-5.514147	2.783768	-0.688642
C	-6.566442	3.036812	0.212340
C	-6.369366	2.824570	1.587764
C	-5.127754	2.363453	2.065537
H	-1.100283	6.069876	1.051636
C	2.217009	2.666983	0.951603
C	2.774111	2.142891	2.275731
C	2.399660	2.707603	3.512344
C	2.856205	2.152431	4.721700
C	3.689555	1.020056	4.708701
C	4.093228	0.467610	3.479090
C	3.650836	1.038059	2.275742
C	3.150106	3.631701	0.224420
C	4.085896	4.432691	0.908189
C	4.908600	5.328009	0.200082
C	4.805167	5.428890	-1.197849
C	3.872061	4.630245	-1.885674
C	3.047729	3.738369	-1.180496
C	0.545803	-2.340451	0.059025
C	1.838265	-2.707476	-0.388661
C	1.968613	-3.932995	-1.068965
C	0.862995	-4.776979	-1.242779
C	-0.403556	-4.396480	-0.775564
C	-0.599698	-3.145015	-0.159619
C	3.047215	-1.840602	-0.035382
C	3.928232	-2.481153	1.050619
C	3.407179	-3.437279	1.949397
C	4.184297	-3.928923	3.012832
C	5.503508	-3.479401	3.193755
C	6.038045	-2.536743	2.297351
C	5.257965	-2.042822	1.238254
C	3.850908	-1.320938	-1.226166
C	3.810913	0.053972	-1.527979
C	4.596984	0.600715	-2.555475
C	5.430730	-0.235730	-3.315095
C	5.474910	-1.614688	-3.032601
C	4.700997	-2.149743	-1.990756
H	0.992110	-5.749102	-1.743298
C	-1.989287	-2.679484	0.281488
C	-2.612443	-3.691113	1.253032
C	-3.668357	-4.551859	0.895153
C	-4.180839	-5.478875	1.822167
C	-3.649278	-5.554144	3.120167
C	-2.598462	-4.692952	3.488997
C	-2.087178	-3.771908	2.562217
C	-2.923121	-2.290801	-0.870192
C	-3.783903	-1.183391	-0.703891
C	-4.704202	-0.815826	-1.696822
C	-4.786522	-1.556176	-2.887307
C	-3.937079	-2.658659	-3.072532
C	-3.016791	-3.021108	-2.073006
H	0.486308	0.686696	3.586523
H	1.000976	-1.960641	2.789068
H	-2.942669	4.404796	1.395921
H	1.274385	5.295094	0.809827

	H -2.420687 0.807859 0.928558 H -3.371884 -0.930245 2.350449 H -3.254474 -1.988357 4.588626 H -2.489829 -0.650322 6.585992 H -1.856458 1.763418 6.288487 H -1.949812 2.814397 4.017603 H -3.463757 2.125713 -0.925856 H -5.642220 2.943584 -1.771265 H -7.539325 3.397668 -0.157925 H -7.188470 3.017856 2.298937 H -4.978718 2.196077 3.143815 H 2.113337 1.781849 0.285354 H 1.715408 3.570707 3.527122 H 2.546910 2.600491 5.679705 H 4.028278 0.569452 5.655158 H 4.741730 -0.421775 3.449979 H 3.977210 0.606625 1.316452 H 4.177956 4.347669 2.002501 H 5.639289 5.946275 0.746038 H 5.453416 6.126813 -1.751580 H 3.783778 4.697904 -2.981888 H 2.321920 3.110732 -1.724894 H 2.956246 -4.247002 -1.433354 H -1.256259 -5.085925 -0.870890 H 2.636602 -0.929584 0.446463 H 2.381212 -3.812881 1.809290 H 3.755244 -4.675252 3.700590 H 6.114763 -3.867484 4.023770 H 7.072271 -2.178489 2.422941 H 5.685538 -1.301446 0.546028 H 3.141360 0.714844 -0.958624 H 4.533850 1.679907 -2.760952 H 6.047232 0.183277 -4.126054 H 6.130707 -2.277312 -3.619737 H 4.789157 -3.219265 -1.745565 H -1.838974 -1.752966 0.869267 H -4.104123 -4.487600 -0.113818 H -5.008821 -6.142625 1.525922 H -4.054707 -6.277274 3.845438 H -2.178072 -4.736121 4.506714 H -1.272734 -3.089492 2.855061 H -3.742038 -0.592605 0.223104 H -5.339070 0.068988 -1.541555 H -5.493310 -1.257993 -3.676785 H -3.978686 -3.239961 -4.007322 H -2.353733 -3.879747 -2.245138
Zero-point correction= 0.571579 (Hartree/Particle) Thermal correction to Energy= 0.610070 Thermal correction to Enthalpy= 0.611014 Thermal correction to Gibbs Free Energy= 0.498768 Sum of electronic and zero-point Energies= -1627.320463 Sum of electronic and thermal Energies= -1627.281972 Sum of electronic and thermal Enthalpies= -1627.281028 Sum of electronic and thermal Free Energies= -1627.393274	Zero-point correction= 1.153688 (Hartree/Particle) Thermal correction to Energy= 1.224797 Thermal correction to Enthalpy= 1.225741 Thermal correction to Gibbs Free Energy= 1.041243 Sum of electronic and zero-point Energies= -3395.366484 Sum of electronic and thermal Energies= -3395.295376 Sum of electronic and thermal Enthalpies= -3395.294431 Sum of electronic and thermal Free Energies= -3395.478929

IMes-XI-XII	**IPR*-XI-XII**
72 IMesXI-XII SCF Done: -1627.88053980 A.U. Pd -0.447783 0.454134 -0.436932 C -0.531546 2.577253 -0.314373 C 0.045197 3.378577 -1.327277 C -1.698914 3.040452 0.339558	146 ItPrXI-XII SCF Done: -3396.51362327 A.U. Pd -0.244060 -1.362032 0.817696 C -0.760513 -3.114158 1.861175 C -1.647344 -3.042999 2.960445 C -0.798395 -4.253039 1.021120

C	-0.569622	4.582572	-1.720787
H	0.984037	3.067732	-1.811706
C	-2.320650	4.233131	-0.060883
H	-2.096772	2.458725	1.187774
C	-1.756016	5.005883	-1.095631
H	-0.115753	5.196283	-2.516292
H	-3.239355	4.574251	0.444157
H	-2.232677	5.951583	-1.400842
C	2.071001	1.657176	0.657679
C	2.612877	1.377261	-0.613439
C	2.929887	2.071531	1.698942
C	3.983364	1.545803	-0.853999
C	4.303489	2.233117	1.460490
C	4.831401	1.983204	0.179765
H	1.937551	0.989785	-1.397369
H	2.490157	2.264095	2.689869
H	4.396308	1.317368	-1.848962
H	4.967827	2.562220	2.275920
H	5.908366	2.117106	-0.010127
C	0.597925	1.498756	0.957269
O	0.175655	1.529485	2.115982
N	0.507066	-2.447652	0.012428
N	-1.644218	-2.262669	0.134222
C	-0.509116	-1.535302	-0.148036
C	0.019693	-3.704157	0.378822
C	-1.345105	-3.586497	0.455970
C	1.903925	-2.110872	-0.082086
C	2.586225	-1.722411	1.092375
C	3.957903	-1.425167	0.977528
C	4.636028	-1.503395	-0.252848
C	3.906530	-1.867383	-1.404005
C	2.534366	-2.168665	-1.345000
C	-2.950089	-1.657783	0.189387
C	-3.775094	-1.719061	-0.953959
C	-5.033048	-1.088171	-0.889179
C	-5.461322	-0.408707	0.268316
C	-4.597629	-0.365549	1.383172
C	-3.330292	-0.976270	1.370665
H	0.686621	-4.554047	0.554068
H	-2.123303	-4.311681	0.713324
H	4.505570	-1.096454	1.875358
H	4.417888	-1.901348	-2.380713
H	-5.691088	-1.120628	-1.773352
H	-4.915715	0.172815	2.291787
C	-6.806504	0.280741	0.322388
H	-7.400668	0.102871	-0.595981
H	-7.404678	-0.069845	1.190219
H	-6.684667	1.379252	0.438389
C	6.113450	-1.199427	-0.345772
H	6.711339	-2.135774	-0.399905
H	6.348045	-0.609247	-1.255794
H	6.466434	-0.623609	0.532593
C	-3.284636	-2.400941	-2.209432
H	-2.346321	-1.924792	-2.568346
H	-3.045873	-3.470988	-2.031048
H	-4.036025	-2.345836	-3.020716
C	-2.384256	-0.855134	2.540387
H	-2.924342	-0.581645	3.467881
H	-1.825835	-1.796156	2.722176
H	-1.622351	-0.067896	2.340716
C	1.854620	-1.581759	2.404659
H	1.213492	-2.461843	2.619612
H	2.562887	-1.451568	3.245436

C	-2.599410	-4.058694	3.171925
H	-1.601284	-2.190541	3.654888
C	-1.760573	-5.254663	1.219878
H	-0.049822	-4.344679	0.217275
C	-2.662529	-5.159410	2.298437
H	-3.291830	-3.990253	4.026990
H	-1.803163	-6.120565	0.539794
H	-3.405857	-5.955295	2.466654
C	1.395736	-1.742616	3.315194
C	0.584233	-0.720573	3.849746
C	2.542327	-2.159633	4.027561
C	0.895792	-0.146624	5.090743
C	2.868350	-1.566130	5.254336
C	2.038921	-0.565160	5.794912
H	-0.277142	-0.360127	3.261405
H	3.169354	-2.949048	3.589486
H	0.247697	0.641218	5.502593
H	3.773468	-1.886236	5.794407
H	2.287046	-0.107832	6.766381
C	1.103914	-2.394159	1.989090
O	1.910726	-3.149926	1.450068
N	-0.205048	0.178332	-1.767777
N	0.328089	1.540856	-0.185167
C	0.023168	0.221490	-0.414816
C	-0.041520	1.428957	-2.365004
C	0.302897	2.294676	-1.360254
C	-0.497324	-1.065327	-2.431761
C	-1.831174	-1.540527	-2.461394
C	-2.071131	-2.734912	-3.169963
C	-1.017606	-3.437912	-3.775706
C	0.309702	-3.002126	-3.631245
C	0.594656	-1.812099	-2.938069
C	-2.921620	-0.849569	-1.633263
C	-3.450834	0.468334	-2.196366
C	-4.346408	1.218483	-1.399018
C	-4.911618	2.406941	-1.880349
C	-4.587864	2.873484	-3.168944
C	-3.691962	2.140911	-3.964954
C	-3.130852	0.942018	-3.482366
C	-4.066105	-1.799219	-1.275240
C	-3.970672	-2.607323	-0.124145
C	-5.008445	-3.491848	0.213973
C	-6.151436	-3.586746	-0.599045
C	-6.251387	-2.789544	-1.753503
C	-5.216601	-1.899313	-2.086359
H	-1.230148	-4.367184	-4.327460
C	2.021292	-1.350843	-2.622131
C	2.424157	-0.097439	-3.393799
C	1.955116	0.152232	-4.699365
C	2.271094	1.356221	-5.355031
C	3.056051	2.327567	-4.708417
C	3.550353	2.076407	-3.414682
C	3.246295	0.865975	-2.773217
C	3.039095	-2.486182	-2.694504
C	3.859354	-2.696773	-3.820326
C	4.763129	-3.774847	-3.851143
C	4.858288	-4.649955	-2.755222
C	4.042909	-4.442131	-1.626793
C	3.137355	-3.369600	-1.596372
C	0.466342	2.039915	1.153005
C	1.745108	2.050869	1.752385
C	1.827340	2.481349	3.089268
C	0.670645	2.851907	3.793241

H	1.185941	-0.694125	2.384611
C	1.727717	-2.488091	-2.580122
H	2.369597	-2.558351	-3.479618
H	1.169014	-3.441806	-2.472874
H	0.966614	-1.694510	-2.749041

C	-0.591121	2.809790	3.178772
C	-0.713495	2.425059	1.830407
C	2.958434	1.657067	0.913675
C	3.707846	2.871456	0.343612
C	3.080761	4.128411	0.206177
C	3.733699	5.194767	-0.437395
C	5.031035	5.026474	-0.950412
C	5.670314	3.781232	-0.809640
C	5.014736	2.715707	-0.170687
C	3.870073	0.614299	1.550909
C	3.836867	-0.706631	1.063438
C	4.703996	-1.688428	1.568526
C	5.610038	-1.361730	2.590057
C	5.646513	-0.048432	3.095609
C	4.791205	0.934481	2.572366
H	0.754170	3.161391	4.846640
C	-2.041895	2.479776	1.074020
C	-2.308431	3.901491	0.577185
C	-2.444004	4.997176	1.458242
C	-2.679892	6.291682	0.966109
C	-2.778205	6.515875	-0.419627
C	-2.639754	5.434291	-1.305558
C	-2.406410	4.140491	-0.809187
C	-3.197166	1.789826	1.803035
C	-4.432659	2.410198	2.067666
C	-5.501607	1.668792	2.608933
C	-5.352834	0.298719	2.880599
C	-4.119828	-0.329568	2.619839
C	-3.053559	0.413611	2.096204
H	-0.140813	1.580696	-3.441836
H	0.533224	3.362772	-1.369698
H	-3.095317	-3.133802	-3.212023
H	1.142098	-3.601698	-4.029937
H	-2.438352	-0.595594	-0.659149
H	-4.606262	0.854839	-0.392376
H	-5.594368	2.982531	-1.236323
H	-5.026785	3.811006	-3.544805
H	-3.432154	2.496550	-4.975061
H	-2.444549	0.359018	-4.117321
H	-3.072906	-2.544546	0.511373
H	-4.912949	-4.106531	1.121710
H	-6.965998	-4.278898	-0.331793
H	-7.144194	-2.855559	-2.395944
H	-5.303971	-1.262118	-2.980986
H	1.990658	-1.053967	-1.550180
H	1.308444	-0.592431	-5.191045
H	1.891422	1.540696	-6.373034
H	3.285296	3.280094	-5.212153
H	4.160969	2.828339	-2.890502
H	3.636593	0.672740	-1.761065
H	3.797215	-2.004368	-4.674824
H	5.401714	-3.926614	-4.736276
H	5.570699	-5.490130	-2.778376
H	4.110827	-5.117178	-0.758582
H	2.502176	-3.217736	-0.706891
H	2.802162	2.496021	3.595888
H	-1.498088	3.064221	3.749175
H	2.540163	1.156160	0.016145
H	2.067982	4.280026	0.611841
H	3.222777	6.166355	-0.532577
H	5.544322	5.862111	-1.451910
H	6.688296	3.634101	-1.204464
H	5.522111	1.743549	-0.072143

	H 3.108337 -0.979326 0.284438 H 4.641915 -2.711123 1.168021 H 6.288908 -2.128829 2.995579 H 6.358065 0.216048 3.894173 H 4.868036 1.973063 2.931706 H -1.918497 1.869563 0.157275 H -2.364924 4.838602 2.544439 H -2.785829 7.132284 1.670456 H -2.961253 7.531529 -0.805156 H -2.719481 5.589920 -2.393258 H -2.303931 3.297937 -1.508766 H -4.574313 3.473471 1.821386 H -6.464272 2.168251 2.803882 H -6.196848 -0.282374 3.284477 H -3.988020 -1.407431 2.802620 H -2.092909 -0.093682 1.861630
Zero-point correction= 0.570933 (Hartree/Particle) Thermal correction to Energy= 0.608825 Thermal correction to Enthalpy= 0.609770 Thermal correction to Gibbs Free Energy= 0.498458 Sum of electronic and zero-point Energies= -1627.309607 Sum of electronic and thermal Energies= -1627.271714 Sum of electronic and thermal Enthalpies= -1627.270770 Sum of electronic and thermal Free Energies= -1627.382082	Zero-point correction= 1.153050 (Hartree/Particle) Thermal correction to Energy= 1.223257 Thermal correction to Enthalpy= 1.224202 Thermal correction to Gibbs Free Energy= 1.043108 Sum of electronic and zero-point Energies= -3395.360574 Sum of electronic and thermal Energies= -3395.290366 Sum of electronic and thermal Enthalpies= -3395.289422 Sum of electronic and thermal Free Energies= -3395.470516

IMes-XII	**IPR*-XII**
72	146
IMesXII SCF Done: -1627.90987812 A.U.	ItPrXII SCF Done: -3396.54422678 A.U.
Pd -0.449695 -0.459977 0.403307	Pd 0.027988 -0.898061 -1.272034
C -0.269678 -2.593233 0.014584	C 0.008922 -2.443231 -2.858445
C -0.044746 -3.319987 1.231014	C -1.223395 -3.181433 -2.759254
C -1.626253 -2.226813 -0.323609	C -0.029438 -1.144087 -3.476341
C -1.115294 -3.684266 2.050309	C -2.402306 -2.667208 -3.294567
H 0.979137 -3.627697 1.491297	H -1.209927 -4.186394 -2.310483
C -2.694502 -2.585600 0.545411	C -1.261858 -0.616784 -3.960256
H -1.843678 -1.870821 -1.342807	H 0.923077 -0.685245 -3.777617
C -2.441405 -3.307443 1.714078	C -2.429758 -1.375939 -3.884274
H -0.926268 -4.267447 2.965432	H -3.328349 -3.259563 -3.242144
H -3.719312 -2.286645 0.275053	H -1.274569 0.390389 -4.404425
H -3.273765 -3.590151 2.378361	H -3.382067 -0.966275 -4.255198
C 2.245099 -2.141013 -0.564927	C 1.460055 -4.238618 -1.666445
C 2.656839 -1.693095 0.712018	C 0.737960 -4.299089 -0.453753
C 3.232326 -2.452082 -1.527486	C 2.355912 -5.283218 -1.988321
C 4.020429 -1.600716 1.028752	C 0.878520 -5.406816 0.396215
C 4.595459 -2.371066 -1.205981	C 2.498323 -6.386788 -1.135475
C 4.993420 -1.957220 0.078565	C 1.750983 -6.455252 0.055488
H 1.899482 -1.372961 1.446376	H 0.091619 -3.454986 -0.159241
H 2.897645 -2.761249 -2.529645	H 2.929738 -5.209464 -2.925220
H 4.324463 -1.229252 2.019811	H 0.302924 -5.442912 1.332173
H 5.354015 -2.634520 -1.960643	H 3.192113 -7.200608 -1.400172
H 6.063093 -1.893552 0.332899	H 1.855372 -7.325420 0.723371
C 0.798060 -2.254452 -0.998021	C 1.350257 -3.090318 -2.635059
O 0.512903 -2.130075 -2.202555	O 2.342983 -2.733817 -3.283670
N 0.458235 2.434553 -0.112924	N 0.055184 0.241730 1.587155
N -1.689371 2.198072 -0.223719	N -0.407853 1.776813 0.152046
C -0.539454 1.517110 0.111468	C -0.086030 0.441580 0.233615
C -0.053262 3.650972 -0.573604	C -0.178000 1.403422 2.323710
C -1.415753 3.499579 -0.646755	C -0.478573 2.381787 1.411673
C 1.856589 2.111710 0.006301	C 0.415521 -1.042256 2.113461
C 2.524162 1.538079 -1.099119	C 1.782640 -1.368570 2.218077
C 3.898827 1.261300 -0.952594	C 2.111500 -2.626312 2.762395
C 4.590716 1.527427 0.242430	C 1.102730 -3.509708 3.174860

C	3.872512	2.061361	1.333762
C	2.502405	2.359689	1.240004
C	-2.958034	1.517840	-0.282270
C	-3.745729	1.434777	0.884739
C	-4.940217	0.690919	0.816448
C	-5.342014	0.037945	-0.365371
C	-4.513739	0.135485	-1.504198
C	-3.312014	0.865638	-1.487871
H	0.595796	4.500704	-0.806916
H	-2.205951	4.190444	-0.957096
H	4.436613	0.799009	-1.796031
H	4.395261	2.249110	2.286858
H	-5.565202	0.605299	1.720971
H	-4.802160	-0.391214	-2.429351
C	-6.629582	-0.753726	-0.424938
H	-7.050006	-0.934312	0.584563
H	-7.401651	-0.216763	-1.018295
H	-6.476330	-1.738598	-0.914145
C	6.072318	1.255706	0.366340
H	6.454097	0.669593	-0.492479
H	6.648739	2.205431	0.413916
H	6.302282	0.690601	1.293980
C	-3.259296	2.051018	2.172841
H	-2.346159	1.516806	2.517377
H	-2.972267	3.114889	2.039614
H	-4.025211	1.989532	2.970067
C	-2.374347	0.885230	-2.670274
H	-2.829896	0.407606	-3.558892
H	-2.070330	1.917433	-2.942870
H	-1.439500	0.335251	-2.418879
C	1.792840	1.173875	-2.368038
H	0.943469	1.854859	-2.574348
H	2.476183	1.187042	-3.240040
H	1.372481	0.146378	-2.290105
C	1.712042	2.887981	2.413254
H	2.354621	3.035069	3.303009
H	1.220557	3.855505	2.175993
H	0.898127	2.178222	2.678208

C	-0.254023	-3.192922	2.979354
C	-0.618935	-1.955901	2.420274
C	2.837977	-0.387274	1.703701
C	3.249840	0.613430	2.778905
C	3.249696	1.993052	2.486977
C	3.619100	2.942591	3.453227
C	3.997188	2.521775	4.740517
C	3.997906	1.148860	5.048180
C	3.623735	0.204055	4.076856
C	3.972766	-1.135692	1.003332
C	3.635302	-1.858743	-0.161151
C	4.601758	-2.589669	-0.861529
C	5.933877	-2.602349	-0.405772
C	6.284227	-1.871979	0.742696
C	5.307417	-1.140483	1.447254
H	1.378084	-4.484366	3.607100
C	-2.057646	-1.563426	2.087374
C	-2.634462	-0.560566	3.083721
C	-2.244084	-0.545044	4.438072
C	-2.735820	0.440167	5.314038
C	-3.619591	1.426817	4.843275
C	-4.025292	1.411810	3.495905
C	-3.542408	0.419709	2.629445
C	-2.938157	-2.771208	1.788540
C	-3.839739	-3.314177	2.723194
C	-4.605001	-4.449322	2.395102
C	-4.477575	-5.050065	1.130393
C	-3.579729	-4.508815	0.190045
C	-2.817212	-3.378515	0.519073
C	-0.575332	2.412878	-1.122516
C	-1.860725	2.405755	-1.713652
C	-1.979503	2.934046	-3.011076
C	-0.857552	3.461750	-3.673807
C	0.398500	3.489356	-3.047635
C	0.567463	2.951924	-1.756285
C	-3.050412	1.920544	-0.889412
C	-3.798622	3.081758	-0.209869
C	-3.217735	4.359769	-0.066149
C	-3.877276	5.377125	0.647200
C	-5.134184	5.137347	1.226720
C	-5.727430	3.869912	1.082147
C	-5.066474	2.854585	0.371998
C	-3.989873	0.938884	-1.582258
C	-3.970728	-0.413533	-1.187858
C	-4.903594	-1.332438	-1.694539
C	-5.845877	-0.917693	-2.650238
C	-5.856139	0.423596	-3.079011
C	-4.948400	1.348121	-2.534842
H	-0.968370	3.869397	-4.690974
C	1.921717	2.940623	-1.045251
C	2.445463	4.364885	-0.853484
C	3.257435	4.994734	-1.819324
C	3.694039	6.317195	-1.633399
C	3.333530	7.026510	-0.473287
C	2.536221	6.402484	0.502638
C	2.096803	5.081485	0.310860
C	2.959868	1.979918	-1.632460
C	4.239506	1.915597	-1.034432
C	5.199040	0.998415	-1.487509
C	4.897078	0.131223	-2.552097
C	3.630057	0.182902	-3.152337
C	2.669776	1.102222	-2.692383
H	-0.129798	1.416223	3.415901

	H -0.764729 3.429780 1.536600 H 3.170603 -2.920579 2.824443 H -1.041041 -3.921923 3.227899 H 2.354165 0.201820 0.896528 H 2.948824 2.326936 1.483812 H 3.606972 4.013371 3.193386 H 4.286698 3.260980 5.504325 H 4.288213 0.810064 6.055695 H 3.613207 -0.867603 4.330914 H 2.595287 -1.821820 -0.532033 H 4.301551 -3.113434 -1.782128 H 6.701603 -3.171425 -0.954465 H 7.327714 -1.867204 1.097425 H 5.589464 -0.561858 2.340817 H -1.984975 -1.017532 1.121524 H -1.526728 -1.297615 4.802308 H -2.416067 0.442013 6.368529 H -3.989904 2.209885 5.523878 H -4.704147 2.186576 3.106828 H -3.863882 0.411734 1.575858 H -3.948146 -2.836064 3.709894 H -5.310109 -4.864298 3.133105 H -5.080175 -5.936372 0.875608 H -3.474306 -4.965116 -0.807615 H -2.124287 -2.944043 -0.222068 H -2.959175 2.932199 -3.509823 H 1.267313 3.921714 -3.566557 H -2.614339 1.344537 -0.047530 H -2.237961 4.568580 -0.523418 H -3.403626 6.367344 0.743250 H -5.652914 5.934685 1.782030 H -6.716024 3.668069 1.525101 H -5.541919 1.867183 0.263837 H -3.199814 -0.753658 -0.480334 H -4.876445 -2.374388 -1.339750 H -6.576401 -1.634241 -3.058063 H -6.596491 0.758725 -3.823012 H -5.017813 2.410622 -2.817633 H 1.725301 2.559107 -0.023107 H 3.570259 4.428558 -2.711207 H 4.329190 6.795127 -2.396340 H 3.681743 8.061105 -0.325764 H 2.259027 6.944981 1.420796 H 1.479052 4.587396 1.079546 H 4.488047 2.597567 -0.206030 H 6.180079 0.942922 -0.991045 H 5.640957 -0.604516 -2.892035 H 3.368277 -0.527949 -3.949780 H 1.675049 1.133901 -3.157276
Zero-point correction= 0.572675 (Hartree/Particle) Thermal correction to Energy= 0.610806 Thermal correction to Enthalpy= 0.611750 Thermal correction to Gibbs Free Energy= 0.500592 Sum of electronic and zero-point Energies= -1627.337203 Sum of electronic and thermal Energies= -1627.299072 Sum of electronic and thermal Enthalpies= -1627.298128 Sum of electronic and thermal Free Energies= -1627.409286	Zero-point correction= 1.155519 (Hartree/Particle) Thermal correction to Energy= 1.226036 Thermal correction to Enthalpy= 1.226981 Thermal correction to Gibbs Free Energy= 1.045163 Sum of electronic and zero-point Energies= -3395.388708 Sum of electronic and thermal Energies= -3395.318190 Sum of electronic and thermal Enthalpies= -3395.317246 Sum of electronic and thermal Free Energies= -3395.499064

B-Ph(oMe)-IPr-IX	**B-Ph(oMeISOMER)-IPr-IX**
103 IPrIX-MeOrto SCF Done: -2943.17774131 A.U.	103 IPrIX-MeOrto180 SCF Done: -2943.17765554 A.U.

Pd	0.135873	0.244631	-0.493705	Pd	-0.099869	-0.340686	-0.439895
K	-0.761579	5.289489	1.092248	K	2.920143	-4.351094	1.486837
O	0.413185	4.481921	-1.065773	O	1.705715	-4.214650	-0.807033
H	0.679309	4.679389	-1.979273	H	1.694613	-4.531198	-1.725676
B	-0.517196	3.327009	-1.068679	B	2.069588	-2.778293	-0.789671
O	-1.877432	3.843914	-1.278272	O	3.537517	-2.683119	-0.736114
H	-2.525958	3.118737	-1.199404	H	3.807276	-1.746040	-0.721116
C	-0.078828	2.149457	-2.159321	C	1.310956	-1.968294	-2.019094
C	-1.063536	1.721751	-3.109745	C	1.936571	-1.262960	-3.108536
C	1.259646	1.644473	-2.360671	C	-0.113152	-2.127976	-2.091882
C	-0.791309	0.837581	-4.155806	C	1.138928	-0.732331	-4.141624
H	-2.083207	2.124798	-3.012050	C	-0.897473	-1.580916	-3.138017
C	1.507286	0.702931	-3.402921	H	-0.604022	-2.792755	-1.362903
C	0.506408	0.303099	-4.289613	C	-0.262436	-0.872299	-4.161260
H	-1.591107	0.542245	-4.853137	H	1.632539	-0.191089	-4.966290
H	2.532331	0.310880	-3.512268	H	-1.989844	-1.719836	-3.128909
C	0.574036	2.606242	1.173262	C	0.456460	-2.649056	1.262321
O	0.821319	3.435917	2.080574	O	0.554954	-3.508307	2.169101
O	-0.548668	2.826078	0.398297	O	1.615415	-2.268189	0.606771
O	1.238688	1.537237	0.925334	O	-0.618415	-2.033487	0.921509
N	1.872038	-1.592180	1.064140	N	-2.587256	0.637240	0.850293
N	-0.177244	-1.833357	1.734662	N	-0.906528	1.736380	1.672977
C	0.585139	-1.206826	0.785798	C	-1.232750	0.810998	0.718442
C	1.910596	-2.432279	2.177712	C	-3.094186	1.432837	1.877334
C	0.618426	-2.582325	2.604727	C	-2.033821	2.123473	2.402012
C	3.022050	-1.245151	0.260677	C	-3.377456	-0.187872	-0.036482
C	3.963646	-0.323804	0.780640	C	-3.830125	-1.448627	0.421933
C	5.092268	-0.039774	-0.018219	C	-4.585060	-2.224966	-0.482752
C	5.250995	-0.624376	-1.280259	C	-4.863379	-1.764260	-1.776053
C	4.287175	-1.517729	-1.775421	C	-4.395493	-0.510095	-2.199674
C	3.151365	-1.860460	-1.016393	C	-3.638556	0.310693	-1.341746
C	3.796789	0.340547	2.144899	C	-3.558916	-1.945634	1.839432
H	6.132290	-0.376374	-1.893193	H	-5.448760	-2.391537	-2.467390
C	2.116131	-2.862693	-1.527706	C	-3.137059	1.684840	-1.782906
C	-1.615904	-1.756603	1.787212	C	0.419619	2.273292	1.854172
C	-2.357115	-2.756101	1.108414	C	0.745359	3.477078	1.180572
C	-3.762332	-2.655792	1.159380	C	2.045810	3.987048	1.372304
C	-4.384569	-1.612633	1.858551	C	2.964054	3.325214	2.198194
C	-3.619021	-0.631608	2.506511	C	2.614759	2.124085	2.833499
C	-2.211769	-0.667772	2.471907	C	1.337714	1.555996	2.662196
C	-1.661810	-3.903411	0.375528	C	-0.276433	4.208950	0.310156
H	-5.483764	-1.547808	1.876853	H	3.976766	3.737845	2.328697
C	-1.356924	0.417921	3.122833	C	0.955196	0.220387	3.297209
H	2.849688	-2.850276	2.549537	H	-4.157176	1.437179	2.132357
H	0.191887	-3.145041	3.439291	H	-1.972850	2.845411	3.220706
H	5.845719	0.672016	0.351365	H	-4.951355	-3.213009	-0.166087
H	4.425326	-1.960218	-2.772406	H	-4.616088	-0.165956	-3.220420
H	2.729746	0.243916	2.429819	H	-2.669432	-1.399420	2.214251
H	1.115423	-2.451876	-1.285672	H	-2.127423	1.819694	-1.344611
H	-4.378119	-3.397869	0.630628	H	2.346353	4.912056	0.858645
H	-4.126068	0.198176	3.020207	H	3.360633	1.600278	3.448966
H	-0.663613	-3.534247	0.057113	H	-1.006512	3.454110	-0.052404
H	-0.442177	0.527605	2.503222	H	0.253986	-0.283885	2.599204
C	-2.035585	1.798965	3.156836	C	2.148097	-0.734340	3.484153
H	-2.879147	1.833725	3.879503	H	2.838407	-0.392089	4.285234
H	-1.287220	2.559301	3.458486	H	1.766529	-1.738303	3.759014
H	-2.408805	2.087493	2.154293	H	2.718420	-0.849153	2.540676
C	-0.912642	-0.000682	4.541396	C	0.212726	0.433902	4.634340
H	-0.341364	-0.950471	4.530527	H	-0.699704	1.049827	4.504070
H	-0.260601	0.779360	4.986757	H	-0.096670	-0.541448	5.064395
H	-1.793666	-0.139408	5.204305	H	0.867917	0.947241	5.370530
C	-2.398912	-4.354536	-0.896288	C	0.342818	4.867921	-0.933905
H	-1.775893	-5.086342	-1.450492	H	-0.461060	5.262992	-1.588312

H	-3.362891	-4.854656	-0.662714	H	0.999767	5.722964	-0.667641
H	-2.591407	-3.499896	-1.570691	H	0.927463	4.138337	-1.523970
C	-1.447576	-5.104834	1.323673	C	-1.048700	5.255740	1.144220
H	-2.424179	-5.510843	1.663566	H	-0.356131	6.032941	1.532201
H	-0.898708	-5.917947	0.803594	H	-1.817623	5.759716	0.521682
H	-0.866730	-4.828889	2.225597	H	-1.563250	4.800203	2.013152
C	4.098149	1.850521	2.102647	C	-3.208499	-3.443451	1.892841
H	3.799945	2.320698	3.061591	H	-2.858599	-3.711028	2.910705
H	5.179408	2.055536	1.948464	H	-4.086008	-4.085613	1.662718
H	3.509296	2.338111	1.304053	H	-2.383595	-3.671890	1.192664
C	4.671724	-0.363423	3.204997	C	-4.763691	-1.633819	2.755373
H	5.749317	-0.279972	2.946513	H	-5.673100	-2.167352	2.404343
H	4.524799	0.100856	4.202964	H	-4.557667	-1.959789	3.796738
H	4.438213	-1.444421	3.295374	H	-5.005967	-0.551508	2.779869
C	2.124258	-3.047182	-3.051001	C	-2.947122	1.815183	-3.300000
H	3.041973	-3.560848	-3.411358	H	-3.912382	1.794342	-3.850760
H	1.253614	-3.663756	-3.351297	H	-2.449232	2.778114	-3.530575
H	2.030827	-2.074876	-3.571734	H	-2.292683	1.008870	-3.682671
C	2.251060	-4.229120	-0.818312	C	-4.048850	2.808697	-1.242601
H	1.460229	-4.922879	-1.174087	H	-3.640262	3.803311	-1.520550
H	3.237477	-4.693190	-1.033662	H	-5.072352	2.726225	-1.667245
H	2.145589	-4.145459	0.281753	H	-4.135814	2.780333	-0.137681
C	-2.579819	-0.394142	-1.370358	C	2.131207	1.391955	-1.188395
C	-2.938309	0.624821	-0.462580	C	2.805543	0.706717	-0.156134
C	-3.569130	-0.946659	-2.213061	C	2.860686	2.256312	-2.034460
C	-4.263804	1.079087	-0.392197	C	4.181865	0.896457	0.040878
C	-4.894172	-0.491732	-2.143816	C	4.237531	2.442592	-1.840206
C	-5.245719	0.523060	-1.232770	C	4.901781	1.766527	-0.798595
H	-2.157888	1.067991	0.178917	H	2.239358	0.007495	0.480345
H	-3.269764	-1.723116	-2.933950	H	2.326507	2.758737	-2.855515
H	-4.531528	1.865118	0.332180	H	4.690828	0.366712	0.862013
H	-5.659387	-0.924701	-2.808096	H	4.801017	3.113436	-2.508359
H	-6.286485	0.881077	-1.180013	H	5.983168	1.913431	-0.646899
C	-1.147144	-0.876547	-1.502654	C	0.647346	1.195644	-1.442264
O	-0.878898	-1.833145	-2.217940	O	0.055439	1.906268	-2.243221
H	0.730542	-0.422308	-5.087793	H	-0.844640	-0.432581	-4.986469
C	2.487036	2.196046	-1.655897	C	3.437813	-1.096981	-3.211848
H	2.237002	2.954691	-0.898218	H	3.722507	-0.649744	-4.185469
H	3.063043	1.386522	-1.166241	H	3.830522	-0.423137	-2.421368
H	3.153878	2.664612	-2.412536	H	3.962343	-2.065082	-3.090155
Zero-point correction= 0.820805 (Hartree/Particle)				Zero-point correction= 0.820987 (Hartree/Particle)			
Thermal correction to Energy= 0.876224				Thermal correction to Energy= 0.876383			
Thermal correction to Enthalpy= 0.877168				Thermal correction to Enthalpy= 0.877327			
Thermal correction to Gibbs Free Energy= 0.734002				Thermal correction to Gibbs Free Energy= 0.733707			
Sum of electronic and zero-point Energies= -2942.356936				Sum of electronic and zero-point Energies= -2942.356669			
Sum of electronic and thermal Energies= -2942.301518				Sum of electronic and thermal Energies= -2942.301273			
Sum of electronic and thermal Enthalpies= -2942.300574				Sum of electronic and thermal Enthalpies= -2942.300329			
Sum of electronic and thermal Free Energies= -2942.443739				Sum of electronic and thermal Free Energies= -2942.443948			

B-Ph(oMe)-IPr-IX-X				**B-Ph(oMeISOMER)-IPr-IX-X**			
103				103			
IPrIX-X-MeOrto SCF Done: -2943.15873355 A.U.				IPrIX-X-MeOrto180 SCF Done: -2943.15791670 A.U.			
Pd	0.241813	0.289546	-0.354077	Pd	-0.241166	-0.277038	-0.342298
K	2.173102	4.405665	2.703431	K	-2.699684	-3.902265	2.937775
O	2.233467	3.782230	0.178813	O	-2.661354	-3.544956	0.391017
H	2.446158	4.017575	-0.743180	H	-2.952527	-3.761025	-0.513013
B	0.937774	3.156699	0.215150	B	-1.331660	-2.964550	0.347773
O	-0.111689	3.943700	-0.262749	O	-0.334028	-3.869126	-0.052143
H	-0.967793	3.472611	-0.209690	H	0.557320	-3.477099	0.042630
C	1.358757	1.786723	-1.501931	C	-1.726813	-1.633890	-1.250556
C	0.711303	2.393960	-2.613851	C	-1.615937	-2.306462	-2.517772
C	2.758177	1.479827	-1.671562	C	-2.972697	-0.969894	-0.998430

C	1.348021	2.658069	-3.837025
H	-0.342110	2.696335	-2.510327
C	3.392863	1.757979	-2.902997
C	2.703823	2.328594	-3.987178
H	0.785937	3.118679	-4.665983
H	4.461933	1.508168	-3.015465
C	1.547356	1.559248	2.073201
O	2.176444	1.916929	3.098702
O	0.699961	2.540505	1.499883
O	1.548978	0.424050	1.522413
N	0.497175	-2.641105	0.156892
N	-1.523637	-2.083851	0.696365
C	-0.341148	-1.557573	0.240876
C	-0.151731	-3.817109	0.529172
C	-1.426871	-3.465957	0.882733
C	1.897413	-2.564751	-0.191104
C	2.844833	-2.560113	0.865846
C	4.206853	-2.548028	0.503761
C	4.596828	-2.513372	-0.843262
C	3.633066	-2.476695	-1.860517
C	2.255980	-2.500866	-1.559817
C	2.419571	-2.586136	2.333431
H	5.667538	-2.493204	-1.102172
C	1.212128	-2.501011	-2.671492
C	-2.676073	-1.294781	1.050553
C	-3.818965	-1.343534	0.215902
C	-4.934893	-0.572335	0.602735
C	-4.905462	0.205325	1.766439
C	-3.753215	0.241311	2.567642
C	-2.604886	-0.498856	2.227020
C	-3.878538	-2.233894	-1.024718
H	-5.786227	0.804434	2.046969
C	-1.335781	-0.448625	3.077314
H	0.354146	-4.785849	0.502558
H	-2.266461	-4.059774	1.253239
H	4.973418	-2.543922	1.293173
H	3.951401	-2.422793	-2.912710
H	1.374821	-2.213614	2.377551
H	0.228681	-2.247633	-2.229050
H	-5.837511	-0.578137	-0.026658
H	-3.740414	0.871919	3.468630
H	-2.835471	-2.495878	-1.300037
H	-0.474017	-0.500286	2.381678
C	-1.163210	0.867510	3.852567
H	-1.901940	0.977240	4.676150
H	-0.149839	0.902509	4.301090
H	-1.249262	1.742249	3.175832
C	-1.242045	-1.670674	4.016061
H	-1.279069	-2.624279	3.450826
H	-0.284297	-1.650452	4.577159
H	-2.076007	-1.674263	4.750541
C	-4.500999	-1.532172	-2.244766
H	-4.432930	-2.191965	-3.134152
H	-5.575485	-1.298819	-2.087378
H	-3.964269	-0.595171	-2.479101
C	-4.642359	-3.539033	-0.706332
H	-5.699010	-3.318050	-0.443539
H	-4.642908	-4.217985	-1.584852
H	-4.198154	-4.087209	0.148974
C	3.260924	-1.651539	3.221222
H	2.836326	-1.629422	4.247018
H	4.311586	-2.001458	3.313337
H	3.244996	-0.617393	2.828720

C	-2.725801	-2.348754	-3.396649
C	-4.049582	-0.987752	-1.893339
H	-3.102997	-0.424931	-0.050685
C	-3.933437	-1.699590	-3.099693
H	-2.623221	-2.887753	-4.354156
H	-4.975355	-0.444205	-1.645998
C	-1.715737	-1.209515	2.149573
O	-2.354037	-1.403044	3.213809
O	-1.039593	-2.325676	1.627042
O	-1.582753	-0.116316	1.523565
N	-0.272894	2.673583	-0.023994
N	1.721831	2.022052	0.515648
C	0.500887	1.547940	0.114144
C	0.458000	3.825916	0.257526
C	1.716372	3.416828	0.612114
C	-1.688461	2.631157	-0.320584
C	-2.598975	2.729520	0.763446
C	-3.971309	2.663961	0.451265
C	-4.405740	2.501415	-0.872400
C	-3.477331	2.389387	-1.916844
C	-2.092525	2.442540	-1.664896
C	-2.126695	2.944873	2.200417
H	-5.484390	2.445164	-1.090720
C	-1.077854	2.322677	-2.797595
C	2.810120	1.173715	0.930352
C	3.949545	1.068771	0.096816
C	4.996983	0.234208	0.539586
C	4.904747	-0.452851	1.756238
C	3.757490	-0.333219	2.556803
C	2.673369	0.472409	2.160050
C	4.076150	1.869546	-1.198130
H	5.731978	-1.103881	2.080517
C	1.405462	0.588162	3.006538
H	0.016643	4.822911	0.179214
H	2.599674	3.978228	0.927541
H	-4.710800	2.730047	1.263372
H	-3.830492	2.231892	-2.946462
H	-1.088328	2.557245	2.266114
H	-0.117322	1.977958	-2.366050
H	5.895731	0.118654	-0.084902
H	3.694597	-0.896234	3.499713
H	3.057889	2.208280	-1.482969
H	0.550561	0.687253	2.307213
C	1.104048	-0.663497	3.846515
H	1.828421	-0.803700	4.678045
H	0.091587	-0.575814	4.290007
H	1.103100	-1.577360	3.217469
C	1.433835	1.859668	3.881519
H	1.565924	2.774893	3.268663
H	0.479062	1.963225	4.438452
H	2.264573	1.818112	4.618565
C	4.615494	1.040729	-2.376654
H	4.626712	1.658981	-3.298028
H	5.654683	0.690591	-2.200564
H	3.970903	0.163614	-2.566839
C	4.956932	3.117266	-0.962696
H	5.993089	2.817726	-0.696167
H	5.006584	3.743218	-1.878438
H	4.575008	3.750198	-0.135731
C	-2.955855	2.181246	3.248234
H	-2.494525	2.308829	4.250567
H	-3.992685	2.574714	3.321334
H	-2.986778	1.098350	3.023331

C	2.445964	-4.028223	2.887689
H	3.479072	-4.436858	2.865916
H	2.093905	-4.047483	3.940827
H	1.802919	-4.717088	2.303953
C	1.483285	-1.424317	-3.736003
H	2.406401	-1.630649	-4.318808
H	0.633878	-1.379625	-4.446134
H	1.581956	-0.425884	-3.267490
C	1.096591	-3.910362	-3.290381
H	0.308041	-3.928128	-4.071991
H	2.053866	-4.221378	-3.761881
H	0.837475	-4.670658	-2.523148
C	-2.266916	1.374119	-1.391967
C	-2.452645	1.905438	-0.098360
C	-3.070074	1.845287	-2.453330
C	-3.444215	2.871223	0.139172
C	-4.043258	2.829846	-2.221384
C	-4.238662	3.339618	-0.923504
H	-1.814001	1.532143	0.718999
H	-2.906632	1.427588	-3.459160
H	-3.595770	3.253305	1.160853
H	-4.656060	3.203975	-3.057302
H	-5.010299	4.104732	-0.741677
C	-1.229970	0.292938	-1.668000
O	-1.388093	-0.463325	-2.619236
H	3.228448	2.520300	-4.937558
C	3.606852	0.902317	-0.561968
H	4.646544	0.722786	-0.900999
H	3.633142	1.595614	0.303100
H	3.202759	-0.051325	-0.176799
Zero-point correction=			0.819107 (Hartree/Particle)
Thermal correction to Energy=			0.874499
Thermal correction to Enthalpy=			0.875444
Thermal correction to Gibbs Free Energy=			0.730305
Sum of electronic and zero-point Energies=			-2942.339627
Sum of electronic and thermal Energies=			-2942.284234
Sum of electronic and thermal Enthalpies=			-2942.283290
Sum of electronic and thermal Free Energies=			-2942.428429

C	-2.106131	4.454172	2.534524
H	-3.135131	4.872110	2.501516
H	-1.700144	4.625132	3.554087
H	-1.490186	5.036714	1.820774
C	-1.467289	1.258664	-3.836008
H	-2.354828	1.553937	-4.435663
H	-0.624116	1.093554	-4.536337
H	-1.686911	0.293651	-3.339272
C	-0.836472	3.703762	-3.442358
H	-0.065934	3.634573	-4.239019
H	-1.770236	4.098076	-3.898346
H	-0.489067	4.445779	-2.692341
C	2.190173	-1.644471	-1.219469
C	2.269997	-2.102502	0.112396
C	3.016596	-2.236211	-2.199820
C	3.170984	-3.119366	0.466003
C	3.903017	-3.266138	-1.851749
C	3.986030	-3.708467	-0.517365
H	1.623316	-1.628896	0.869140
H	2.934073	-1.881810	-3.238949
H	3.236694	-3.446350	1.515565
H	4.534522	-3.731512	-2.625633
H	4.687105	-4.513809	-0.245648
C	1.225166	-0.541062	-1.629711
O	1.419986	0.080123	-2.670407
H	-4.773179	-1.740334	-3.812904
C	-0.332227	-2.937030	-2.999612
H	0.255883	-3.348788	-2.162917
H	-0.525435	-3.751520	-3.727798
H	0.289381	-2.173730	-3.514195
Zero-point correction=			0.819134 (Hartree/Particle)
Thermal correction to Energy=			0.874441
Thermal correction to Enthalpy=			0.875385
Thermal correction to Gibbs Free Energy=			0.731225
Sum of electronic and zero-point Energies=			-2942.338783
Sum of electronic and thermal Energies=			-2942.283476
Sum of electronic and thermal Enthalpies=			-2942.282532
Sum of electronic and thermal Free Energies=			-2942.426691

B-Ph(oMe)-IPr-X			
103			
IPrX-MeOrto SCF Done: -2943.18504001 A.U.			
Pd	0.241411	0.379543	-0.429521
K	3.974756	2.168031	1.074474
O	1.776426	3.778950	1.370740
H	1.623364	4.420006	0.642456
B	0.551219	3.213950	1.724677
O	-0.597863	3.924205	1.496858
H	-1.389971	3.354644	1.521791
C	1.119835	2.083762	-1.278897
C	0.477089	3.341155	-1.396874
C	2.503005	2.040020	-1.657922
C	1.155724	4.521364	-1.766958
H	-0.590358	3.426116	-1.145915
C	3.180086	3.224120	-2.044327
C	2.525428	4.469962	-2.078579
H	0.607393	5.477109	-1.817184
H	4.241607	3.164389	-2.350227
C	1.707740	1.205848	2.280052
O	2.558551	1.400718	3.166651
O	0.517679	1.971623	2.326373
O	1.813679	0.423687	1.279020

B-Ph(oMeISOMER)-IPr-X			
103			
IPrX-MeOrto180 SCF Done: -2943.18422570 A.U.			
Pd	-0.234588	0.482352	0.375492
K	-4.088034	1.092401	-1.623908
O	-2.185205	3.235619	-1.665201
H	-2.244690	3.882698	-0.930915
B	-0.845084	2.955318	-1.922498
O	0.109243	3.892352	-1.628012
H	1.012750	3.516685	-1.636598
C	-1.521917	1.983916	1.055806
C	-1.368047	3.346120	1.459591
C	-2.842779	1.459931	1.103633
C	-2.513883	4.133845	1.739422
C	-3.973763	2.228223	1.448129
H	-2.996594	0.391244	0.876336
C	-3.813998	3.596533	1.728037
H	-2.374880	5.196156	2.005645
H	-4.970117	1.753878	1.519471
C	-1.525505	0.773580	-2.550438
O	-2.252143	0.698701	-3.557859
O	-0.512690	1.760143	-2.538222
O	-1.636967	0.083625	-1.482280

N	0.423561	-2.616559	-0.097892	N	-0.377586	-2.493627	0.523163
N	-1.565054	-2.072055	0.536599	N	1.653076	-2.082710	-0.087711
C	-0.372286	-1.518340	0.134626	C	0.456675	-1.458734	0.156312
C	-0.260209	-3.812611	0.114873	C	0.290801	-3.716844	0.536072
C	-1.517359	-3.469156	0.528982	C	1.575026	-3.460663	0.138745
C	1.799545	-2.556589	-0.525207	C	-1.781314	-2.317401	0.809705
C	2.814451	-2.543956	0.467404	C	-2.715150	-2.574309	-0.228583
C	4.148937	-2.546620	0.014279	C	-4.079929	-2.376086	0.070335
C	4.449439	-2.579193	-1.357699	C	-4.486810	-1.947299	1.345245
C	3.420944	-2.582366	-2.309708	C	-3.537005	-1.707395	2.349686
C	2.067391	-2.550178	-1.914873	C	-2.158450	-1.878287	2.104141
C	2.472429	-2.566641	1.956584	C	-2.273618	-3.141355	-1.576709
H	5.500931	-2.595484	-1.687070	H	-5.558509	-1.805865	1.561087
C	0.944555	-2.530981	-2.948962	C	-1.126126	-1.639055	3.202971
C	-2.707303	-1.336645	1.015972	C	2.820123	-1.425539	-0.619504
C	-3.865645	-1.284556	0.201537	C	3.940409	-1.247426	0.227354
C	-4.991852	-0.612915	0.720453	C	5.080973	-0.633714	-0.331416
C	-4.953679	-0.016964	1.986019	C	5.095693	-0.228058	-1.670707
C	-3.780968	-0.059450	2.757652	C	3.964324	-0.409869	-2.482277
C	-2.623001	-0.715327	2.294000	C	2.790958	-1.000816	-1.976996
C	-3.914052	-1.930557	-1.182812	C	3.955390	-1.751858	1.670419
H	-5.842915	0.505537	2.373092	H	5.995061	0.251995	-2.087657
C	-1.323303	-0.721968	3.105001	C	1.530700	-1.152853	-2.833340
H	0.209672	-4.786012	-0.050823	H	-0.204128	-4.647378	0.826116
H	-2.369340	-4.077772	0.841987	H	2.431765	-4.122294	-0.014172
H	4.968543	-2.535337	0.748310	H	-4.836552	-2.586970	-0.702276
H	3.669394	-2.591178	-3.382370	H	-3.866841	-1.361418	3.340200
H	1.516759	-2.014401	2.071705	H	-1.210490	-2.857389	-1.721529
H	0.000991	-2.271332	-2.427942	H	-0.145037	-1.457532	2.720187
H	-5.906502	-0.544177	0.112813	H	5.969512	-0.471943	0.297616
H	-3.767584	0.435029	3.739175	H	3.990286	-0.062680	-3.525046
H	-2.865241	-2.074924	-1.517839	H	2.905834	-1.962408	1.964974
H	-0.514552	-0.461059	2.387949	H	0.673721	-0.869507	-2.184588
C	-1.288401	0.336116	4.218294	C	1.492755	-0.213917	-4.049141
H	-1.989841	0.092545	5.045625	H	2.238495	-0.500946	-4.821662
H	-0.267752	0.391512	4.647339	H	0.489506	-0.253565	-4.519597
H	-1.525775	1.346489	3.831662	H	1.667811	0.840339	-3.756941
C	-0.998961	-2.115746	3.689162	C	1.307561	-2.616271	-3.275847
H	-0.899343	-2.894534	2.908127	H	1.242982	-3.311265	-2.414950
H	-0.037670	-2.079597	4.243163	H	0.359635	-2.701192	-3.847456
H	-1.790738	-2.439303	4.398301	H	2.136396	-2.960655	-3.930687
C	-4.602597	-1.040089	-2.234367	C	4.498239	-0.716667	2.671404
H	-4.465050	-1.476902	-3.244447	H	4.458969	-1.131607	3.699988
H	-5.695944	-0.959063	-2.054552	H	5.555361	-0.448383	2.462469
H	-4.174179	-0.021104	-2.245997	H	3.885140	0.202334	2.657340
C	-4.609453	-3.309068	-1.122682	C	4.759420	-3.068499	1.761499
H	-5.665468	-3.198026	-0.795424	H	5.825977	-2.893383	1.504379
H	-4.611277	-3.789068	-2.123819	H	4.720380	-3.483554	2.790579
H	-4.114693	-4.003751	-0.415188	H	4.377529	-3.842703	1.065051
C	3.512185	-1.856362	2.837225	C	-3.053613	-2.596831	-2.784925
H	3.138722	-1.785645	3.879097	H	-2.658691	-3.048893	-3.718600
H	4.476881	-2.407074	2.871411	H	-4.132751	-2.860620	-2.739382
H	3.685107	-0.820503	2.491004	H	-2.939005	-1.500230	-2.882784
C	2.261887	-4.014628	2.454693	C	-2.364048	-4.685260	-1.541527
H	3.195767	-4.606163	2.343539	H	-3.421429	-5.009511	-1.434675
H	1.979605	-4.016061	3.528469	H	-1.963706	-5.123203	-2.479880
H	1.459540	-4.537627	1.899314	H	-1.798136	-5.119357	-0.693896
C	1.143416	-1.438338	-4.013537	C	-1.418006	-0.386381	4.045190
H	2.069289	-1.590513	-4.608859	H	-2.334720	-0.495946	4.663689
H	0.283379	-1.434507	-4.712154	H	-0.567773	-0.194221	4.729103
H	1.172337	-0.438677	-3.536351	H	-1.528120	0.502847	3.393222
C	0.775134	-3.928279	-3.581330	C	-0.995524	-2.905340	4.077376
H	-0.069241	-3.930200	-4.302205	H	-0.216172	-2.761633	4.854861

H	1.692429	-4.236052	-4.128168
H	0.569325	-4.700121	-2.810139
C	-2.276285	1.559132	-1.365820
C	-2.602553	1.840405	-0.023486
C	-2.954907	2.242213	-2.397927
C	-3.612335	2.764646	0.285817
C	-3.932335	3.202413	-2.088231
C	-4.270297	3.459774	-0.746527
H	-2.064840	1.299309	0.771125
H	-2.698155	2.005008	-3.442051
H	-3.896401	2.933382	1.337431
H	-4.441754	3.748730	-2.898373
H	-5.050683	4.198987	-0.505048
C	-1.233526	0.514732	-1.730535
O	-1.382343	-0.151761	-2.750937
H	3.072219	5.378920	-2.377912
C	3.265499	0.728346	-1.688873
H	4.361964	0.871571	-1.814817
H	3.076753	0.097573	-0.794636
H	2.932894	0.110015	-2.545332
Zero-point correction=		0.820423 (Hartree/Particle)	
Thermal correction to Energy=		0.876380	
Thermal correction to Enthalpy=		0.877324	
Thermal correction to Gibbs Free Energy=		0.731385	
Sum of electronic and zero-point Energies=		-2942.364617	
Sum of electronic and thermal Energies=		-2942.308660	
Sum of electronic and thermal Enthalpies=		-2942.307716	
Sum of electronic and thermal Free Energies=		-2942.453655	

H	-1.954108	-3.136940	4.590006
H	-0.715257	-3.791764	3.469907
C	2.320760	1.800014	0.844455
C	2.374924	1.887511	-0.562689
C	3.250472	2.531941	1.612433
C	3.349419	2.676802	-1.192841
C	4.210067	3.342986	0.985026
C	4.264807	3.416389	-0.418828
H	1.636611	1.317668	-1.151584
H	3.189265	2.468041	2.710119
H	3.403598	2.703070	-2.293310
H	4.920616	3.924286	1.594580
H	5.023274	4.045898	-0.911015
C	1.263225	0.960336	1.555267
O	1.431623	0.631960	2.725833
H	-4.680533	4.229873	1.977834
C	-0.002091	3.966416	1.629840
H	0.540182	3.468546	2.460731
H	0.611985	3.837969	0.720887
H	-0.061465	5.049282	1.860714
Zero-point correction=		0.820620 (Hartree/Particle)	
Thermal correction to Energy=		0.876495	
Thermal correction to Enthalpy=		0.877439	
Thermal correction to Gibbs Free Energy=		0.732282	
Sum of electronic and zero-point Energies=		-2942.363606	
Sum of electronic and thermal Energies=		-2942.307731	
Sum of electronic and thermal Enthalpies=		-2942.306787	
Sum of electronic and thermal Free Energies=		-2942.451943	

B-Ph(oMe)-IPr-XI			
93			
IPrXI-MeOrto SCF Done: -1902.90040782 A.U.			
Pd	0.435654	0.877505	-0.149808
C	0.837409	2.898754	-0.323337
C	-0.020616	3.950276	-0.728658
C	2.187742	3.243838	-0.015306
C	0.414261	5.285889	-0.809999
H	-1.068129	3.734913	-0.993948
C	2.620030	4.585675	-0.096110
C	1.742703	5.610108	-0.487622
H	-0.287348	6.073734	-1.131736
H	3.670170	4.827347	0.146735
N	1.438614	-2.007002	-0.062729
N	-0.715463	-2.083884	0.052310
C	0.332309	-1.192292	-0.005849
C	1.099495	-3.359071	-0.049907
C	-0.266465	-3.407415	0.023565
C	2.788723	-1.507972	-0.015521
C	3.373595	-1.305420	1.260336
C	4.692509	-0.811445	1.293113
C	5.385650	-0.530814	0.105920
C	4.770775	-0.724157	-1.140010
C	3.453524	-1.217329	-1.231682
C	2.581679	-1.529140	2.547494
H	6.413584	-0.137895	0.152872
C	2.745629	-1.338402	-2.577315
C	-2.103288	-1.725598	0.227781
C	-2.996412	-1.918781	-0.855760
C	-4.352425	-1.600189	-0.639797
C	-4.787577	-1.091237	0.589419
C	-3.878471	-0.897694	1.639339
C	-2.515340	-1.217020	1.491421

B-Ph(oMeISOMER)-IPr-XI			
93			
IPrXI-MeOrto180 SCF Done: -1902.89979882 A.U.			
Pd	0.593407	0.715791	-0.128405
C	1.675301	2.447163	-0.156040
C	1.612005	3.680618	-0.862197
C	2.827594	2.179870	0.623973
C	2.686248	4.592910	-0.748762
C	3.898579	3.089520	0.722052
H	2.918110	1.221197	1.170860
C	3.820454	4.310579	0.033683
H	2.635042	5.549123	-1.298080
H	4.781578	2.842456	1.334752
N	1.060168	-2.218269	-0.100683
N	-1.090807	-2.013564	-0.049855
C	0.064496	-1.273734	-0.058445
C	0.550493	-3.514430	-0.125119
C	-0.814650	-3.385007	-0.094213
C	2.443709	-1.821410	0.001054
C	2.994794	-1.676775	1.300588
C	4.321804	-1.211229	1.390523
C	5.052269	-0.889148	0.237117
C	4.472825	-1.027635	-1.032185
C	3.153585	-1.499773	-1.183105
C	2.170104	-1.926673	2.561844
H	6.081110	-0.507441	0.329559
C	2.505897	-1.585808	-2.561900
C	-2.413823	-1.459415	0.118541
C	-3.301009	-1.470353	-0.984548
C	-4.608066	-0.985836	-0.768367
C	-4.994398	-0.485990	0.480764
C	-4.080851	-0.450937	1.544931
C	-2.770429	-0.941650	1.395758

C	-2.543010	-2.483613	-2.201697
H	-5.846261	-0.822744	0.728422
C	-1.519759	-1.030763	2.638707
H	1.856807	-4.147729	-0.085018
H	-0.958685	-4.252176	0.072203
H	5.178494	-0.628203	2.263777
H	5.317421	-0.470618	-2.061277
H	1.681169	-2.125393	2.293689
H	1.826085	-1.940779	-2.418857
H	-5.074560	-1.733049	-1.459489
H	-4.238338	-0.476317	2.587917
H	-1.438230	-2.381480	-2.253384
H	-0.620472	-0.553083	2.192695
C	-2.014946	-0.098387	3.754686
H	-2.844891	-0.552558	4.337432
H	-1.188644	0.104436	4.466930
H	-2.365553	0.872400	3.355188
C	-1.089335	-2.386002	3.244825
H	-0.642441	-3.066437	2.494120
H	-0.333508	-2.228247	4.042958
H	-1.960681	-2.904748	3.698335
C	-3.123549	-1.712081	-3.402707
H	-2.692822	-2.104008	-4.347655
H	-4.225771	-1.828430	-3.475120
H	-2.875565	-0.636069	-3.333589
C	-2.902445	-3.983282	-2.303394
H	-4.004283	-4.121070	-2.270862
H	-2.533028	-4.413215	-3.258115
H	-2.472627	-4.577910	-1.471974
C	2.083917	-0.182180	3.113701
H	1.450427	-0.345783	4.010578
H	2.935761	0.466872	3.406692
H	1.476037	0.372659	2.365169
C	3.370332	-2.325584	3.603700
H	4.246384	-1.757129	3.981070
H	2.724221	-2.547923	4.478505
H	3.741221	-3.287881	3.194388
C	2.298224	0.058867	-3.060070
H	3.174417	0.722427	-3.219402
H	1.734458	-0.015659	-4.012309
H	1.633329	0.545371	-2.308090
C	3.598697	-2.064801	-3.634236
H	3.010390	-2.214975	-4.563125
H	4.499188	-1.477454	-3.912856
H	3.939626	-3.058393	-3.275322
C	-2.448812	1.629841	-0.378604
C	-2.335887	2.146170	0.927864
C	-3.700165	1.662101	-1.032789
C	-3.455340	2.691998	1.571351
C	-4.821443	2.201191	-0.384975
C	-4.701534	2.718563	0.917866
H	-1.344466	2.124084	1.410698
H	-3.773163	1.253762	-2.051630
H	-3.355755	3.106726	2.587001
H	-5.795864	2.218110	-0.898748
C	-1.265687	1.059289	-1.122867
O	-1.342029	0.693188	-2.282998
H	2.097453	6.651860	-0.550025
C	3.171020	2.176906	0.424471
H	3.214229	2.079862	1.530321
H	2.897656	1.175186	0.021963
H	4.203360	2.381919	0.073060
H	-5.581013	3.148394	1.423847

C	-2.886333	-2.000091	-2.356115
H	-6.013549	-0.094265	0.624109
C	-1.775814	-0.936687	2.557152
H	1.197169	-4.396364	-0.155483
H	-1.610981	-4.134424	-0.084913
H	4.780778	-1.074486	2.382112
H	5.048738	-0.743939	-1.926468
H	1.206217	-2.383164	2.256397
H	1.516638	-2.074821	-2.437758
H	-5.326996	-0.984437	-1.601831
H	-4.394054	-0.023780	2.507676
H	-1.776982	-2.053383	-2.369508
H	-0.800202	-0.622915	2.127744
C	-2.116622	0.070081	3.666002
H	-3.013861	-0.235835	4.246057
H	-1.272175	0.135742	4.382608
H	-2.297127	1.082361	3.255014
C	-1.600491	-2.349195	3.159175
H	-1.280144	-3.094951	2.405237
H	-0.832731	-2.333727	3.961371
H	-2.553677	-2.704301	3.605839
C	-3.307671	-1.061267	-3.503476
H	-2.898844	-1.432623	-4.466303
H	-4.411976	-1.015040	-3.614797
H	-2.917245	-0.039132	-3.335966
C	-3.444805	-3.422428	-2.582072
H	-4.555667	-3.410379	-2.579044
H	-3.111322	-3.825634	-3.561389
H	-3.120506	-4.131334	-1.793067
C	1.835181	-0.592129	3.260431
H	1.192570	-0.765833	4.148948
H	2.755570	-0.071441	3.599046
H	1.293529	0.093418	2.573371
C	2.855594	-2.915584	3.524319
H	3.804493	-2.505092	3.929762
H	2.194510	-3.133607	4.389123
H	3.091677	-3.875104	3.019532
C	2.244131	-0.173163	-3.126755
H	3.193397	0.382864	-3.277639
H	1.716420	-0.234749	-4.100828
H	1.613076	0.416464	-2.423124
C	3.332966	-2.451202	-3.533207
H	2.802183	-2.556173	-4.502388
H	4.321550	-1.993387	-3.748927
H	3.513401	-3.467701	-3.125070
C	-2.056443	2.061911	-0.191131
C	-1.732851	2.636311	1.055195
C	-3.369095	2.185568	-0.696779
C	-2.712374	3.320214	1.790915
C	-4.350786	2.854034	0.048267
C	-4.025877	3.421931	1.293854
H	-0.694838	2.545978	1.417724
H	-3.602851	1.735988	-1.673004
H	-2.450255	3.778897	2.757541
H	-5.377759	2.931302	-0.343042
C	-1.036810	1.332481	-1.029072
O	-1.241503	1.056649	-2.200936
H	4.641406	5.043132	0.099591
C	0.434454	4.017429	-1.749684
H	0.289963	3.239939	-2.527787
H	-0.510876	4.055825	-1.168850
H	0.561797	4.996602	-2.254536
H	-4.796210	3.952992	1.875945

Zero-point correction= 0.766624 (Hartree/Particle)	Zero-point correction= 0.766828 (Hartree/Particle)
Thermal correction to Energy= 0.813105	Thermal correction to Energy= 0.813376
Thermal correction to Enthalpy= 0.814049	Thermal correction to Enthalpy= 0.814320
Thermal correction to Gibbs Free Energy= 0.688359	Thermal correction to Gibbs Free Energy= 0.687672
Sum of electronic and zero-point Energies= -1902.133784	Sum of electronic and zero-point Energies= -1902.132971
Sum of electronic and thermal Energies= -1902.087303	Sum of electronic and thermal Energies= -1902.086423
Sum of electronic and thermal Enthalpies= -1902.086358	Sum of electronic and thermal Enthalpies= -1902.085479
Sum of electronic and thermal Free Energies= -1902.212049	Sum of electronic and thermal Free Energies= -1902.212127

B-Ph(oMe)-IPr-XI-XII				**B-Ph(oMeISOMER)-IPr-XI-XII**			
93				93			
IPrXI-XII-MeOrto SCF Done: -1902.88990799 A.U.				IPrXI-XII-MeOrto180 SCF Done: -1902.89551951 A.U.			
Pd	0.368952	0.708141	0.094487	Pd	0.308528	0.700672	0.254037
C	0.361944	2.838277	-0.051185	C	0.383629	2.822773	0.194463
C	0.116663	3.573059	1.150070	C	-0.336782	3.543414	1.178861
C	1.359338	3.290439	-0.949016	C	1.639691	3.337301	-0.265442
C	0.901307	4.724489	1.394443	C	0.168894	4.727112	1.741320
C	2.148056	4.414627	-0.670365	H	-1.320257	3.174956	1.505656
H	1.476489	2.749172	-1.902034	C	2.121490	4.534162	0.304399
C	1.907886	5.141918	0.508831	C	1.404218	5.225088	1.297591
H	0.723244	5.300827	2.318240	H	-0.406133	5.260860	2.515044
H	2.931747	4.733167	-1.376481	H	3.090735	4.932919	-0.040253
H	2.501261	6.041690	0.739196	H	1.811062	6.159173	1.718021
N	1.691464	-1.977955	0.157565	N	1.559453	-2.029994	0.217806
N	-0.443312	-2.307728	0.136376	N	-0.587004	-2.283731	0.258654
C	0.493089	-1.302748	0.126242	C	0.384286	-1.312805	0.220501
C	1.512373	-3.360105	0.194033	C	1.330749	-3.405016	0.266001
C	0.157215	-3.570171	0.180646	C	-0.030993	-3.566639	0.291682
C	2.948253	-1.285705	0.026319	C	2.833932	-1.389056	0.012436
C	3.578625	-0.787539	1.192222	C	3.523072	-0.857425	1.129220
C	4.781175	-0.073642	1.019517	C	4.735745	-0.183855	0.879488
C	5.319873	0.132051	-0.259633	C	5.234208	-0.055616	-0.425591
C	4.659287	-0.357491	-1.396826	C	4.523354	-0.586941	-1.512131
C	3.450980	-1.072712	-1.281713	C	3.300704	-1.260968	-1.319957
C	2.930919	-0.926701	2.567798	C	2.936608	-0.931113	2.536404
H	6.259472	0.695855	-0.373032	H	6.181562	0.478743	-0.599641
C	2.668665	-1.502124	-2.521098	C	2.475051	-1.738154	-2.512788
C	-1.866688	-2.089095	0.065691	C	-2.001914	-2.010822	0.190237
C	-2.440816	-1.731797	-1.182815	C	-2.564560	-1.654261	-1.064318
C	-3.841234	-1.576490	-1.216235	C	-3.957890	-1.449428	-1.101978
C	-4.621683	-1.773414	-0.068747	C	-4.744136	-1.594772	0.049689
C	-4.020450	-2.096880	1.156168	C	-4.153043	-1.912041	1.281006
C	-2.622890	-2.246845	1.254468	C	-2.761761	-2.114678	1.381419
C	-1.576011	-1.515205	-2.426184	C	-1.690612	-1.487773	-2.308440
H	-5.713771	-1.643013	-0.123838	H	-5.831094	-1.427311	-0.008017
C	-1.928359	-2.472230	2.599003	C	-2.074608	-2.336497	2.729221
H	2.356133	-4.056246	0.214682	H	2.148836	-4.131489	0.264959
H	-0.434463	-4.490750	0.189858	H	-0.654180	-4.465681	0.322724
H	5.296885	0.339888	1.899988	H	5.293719	0.256523	1.720383
H	5.078929	-0.163098	-2.396274	H	4.911576	-0.454419	-2.533848
H	2.134277	-1.696862	2.486168	H	2.108449	-1.671183	2.513087
H	1.853020	-2.179803	-2.193437	H	1.653664	-2.378123	-2.129350
H	-4.330545	-1.279403	-2.154115	H	-4.436252	-1.152860	-2.045798
H	-4.646426	-2.214750	2.053022	H	-4.781177	-1.987511	2.180956
H	-0.684646	-0.942241	-2.092199	H	-0.773642	-0.957875	-1.973613
H	-1.030162	-3.100419	2.413710	H	-1.185632	-2.980151	2.552937
C	-1.425701	-1.124039	3.166190	C	-1.555690	-0.986883	3.277490
H	-2.281580	-0.447225	3.374290	H	-2.403044	-0.292708	3.461866
H	-0.869732	-1.277508	4.115088	H	-1.012588	-1.131268	4.235203
H	-0.751550	-0.607635	2.450022	H	-0.866691	-0.493525	2.558314
C	-2.796002	-3.214960	3.628610	C	-2.956432	-3.054230	3.764688
H	-3.204027	-4.161875	3.218088	H	-3.378166	-3.999094	3.363204

H	-2.195943	-3.459386	4.529431	H	-2.362504	-3.298198	4.669700
H	-3.651970	-2.595463	3.971164	H	-3.803518	-2.418017	4.098523
C	-2.258659	-0.666715	-3.508879	C	-2.326339	-0.612941	-3.398508
H	-1.523854	-0.418823	-4.301070	H	-1.573794	-0.394043	-4.182575
H	-3.102612	-1.205803	-3.991620	H	-3.185773	-1.117360	-3.891231
H	-2.628233	0.292475	-3.096941	H	-2.669856	0.357176	-2.990399
C	-1.082119	-2.853783	-3.018378	C	-1.263421	-2.852599	-2.892761
H	-1.937380	-3.469206	-3.370986	H	-2.148993	-3.426053	-3.240906
H	-0.416187	-2.663895	-3.886484	H	-0.589655	-2.701808	-3.762256
H	-0.508639	-3.454837	-2.284776	H	-0.720537	-3.477093	-2.155574
C	2.243515	0.398491	2.961013	C	2.321923	0.428797	2.926343
H	1.708410	0.298322	3.928402	H	1.842429	0.379712	3.925968
H	2.980246	1.224139	3.047945	H	3.089058	1.230741	2.939288
H	1.495093	0.703761	2.186152	H	1.537637	0.742218	2.189345
C	3.920358	-1.396065	3.650780	C	3.959544	-1.411849	3.582942
H	4.706147	-0.636521	3.847582	H	4.782046	-0.678834	3.721986
H	3.389334	-1.570280	4.609827	H	3.469319	-1.541778	4.570295
H	4.426896	-2.339204	3.358616	H	4.415380	-2.380912	3.292116
C	1.996662	-0.272645	-3.170491	C	1.814511	-0.531402	-3.211856
H	2.757881	0.440061	-3.553683	H	2.580832	0.155043	-3.630243
H	1.354504	-0.580304	-4.022259	H	1.165960	-0.869906	-4.047037
H	1.357420	0.269636	-2.441792	H	1.189387	0.054068	-2.508173
C	3.533124	-2.282187	-3.528970	C	3.296066	-2.593009	-3.496414
H	2.908081	-2.643354	-4.372254	H	2.639719	-2.991612	-4.298046
H	4.332646	-1.646129	-3.964175	H	4.093262	-1.999792	-3.992339
H	4.019240	-3.161569	-3.057417	H	3.780570	-3.451859	-2.986876
C	-2.354093	1.901310	-0.636192	C	-2.210374	2.009676	-0.740637
C	-2.832249	1.259617	0.521562	C	-2.765125	1.451296	0.428133
C	-3.263353	2.602984	-1.460072	C	-3.056332	2.666195	-1.660496
C	-4.190265	1.329102	0.865815	C	-4.138767	1.561221	0.687603
C	-4.619620	2.684607	-1.109698	C	-4.431942	2.774653	-1.403043
C	-5.086915	2.048961	0.056854	C	-4.976263	2.226164	-0.226017
H	-2.122241	0.684578	1.134658	H	-2.092573	0.901838	1.109618
H	-2.880659	3.078061	-2.376620	H	-2.610281	3.081012	-2.577748
H	-4.550054	0.805547	1.765021	H	-4.558039	1.106735	1.598332
H	-5.319195	3.245695	-1.750179	H	-5.085983	3.291914	-2.123599
H	-6.152570	2.110666	0.330616	H	-6.056382	2.311947	-0.025042
C	-0.914046	1.810049	-1.093087	C	-0.736168	1.877906	-1.082269
O	-0.666534	1.848483	-2.302828	O	-0.373801	1.951846	-2.260023
C	-0.905960	3.163593	2.187046	C	2.462764	2.619635	-1.309009
H	-1.940456	3.297057	1.808732	H	3.348656	3.214617	-1.608960
H	-0.800860	2.093141	2.455774	H	2.819641	1.637409	-0.932494
H	-0.799347	3.765538	3.111602	H	1.840516	2.405536	-2.201142
Zero-point correction= 0.765891 (Hartree/Particle)				Zero-point correction= 0.766492 (Hartree/Particle)			
Thermal correction to Energy= 0.811819				Thermal correction to Energy= 0.812077			
Thermal correction to Enthalpy= 0.812763				Thermal correction to Enthalpy= 0.813021			
Thermal correction to Gibbs Free Energy= 0.687337				Thermal correction to Gibbs Free Energy= 0.690038			
Sum of electronic and zero-point Energies= -1902.124017				Sum of electronic and zero-point Energies= -1902.129028			
Sum of electronic and thermal Energies= -1902.078089				Sum of electronic and thermal Energies= -1902.083442			
Sum of electronic and thermal Enthalpies= -1902.077145				Sum of electronic and thermal Enthalpies= -1902.082498			
Sum of electronic and thermal Free Energies= -1902.202571				Sum of electronic and thermal Free Energies= -1902.205482			

B-Ph(oMe)-IPr-XII			**B-Ph(oMeISOMER)-IPr-XII**		
93			93		
IPrXII-MeOrto SCF Done: -1902.92116053 A.U.			IPrXII-MeOrto180 SCF Done: -1902.92174621 A.U.		
Pd	0.212459	-0.676832 -0.269252	Pd	0.301872	-0.312570 -0.779839
C	-0.015161	-2.832531 -0.598080	C	-0.357180	-1.784621 -2.289179
C	-0.290711	-3.162189 -1.983305	C	-1.110163	-1.168397 -3.351043
C	1.357294	-2.587593 -0.201535	C	1.097872	-1.694298 -2.316947
C	0.785315	-3.197217 -2.882288	C	-0.493377	-0.450206 -4.369733
C	2.408493	-2.630965 -1.156734	H	-2.200175	-1.312120 -3.371664
H	1.606136	-2.602456 0.870647	C	1.673078	-0.877288 -3.350137

C	2.117981	-2.923743	-2.487412
H	0.584386	-3.476397	-3.929967
H	3.438853	-2.435212	-0.823499
H	2.924430	-2.964633	-3.237026
N	1.765701	1.722210	0.699531
N	-0.239963	2.354707	0.213169
C	0.568750	1.242280	0.216105
C	1.704896	3.084309	0.991955
C	0.431871	3.488662	0.679367
C	2.900287	0.855570	0.886565
C	3.847622	0.749301	-0.161454
C	4.905422	-0.163636	0.016218
C	4.999766	-0.940623	1.182126
C	4.040878	-0.815610	2.198349
C	2.968590	0.091573	2.076602
C	3.666070	1.517363	-1.469169
H	5.828682	-1.657203	1.296604
C	1.929800	0.225985	3.188498
C	-1.615974	2.343541	-0.208652
C	-2.623592	2.268262	0.787933
C	-3.962009	2.350744	0.358379
C	-4.276853	2.473809	-1.004243
C	-3.260416	2.477922	-1.969788
C	-1.901796	2.415585	-1.593661
C	-2.266442	1.997132	2.248095
H	-5.330991	2.539156	-1.318046
C	-0.800768	2.373890	-2.651355
H	2.563452	3.633658	1.389917
H	-0.056598	4.465726	0.743483
H	5.657167	-0.282722	-0.778791
H	4.122583	-1.436748	3.104202
H	3.018448	2.394104	-1.252633
H	1.184082	0.980917	2.863367
H	-4.773800	2.296987	1.098393
H	-3.523332	2.537007	-3.037518
H	-1.260014	2.430548	2.435549
H	0.171880	2.508780	-2.133036
C	-0.763171	0.983335	-3.320632
H	-1.730736	0.747191	-3.812502
H	0.038050	0.936638	-4.087044
H	-0.549118	0.194209	-2.561437
C	-0.934051	3.504621	-3.689329
H	-0.973079	4.501602	-3.203336
H	-0.068366	3.492077	-4.384047
H	-1.850110	3.393212	-4.307289
C	-2.158298	0.471220	2.475731
H	-1.863015	0.251341	3.522706
H	-3.127902	-0.029289	2.270680
H	-1.402276	0.012516	1.802099
C	-3.238421	2.643756	3.249865
H	-4.240821	2.166668	3.216920
H	-2.858358	2.518215	4.284660
H	-3.369549	3.729308	3.058325
C	2.915331	0.642324	-2.497083
H	2.685036	1.223884	-3.414704
H	3.527474	-0.237312	-2.786270
H	1.964299	0.252787	-2.071344
C	4.987436	2.057327	-2.044847
H	5.656426	1.237632	-2.383062
H	4.787679	2.695671	-2.930594
H	5.543575	2.663087	-1.299413
C	1.161266	-1.089360	3.414624
H	1.838165	-1.919094	3.707891

C	0.912184	-0.274827	-4.348704
H	-1.097717	-0.011160	-5.178659
H	2.769697	-0.772573	-3.360723
H	1.407133	0.325836	-5.128278
N	1.698705	0.929141	1.602108
N	-0.242047	1.849007	1.381753
C	0.561997	0.879120	0.826963
C	1.609795	1.898834	2.601190
C	0.378042	2.485264	2.459871
C	2.823347	0.060559	1.364233
C	3.864736	0.525587	0.522734
C	4.919848	-0.366993	0.249687
C	4.929588	-1.660418	0.796514
C	3.886855	-2.086225	1.631785
C	2.807983	-1.232731	1.939530
C	3.802344	1.909293	-0.122621
H	5.759279	-2.346588	0.563508
C	1.652612	-1.715007	2.814134
C	-1.572989	2.136787	0.914887
C	-2.668847	1.638976	1.669763
C	-3.961583	1.960942	1.215556
C	-4.150704	2.712603	0.044504
C	-3.048850	3.157367	-0.697815
C	-1.729474	2.891510	-0.272866
C	-2.442682	0.725455	2.875328
H	-5.172076	2.944804	-0.297558
C	-0.542157	3.396885	-1.090469
H	2.423980	2.080441	3.309225
H	-0.111333	3.289916	3.017281
H	5.742033	-0.048519	-0.409237
H	3.902119	-3.106682	2.045354
H	3.100292	2.526190	0.478075
H	1.003247	-0.839954	3.028589
H	-4.837683	1.596937	1.771431
H	-3.211429	3.734054	-1.621810
H	-1.511620	1.063886	3.379726
H	0.384067	3.168605	-0.522956
C	-0.441651	2.638820	-2.429491
H	-1.352245	2.780191	-3.048873
H	0.434883	2.985825	-3.014782
H	-0.312930	1.546090	-2.239013
C	-0.593484	4.924126	-1.295156
H	-0.665269	5.463635	-0.327736
H	0.321639	5.272664	-1.818409
H	-1.462523	5.228158	-1.916332
C	-2.204169	-0.729664	2.410286
H	-1.914499	-1.367821	3.271010
H	-3.123116	-1.153741	1.956716
H	-1.403353	-0.792057	1.646041
C	-3.570784	0.788622	3.918656
H	-4.510460	0.338589	3.533904
H	-3.285729	0.209745	4.821299
H	-3.791482	1.830535	4.231528
C	3.210219	1.808202	-1.544158
H	3.071214	2.816168	-1.988854
H	3.883455	1.225792	-2.208430
H	2.225641	1.288531	-1.529301
C	5.160249	2.634904	-0.123406
H	5.896464	2.132630	-0.786096
H	5.041444	3.671990	-0.500790
H	5.599566	2.684395	0.894598
C	0.788813	-2.739810	2.054071
H	1.375013	-3.640802	1.777103

H	0.410156	-0.967595	4.222471
H	0.621014	-1.397559	2.497242
C	2.578969	0.745794	4.488096
H	1.808105	0.908681	5.270480
H	3.315958	0.019856	4.892593
H	3.110556	1.706040	4.321341
C	-2.416889	-2.480095	0.433111
C	-2.804904	-1.449076	-0.452348
C	-3.372522	-3.001937	1.332968
C	-4.121105	-0.965907	-0.452658
C	-4.691151	-2.522741	1.331419
C	-5.069560	-1.504310	0.435542
H	-2.047849	-0.983196	-1.112189
H	-3.046902	-3.779496	2.040905
H	-4.396801	-0.152073	-1.138009
H	-5.428443	-2.940947	2.035358
H	-6.103453	-1.122828	0.435884
C	-0.993854	-2.974229	0.552354
O	-0.616071	-3.471786	1.621913
C	-1.667289	-3.550969	-2.474609
H	-2.230527	-4.137030	-1.721219
H	-2.292698	-2.662157	-2.703168
H	-1.593162	-4.152850	-3.402511
Zero-point correction=	0.767295 (Hartree/Particle)		
Thermal correction to Energy=	0.813611		
Thermal correction to Enthalpy=	0.814555		
Thermal correction to Gibbs Free Energy=	0.688034		
Sum of electronic and zero-point Energies=	-1902.153866		
Sum of electronic and thermal Energies=	-1902.107549		
Sum of electronic and thermal Enthalpies=	-1902.106605		
Sum of electronic and thermal Free Energies=	-1902.233127		

H	-0.072679	-3.068438	2.670669
H	0.390012	-2.292041	1.120161
C	2.142213	-2.266047	4.167747
H	1.277016	-2.526183	4.812835
H	2.745129	-3.190012	4.041268
H	2.767904	-1.525841	4.708849
C	-2.468224	-2.353857	-0.846129
C	-3.074418	-1.077690	-0.938185
C	-3.209845	-3.414368	-0.274657
C	-4.402464	-0.890824	-0.523156
C	-4.527442	-3.220236	0.163298
C	-5.134837	-1.957873	0.026436
H	-2.493383	-0.212396	-1.294373
H	-2.717022	-4.394801	-0.187448
H	-4.855329	0.106862	-0.610493
H	-5.088563	-4.059211	0.605355
H	-6.174381	-1.803026	0.357705
C	-1.058253	-2.688650	-1.301724
O	-0.529946	-3.736835	-0.906869
C	2.053454	-2.603923	-1.562301
H	2.999706	-2.064386	-1.351634
H	1.642099	-2.984670	-0.615121
H	2.288896	-3.493001	-2.188913
Zero-point correction=	0.767744 (Hartree/Particle)		
Thermal correction to Energy=	0.813932		
Thermal correction to Enthalpy=	0.814877		
Thermal correction to Gibbs Free Energy=	0.689411		
Sum of electronic and zero-point Energies=	-1902.154003		
Sum of electronic and thermal Energies=	-1902.107814		
Sum of electronic and thermal Enthalpies=	-1902.106870		
Sum of electronic and thermal Free Energies=	-1902.232336		

B-Ph(pCF3)-IPr-IX			
103			
IPrIX-CF3 SCF Done: -3240.69205384 A.U.			
Pd	0.107554	0.080692	-0.353096
K	-3.492687	0.942292	-4.293827
O	-1.016886	0.177646	-4.506914
H	-0.426461	-0.328970	-5.090371
B	-1.239684	-0.590488	-3.258992
O	-2.239953	-1.634334	-3.523602
H	-2.416640	-2.142545	-2.709098
C	0.182376	-1.172345	-2.659018
C	0.395516	-2.571323	-2.480941
C	1.314681	-0.325058	-2.442815
C	1.634769	-3.093754	-2.108043
H	-0.445343	-3.259989	-2.658746
C	2.573293	-0.846020	-2.044126
H	1.241071	0.745573	-2.693901
C	2.729935	-2.226641	-1.880459
H	1.768142	-4.180058	-1.987217
H	3.419420	-0.164059	-1.875403
C	-1.556238	1.714935	-2.142248
O	-2.293406	2.590396	-2.652247
O	-1.938414	0.391929	-2.300775
O	-0.506145	1.929659	-1.435808
N	0.808979	2.188594	1.612033
N	-0.909420	1.102394	2.372946
C	-0.004792	1.117323	1.346491
C	0.417550	2.832801	2.783953

B-Ph(pOMe)-IPr-IX			
104			
IPrIX-OMe SCF Done: -3018.33791272 A.U.			
Pd	-0.072405	0.283664	0.336427
K	2.983259	4.693787	0.406194
O	1.172773	3.980035	2.096424
H	0.837985	4.059040	3.005336
B	1.573476	2.571575	1.854012
O	2.937888	2.377570	2.358049
H	3.239081	1.469513	2.163999
C	0.469398	1.523058	2.486807
C	0.843512	0.550403	3.459768
C	-0.943485	1.666463	2.268920
C	-0.084701	-0.255786	4.128707
H	1.912812	0.427520	3.694813
C	-1.893728	0.868735	2.934771
H	-1.301933	2.462034	1.595460
C	-1.465507	-0.113064	3.848747
H	0.271799	-1.006640	4.847355
H	-2.968291	0.972874	2.723523
C	0.763852	2.942507	-0.569234
O	1.042017	3.982021	-1.211513
O	1.716215	2.463583	0.312796
O	-0.307256	2.243274	-0.691071
N	-2.033201	-0.356933	-1.800883
N	-0.100918	-1.188182	-2.338507
C	-0.764048	-0.556188	-1.321259
C	-2.152453	-0.839294	-3.104627

C	-0.671553	2.153271	3.262791
C	1.964269	2.510517	0.802713
C	1.879777	3.582023	-0.119817
C	3.006228	3.806718	-0.938422
C	4.145035	2.995182	-0.843768
C	4.197872	1.946206	0.087963
C	3.108450	1.679975	0.940065
C	0.651690	4.484324	-0.203521
H	5.005914	3.180988	-1.505950
C	3.165213	0.575443	1.994249
C	-1.947266	0.112027	2.527038
C	-1.680284	-1.007471	3.353926
C	-2.707394	-1.963702	3.491413
C	-3.936105	-1.798390	2.839423
C	-4.160647	-0.686968	2.012911
C	-3.163333	0.288355	1.818307
C	-0.352312	-1.158975	4.095582
H	-4.723529	-2.559356	2.957032
C	-3.364324	1.471717	0.872103
H	0.950093	3.706602	3.168042
H	-1.300940	2.318555	4.141127
H	2.980383	4.623982	-1.674371
H	5.098777	1.318432	0.147912
H	-0.213964	3.887370	0.151246
H	2.154495	0.123041	2.057497
H	-2.536220	-2.856084	4.111143
H	-5.120179	-0.593280	1.483726
H	0.412354	-0.586847	3.527954
H	-2.381710	1.679317	0.397497
C	-4.351957	1.182148	-0.271615
H	-5.399868	1.104947	0.090124
H	-4.297592	2.009757	-1.007268
H	-4.082319	0.249457	-0.806319
C	-3.787461	2.742033	1.641756
H	-3.041982	3.027315	2.410561
H	-3.892395	3.597369	0.942358
H	-4.762541	2.586546	2.151236
C	0.140771	-2.614430	4.172922
H	1.168137	-2.640185	4.589929
H	-0.499469	-3.234700	4.835600
H	0.174506	-3.081255	3.171387
C	-0.454000	-0.551624	5.512735
H	-1.213991	-1.094913	6.113833
H	0.519978	-0.626978	6.040233
H	-0.745648	0.516800	5.489502
C	0.320912	4.932085	-1.637769
H	-0.659223	5.450928	-1.652187
H	1.077306	5.642260	-2.036537
H	0.239183	4.055695	-2.307205
C	0.830234	5.711697	0.718883
H	1.685834	6.334784	0.380294
H	-0.080400	6.347265	0.706223
H	1.030224	5.424894	1.771362
C	4.110843	-0.574439	1.630274
H	5.178856	-0.269087	1.651795
H	3.984030	-1.407818	2.349083
H	3.876046	-0.972746	0.627978
C	3.514630	1.166440	3.378067
H	3.512531	0.369065	4.151018
H	4.524750	1.628767	3.363589
H	2.789732	1.943917	3.694211
C	-0.836906	-2.579996	0.405924
C	-2.067395	-2.132842	-0.118597
C	-0.933082	-1.362031	-3.446612
C	-3.115410	0.196833	-1.016030
C	-3.532509	1.525405	-1.273324
C	-4.592460	2.027977	-0.489102
C	-5.193101	1.244423	0.504135
C	-4.746383	-0.065220	0.742167
C	-3.695119	-0.624736	-0.009455
C	-2.897872	2.384300	-2.364114
H	-6.014927	1.660073	1.109036
C	-3.187954	-2.042453	0.255804
C	1.254503	-1.668388	-2.225606
C	1.448798	-2.993425	-1.759840
C	2.779900	-3.443763	-1.646546
C	3.853452	-2.607265	-1.980648
C	3.625446	-1.293032	-2.415142
C	2.317945	-0.782585	-2.531238
C	0.266048	-3.899539	-1.415687
H	4.885732	-2.975968	-1.874312
C	2.047520	0.663979	-2.940003
H	-3.093821	-0.777630	-3.656958
H	-0.581114	-1.836484	-4.366519
H	-4.942824	3.057267	-0.658619
H	-5.216282	-0.660267	1.537605
H	-1.898434	1.956009	-2.581826
H	-2.080351	-1.987144	0.252162
H	2.978808	-4.459279	-1.274048
H	4.482111	-0.639336	-2.635042
H	-0.573645	-3.243682	-1.102436
H	1.130783	0.987585	-2.403290
C	3.166730	1.636925	-2.527407
H	4.091399	1.489431	-3.126088
H	2.814812	2.677000	-2.680112
H	3.411170	1.531323	-1.451455
C	1.764658	0.772173	-4.454316
H	0.899129	0.149455	-4.757355
H	1.535638	1.822840	-4.729235
H	2.646214	0.441846	-5.044730
C	0.548246	-4.853266	-0.242663
H	-0.386286	-5.375248	0.048777
H	1.291372	-5.633726	-0.511754
H	0.914433	-4.301681	0.643053
C	-0.191522	-4.697030	-2.657232
H	0.620673	-5.368250	-3.009231
H	-1.075669	-5.322775	-2.413135
H	-0.470434	-4.033632	-3.499201
C	-2.658595	3.836615	-1.912644
H	-2.047330	4.369521	-2.669079
H	-3.609544	4.399162	-1.791893
H	-2.090571	3.855153	-0.963968
C	-3.755334	2.345129	-3.648638
H	-4.763163	2.775089	-3.462642
H	-3.276192	2.937795	-4.456314
H	-3.902788	1.312330	-4.026234
C	-3.566070	-2.585823	1.640755
H	-4.653740	-2.802440	1.723477
H	-3.022675	-3.535290	1.822451
H	-3.283452	-1.881570	2.446802
C	-3.624044	-3.032200	-0.847278
H	-3.209048	-4.041040	-0.638472
H	-4.731167	-3.119006	-0.886248
H	-3.268951	-2.732362	-1.852936
C	1.964648	-1.560434	1.337886
C	2.856111	-0.637970	0.750212

C	-0.667247	-3.949833	0.706380
C	-3.119369	-3.037547	-0.326173
C	-1.715562	-4.855856	0.487519
C	-2.945337	-4.401815	-0.027327
H	-2.184115	-1.068026	-0.377433
H	0.308284	-4.285268	1.091510
H	-4.083004	-2.671322	-0.715339
H	-1.574728	-5.924768	0.714748
H	-3.768768	-5.114128	-0.196570
C	0.335138	-1.638777	0.605423
O	1.324892	-1.994578	1.228178
C	4.051985	-2.829298	-1.472196
F	5.045191	-1.903655	-1.393676
F	3.977137	-3.439194	-0.257018
F	4.459364	-3.782209	-2.356305

Zero-point correction= 0.798236 (Hartree/Particle)
Thermal correction to Energy= 0.856131
Thermal correction to Enthalpy= 0.857075
Thermal correction to Gibbs Free Energy= 0.704503
Sum of electronic and zero-point Energies= -3239.893818
Sum of electronic and thermal Energies= -3239.835923
Sum of electronic and thermal Enthalpies= -3239.834978
Sum of electronic and thermal Free Energies= -3239.987551

C	2.479699	-2.602059	2.141080
C	4.239333	-0.760497	0.951091
C	3.862401	-2.723408	2.343586
C	4.746851	-1.803208	1.747837
H	2.447445	0.187067	0.142731
H	1.769794	-3.299282	2.612675
H	4.923129	-0.040333	0.473990
H	4.256689	-3.536794	2.973923
H	5.832861	-1.899329	1.907496
C	0.461875	-1.434565	1.168170
O	-0.284659	-2.303061	1.604788
O	-2.445933	-0.882478	4.412154
C	-2.056662	-2.043648	5.134115
H	-1.412614	-2.707817	4.514490
H	-1.520449	-1.789390	6.077490
H	-2.991680	-2.577940	5.390359

Zero-point correction= 0.825512 (Hartree/Particle)
Thermal correction to Energy= 0.882101
Thermal correction to Enthalpy= 0.883045
Thermal correction to Gibbs Free Energy= 0.735162
Sum of electronic and zero-point Energies= -3017.512401
Sum of electronic and thermal Energies= -3017.455811
Sum of electronic and thermal Enthalpies= -3017.454867
Sum of electronic and thermal Free Energies= -3017.602751

B-Ph(pCF3)-IPr-IX-X

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IPrIX-X-CF3 SCF Done: -3240.67441959 A.U.

Pd	0.071106	-0.175822	0.109375
K	-1.315150	-0.962927	5.392997
O	-2.215325	-1.805832	3.111608
H	-2.849908	-2.350793	2.611059
B	-0.949679	-1.797441	2.422402
O	-0.427065	-3.055181	2.132570
H	0.421770	-2.988959	1.649804
C	-1.824754	-1.132675	0.514974
C	-2.262398	-2.308013	-0.153672
C	-2.782530	-0.080194	0.641893
C	-3.548202	-2.420631	-0.709126
H	-1.567474	-3.159069	-0.239915
C	-4.067381	-0.179084	0.096634
H	-2.501093	0.850286	1.161947
C	-4.449021	-1.344875	-0.599258
H	-3.849635	-3.330899	-1.249363
H	-4.770822	0.663610	0.182419
C	-0.275148	0.553477	3.053443
O	-0.424322	1.060385	4.191609
O	-0.051253	-0.842650	3.026816
O	-0.262081	1.156563	1.941931
N	0.687360	2.380486	-1.278378
N	2.557362	1.300452	-1.089837
C	1.228960	1.228583	-0.766686
C	1.652996	3.142640	-1.932657
C	2.839949	2.468542	-1.804801
C	-0.684139	2.774529	-1.030807
C	-0.941837	3.607438	0.089995
C	-2.287926	3.932887	0.346662
C	-3.319466	3.447219	-0.471565
C	-3.029864	2.619409	-1.564740
C	-1.701991	2.255800	-1.866854
C	0.186907	4.166201	0.955753
H	-4.365874	3.707875	-0.244717

B-Ph(pOMe)-IPr-IX-X

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IPrIX-X-OMe SCF Done: -3018.31766681 A.U.

Pd	-0.159006	-0.182105	-0.046062
K	-2.614361	-0.848479	4.875285
O	-2.995390	-1.798012	2.504301
H	-3.511084	-2.319538	1.861579
B	-1.615679	-1.782512	2.096282
O	-1.023960	-3.032383	1.948117
H	-0.100216	-2.961230	1.632588
C	-2.065249	-1.154637	-0.000085
C	-2.388197	-2.378292	-0.640597
C	-3.079294	-0.144958	-0.047519
C	-3.622913	-2.610947	-1.276206
H	-1.654230	-3.200245	-0.617153
C	-4.310510	-0.347712	-0.675562
H	-2.888795	0.834275	0.421728
C	-4.593668	-1.584290	-1.302359
H	-3.809732	-3.583358	-1.754845
H	-5.071593	0.447155	-0.716295
C	-1.100414	0.600751	2.768619
O	-1.476251	1.138228	3.840483
O	-0.870932	-0.792419	2.831581
O	-0.866617	1.172308	1.667124
N	0.754999	2.389745	-1.228447
N	2.541018	1.278648	-0.705164
C	1.174499	1.223308	-0.637212
C	1.837031	3.143251	-1.679571
C	2.969620	2.449152	-1.339936
C	-0.633610	2.801320	-1.224387
C	-1.071152	3.646651	-0.171297
C	-2.438304	3.985157	-0.149100
C	-3.322246	3.491227	-1.119973
C	-2.859660	2.644350	-2.136757
C	-1.502594	2.272695	-2.209856
C	-0.103460	4.194631	0.875653
H	-4.390301	3.758548	-1.073922

C	-1.386219	1.364439	-3.062901	C	-0.992425	1.361501	-3.320709
C	3.536250	0.365761	-0.596240	C	3.394286	0.330568	-0.036115
C	4.119506	-0.555580	-1.498555	C	4.130772	-0.596056	-0.812299
C	5.087895	-1.441320	-0.980996	C	4.977554	-1.488177	-0.121843
C	5.436939	-1.416053	0.375008	C	5.062668	-1.464999	1.276009
C	4.813028	-0.514775	1.252850	C	4.285294	-0.563046	2.020894
C	3.841027	0.396080	0.793692	C	3.423966	0.353852	1.386641
C	3.732056	-0.592791	-2.975067	C	4.017017	-0.635059	-2.334470
H	6.191689	-2.120525	0.759342	H	5.726589	-2.174064	1.795779
C	3.143214	1.367670	1.745572	C	2.551948	1.320083	2.189061
H	1.406438	4.085927	-2.427149	H	1.702073	4.097041	-2.196694
H	3.851173	2.710730	-2.142510	H	4.029245	2.680501	-1.478239
H	-2.532356	4.568360	1.210671	H	-2.819066	4.631364	0.655683
H	-3.849382	2.220559	-2.181120	H	-3.567541	2.242050	-2.876209
H	1.036145	3.454481	0.887403	H	0.741280	3.478181	0.945688
H	-0.368201	0.948103	-2.923521	H	-0.061722	0.875201	-2.967681
H	5.561568	-2.174383	-1.651152	H	5.562274	-2.226477	-0.690946
H	5.079432	-0.525861	2.319908	H	4.340221	-0.579272	3.119345
H	2.756184	-0.073184	-3.074839	H	3.073933	-0.116235	-2.607860
H	2.099827	1.484346	1.388415	H	1.599034	1.435192	1.632508
C	3.020757	0.840141	3.183755	C	2.150214	0.786414	3.573004
H	4.000211	0.795083	3.707500	H	3.007455	0.743342	4.279680
H	2.355980	1.508053	3.768005	H	1.381140	1.451719	4.015553
H	2.560859	-0.169407	3.196432	H	1.699669	-0.224003	3.493000
C	3.805382	2.761050	1.702153	C	3.207131	2.714112	2.285279
H	3.805276	3.180018	0.674923	H	3.407935	3.141063	1.281218
H	3.252259	3.469343	2.353950	H	2.535952	3.417643	2.821108
H	4.858334	2.714183	2.054041	H	4.170788	2.665424	2.836788
C	3.533780	-2.026199	-3.502645	C	3.915649	-2.069434	-2.886296
H	3.117372	-1.995164	-4.530184	H	3.688380	-2.040294	-3.971532
H	4.491801	-2.586183	-3.550420	H	4.867140	-2.629351	-2.761691
H	2.826934	-2.594716	-2.869535	H	3.106989	-2.637042	-2.388114
C	4.775603	0.160538	-3.829055	C	5.195679	0.117790	-2.989523
H	5.769239	-0.331309	-3.755720	H	6.160764	-0.373472	-2.740614
H	4.475949	0.168678	-4.898037	H	5.090695	0.125505	-4.094822
H	4.902272	1.212775	-3.502660	H	5.260970	1.170027	-2.646176
C	-0.172098	4.291039	2.446575	C	-0.709749	4.310979	2.285256
H	0.728615	4.596970	3.020005	H	0.082842	4.601866	3.007298
H	-0.942387	5.072709	2.622164	H	-1.489947	5.101200	2.334051
H	-0.525713	3.325673	2.855714	H	-1.143150	3.348566	2.618512
C	0.657691	5.531905	0.404883	C	0.460225	5.561102	0.423451
H	-0.161575	6.279524	0.470025	H	-0.354891	6.313762	0.362448
H	1.518811	5.914545	0.992687	H	1.215941	5.932481	1.147833
H	0.970265	5.473895	-0.656514	H	0.940951	5.511003	-0.573808
C	-2.326671	0.152568	-3.163022	C	-1.961396	0.214553	-3.653321
H	-3.382789	0.438628	-3.348649	H	-2.889175	0.573978	-4.148092
H	-2.001292	-0.508164	-3.991506	H	-1.466951	-0.502196	-4.339132
H	-2.292270	-0.440312	-2.230248	H	-2.245678	-0.337912	-2.736245
C	-1.386245	2.202967	-4.358991	C	-0.642055	2.199040	-4.569344
H	-1.110823	1.573724	-5.231518	H	-0.225031	1.552777	-5.370497
H	-2.391472	2.635657	-4.552026	H	-1.543869	2.709257	-4.971806
H	-0.664066	3.044828	-4.299836	H	0.109934	2.982098	-4.334684
C	1.216582	-2.721627	-0.772919	C	1.113860	-2.743467	-0.669458
C	2.112222	-2.692324	0.318401	C	1.789787	-2.713411	0.569507
C	0.935350	-3.951080	-1.408502	C	0.944418	-3.976953	-1.335909
C	2.732457	-3.874543	0.756061	C	2.299402	-3.897796	1.127736
C	1.526879	-5.136386	-0.943779	C	1.419497	-5.164567	-0.756860
C	2.432093	-5.100276	0.134135	C	2.103393	-5.127930	0.473149
H	2.338265	-1.728755	0.801125	H	1.936265	-1.746382	1.075417
H	0.247397	-3.954321	-2.268164	H	0.432268	-3.981704	-2.310628
H	3.452834	-3.831490	1.587893	H	2.851943	-3.852890	2.079400
H	1.286416	-6.096280	-1.428350	H	1.261619	-6.126959	-1.269987
H	2.904729	-6.030194	0.488280	H	2.486401	-6.059312	0.919823

C	0.567738	-1.457387	-1.308268
O	0.385137	-1.339305	-2.513913
C	-5.790431	-1.371006	-1.283383
F	-5.817419	-0.519907	-2.355324
F	-6.123864	-2.601409	-1.749232
F	-6.794605	-0.965434	-0.455599

Zero-point correction= 0.795971 (Hartree/Particle)
Thermal correction to Energy= 0.853898
Thermal correction to Enthalpy= 0.854842
Thermal correction to Gibbs Free Energy= 0.702574
Sum of electronic and zero-point Energies= -3239.878448
Sum of electronic and thermal Energies= -3239.820522
Sum of electronic and thermal Enthalpies= -3239.819578
Sum of electronic and thermal Free Energies= -3239.971845

C	0.583793	-1.479384	-1.326535
O	0.634322	-1.376444	-2.548502
O	-5.819994	-1.685949	-1.901345
C	-6.138156	-2.884223	-2.589243
H	-5.425720	-3.090681	-3.421545
H	-6.151909	-3.768350	-1.909278
H	-7.152051	-2.744050	-3.011775

Zero-point correction= 0.823571 (Hartree/Particle)
Thermal correction to Energy= 0.880053
Thermal correction to Enthalpy= 0.880997
Thermal correction to Gibbs Free Energy= 0.734061
Sum of electronic and zero-point Energies= -3017.494096
Sum of electronic and thermal Energies= -3017.437614
Sum of electronic and thermal Enthalpies= -3017.436670
Sum of electronic and thermal Free Energies= -3017.583605

B-Ph(pCF3)-IPr-X

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IPrX-CF3 SCF Done: -3240.70165177 A.U.

Pd	-0.068313	-0.076669	0.370433
K	3.931425	0.667413	-1.928866
O	2.970118	-1.841897	-2.231857
H	3.431279	-2.587977	-1.801964
B	1.593277	-2.080205	-2.158375
O	1.181644	-3.333469	-1.799448
H	0.247259	-3.358105	-1.499213
C	1.815685	-0.720042	0.910257
C	2.379863	-2.019239	0.890744
C	2.719124	0.360762	1.143290
C	3.773259	-2.225694	0.901003
H	1.721059	-2.895555	0.782047
C	4.108107	0.169996	1.196201
H	2.328118	1.387438	1.247981
C	4.645337	-1.124883	1.007356
H	4.190673	-3.240376	0.794231
H	4.788284	1.023552	1.361398
C	1.186682	0.270651	-2.487876
O	1.834503	0.624144	-3.491226
O	0.703739	-1.067605	-2.443800
O	0.935713	0.958540	-1.450514
N	-1.678193	2.419081	0.601891
N	-3.080305	0.903864	-0.038502
C	-1.745876	1.104816	0.200614
C	-2.939816	3.009348	0.644256
C	-3.830198	2.053279	0.231193
C	-0.424679	3.092141	0.854409
C	0.187874	3.786809	-0.221172
C	1.421917	4.415577	0.041650
C	2.012614	4.346485	1.312859
C	1.387969	3.636091	2.349428
C	0.156783	2.980225	2.141453
C	-0.476249	3.877434	-1.593333
H	2.976071	4.848978	1.497563
C	-0.526924	2.201299	3.260316
C	-3.609261	-0.297225	-0.633110
C	-4.331982	-1.198678	0.185455
C	-4.867381	-2.347551	-0.433326
C	-4.663629	-2.590645	-1.796903
C	-3.900741	-1.702268	-2.572345
C	-3.346997	-0.533020	-2.012631
C	-4.516521	-0.955072	1.681936
H	-5.084313	-3.497066	-2.260743

B-Ph(pOMe)-IPr-X

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IPrX-OMe SCF Done: -3018.34080876 A.U.

Pd	0.193319	-0.250521	0.196284
K	3.753567	0.948638	-1.607759
O	2.823326	-1.676477	-2.505979
H	3.174164	-2.449522	-2.014661
B	1.450104	-1.843872	-2.663514
O	0.913930	-3.103270	-2.624520
H	-0.051950	-3.087014	-2.477727
C	1.878428	-1.432695	0.464642
C	2.034367	-2.831493	0.276597
C	3.052764	-0.741821	0.857437
C	3.278996	-3.475613	0.378858
H	1.162129	-3.444115	0.001185
C	4.317402	-1.364693	0.995256
H	2.991856	0.336886	1.095636
C	4.438455	-2.746671	0.731392
H	3.378558	-4.559769	0.208914
H	5.180428	-0.772144	1.338768
C	1.253557	0.517817	-2.655214
O	1.872879	1.064506	-3.583827
O	0.653339	-0.734135	-2.893565
O	1.151645	0.956284	-1.456888
N	-0.816167	2.456996	0.953705
N	-2.561470	1.324696	0.365415
C	-1.194373	1.243605	0.422464
C	-1.920491	3.258399	1.243535
C	-3.026946	2.546103	0.863352
C	0.569708	2.833690	1.099375
C	1.159665	3.621897	0.078503
C	2.528968	3.937042	0.217588
C	3.271484	3.461776	1.311524
C	2.657597	2.673642	2.300115
C	1.288551	2.343382	2.220392
C	0.337836	4.155908	-1.092470
H	4.338899	3.723228	1.405923
C	0.588966	1.547082	3.318478
C	-3.383639	0.323069	-0.265517
C	-4.182540	-0.516236	0.548512
C	-4.983075	-1.476974	-0.103486
C	-4.973219	-1.595059	-1.498204
C	-4.150815	-0.765195	-2.277177
C	-3.327489	0.211011	-1.683372
C	-4.204508	-0.376988	2.069674
H	-5.600475	-2.357008	-1.987454

C	-2.475405	0.416609	-2.839664
H	-3.087000	4.044543	0.963903
H	-4.913141	2.087373	0.084951
H	1.927628	4.968247	-0.764534
H	1.870538	3.576227	3.336467
H	-1.105600	2.970511	-1.705929
H	-1.203233	1.457335	2.793531
H	-5.431484	-3.073272	0.171216
H	-3.725670	-1.929852	-3.633599
H	-3.715879	-0.255881	2.003273
H	-1.609446	0.685126	-2.195720
C	-1.894136	-0.226321	-4.108608
H	-2.674634	-0.414624	-4.877350
H	-1.141183	0.453036	-4.557469
H	-1.374031	-1.176777	-3.880436
C	-3.221897	1.722486	-3.193269
H	-3.565662	2.270256	-2.293814
H	-2.552877	2.402591	-3.760959
H	-4.109715	1.508363	-3.825973
C	-4.351478	-2.239019	2.517403
H	-4.315179	-1.984077	3.595892
H	-5.200753	-2.940005	2.370047
H	-3.413497	-2.769771	2.266274
C	-5.884590	-0.298765	1.968947
H	-6.712596	-0.967833	1.650698
H	-6.003050	-0.100068	3.054775
H	-6.007846	0.663096	1.432272
C	0.517554	3.883421	-2.767278
H	-0.037849	3.832456	-3.727082
H	1.121485	4.816165	-2.795782
H	1.192224	3.007405	-2.725688
C	-1.398693	5.115024	-1.670106
H	-0.805360	6.049187	-1.571637
H	-1.928565	5.145608	-2.645449
H	-2.164199	5.117885	-0.869696
C	0.460555	1.389276	4.113652
H	1.124193	2.036589	4.726232
H	-0.100638	0.727691	4.802822
H	1.087116	0.739914	3.470159
C	-1.383616	3.152390	4.123147
H	-1.917996	2.586276	4.914722
H	-0.750228	3.920993	4.616436
H	-2.142872	3.683687	3.511495
C	-1.043907	-2.685866	1.181579
C	-1.472441	-2.953440	-0.137835
C	-0.781827	-3.763393	2.054019
C	-1.667482	-4.277597	-0.565628
C	-0.922785	-5.088751	1.606307
C	-1.375480	-5.349832	0.300648
H	-1.676715	-2.111464	-0.816587
H	-0.467446	-3.541191	3.085607
H	-2.053106	-4.468533	-1.579986
H	-0.689959	-5.924710	2.285454
H	-1.506492	-6.388407	-0.042173
C	-0.889384	-1.265884	1.703845
O	-1.248526	-1.000729	2.846402
C	6.106516	-1.253824	0.709377
F	6.575275	-2.516519	0.782613
F	6.347267	-0.832586	-0.611488
F	6.892392	-0.463472	1.478095

Zero-point correction=	0.797612 (Hartree/Particle)
Thermal correction to Energy=	0.855988
Thermal correction to Enthalpy=	0.856932

C	-2.395402	1.092642	-2.519360
H	-1.819915	4.250781	1.690983
H	-4.090618	2.797351	0.886686
H	3.016040	4.570039	-0.541073
H	3.249760	2.309372	3.152595
H	-0.526606	3.471820	-1.221338
H	-0.249906	0.990028	2.854241
H	-5.610283	-2.153333	0.496127
H	-4.139594	-0.890583	-3.369319
H	-3.272819	0.149114	2.366983
H	-1.431112	1.140963	-1.967529
C	-2.080528	0.516520	-3.908704
H	-2.962899	0.547668	-4.583976
H	-1.274806	1.111198	-4.385236
H	-1.713002	-0.526027	-3.843909
C	-2.933753	2.535555	-2.646126
H	-3.091718	3.015112	-1.659739
H	-2.214460	3.163528	-3.212726
H	-3.902167	2.547014	-3.190738
C	-4.206405	-1.731908	2.799910
H	-4.084066	-1.571245	3.890590
H	-5.160381	-2.281649	2.651675
H	-3.372070	-2.371830	2.458935
C	-5.413766	0.474610	2.517051
H	-6.366394	-0.027905	2.244203
H	-5.406182	0.618807	3.617926
H	-5.421669	1.476392	2.042488
C	1.096602	4.185491	-2.430055
H	0.409795	4.506578	-3.240943
H	1.932986	4.917730	-2.416725
H	1.489590	3.187605	-2.705356
C	-0.205041	5.564867	-0.759321
H	0.632995	6.285797	-0.646794
H	-0.865594	5.931718	-1.572782
H	-0.785363	5.580087	0.184205
C	1.476066	0.481166	3.977476
H	2.312096	0.922447	4.562693
H	0.863426	-0.126886	4.672309
H	1.891072	-0.209849	3.217558
C	-0.002293	2.519079	4.363991
H	-0.567745	1.957870	5.136893
H	0.801286	3.094259	4.872814
H	-0.696581	3.248803	3.897589
C	-1.308887	-2.684237	0.707126
C	-1.670787	-2.637582	-0.655618
C	-1.473169	-3.889131	1.422771
C	-2.212345	-3.767332	-1.288324
C	-1.975159	-5.033094	0.779510
C	-2.352609	-4.973865	-0.574689
H	-1.534435	-1.689179	-1.201000
H	-1.193074	-3.907600	2.487780
H	-2.539789	-3.702641	-2.339061
H	-2.078999	-5.977063	1.338591
H	-2.761329	-5.866976	-1.073903
C	-0.754995	-1.461164	1.420455
O	-0.928879	-1.330320	2.629538
O	5.606159	-3.463195	0.810328
C	6.780542	-2.788430	1.219982
H	7.063005	-1.966592	0.518210
H	6.682621	-2.356660	2.243992
H	7.592282	-3.541427	1.226911

Zero-point correction=	0.824028 (Hartree/Particle)
Thermal correction to Energy=	0.881412
Thermal correction to Enthalpy=	0.882356

Thermal correction to Gibbs Free Energy= 0.703302	Thermal correction to Gibbs Free Energy= 0.731638
Sum of electronic and zero-point Energies= -3239.904040	Sum of electronic and zero-point Energies= -3017.516781
Sum of electronic and thermal Energies= -3239.845664	Sum of electronic and thermal Energies= -3017.459397
Sum of electronic and thermal Enthalpies= -3239.844719	Sum of electronic and thermal Enthalpies= -3017.458453
Sum of electronic and thermal Free Energies= -3239.998350	Sum of electronic and thermal Free Energies= -3017.609171

B-Ph(pCF3)-IPr-XI				**B-Ph(pOMe)-IPr-XI**			
93				94			
IPrXI-CF3 SCF Done: -2200.41319811 A.U.				IPrXI-OMe SCF Done: -1978.05463001 A.U.			
Pd	-0.319730	-0.040766	-0.123805	Pd	0.527089	0.333770	-0.146171
C	-2.163339	-0.898527	-0.235334	C	2.041004	1.681355	-0.346217
C	-2.598665	-2.201637	-0.572603	C	2.075610	3.079913	-0.568022
C	-3.163074	0.052488	0.104763	C	3.288337	1.030399	-0.182424
C	-3.960227	-2.548083	-0.563055	C	3.282643	3.792756	-0.599337
H	-1.861020	-2.974132	-0.846475	H	1.135810	3.636500	-0.720872
C	-4.527160	-0.281040	0.121716	C	4.515060	1.727308	-0.204430
H	-2.882391	1.090961	0.365275	H	3.331791	-0.066006	-0.034080
C	-4.930231	-1.588404	-0.214042	C	4.513020	3.122808	-0.414498
H	-4.278106	-3.569995	-0.823021	H	3.305785	4.880831	-0.770400
H	-5.283717	0.470570	0.396778	H	5.454027	1.170798	-0.067557
N	1.052180	2.594068	0.100794	N	-0.001306	-2.585147	0.160578
N	2.637885	1.126771	0.133123	N	-1.946267	-1.644657	0.209555
C	1.274837	1.241468	0.056398	C	-0.609706	-1.355735	0.105552
C	2.241454	3.314247	0.193031	C	-0.926822	-3.619457	0.287828
C	3.248934	2.382628	0.210651	C	-2.162058	-3.022865	0.315985
C	-0.292466	3.116017	0.148540	C	1.436666	-2.696476	0.171601
C	-0.933427	3.185430	1.412774	C	2.104448	-2.557185	1.415901
C	-2.263514	3.651474	1.437337	C	3.512288	-2.620254	1.404641
C	-2.921770	4.014809	0.252888	C	4.215939	-2.802639	0.204807
C	-2.268697	3.908158	-0.984235	C	3.527366	-2.910130	-1.012825
C	-0.937391	3.453902	-1.067594	C	2.119836	-2.855894	-1.059729
C	-0.256973	2.689257	2.688631	C	1.347553	-2.256095	2.707205
H	-3.964786	4.366398	0.292294	H	5.316690	-2.840847	0.216285
C	-0.266072	3.233311	-2.419017	C	1.378551	-2.865274	-2.392933
C	3.327652	-0.138703	0.218216	C	-2.971150	-0.631551	0.289987
C	4.045714	-0.593187	-0.914281	C	-3.803536	-0.422584	-0.836539
C	4.727852	-1.821465	-0.797176	C	-4.799921	0.568670	-0.729509
C	4.666975	-2.568838	0.384809	C	-4.933400	1.331819	0.436334
C	3.922212	-2.107384	1.480595	C	-4.075428	1.121513	1.526344
C	3.234653	-0.880140	1.430043	C	-3.073093	0.133701	1.485800
C	4.104642	0.209176	-2.212928	C	-3.652245	-1.241560	-2.117219
H	5.187097	-3.537112	0.449408	H	-5.700060	2.120086	0.491509
C	2.414268	-0.368122	2.617228	C	-2.117516	-0.093277	2.659929
H	2.260728	4.407113	0.240414	H	-0.624583	-4.669139	0.349761
H	4.334329	2.494044	0.284738	H	-3.165614	-3.445771	0.415537
H	-2.798152	3.711101	2.397939	H	4.065992	-2.505093	2.349366
H	-2.809464	4.163633	-1.908408	H	4.093723	-3.018297	-1.950606
H	0.805689	2.477383	2.450610	H	0.263977	-2.379296	2.503604
H	0.810944	3.036349	-2.232186	H	0.294991	-2.973392	-2.174477
H	5.297396	-2.206154	-1.656718	H	-5.464537	0.760746	-1.585342
H	3.863020	-2.726224	2.386147	H	-4.177683	1.756162	2.417049
H	3.282413	0.955301	-2.181124	H	-2.645131	-1.709705	-2.094185
H	1.447189	-0.019460	2.192516	H	-1.100609	-0.151987	2.212104
C	2.077917	-1.446815	3.657803	C	-2.091728	1.056429	3.678392
H	2.978178	-1.779079	4.218370	H	-3.038564	1.120098	4.256685
H	1.363524	-1.037703	4.401767	H	-1.273586	0.890115	4.409295
H	1.612486	-2.336908	3.192872	H	-1.918130	2.035370	3.192232
C	3.090137	0.833925	3.314326	C	-2.394577	-1.426627	3.389918
H	3.273279	1.680303	2.624458	H	-2.332261	-2.303732	2.717170
H	2.447074	1.209454	4.138192	H	-1.653321	-1.578441	4.202906
H	4.065442	0.533352	3.752894	H	-3.406439	-1.418838	3.848438

C	3.869992	-0.663571	-3.460613
H	3.820327	-0.024564	-4.366762
H	4.694938	-1.390032	-3.619836
H	2.913835	-1.215244	-3.377857
C	5.444106	0.970981	-2.318563
H	6.295882	0.259095	-2.362180
H	5.472679	1.593183	-3.237711
H	5.615250	1.637374	-1.448560
C	-0.892563	1.358107	3.144113
H	-0.359631	0.950774	4.028702
H	-1.961689	1.489836	3.412790
H	-0.845435	0.591007	2.335706
C	-0.271521	3.742033	3.813021
H	-1.304178	3.965555	4.154558
H	0.293957	3.372547	4.693938
H	0.189517	4.695393	3.481848
C	-0.851578	1.970769	-3.089035
H	-1.930933	2.104977	-3.313177
H	-0.322084	1.747529	-4.038063
H	-0.750505	1.086326	-2.421001
C	-0.357794	4.468596	-3.335102
H	0.209330	4.293263	-4.272758
H	-1.406596	4.689416	-3.625738
H	0.055314	5.374635	-2.844605
C	0.968293	-2.704222	-0.498759
C	0.488552	-3.042900	0.782857
C	1.841861	-3.588065	-1.171572
C	0.871762	-4.251541	1.382893
C	2.235651	-4.788597	-0.563618
C	1.750718	-5.123834	0.713984
H	-0.197441	-2.340910	1.285739
H	2.209160	-3.307860	-2.169992
H	0.480215	-4.517764	2.377447
H	2.926622	-5.467699	-1.088002
C	0.575187	-1.427110	-1.196946
O	0.842273	-1.218725	-2.367903
C	-6.396262	-1.934626	-0.270359
F	-6.625838	-3.250192	-0.009226
F	-7.129596	-1.211835	0.621334
F	-6.932217	-1.685264	-1.500902
H	2.054244	-6.071022	1.188065

C	-3.718132	-0.377020	-3.390552
H	-3.509331	-1.002360	-4.283548
H	-4.724494	0.070216	-3.535196
H	-2.963662	0.432366	-3.355036
C	-4.708424	-2.367953	-2.166304
H	-5.733335	-1.940137	-2.196492
H	-4.573831	-2.995550	-3.072322
H	-4.654217	-3.031645	-1.279386
C	1.567383	-0.784944	3.119950
H	0.956195	-0.530983	4.011392
H	2.633084	-0.587458	3.360738
H	1.279120	-0.088120	2.298406
C	1.709663	-3.227759	3.846352
H	2.769700	-3.120312	4.159384
H	1.081392	-3.025732	4.739037
H	1.551062	-4.283757	3.544701
C	1.567387	-1.508284	-3.106039
H	2.636459	-1.334590	-3.351664
H	0.982228	-1.476416	-4.048081
H	1.226267	-0.669433	-2.459809
C	1.791503	-4.049818	-3.287311
H	1.175378	-4.067443	-4.210289
H	2.852724	-3.973971	-3.605711
H	1.663293	-5.021848	-2.766675
C	-1.489957	2.480044	-0.578733
C	-1.147539	2.946751	0.706171
C	-2.562736	3.081783	-1.273895
C	-1.859823	4.006833	1.286064
C	-3.283508	4.131850	-0.687078
C	-2.931986	4.598983	0.592875
H	-0.304378	2.461133	1.226635
H	-2.818852	2.703439	-2.274906
H	-1.575515	4.378316	2.283453
H	-4.125719	4.589699	-1.230141
C	-0.740840	1.354817	-1.251185
O	-0.950052	1.041996	-2.411528
O	5.638468	3.908231	-0.463103
C	6.898125	3.284270	-0.304827
H	7.001535	2.785527	0.688388
H	7.096329	2.525418	-1.098850
H	7.659386	4.085288	-0.380818
H	-3.493014	5.429892	1.050170

Zero-point correction=	0.744529 (Hartree/Particle)
Thermal correction to Energy=	0.793325
Thermal correction to Enthalpy=	0.794269
Thermal correction to Gibbs Free Energy=	0.660100
Sum of electronic and zero-point Energies=	-2199.668669
Sum of electronic and thermal Energies=	-2199.619873
Sum of electronic and thermal Enthalpies=	-2199.618929
Sum of electronic and thermal Free Energies=	-2199.753098

Zero-point correction=	0.770650 (Hartree/Particle)
Thermal correction to Energy=	0.818623
Thermal correction to Enthalpy=	0.819568
Thermal correction to Gibbs Free Energy=	0.687811
Sum of electronic and zero-point Energies=	-1977.283980
Sum of electronic and thermal Energies=	-1977.236007
Sum of electronic and thermal Enthalpies=	-1977.235062
Sum of electronic and thermal Free Energies=	-1977.366819

B-Ph(pCF3)-IPr-XI-XII			
93			
IPrXI-XII-CF3 SCF Done: -2200.40290996 A.U.			
Pd	-0.241072	-0.003164	-0.020045
C	-1.913233	-1.241561	-0.372319
C	-2.369889	-2.083100	0.668062
C	-2.862963	-0.635875	-1.230441
C	-3.746095	-2.256493	0.892949
H	-1.647986	-2.607064	1.312993
C	-4.235413	-0.790048	-1.000216
H	-2.502021	-0.053601	-2.093836

B-Ph(pOMe)-IPr-XI-XII			
94			
IPrXI-XII-OMe SCF Done: -1978.04890257 A.U.			
Pd	0.479220	0.280781	0.083517
C	1.551064	2.083009	-0.095172
C	1.546623	3.014378	0.974377
C	2.701723	2.015656	-0.912024
C	2.676378	3.790174	1.258906
H	0.645181	3.136729	1.594724
C	3.847861	2.778206	-0.636154
H	2.681897	1.364265	-1.801602

C	-4.677829	-1.599338	0.068347	C	3.839659	3.670140	0.462729
H	-4.101751	-2.896360	1.714656	H	2.688279	4.510162	2.091852
H	-4.972709	-0.289568	-1.646789	H	4.728051	2.688328	-1.289056
N	1.158605	2.647428	0.305039	N	0.165776	-2.718982	0.245126
N	2.647282	1.083314	0.371023	N	-1.801676	-1.829637	0.296203
C	1.297055	1.282732	0.223642	C	-0.471084	-1.500250	0.198585
C	2.382747	3.284024	0.507026	C	-0.734931	-3.775610	0.375601
C	3.328444	2.290947	0.547697	C	-1.984282	-3.211114	0.409114
C	-0.114732	3.291018	0.101762	C	1.585714	-2.843634	0.037935
C	-0.983883	3.441182	1.209137	C	2.447731	-2.768451	1.158448
C	-2.241322	4.030272	0.967025	C	3.832306	-2.863289	0.914516
C	-2.608951	4.438791	-0.323605	C	4.324938	-3.018328	-0.390425
C	-1.733620	4.252595	-1.404776	C	3.444599	-3.065810	-1.482022
C	-0.466120	3.665856	-1.219563	C	2.051057	-2.972860	-1.294315
C	-0.621939	2.898781	2.589654	C	1.904393	-2.488742	2.557477
H	-3.598036	4.893458	-0.492429	H	5.411303	-3.087752	-0.559954
C	0.436266	3.343779	-2.408553	C	1.098746	-2.915302	-2.486029
C	3.266065	-0.218724	0.319696	C	-2.871056	-0.864566	0.228280
C	3.427777	-0.845203	-0.944600	C	-3.206956	-0.310938	-1.035941
C	4.027863	-2.120575	-0.949240	C	-4.263270	0.621738	-1.060310
C	4.454018	-2.726353	0.240922	C	-4.952570	0.968720	0.109809
C	4.271877	-2.083909	1.473655	C	-4.588994	0.411335	1.343685
C	3.659146	-0.817607	1.542457	C	-3.527499	-0.510063	1.433351
C	2.964429	-0.165108	-2.234961	C	-2.448535	-0.705888	-2.305676
H	4.912761	-3.726688	0.207813	H	-5.769259	1.705696	0.062197
C	3.342222	-0.151739	2.882788	C	-3.039063	-1.043336	2.781609
H	2.465970	4.371678	0.591008	H	-0.405653	-4.817969	0.421022
H	4.414245	2.328443	0.678845	H	-2.979945	-3.657284	0.493578
H	-2.949991	4.155467	1.800293	H	4.537009	-2.801183	1.758063
H	-2.048478	4.550061	-2.417013	H	3.846498	-3.158686	-2.503114
H	0.461471	2.654469	2.582681	H	0.816286	-2.713341	2.545138
H	1.446164	3.099711	-2.016476	H	0.061307	-2.990512	-2.099053
H	4.151383	-2.658472	-1.899198	H	-4.544124	1.096910	-2.010183
H	4.589375	-2.587242	2.398729	H	-5.124264	0.715886	2.254999
H	1.961196	0.261882	-2.021529	H	-1.370265	-0.704228	-2.037450
H	3.386958	0.948660	2.732503	H	-2.652405	-2.072424	2.617964
C	1.896706	-0.489565	3.312872	C	-1.853052	-0.192802	3.291065
H	1.788708	-1.582116	3.482292	H	-2.177180	0.854159	3.472495
H	1.632045	0.032986	4.256145	H	-1.454903	-0.599575	4.244614
H	1.162937	-0.194424	2.533771	H	-1.024548	-0.166495	2.552264
C	4.346068	-0.496311	3.996095	C	-4.146115	-1.140127	3.845357
H	5.393132	-0.313044	3.677490	H	-5.026285	-1.704699	3.473705
H	4.145580	0.119998	4.896808	H	-3.762683	-1.653878	4.751101
H	4.266469	-1.558822	4.309489	H	-4.497171	-0.137189	4.168553
C	2.788822	-1.131140	-3.415460	C	-2.616442	0.291061	-3.461388
H	2.317791	-0.595907	-4.264658	H	-1.926513	0.021282	-4.286311
H	3.761749	-1.532204	-3.773294	H	-3.649143	0.280393	-3.872544
H	2.123058	-1.975103	-3.153479	H	-2.362250	1.321267	-3.148229
C	3.898727	0.998200	-2.637263	C	-2.819013	-2.129944	-2.777794
H	4.918967	0.622033	-2.865108	H	-3.893128	-2.185178	-3.056697
H	3.508668	1.501077	-3.547198	H	-2.219646	-2.401656	-3.672382
H	3.986935	1.767759	-1.845327	H	-2.626738	-2.899799	-2.004914
C	-1.382063	1.581394	2.852699	C	2.056506	-0.988091	2.884956
H	-1.084059	1.138606	3.825862	H	1.612587	-0.747806	3.873538
H	-2.480064	1.744298	2.861253	H	3.124842	-0.687113	2.893584
H	-1.164258	0.827086	2.055756	H	1.541724	-0.353725	2.120140
C	-0.857862	3.925412	3.713605	C	2.548054	-3.372237	3.642138
H	-1.934751	4.170992	3.828029	H	3.625301	-3.139303	3.778231
H	-0.510203	3.520115	4.686704	H	2.053736	-3.202892	4.621360
H	-0.314042	4.872953	3.519003	H	2.463441	-4.450324	3.392978
C	-0.084840	2.080651	-3.129436	C	1.217008	-1.546201	-3.189740
H	-1.082326	2.266861	-3.581658	H	2.222826	-1.417368	-3.643994
H	0.609028	1.773037	-3.939577	H	0.462081	-1.455343	-3.998721

H	-0.185418	1.226922	-2.425307
C	0.598765	4.528986	-3.378409
H	1.328081	4.274956	-4.175554
H	-0.357144	4.784445	-3.882836
H	0.960141	5.439233	-2.856158
C	0.485846	-2.829342	-0.774582
C	0.884866	-2.928483	0.573277
C	0.780443	-3.886980	-1.662926
C	1.562368	-4.066505	1.032521
C	1.457770	-5.026830	-1.203600
C	1.847485	-5.120761	0.145900
H	0.679675	-2.075267	1.242031
H	0.461591	-3.793600	-2.712753
H	1.884758	-4.123695	2.083943
H	1.681949	-5.850373	-1.900510
H	2.379278	-6.016241	0.505680
C	-0.217452	-1.605958	-1.314676
O	-0.298976	-1.396800	-2.524380
C	-6.160058	-1.813466	0.270636
F	-6.649980	-2.766260	-0.570233
F	-6.454089	-2.214459	1.535246
F	-6.870595	-0.678672	0.028855

Zero-point correction= 0.743311 (Hartree/Particle)
Thermal correction to Energy= 0.791607
Thermal correction to Enthalpy= 0.792551
Thermal correction to Gibbs Free Energy= 0.659164
Sum of electronic and zero-point Energies= -2199.659599
Sum of electronic and thermal Energies= -2199.611303
Sum of electronic and thermal Enthalpies= -2199.610359
Sum of electronic and thermal Free Energies= -2199.743746

H	1.051794	-0.709665	-2.478817
C	1.303250	-4.084749	-3.467611
H	0.542147	-4.044841	-4.274683
H	2.300050	-4.044008	-3.955786
H	1.215554	-5.066949	-2.958104
C	-1.263418	2.614828	-0.704168
C	-1.763530	2.500217	0.607745
C	-1.869566	3.524336	-1.598260
C	-2.845665	3.285992	1.027690
C	-2.953757	4.310760	-1.179212
C	-3.442325	4.196150	0.136147
H	-1.300914	1.753370	1.274875
H	-1.466510	3.600394	-2.620264
H	-3.237749	3.174224	2.050752
H	-3.420872	5.021036	-1.880513
H	-4.293577	4.814018	0.464768
C	-0.114507	1.766913	-1.200887
O	0.120016	1.654912	-2.403012
O	4.888529	4.470042	0.817997
C	6.076743	4.416503	0.044774
H	6.538337	3.401674	0.055623
H	5.899928	4.714446	-1.014874
H	6.782042	5.135002	0.505175

Zero-point correction= 0.770462 (Hartree/Particle)
Thermal correction to Energy= 0.817464
Thermal correction to Enthalpy= 0.818409
Thermal correction to Gibbs Free Energy= 0.690361
Sum of electronic and zero-point Energies= -1977.278441
Sum of electronic and thermal Energies= -1977.231438
Sum of electronic and thermal Enthalpies= -1977.230494
Sum of electronic and thermal Free Energies= -1977.358541

B-Ph(pCF3)-IPr-XII

93
IPrXII-CF3 SCF Done: -2200.43852643 A.U.

Pd	-0.025855	-0.362394	-0.330412
C	-0.339188	-2.274211	-1.286882
C	-0.548709	-3.234682	-0.237157
C	-1.452445	-1.441617	-1.677647
C	-1.802639	-3.389408	0.349292
H	0.283409	-3.885068	0.070715
C	-2.718986	-1.606173	-1.055292
H	-1.373633	-0.848310	-2.600896
C	-2.891172	-2.570223	-0.059961
H	-1.954115	-4.141758	1.137584
H	-3.557021	-0.963965	-1.359597
N	-0.625846	2.548805	0.230266
N	1.310334	2.059594	1.052794
C	0.248370	1.499329	0.386106
C	-0.128103	3.727576	0.784230
C	1.102430	3.417546	1.308201
C	-1.897538	2.359243	-0.420371
C	-2.993259	1.931680	0.367989
C	-4.196785	1.637694	-0.303000
C	-4.292364	1.763399	-1.697565
C	-3.187653	2.190944	-2.450248
C	-1.961471	2.500732	-1.827743
C	-2.859676	1.711180	1.872765
H	-5.238251	1.515842	-2.205232
C	-0.746776	2.918198	-2.654181
C	2.472323	1.310791	1.458379
C	3.610108	1.312981	0.612043

B-Ph(pOMe)-IPr-XII

94
IPrXII-OMe SCF Done: -1978.08208078 A.U.

Pd	0.143021	0.496744	-0.306767
C	0.099430	2.488705	-1.146518
C	0.095522	3.336414	0.009579
C	1.377201	1.983905	-1.592638
C	1.283990	3.719360	0.639657
H	-0.860238	3.739624	0.376079
C	2.571909	2.371849	-0.950209
H	1.421735	1.448217	-2.552798
C	2.531524	3.232164	0.160923
H	1.232505	4.385456	1.511410
H	3.543260	1.982627	-1.287986
N	1.319841	-2.232417	0.202300
N	-0.715946	-2.195203	0.926195
C	0.233041	-1.395917	0.332295
C	1.057791	-3.509276	0.699222
C	-0.234705	-3.486453	1.160162
C	2.553436	-1.770900	-0.382961
C	3.495700	-1.124634	0.453827
C	4.650740	-0.597734	-0.157280
C	4.851327	-0.713237	-1.540765
C	3.898467	-1.358677	-2.343616
C	2.725436	-1.902751	-1.783016
C	3.236349	-0.912098	1.942947
H	5.757139	-0.286944	-2.000796
C	1.648106	-2.524712	-2.668446
C	-2.024314	-1.723828	1.302092
C	-3.096631	-1.888503	0.389313

C	4.749694	0.616586	1.059328	C	-4.373477	-1.466137	0.808737
C	4.746302	-0.059110	2.288890	C	-4.565667	-0.895210	2.075382
C	3.587808	-0.089147	3.077757	C	-3.476142	-0.695360	2.934894
C	2.418956	0.591308	2.677008	C	-2.177158	-1.101397	2.565368
C	3.562466	1.942111	-0.778063	C	-2.857951	-2.389718	-1.031702
H	5.651146	-0.591516	2.622822	H	-5.574028	-0.576744	2.384520
C	1.136742	0.482122	3.498906	C	-0.983686	-0.801674	3.468730
H	-0.688329	4.666952	0.755333	H	1.805701	-4.307621	0.677128
H	1.843333	4.028408	1.832764	H	-0.852480	-4.259895	1.626456
H	-5.062117	1.272897	0.271142	H	5.394439	-0.067666	0.457729
H	-3.273933	2.275745	-3.544905	H	4.060683	-1.428458	-3.430366
H	-1.892479	2.152206	2.193993	H	2.370097	-1.546205	2.227663
H	0.050008	3.232328	-1.947049	H	0.945901	-3.075345	-2.006837
H	5.649373	0.587543	0.426925	H	-5.228947	-1.568940	0.124628
H	3.586002	-0.655559	4.022254	H	-3.633793	-0.209688	3.910728
H	2.761041	2.712321	-0.773975	H	-1.905356	-2.962596	-1.030743
H	0.399939	1.199287	3.080130	H	-0.102206	-1.338565	3.059599
C	0.532662	-0.928947	3.334844	C	-0.659286	0.706766	3.413929
H	1.240015	-1.711797	3.682132	H	-1.520195	1.312808	3.768587
H	-0.405924	-1.027034	3.918125	H	0.216660	0.944722	4.052639
H	0.289845	-1.123535	2.266246	H	-0.417646	1.013580	2.371962
C	1.348323	0.848518	4.980205	C	-1.193129	-1.293267	4.913511
H	1.789072	1.861113	5.089329	H	-1.442644	-2.374228	4.942208
H	0.380026	0.832200	5.522584	H	-0.271915	-1.134702	5.512346
H	2.022362	0.129324	5.491752	H	-2.012829	-0.743719	5.422954
C	3.157474	0.862285	-1.806295	C	-2.662749	-1.173837	-1.964238
H	3.083329	1.291308	-2.826917	H	-2.445144	-1.497222	-3.002911
H	3.894839	0.032383	-1.824555	H	-3.566537	-0.528726	-1.976748
H	2.169930	0.420719	-1.548596	H	-1.812640	-0.545609	-1.615411
C	4.872504	2.643038	-1.179215	C	-3.963343	-3.329196	-1.545232
H	5.701157	1.918245	-1.324527	H	-4.925690	-2.793572	-1.687469
H	4.739970	3.175958	-2.143410	H	-3.679886	-3.747362	-2.533258
H	5.195266	3.381664	-0.416136	H	-4.143046	-4.174854	-0.848963
C	-2.802726	0.202095	2.184896	C	2.832052	0.554752	2.195023
H	-2.631638	0.029971	3.268001	H	2.577441	0.716651	3.263488
H	-3.753488	-0.293108	1.906357	H	3.654140	1.247124	1.918513
H	-1.980915	-0.284443	1.615337	H	1.947191	0.816792	1.572089
C	-3.973468	2.417412	2.669095	C	4.428557	-1.338907	2.819500
H	-4.971870	1.984565	2.448323	H	5.318987	-0.699565	2.641107
H	-3.801207	2.302002	3.759673	H	4.169676	-1.244752	3.895055
H	-4.015989	3.502144	2.437848	H	4.723468	-2.391107	2.625130
C	-0.189345	1.725264	-3.457318	C	0.835210	-1.416807	-3.370598
H	-0.945636	1.324587	-4.165217	H	1.481216	-0.813392	-4.042911
H	0.700351	2.028802	-4.047315	H	0.015184	-1.850860	-3.979478
H	0.114706	0.900904	-2.779612	H	0.384169	-0.728469	-2.622934
C	-1.058501	4.123604	-3.563566	C	2.221206	-3.539523	-3.675903
H	-0.139955	4.460108	-4.088364	H	1.398448	-4.036752	-4.230809
H	-1.805634	3.865329	-4.343492	H	2.870872	-3.048361	-4.431147
H	-1.459730	4.980200	-2.982909	H	2.822770	-4.323848	-3.170800
C	2.254622	-2.552686	-1.543905	C	-2.500270	2.314746	-1.442285
C	2.575228	-2.427139	-0.171944	C	-2.839069	1.989634	-0.108719
C	3.268675	-2.935390	-2.450893	C	-3.531458	2.664161	-2.343095
C	3.876656	-2.694448	0.280657	C	-4.176039	2.036207	0.316738
C	4.566097	-3.210788	-1.996614	C	-4.866057	2.717840	-1.915585
C	4.873495	-3.091699	-0.627369	C	-5.192137	2.406222	-0.581631
H	1.815679	-2.063017	0.540141	H	-2.053564	1.636300	0.582064
H	3.012784	-2.994359	-3.519782	H	-3.258334	2.876612	-3.388093
H	4.112225	-2.571710	1.347936	H	-4.421296	1.759513	1.352765
H	5.345954	-3.515222	-2.712888	H	-5.659733	2.998679	-2.626537
H	5.894338	-3.301532	-0.269460	H	-6.241091	2.442380	-0.245636
C	0.911061	-2.181574	-2.127329	C	-1.101077	2.196458	-2.007356
O	0.838483	-1.795017	-3.301039	O	-0.953352	1.879395	-3.196459
C	-4.236481	-2.776360	0.587244	O	3.737717	3.526205	0.734066

F	-4.846530	-3.911254	0.149802	C	3.759478	4.335822	1.900430
F	-4.130773	-2.893108	1.942119	H	3.349656	5.354483	1.710559
F	-5.095196	-1.746068	0.342699	H	3.191712	3.868667	2.738064
				H	4.822300	4.428330	2.195314

Zero-point correction=	0.745314 (Hartree/Particle)
Thermal correction to Energy=	0.793912
Thermal correction to Enthalpy=	0.794856
Thermal correction to Gibbs Free Energy=	0.660953
Sum of electronic and zero-point Energies=	-2199.693213
Sum of electronic and thermal Energies=	-2199.644615
Sum of electronic and thermal Enthalpies=	-2199.643671
Sum of electronic and thermal Free Energies=	-2199.777574

Zero-point correction=	0.772260 (Hartree/Particle)
Thermal correction to Energy=	0.819669
Thermal correction to Enthalpy=	0.820614
Thermal correction to Gibbs Free Energy=	0.690713
Sum of electronic and zero-point Energies=	-1977.309821
Sum of electronic and thermal Energies=	-1977.262411
Sum of electronic and thermal Enthalpies=	-1977.261467
Sum of electronic and thermal Free Energies=	-1977.391368

B-Ph(pF)-IPr-IX				**B-Ph(pMe)-IPr-IX**			
100				103			
IPrIX-F SCF Done: -3003.05494938 A.U.				IPrIX-Me SCF Done: -2943.17974005 A.U.			
Pd	-0.095165	0.314827	0.382902	Pd	-0.125217	0.285530	0.441080
K	2.574088	4.804841	-0.753669	K	2.498498	4.849610	-0.683160
O	1.045784	4.350819	1.280884	O	1.094543	4.272398	1.419337
H	0.856381	4.597914	2.201747	H	0.963328	4.469025	2.362158
B	1.514638	2.944825	1.246706	B	1.616629	2.891402	1.284445
O	2.943142	2.914572	1.576330	O	3.074305	2.922141	1.481736
H	3.283609	2.002559	1.498388	H	3.443142	2.024181	1.379299
C	0.583818	1.980728	2.212612	C	0.830763	1.848099	2.289586
C	1.152959	1.267253	3.311418	C	1.534388	1.098179	3.279197
C	-0.846677	1.956510	2.117687	C	-0.597776	1.768153	2.348953
C	0.373728	0.561493	4.234440	C	0.875710	0.321212	4.233797
H	2.247417	1.280358	3.435705	H	2.635177	1.145689	3.291890
C	-1.652164	1.242635	3.036935	C	-1.264206	0.965705	3.311890
H	-1.345332	2.568868	1.349268	H	-1.200613	2.415604	1.690437
C	-1.023115	0.553220	4.073455	C	-0.540167	0.229863	4.263018
H	0.820513	0.004162	5.071242	H	1.463963	-0.243485	4.977051
H	-2.746726	1.215329	2.936489	H	-2.366010	0.924274	3.300625
C	0.371788	2.801014	-1.072828	C	0.298233	2.841027	-0.936171
O	0.492493	3.720933	-1.914175	O	0.364067	3.781156	-1.762779
O	1.455417	2.541405	-0.248897	O	1.441764	2.547029	-0.213734
O	-0.645782	2.029252	-0.934259	O	-0.720063	2.084609	-0.734414
N	-2.203026	-0.881478	-1.336183	N	-2.280068	-0.746920	-1.313573
N	-0.273566	-1.683138	-1.925447	N	-0.387042	-1.547051	-2.011341
C	-0.877147	-0.890012	-0.987391	C	-0.944128	-0.803484	-1.006495
C	-2.419161	-1.643380	-2.484622	C	-2.548520	-1.433338	-2.497175
C	-1.201774	-2.146864	-2.860678	C	-1.353873	-1.935451	-2.942062
C	-3.233604	-0.237975	-0.550922	C	-3.267368	-0.144922	-0.444524
C	-3.781902	0.983467	-1.013304	C	-3.813762	1.114080	-0.793452
C	-4.775131	1.583602	-0.210604	C	-4.750757	1.673798	0.100750
C	-5.187840	0.995021	0.991606	C	-5.111327	1.011657	1.281363
C	-4.617685	-0.212909	1.424633	C	-4.548596	-0.235029	1.597753
C	-3.622956	-0.860882	0.667001	C	-3.612246	-0.847292	0.742617
C	-3.355667	1.620028	-2.333640	C	-3.445048	1.830654	-2.089516
H	-5.960875	1.485164	1.605044	H	-5.838289	1.473670	1.968580
C	-2.996253	-2.177232	1.128173	C	-3.015005	-2.217664	1.061486
C	1.127096	-2.025384	-1.898959	C	1.007563	-1.909431	-2.058697
C	1.508257	-3.205681	-1.211817	C	1.394241	-3.138845	-1.468243
C	2.882330	-3.519805	-1.193801	C	2.763374	-3.470516	-1.517341
C	3.817977	-2.695339	-1.833489	C	3.689584	-2.614941	-2.128690
C	3.408499	-1.520151	-2.481234	C	3.275351	-1.395211	-2.684547
C	2.051724	-1.142877	-2.511678	C	1.923656	-1.001049	-2.646051
C	0.472495	-4.101960	-0.531795	C	0.368768	-4.072768	-0.824990
H	4.887230	-2.957187	-1.801702	H	4.755867	-2.889707	-2.148012
C	1.590810	0.167011	-3.149114	C	1.458573	0.348032	-3.191449
H	-3.415813	-1.764026	-2.917028	H	-3.560145	-1.504680	-2.905226
H	-0.909131	-2.783466	-3.699901	H	-1.100290	-2.522807	-3.828618
H	-5.224351	2.534403	-0.534617	H	-5.193589	2.653888	-0.131225

H	-4.944206	-0.655572	2.376413
H	-2.347485	1.226456	-2.576210
H	-1.908421	-2.108142	0.923254
H	3.226072	-4.416812	-0.658579
H	4.162664	-0.866120	-2.942970
H	-0.375290	-3.452410	-0.225467
H	0.711933	0.521560	-2.569733
C	2.644153	1.287208	-3.074514
H	3.503921	1.100531	-3.753467
H	2.172289	2.247157	-3.365787
H	3.021618	1.410885	-2.039653
C	1.133021	-0.055240	-4.606910
H	0.311391	-0.796636	-4.670870
H	0.764858	0.895321	-5.046082
H	1.974891	-0.424451	-5.231118
C	0.998837	-4.781536	0.743598
H	0.162970	-5.279665	1.275789
H	1.755438	-5.561907	0.514177
H	1.446300	-4.045064	1.436639
C	-0.069717	-5.161679	-1.516789
H	0.747254	-5.836816	-1.849684
H	-0.851347	-5.780983	-1.028766
H	-0.518644	-4.702687	-2.419150
C	-3.217435	3.150717	-2.245019
H	-2.747032	3.538661	-3.171448
H	-4.202869	3.653046	-2.136151
H	-2.558617	3.431650	-1.402369
C	-4.337060	1.228212	-3.461000
H	-5.356461	1.614696	-3.245740
H	-4.008219	1.656591	-4.431346
H	-4.421894	0.129286	-3.585758
C	-3.117214	-2.428027	2.637711
H	-4.166333	-2.626843	2.947352
H	-2.515330	-3.317512	2.912364
H	-2.728748	-1.577521	3.229095
C	-3.556048	-3.378563	0.333832
H	-3.054980	-4.316179	0.655056
H	-4.647007	-3.495119	0.509449
H	-3.394884	-3.274587	-0.757652
C	2.210351	-1.130238	1.451898
C	2.945047	-0.303823	0.575950
C	2.900352	-1.923959	2.395178
C	4.347129	-0.279921	0.631873
C	4.301475	-1.897191	2.453101
C	5.029437	-1.075765	1.570284
H	2.402521	0.329613	-0.144965
H	2.310453	-2.544223	3.087797
H	4.907243	0.359268	-0.069151
H	4.832838	-2.515797	3.194155
H	6.130107	-1.055530	1.616690
C	0.693365	-1.160640	1.440481
O	0.084732	-1.978882	2.116532
F	-1.777766	-0.149483	4.953498

H	-4.840851	-0.739298	2.530112
H	-2.451932	1.447916	-2.402012
H	-1.948188	-2.192161	0.759391
H	3.110707	-4.406649	-1.056647
H	4.023125	-0.720813	-3.126860
H	-0.468646	-3.441233	-0.458485
H	0.606171	0.678764	-2.560685
C	2.529394	1.449352	-3.098131
H	3.364097	1.283221	-3.812868
H	2.060722	2.426741	-3.330854
H	2.938821	1.520434	-2.070894
C	0.944748	0.212425	-4.641522
H	0.113533	-0.516881	-4.718281
H	0.571178	1.189825	-5.011793
H	1.759641	-0.127539	-5.316142
C	0.918601	-4.839177	0.389980
H	0.091478	-5.370408	0.903812
H	1.666854	-5.604619	0.092615
H	1.383524	-4.153759	1.122505
C	-0.200274	-5.062958	-1.866090
H	0.606349	-5.715665	-2.262810
H	-0.972300	-5.712593	-1.402684
H	-0.667955	-4.543741	-2.725297
C	-3.292497	3.352173	-1.912831
H	-2.859850	3.795264	-2.832731
H	-4.269477	3.849853	-1.729478
H	-2.596302	3.575795	-1.083272
C	-4.481081	1.513336	-3.191204
H	-5.485861	1.893304	-2.906289
H	-4.193155	1.996586	-4.148703
H	-4.581987	0.424313	-3.376962
C	-3.008305	-2.551467	2.558530
H	-4.030047	-2.728833	2.958583
H	-2.414747	-3.470997	2.733022
H	-2.531795	-1.738608	3.137418
C	-3.714071	-3.330596	0.249986
H	-3.236709	-4.313002	0.451565
H	-4.787684	-3.406134	0.525982
H	-3.655112	-3.148612	-0.841945
C	2.212616	-1.253178	1.292304
C	2.915625	-0.364223	0.452756
C	2.936483	-2.123254	2.137054
C	4.318651	-0.352220	0.448254
C	4.339070	-2.107244	2.137062
C	5.035027	-1.221916	1.291319
H	2.347884	0.332639	-0.185385
H	2.372748	-2.792841	2.805115
H	4.853319	0.336189	-0.225843
H	4.896521	-2.784462	2.804078
H	6.136839	-1.209897	1.291434
C	0.695797	-1.268999	1.351311
O	0.109375	-2.133181	1.989297
C	-1.219282	-0.654622	5.281382
H	-2.316745	-0.500820	5.298085
H	-1.031688	-1.725823	5.051556
H	-0.829396	-0.468162	6.304682

Zero-point correction=	0.785996 (Hartree/Particle)
Thermal correction to Energy=	0.840825
Thermal correction to Enthalpy=	0.841769
Thermal correction to Gibbs Free Energy=	0.698124
Sum of electronic and zero-point Energies=	-3002.268954
Sum of electronic and thermal Energies=	-3002.214125
Sum of electronic and thermal Enthalpies=	-3002.213181
Sum of electronic and thermal Free Energies=	-3002.356825

Zero-point correction=	0.820190 (Hartree/Particle)
Thermal correction to Energy=	0.875117
Thermal correction to Enthalpy=	0.876061
Thermal correction to Gibbs Free Energy=	0.733018
Sum of electronic and zero-point Energies=	-2942.359550
Sum of electronic and thermal Energies=	-2942.304624
Sum of electronic and thermal Enthalpies=	-2942.303679
Sum of electronic and thermal Free Energies=	-2942.446722

B-Ph(pF)-IPr-IX-X				B-Ph(pMe)-IPr-IX-X			
100				103			
IPrIX-X-F SCF Done: -3003.03625502 A.U.				IPrIX-X-Me SCF Done: -2943.16102026 A.U.			
Pd	-0.216653	-0.254824	-0.200274	Pd	-0.218064	-0.262744	-0.179115
K	-2.639013	-2.874600	4.020070	K	-2.569549	-2.764228	4.142682
O	-2.745296	-3.070918	1.434698	O	-2.719844	-3.014284	1.568682
H	-3.080491	-3.522241	0.638374	H	-3.080667	-3.450710	0.775050
B	-1.379096	-2.673595	1.215844	B	-1.354661	-2.632846	1.318068
O	-0.515537	-3.702397	0.849126	O	-0.504884	-3.674310	0.956512
H	0.395443	-3.377207	0.700007	H	0.403222	-3.356934	0.776620
C	-1.797291	-1.631359	-0.696695	C	-1.815984	-1.630278	-0.614035
C	-1.702040	-2.649880	-1.684803	C	-1.757432	-2.671810	-1.578712
C	-3.023917	-0.899795	-0.663132	C	-3.035944	-0.890261	-0.569777
C	-2.746706	-2.936757	-2.580762	C	-2.829126	-2.955800	-2.442114
H	-0.783962	-3.257177	-1.738296	H	-0.849603	-3.294397	-1.636934
C	-4.081123	-1.162705	-1.547570	C	-4.105787	-1.167004	-1.432639
H	-3.152640	-0.094524	0.078420	H	-3.144346	-0.071028	0.159872
C	-3.925235	-2.180760	-2.500055	C	-4.022071	-2.200815	-2.393427
H	-2.662982	-3.724820	-3.344997	H	-2.735708	-3.772258	-3.179308
H	-5.015874	-0.581774	-1.523336	H	-5.022431	-0.554750	-1.372586
C	-1.521886	-0.541653	2.549272	C	-1.456826	-0.474297	2.610790
O	-2.079016	-0.446395	3.670402	O	-1.986843	-0.348169	3.742331
O	-0.927598	-1.794951	2.265159	O	-0.877806	-1.738148	2.343698
O	-1.395822	0.360296	1.674340	O	-1.346303	0.405501	1.711623
N	0.099297	2.683897	-0.528481	N	0.110386	2.664962	-0.595731
N	2.058580	1.899123	-0.037656	N	2.073150	1.880896	-0.117711
C	0.753414	1.520376	-0.208003	C	0.762360	1.506652	-0.251904
C	0.981455	3.761089	-0.581323	C	0.998981	3.733340	-0.698157
C	2.220628	3.270306	-0.259494	C	2.240674	3.243265	-0.385231
C	-1.341891	2.747038	-0.644947	C	-1.332918	2.738341	-0.676981
C	-2.082599	3.136056	0.501709	C	-2.039015	3.162885	0.478856
C	-3.486630	3.119125	0.391220	C	-3.445539	3.156669	0.407341
C	-4.113880	2.722094	-0.799174	C	-4.108638	2.735729	-0.754959
C	-3.351239	2.335333	-1.910062	C	-3.379845	2.313747	-1.875570
C	-1.943085	2.333007	-1.858441	C	-1.970985	2.299122	-1.862467
C	-1.395606	3.591335	1.788217	C	-1.313423	3.644206	1.734363
H	-5.214156	2.704006	-0.857575	H	-5.210206	2.725170	-0.782574
C	-1.111096	1.943299	-3.076194	C	-1.176499	1.869470	-3.091810
C	3.069429	1.012603	0.479265	C	3.088722	1.001039	0.401644
C	4.077624	0.538515	-0.394141	C	4.077416	0.500545	-0.479200
C	5.060896	-0.309953	0.155834	C	5.066521	-0.340627	0.071520
C	5.024234	-0.674716	1.507573	C	5.052973	-0.674724	1.431516
C	3.990050	-0.217145	2.340178	C	4.037191	-0.191929	2.272559
C	2.978864	0.630834	1.847105	C	3.022208	0.651620	1.779610
C	4.112687	0.934313	-1.868682	C	4.086748	0.861356	-1.963144
H	5.799823	-1.342520	1.915178	H	5.832227	-1.337912	1.839709
C	1.832190	1.111541	2.737239	C	1.897810	1.163394	2.680429
H	0.648627	4.769545	-0.840994	H	0.668354	4.736166	-0.981298
H	3.190841	3.763820	-0.157367	H	3.216129	3.732297	-0.317425
H	-4.098363	3.405263	1.259707	H	-4.030270	3.469760	1.285068
H	-3.855655	2.008273	-2.831274	H	-3.911945	1.966319	-2.773372
H	-0.389865	3.121602	1.807281	H	-0.310538	3.168388	1.736593
H	-0.100228	1.652033	-2.728508	H	-0.160610	1.573204	-2.763726
H	5.857518	-0.704031	-0.492890	H	5.848536	-0.754031	-0.582961
H	3.960446	-0.536611	3.392253	H	4.025813	-0.487050	3.332047
H	3.095128	1.286432	-2.139660	H	3.066636	1.214393	-2.222936
H	0.929600	1.186172	2.096907	H	0.980383	1.217869	2.059395
C	1.458738	0.119708	3.850783	C	1.550504	0.211122	3.836084
H	2.241195	0.045291	4.636878	H	2.351685	0.163860	4.605248
H	0.519626	0.449322	4.339688	H	0.623138	0.558558	4.334846
H	1.269788	-0.891039	3.434221	H	1.351642	-0.813265	3.459490

C	2.117311	2.519641	3.301053
H	2.299372	3.254097	2.489737
H	1.249184	2.879774	3.892066
H	3.009610	2.511161	3.963432
C	4.439360	-0.248472	-2.798729
H	4.319636	0.061012	-3.857148
H	5.485946	-0.599276	-2.672866
H	3.758286	-1.101195	-2.619063
C	5.107755	2.093635	-2.096402
H	6.141052	1.778790	-1.836065
H	5.104405	2.409966	-3.160635
H	4.865592	2.980712	-1.477011
C	-2.119467	3.150934	3.072763
H	-1.504943	3.423795	3.957074
H	-3.096972	3.665899	3.193293
H	-2.280043	2.056038	3.087747
C	-1.208661	5.125880	1.778039
H	-2.195759	5.635889	1.772748
H	-0.655146	5.459870	2.681161
H	-0.650416	5.476894	0.887205
C	-1.667884	0.719078	-3.821137
H	-2.646768	0.925951	-4.304022
H	-0.958330	0.409238	-4.614227
H	-1.791315	-0.137074	-3.129742
C	-0.951161	3.163608	-4.008813
H	-0.307739	2.911514	-4.878163
H	-1.936751	3.501133	-4.396065
H	-0.488560	4.021499	-3.476051
C	1.754125	-2.176218	-1.188734
C	2.214114	-2.342054	0.135516
C	2.046701	-3.165214	-2.153319
C	2.972129	-3.471416	0.486664
C	2.770575	-4.312413	-1.790656
C	3.240985	-4.465317	-0.472543
H	1.989883	-1.559466	0.877410
H	1.692987	-3.014046	-3.185127
H	3.351149	-3.570630	1.515913
H	2.976027	-5.092225	-2.541624
H	3.820046	-5.360209	-0.194034
C	0.967952	-0.946280	-1.613142
O	1.101044	-0.510432	-2.751480
F	-4.936412	-2.438652	-3.363977

Zero-point correction= 0.783807 (Hartree/Particle)
Thermal correction to Energy= 0.838702
Thermal correction to Enthalpy= 0.839646
Thermal correction to Gibbs Free Energy= 0.695882
Sum of electronic and zero-point Energies= -3002.252448
Sum of electronic and thermal Energies= -3002.197553
Sum of electronic and thermal Enthalpies= -3002.196609
Sum of electronic and thermal Free Energies= -3002.340373

C	2.198129	2.589233	3.189377
H	2.359062	3.295922	2.349507
H	1.345836	2.969900	3.790400
H	3.107548	2.601753	3.827914
C	4.386780	-0.345593	-2.870789
H	4.248149	-0.060520	-3.933746
H	5.433233	-0.700951	-2.757102
H	3.703652	-1.188655	-2.657121
C	5.085509	2.007226	-2.238161
H	6.121647	1.690717	-1.991385
H	5.062840	2.298546	-3.309315
H	4.862780	2.910649	-1.635267
C	-2.003010	3.239110	3.049002
H	-1.360426	3.525579	3.908755
H	-2.972099	3.765648	3.186729
H	-2.172344	2.146290	3.092606
C	-1.117518	5.176721	1.681856
H	-2.101376	5.692924	1.693018
H	-0.535756	5.528660	2.560112
H	-0.583676	5.502424	0.766748
C	-1.768131	0.635433	-3.792269
H	-2.754929	0.846401	-4.257702
H	-1.082109	0.296419	-4.594212
H	-1.889781	-0.201412	-3.077610
C	-1.026371	3.064614	-4.058093
H	-0.410996	2.782269	-4.938429
H	-2.018024	3.406172	-4.426122
H	-0.537686	3.928913	-3.560114
C	1.715453	-2.217256	-1.182865
C	2.215290	-2.361013	0.129515
C	1.970860	-3.226855	-2.136463
C	2.976258	-3.489056	0.478769
C	2.698158	-4.372022	-1.774375
C	3.208797	-4.502937	-0.468906
H	2.019323	-1.563413	0.863495
H	1.585551	-3.093101	-3.159278
H	3.386233	-3.571438	1.497614
H	2.874420	-5.167804	-2.516004
H	3.790346	-5.396501	-0.191227
C	0.928247	-0.988041	-1.607286
O	1.041811	-0.569232	-2.754506
C	-5.151547	-2.452506	-3.366077
H	-5.147081	-3.494881	-3.745944
H	-6.143004	-2.254797	-2.907850
H	-5.064797	-1.782559	-4.250850

Zero-point correction= 0.817972 (Hartree/Particle)
Thermal correction to Energy= 0.873941
Thermal correction to Enthalpy= 0.874885
Thermal correction to Gibbs Free Energy= 0.728196
Sum of electronic and zero-point Energies= -2942.343049
Sum of electronic and thermal Energies= -2942.287079
Sum of electronic and thermal Enthalpies= -2942.286135
Sum of electronic and thermal Free Energies= -2942.432824

B-Ph(pF)-IPr-X			
100			
IPrX-F SCF Done: -3003.06063510 A.U.			
Pd	-0.205944	0.382173	0.271467
K	-4.100391	0.239598	-1.520238
O	-2.459433	2.541158	-2.279039
H	-2.572133	3.362357	-1.756638
B	-1.095580	2.322035	-2.465417

B-Ph(pMe)-IPr-X			
103			
IPrX-Me SCF Done: -2943.18612277 A.U.			
Pd	-0.211274	0.374091	0.268609
K	-4.096672	0.113514	-1.505318
O	-2.532367	2.455830	-2.262386
H	-2.659166	3.250095	-1.700739
B	-1.166069	2.279388	-2.471131

O	-0.225961	3.373879	-2.355079
H	0.695981	3.080364	-2.215012
C	-1.540403	1.935104	0.658626
C	-1.347194	3.335523	0.553623
C	-2.844539	1.516579	1.045046
C	-2.397560	4.261478	0.730027
H	-0.354140	3.730509	0.288916
C	-3.911034	2.419027	1.251245
H	-3.039542	0.441978	1.217800
C	-3.674325	3.788762	1.065400
H	-2.236962	5.346176	0.625372
H	-4.908820	2.084083	1.581049
C	-1.581997	0.006834	-2.586825
O	-2.351253	-0.296621	-3.515724
O	-0.657282	1.051267	-2.796832
O	-1.579208	-0.498495	-1.412290
N	0.082203	-2.537790	0.868742
N	2.030932	-1.886392	0.193946
C	0.743610	-1.444682	0.351902
C	0.944638	-3.617143	1.056941
C	2.177989	-3.209675	0.622249
C	-1.344524	-2.539208	1.095610
C	-2.181517	-3.095064	0.094298
C	-3.575066	-3.030195	0.309867
C	-4.100311	-2.421659	1.461691
C	-3.242700	-1.879578	2.433525
C	-1.842046	-1.927818	2.275309
C	-1.602906	-3.789089	-1.136349
H	-5.191868	-2.385105	1.614969
C	-0.897036	-1.403734	3.352558
C	3.059355	-1.118443	-0.462609
C	4.101297	-0.567982	0.322037
C	5.106868	0.154868	-0.353238
C	5.060267	0.327606	-1.741296
C	3.996089	-0.202455	-2.488669
C	2.961975	-0.933755	-1.871199
C	4.159389	-0.756133	1.836902
H	5.852471	0.900268	-2.249183
C	1.771825	-1.472214	-2.671208
H	0.607022	-4.567304	1.479215
H	3.133345	-3.737818	0.561244
H	-4.255900	-3.472430	-0.434624
H	-3.666508	-1.409892	3.333325
H	-0.592928	-3.361573	-1.306526
H	0.045539	-1.094228	2.858106
H	5.929482	0.602297	0.224287
H	3.964692	-0.032190	-3.574244
H	3.138369	-1.027346	2.178508
H	0.863812	-1.245262	-2.070375
C	1.583268	-0.786182	-4.033292
H	2.385713	-1.059671	-4.752196
H	0.616235	-1.099467	-4.476185
H	1.547645	0.316134	-3.934501
C	1.843486	-3.005179	-2.852298
H	1.882385	-3.544696	-1.885488
H	0.947925	-3.365799	-3.400377
H	2.742678	-3.290160	-3.439296
C	4.556515	0.530445	2.584271
H	4.447138	0.379562	3.677623
H	5.614236	0.810431	2.392587
H	3.908731	1.378898	2.295831
C	5.119766	-1.909726	2.202942
H	6.156068	-1.671563	1.880733

O	-0.325025	3.355670	-2.373109
H	0.605290	3.086690	-2.240848
C	-1.579388	1.895068	0.653196
C	-1.419168	3.299060	0.545704
C	-2.878531	1.455089	1.030161
C	-2.496336	4.192653	0.711118
H	-0.434381	3.716274	0.283116
C	-3.956766	2.344354	1.223172
H	-3.055583	0.376494	1.200057
C	-3.792524	3.735886	1.043296
H	-2.323942	5.276634	0.588095
H	-4.942752	1.953587	1.538660
C	-1.582869	-0.049373	-2.593704
O	-2.349039	-0.380211	-3.516212
O	-0.693985	1.023217	-2.814861
O	-1.555491	-0.551117	-1.418089
N	0.147312	-2.541158	0.863572
N	2.080862	-1.839303	0.195563
C	0.782080	-1.430648	0.350211
C	1.036151	-3.599016	1.051375
C	2.259866	-3.159788	0.620588
C	-1.278742	-2.578030	1.091293
C	-2.102236	-3.160227	0.093894
C	-3.496830	-3.130949	0.310801
C	-4.036826	-2.529633	1.459511
C	-3.192646	-1.959378	2.426856
C	-1.791394	-1.972581	2.267745
C	-1.508177	-3.844480	-1.134907
H	-5.128871	-2.520307	1.613545
C	-0.860833	-1.420252	3.343574
C	3.093627	-1.040725	-0.448987
C	4.114299	-0.467481	0.347473
C	5.105263	0.286553	-0.315056
C	5.065765	0.465766	-1.702465
C	4.022237	-0.087791	-2.461617
C	3.002118	-0.848709	-1.856891
C	4.166848	-0.666410	1.861254
H	5.846184	1.062813	-2.200383
C	1.829334	-1.407398	-2.668666
H	0.721701	-4.557983	1.471598
H	3.228246	-3.663797	0.561693
H	-4.166480	-3.594660	-0.430772
H	-3.627550	-1.494518	3.323821
H	-0.508836	-3.393538	-1.308106
H	0.073332	-1.086950	2.848996
H	5.910279	0.753183	0.271943
H	3.994596	0.089147	-3.546222
H	3.149696	-0.962580	2.193638
H	0.912567	-1.201143	-2.073830
C	1.636539	-0.717999	-4.028351
H	2.451407	-0.968023	-4.741878
H	0.680819	-1.051044	-4.481207
H	1.573959	0.382621	-3.923385
C	1.932033	-2.937719	-2.856447
H	1.978122	-3.480523	-1.891819
H	1.045778	-3.313581	-3.409411
H	2.838934	-3.202296	-3.441186
C	4.531234	0.621626	2.622415
H	4.423740	0.456685	3.713952
H	5.582184	0.929120	2.435639
H	3.862861	1.456483	2.341751
C	5.150418	-1.801503	2.223895
H	6.183356	-1.536852	1.911664

H	5.132755	-2.076114	3.300584
H	4.833777	-2.864457	1.717360
C	-2.413268	-3.565735	-2.424191
H	-1.885776	-4.031430	-3.282707
H	-3.415388	-4.044431	-2.372337
H	-2.534015	-2.489661	-2.653763
C	-1.447359	-5.303602	-0.865199
H	-2.442541	-5.775037	-0.717244
H	-0.954569	-5.805911	-1.723977
H	-0.845107	-5.509475	0.041434
C	-1.415007	-0.152813	4.077556
H	-2.308901	-0.361920	4.704249
H	-0.621467	0.241239	4.742819
H	-1.661594	0.647655	3.352155
C	-0.563877	-2.540928	4.343934
H	0.169450	-2.192211	5.100833
H	-1.475884	-2.883793	4.878670
H	-0.127181	-3.420131	3.825502
C	1.900602	2.331299	0.782028
C	2.257015	2.237058	-0.580633
C	2.315742	3.454936	1.527870
C	3.032751	3.239648	-1.183816
C	3.055493	4.479533	0.912640
C	3.420822	4.372392	-0.441710
H	1.940004	1.349720	-1.151952
H	2.042119	3.508623	2.593194
H	3.345259	3.129290	-2.234967
H	3.355253	5.365835	1.494849
H	4.013771	5.169024	-0.918666
C	1.089854	1.245115	1.472180
O	1.282035	1.003742	2.660021
F	-4.693411	4.669186	1.233267

Zero-point correction= 0.785201 (Hartree/Particle)
Thermal correction to Energy= 0.840662
Thermal correction to Enthalpy= 0.841607
Thermal correction to Gibbs Free Energy= 0.695889
Sum of electronic and zero-point Energies= -3002.275434
Sum of electronic and thermal Energies= -3002.219973
Sum of electronic and thermal Enthalpies= -3002.219029
Sum of electronic and thermal Free Energies= -3002.364746

H	5.159093	-1.978017	3.320024
H	4.890008	-2.757846	1.727316
C	-2.325394	-3.644374	-2.422303
H	-1.787726	-4.099237	-3.280336
H	-3.315495	-4.147413	-2.367834
H	-2.472983	-2.572098	-2.654448
C	-1.316693	-5.353984	-0.858812
H	-2.300237	-5.847945	-0.706659
H	-0.814325	-5.847936	-1.716910
H	-0.707735	-5.542284	0.047175
C	-1.412755	-0.182163	4.065518
H	-2.296987	-0.415745	4.697420
H	-0.628189	0.238120	4.725361
H	-1.687102	0.607202	3.337901
C	-0.497094	-2.545658	4.337687
H	0.224461	-2.174599	5.095349
H	-1.400033	-2.913330	4.871349
H	-0.034414	-3.412896	3.821581
C	1.855072	2.369857	0.766206
C	2.190494	2.281059	-0.601891
C	2.273842	3.495092	1.507387
C	2.949881	3.289441	-1.215603
C	2.997969	4.525176	0.882909
C	3.342991	4.422841	-0.477194
H	1.868044	1.392354	-1.168486
H	2.014953	3.545312	2.576592
H	3.246577	3.183249	-2.271792
H	3.301128	5.412467	1.461914
H	3.923607	5.224023	-0.961749
C	1.063312	1.274729	1.464716
O	1.260365	1.045826	2.654601
C	-4.932302	4.705653	1.267379
H	-4.901843	5.130160	2.295555
H	-4.885495	5.563638	0.564626
H	-5.921165	4.216615	1.146207

Zero-point correction= 0.819293 (Hartree/Particle)
Thermal correction to Energy= 0.875889
Thermal correction to Enthalpy= 0.876833
Thermal correction to Gibbs Free Energy= 0.727515
Sum of electronic and zero-point Energies= -2942.366830
Sum of electronic and thermal Energies= -2942.310234
Sum of electronic and thermal Enthalpies= -2942.309289
Sum of electronic and thermal Free Energies= -2942.458607

B-Ph(pF)-IPr-XI			
90			
IPrXI-F SCF Done: -1962.77484202 A.U.			
Pd	0.578430	0.535984	-0.206510
C	1.727919	2.199669	-0.465698
C	1.426318	3.538011	-0.809392
C	3.089520	1.887661	-0.206941
C	2.423468	4.530409	-0.873105
H	0.386336	3.829081	-1.032350
C	4.103268	2.863621	-0.258824
H	3.388753	0.851383	0.041572
C	3.750436	4.178489	-0.592050
H	2.190215	5.573430	-1.138450
H	5.157816	2.621509	-0.054139
N	0.736616	-2.411759	0.233180
N	-1.369753	-1.934575	0.304763
C	-0.137700	-1.357965	0.139301
C	0.074185	-3.620044	0.442652

B-Ph(pMe)-IPr-XI			
93			
IPrXI-Me SCF Done: -1902.89964382 A.U.			
Pd	0.580745	0.515136	-0.223238
C	1.765792	2.149822	-0.484482
C	1.511148	3.495217	-0.829048
C	3.115592	1.799041	-0.214978
C	2.546204	4.448581	-0.878025
H	0.483449	3.818869	-1.065274
C	4.149469	2.751007	-0.258928
H	3.383149	0.752978	0.030972
C	3.882165	4.098511	-0.588939
H	2.310907	5.492584	-1.150207
H	5.186721	2.440360	-0.041047
N	0.671162	-2.437312	0.244483
N	-1.420937	-1.903140	0.326987
C	-0.175333	-1.361522	0.143860
C	-0.021424	-3.624805	0.474585

C	-1.263513	-3.317840	0.484334	C	-1.350245	-3.286358	0.523325
C	2.162260	-2.190150	0.211821	C	2.101839	-2.253832	0.211570
C	2.794002	-1.806231	1.423347	C	2.751901	-1.879186	1.416100
C	4.176409	-1.534932	1.372765	C	4.140395	-1.644168	1.354105
C	4.886779	-1.634166	0.167532	C	4.838997	-1.767897	0.144294
C	4.228951	-1.998937	-1.017068	C	4.163235	-2.121185	-1.033611
C	2.849108	-2.284270	-1.024524	C	2.776481	-2.370606	-1.029469
C	2.010289	-1.610729	2.719521	C	1.982321	-1.654028	2.715774
H	5.964424	-1.407521	0.147179	H	5.921847	-1.568746	0.114818
C	2.110070	-2.571420	-2.327703	C	2.020152	-2.642995	-2.325838
C	-2.595538	-1.175833	0.374912	C	-2.626185	-1.111967	0.396877
C	-3.482616	-1.222273	-0.727949	C	-3.522501	-1.149699	-0.698585
C	-4.675522	-0.477335	-0.629752	C	-4.697414	-0.376732	-0.599826
C	-4.948990	0.297327	0.503651	C	-4.944348	0.416378	0.526883
C	-4.038453	0.344544	1.569761	C	-4.024288	0.454754	1.585196
C	-2.839435	-0.392420	1.537916	C	-2.842647	-0.309640	1.552384
C	-3.182228	-2.051548	-1.975337	C	-3.251170	-1.998680	-1.939293
H	-5.873496	0.893344	0.551008	H	-5.854496	1.034085	0.574632
C	-1.834949	-0.343957	2.692248	C	-1.827450	-0.271606	2.697597
H	0.608735	-4.569106	0.544947	H	0.488260	-4.586621	0.584284
H	-2.142047	-3.950794	0.637553	H	-2.244160	-3.893774	0.690488
H	4.699396	-1.222277	2.289959	H	4.677778	-1.338864	2.265448
H	4.794167	-2.043993	-1.960377	H	4.719927	-2.184732	-1.981023
H	0.977683	-1.981508	2.554437	H	0.939741	-2.000379	2.560730
H	1.116617	-2.993458	-2.064838	H	1.016226	-3.033119	-2.053639
H	-5.388792	-0.485901	-1.467818	H	-5.416889	-0.378057	-1.432618
H	-4.261471	0.984586	2.434293	H	-4.225601	1.109553	2.443984
H	-2.095637	-2.282318	-1.966624	H	-2.171589	-2.259979	-1.932900
H	-0.837063	-0.195266	2.223170	H	-0.830434	-0.155924	2.217502
C	-2.050394	0.829381	3.660249	C	-2.003117	0.920565	3.650378
H	-2.979407	0.709334	4.258117	H	-2.929956	0.834106	4.257433
H	-1.205055	0.882021	4.376878	H	-1.150557	0.960300	4.359274
H	-2.105657	1.798243	3.128213	H	-2.036761	1.883010	3.105133
C	-1.795453	-1.669807	3.485331	C	-1.816330	-1.586640	3.509232
H	-1.558187	-2.543051	2.847345	H	-1.613788	-2.475458	2.880909
H	-1.019937	-1.618029	4.278559	H	-1.028988	-1.546697	4.291450
H	-2.773466	-1.861361	3.976103	H	-2.792953	-1.742128	4.015391
C	-3.468835	-1.287809	-3.282294	C	-3.521628	-1.238060	-3.251510
H	-3.142164	-1.892798	-4.153663	H	-3.219331	-1.860692	-4.119287
H	-4.552989	-1.086223	-3.414678	H	-4.599797	-1.003771	-3.379202
H	-2.917079	-0.328303	-3.304742	H	-2.940272	-0.296459	-3.285317
C	-3.960423	-3.385442	-1.938200	C	-4.066348	-3.309712	-1.886665
H	-5.055478	-3.198274	-1.945039	H	-5.155772	-3.092040	-1.891153
H	-3.715337	-4.009768	-2.823075	H	-3.842327	-3.948838	-2.766549
H	-3.733282	-3.977732	-1.028366	H	-3.851781	-3.899466	-0.972086
C	1.903737	-0.109105	3.059057	C	1.914494	-0.147529	3.043621
H	1.275699	0.045778	3.961275	H	1.298458	0.029255	3.950135
H	2.902710	0.335872	3.249876	H	2.925350	0.275380	3.221801
H	1.441699	0.461735	2.219492	H	1.459026	0.427441	2.203606
C	2.601317	-2.419752	3.890023	C	2.561301	-2.467744	3.888996
H	3.620082	-2.070093	4.160155	H	3.589893	-2.140451	4.149841
H	1.965237	-2.311083	4.793359	H	1.933930	-2.336722	4.795479
H	2.668780	-3.499380	3.642981	H	2.601413	-3.550629	3.650263
C	1.860023	-1.248379	-3.085074	C	1.804793	-1.317738	-3.089923
H	2.821184	-0.772955	-3.373665	H	2.777617	-0.872500	-3.387418
H	1.267172	-1.428103	-4.005598	H	1.200797	-1.485533	-4.005449
H	1.302002	-0.524155	-2.450780	H	1.272506	-0.573269	-2.456787
C	2.833288	-3.607561	-3.208395	C	2.705495	-3.706042	-3.204925
H	2.213148	-3.856005	-4.094544	H	2.072673	-3.939668	-4.086160
H	3.801390	-3.220039	-3.590260	H	3.682935	-3.350839	-3.594403
H	3.038731	-4.547374	-2.654566	H	2.884752	-4.648876	-2.647098
C	-1.887168	2.154962	-0.651250	C	-1.845356	2.195040	-0.675135
C	-1.626509	2.761810	0.593893	C	-1.563548	2.809740	0.561338

C	-3.085196	2.459972	-1.335540
C	-2.546430	3.665507	1.145944
C	-4.009823	3.353892	-0.776542
C	-3.742184	3.960046	0.464678
H	-0.680639	2.515206	1.105031
H	-3.275626	1.978197	-2.306267
H	-2.328395	4.147627	2.112123
H	-4.946350	3.579566	-1.311080
C	-0.922720	1.190986	-1.297141
O	-1.085081	0.776912	-2.432812
F	4.716912	5.129493	-0.648203
H	-4.465416	4.668018	0.900541

Zero-point correction= 0.731819 (Hartree/Particle)
Thermal correction to Energy= 0.777790
Thermal correction to Enthalpy= 0.778734
Thermal correction to Gibbs Free Energy= 0.652576
Sum of electronic and zero-point Energies= -1962.043023
Sum of electronic and thermal Energies= -1961.997052
Sum of electronic and thermal Enthalpies= -1961.996108
Sum of electronic and thermal Free Energies= -1962.122266

C	-3.041285	2.517876	-1.354811
C	-2.460816	3.738145	1.109801
C	-3.943684	3.436389	-0.799300
C	-3.655027	4.050054	0.433537
H	-0.619235	2.548451	1.067962
H	-3.247915	2.030184	-2.319306
H	-2.226064	4.226133	2.069157
H	-4.879204	3.675657	-1.329775
H	-4.360512	4.777326	0.866785
C	-0.905310	1.202783	-1.315284
O	-1.083178	0.783701	-2.447426
C	4.993987	5.125306	-0.611999
H	5.310310	5.402907	0.418323
H	5.897134	4.739305	-1.130973
H	4.681323	6.058625	-1.123338

Zero-point correction= 0.765950 (Hartree/Particle)
Thermal correction to Energy= 0.813027
Thermal correction to Enthalpy= 0.813971
Thermal correction to Gibbs Free Energy= 0.684785
Sum of electronic and zero-point Energies= -1902.133694
Sum of electronic and thermal Energies= -1902.086617
Sum of electronic and thermal Enthalpies= -1902.085673
Sum of electronic and thermal Free Energies= -1902.214859

B-Ph(pF)-IPr-XI-XII

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IPrXI-XII-F SCF Done: -1962.76720178 A.U.

Pd	0.386715	0.612980	0.072892
C	0.586627	2.702380	-0.131197
C	0.205470	3.536893	0.946127
C	1.678896	3.095563	-0.942635
C	0.936698	4.697943	1.253142
H	-0.674490	3.282933	1.556704
C	2.428136	4.242174	-0.642909
H	1.919956	2.494895	-1.835010
C	2.045451	5.025196	0.459289
H	0.661439	5.356492	2.090964
H	3.289978	4.555269	-1.251745
N	1.388871	-2.227615	0.249960
N	-0.770662	-2.269186	0.298749
C	0.290665	-1.401289	0.199088
C	1.028789	-3.567749	0.387507
C	-0.341930	-3.594473	0.418735
C	2.726931	-1.732721	0.048665
C	3.466297	-1.289901	1.171816
C	4.761437	-0.787535	0.934341
C	5.282335	-0.726050	-0.367245
C	4.512834	-1.148734	-1.461892
C	3.211734	-1.658419	-1.280922
C	2.844090	-1.253774	2.565382
H	6.296446	-0.328535	-0.532134
C	2.333736	-2.016689	-2.477313
C	-2.151069	-1.857432	0.221789
C	-2.681240	-1.494221	-1.045269
C	-4.034179	-1.101295	-1.078184
C	-4.814781	-1.087493	0.085723
C	-4.258478	-1.443962	1.322163
C	-2.905912	-1.823977	1.421081
C	-1.818699	-1.524578	-2.308969
H	-5.867295	-0.768864	0.031241
C	-2.246274	-2.102676	2.773257
H	1.773697	-4.367470	0.436982

B-Ph(pMe)-IPr-XI-XII

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IPrXI-XII-Me SCF Done: -1902.89264340 A.U.

Pd	0.396923	0.587477	0.058665
C	0.671381	2.667158	-0.157843
C	0.323853	3.519062	0.914390
C	1.771774	3.025616	-0.973459
C	1.099190	4.656437	1.204295
H	-0.558762	3.296592	1.533687
C	2.548850	4.151659	-0.673090
H	1.994893	2.412865	-1.862610
C	2.227842	4.986924	0.424755
H	0.819215	5.304171	2.052626
H	3.415892	4.403602	-1.307741
N	1.313784	-2.279948	0.264109
N	-0.845793	-2.255514	0.316973
C	0.240890	-1.421222	0.206153
C	0.913685	-3.607069	0.416880
C	-0.457319	-3.591801	0.451018
C	2.664589	-1.824151	0.056613
C	3.416975	-1.390267	1.174694
C	4.724138	-0.923491	0.930937
C	5.243766	-0.885464	-0.372019
C	4.461626	-1.297059	-1.461826
C	3.148536	-1.772373	-1.274422
C	2.797976	-1.324049	2.568566
H	6.267102	-0.514573	-0.542021
C	2.259364	-2.116604	-2.466575
C	-2.211694	-1.798518	0.241841
C	-2.734820	-1.428803	-1.026243
C	-4.071868	-0.984808	-1.056152
C	-4.844443	-0.928055	0.112018
C	-4.294699	-1.291402	1.349348
C	-2.957111	-1.721810	1.444900
C	-1.879330	-1.502476	-2.293078
H	-5.884035	-0.569232	0.059730
C	-2.299681	-2.006672	2.796792
H	1.633932	-4.428588	0.473863

H	-1.048816	-4.425637	0.502870
H	5.366150	-0.425450	1.780032
H	4.923737	-1.066185	-2.480195
H	1.948356	-1.911082	2.550430
H	1.429770	-2.535385	-2.095787
H	-4.484126	-0.786418	-2.029624
H	-4.881439	-1.401788	2.227544
H	-0.849590	-1.056845	-2.033338
H	-1.466263	-2.878675	2.615743
C	-1.523338	-0.834829	3.283024
H	-2.254828	-0.018520	3.463605
H	-0.993524	-1.038882	4.237298
H	-0.780518	-0.464897	2.545466
C	-3.217402	-2.647218	3.834476
H	-3.784369	-3.525728	3.462586
H	-2.659098	-2.955460	4.742490
H	-3.951765	-1.877681	4.153656
C	-2.391051	-0.699979	-3.470656
H	-1.646314	-0.649450	-4.290532
H	-3.316035	-1.153840	-3.887949
H	-2.605501	0.340983	-3.163223
C	-1.530656	-2.969220	-2.776011
H	-2.471273	-3.486520	-3.062432
H	-0.864449	-2.955580	-3.664396
H	-1.029949	-3.577352	-1.997315
C	2.353251	0.176106	2.877625
H	1.833329	0.215139	3.857553
H	3.199054	0.894650	2.896558
H	1.634049	0.534164	2.098384
C	3.788315	-1.779281	3.662457
H	4.670095	-1.118246	3.798243
H	3.260878	-1.821053	4.638126
H	4.161241	-2.797424	3.426374
C	1.848367	-0.730025	-3.179209
H	2.699616	-0.172549	-3.625405
H	1.134267	-0.973622	-3.993577
H	1.330468	-0.053264	-2.467716
C	3.028185	-2.979212	-3.458973
H	2.328493	-3.269667	-4.270328
H	3.911753	-2.510949	-3.942459
H	3.371101	-3.904566	-2.950950
C	-2.183925	1.980687	-0.701582
C	-2.573246	1.657733	0.613167
C	-3.131877	2.536745	-1.587972
C	-3.885599	1.894938	1.044458
C	-4.446344	2.773815	-1.157430
C	-4.825064	2.457601	0.161204
H	-1.825802	1.181534	1.270787
H	-2.810711	2.780554	-2.612730
H	-4.182545	1.621923	2.069194
H	-5.181517	3.211462	-1.851923
H	-5.857241	2.644567	0.498750
C	-0.783861	1.717744	-1.207981
O	-0.529522	1.716555	-2.411197
F	2.753721	6.139378	0.748199

Zero-point correction=	0.730800 (Hartree/Particle)
Thermal correction to Energy=	0.776151
Thermal correction to Enthalpy=	0.777095
Thermal correction to Gibbs Free Energy=	0.652453
Sum of electronic and zero-point Energies=	-1962.036402
Sum of electronic and thermal Energies=	-1961.991051
Sum of electronic and thermal Enthalpies=	-1961.990107

H	-1.189028	-4.399959	0.546415
H	5.339367	-0.569664	1.772552
H	4.871963	-1.231954	-2.481684
H	1.884045	-1.955919	2.560712
H	1.340064	-2.603011	-2.079371
H	-4.515003	-0.661917	-2.008111
H	-4.909477	-1.213967	2.258120
H	-0.894407	-1.062634	-2.026307
H	-1.542267	-2.805508	2.643582
C	-1.539554	-0.754907	3.291969
H	-2.246921	0.083890	3.465363
H	-1.013655	-0.964333	4.247289
H	-0.788271	-0.414114	2.548837
C	-3.281748	-2.514268	3.866401
H	-3.875408	-3.379044	3.504014
H	-2.728882	-2.830801	4.774948
H	-3.992527	-1.721403	4.181961
C	-2.429475	-0.673918	-3.462599
H	-1.688044	-0.660107	-4.286924
H	-3.371944	-1.101145	-3.868894
H	-2.606084	0.377821	-3.168147
C	-1.640828	-2.961124	-2.743897
H	-2.599200	-3.450058	-3.021259
H	-0.977587	-2.980049	-3.634453
H	-1.158103	-3.576540	-1.959630
C	2.348107	0.121870	2.868283
H	1.827153	0.183383	3.846519
H	3.214111	0.816017	2.883833
H	1.641693	0.494865	2.084448
C	3.728506	-1.866394	3.669132
H	4.629553	-1.230134	3.796993
H	3.201989	-1.883313	4.646079
H	4.071218	-2.897228	3.442329
C	1.813360	-0.823412	-3.182417
H	2.680850	-0.297944	-3.636215
H	1.090475	-1.054025	-3.992852
H	1.318383	-0.122658	-2.477918
C	2.924271	-3.110307	-3.437600
H	2.215988	-3.388333	-4.245855
H	3.821314	-2.673467	-3.925644
H	3.239579	-4.039946	-2.919545
C	-2.128192	2.035093	-0.717676
C	-2.518935	1.751150	0.605839
C	-3.064990	2.600680	-1.609804
C	-3.821350	2.035219	1.038828
C	-4.369777	2.884226	-1.177689
C	-4.749785	2.605866	0.149049
H	-1.781471	1.269900	1.270977
H	-2.742332	2.814538	-2.640791
H	-4.119461	1.794056	2.071254
H	-5.096178	3.328382	-1.877338
H	-5.774300	2.828959	0.488137
C	-0.739623	1.718975	-1.226270
O	-0.490797	1.699863	-2.430623
C	3.054858	6.218444	0.717589
H	4.139886	5.981270	0.739501
H	2.912761	6.993062	-0.067829
H	2.784000	6.675835	1.690405

Zero-point correction=	0.765370 (Hartree/Particle)
Thermal correction to Energy=	0.811699
Thermal correction to Enthalpy=	0.812643
Thermal correction to Gibbs Free Energy=	0.685159
Sum of electronic and zero-point Energies=	-1902.127274
Sum of electronic and thermal Energies=	-1902.080944
Sum of electronic and thermal Enthalpies=	-1902.080000

Sum of electronic and thermal Free Energies= -1962.114749	Sum of electronic and thermal Free Energies= -1902.207484

B-Ph(pF)-IPr-XII				**B-Ph(pMe)-IPr-XII**			
90				93			
IPrXII-F SCF Done: -1962.79975881 A.U.				IPrXII-Me SCF Done: -1902.92537588 A.U.			
Pd	-0.136980	0.666080	-0.071276	Pd	-0.188199	0.702502	-0.018094
C	0.067765	2.797860	-0.365838	C	0.037223	2.863972	0.007354
C	0.214114	2.986596	-1.783467	C	0.207541	3.305505	-1.348760
C	-1.267539	2.616778	0.157701	C	-1.305501	2.612763	0.461225
C	-0.902186	3.062442	-2.617734	C	-0.900272	3.522301	-2.168621
H	1.220147	3.124151	-2.206844	H	1.220104	3.517077	-1.722661
C	-2.396552	2.693595	-0.700362	C	-2.408693	2.830340	-0.395365
H	-1.414900	2.645837	1.247733	H	-1.476347	2.461575	1.535249
C	-2.192049	2.914509	-2.058319	C	-2.229236	3.286649	-1.710301
H	-0.803656	3.228075	-3.700421	H	-0.745438	3.885049	-3.199024
H	-3.413820	2.556087	-0.307861	H	-3.420997	2.624306	-0.012819
N	-1.640175	-1.844707	0.693460	N	-1.548996	-1.957106	0.519993
N	0.399530	-2.357597	0.199315	N	0.517380	-2.322715	-0.036814
C	-0.455507	-1.284571	0.273537	C	-0.387836	-1.300007	0.135152
C	-1.527254	-3.223132	0.877481	C	-1.357453	-3.337815	0.588667
C	-0.231798	-3.550011	0.561749	C	-0.052978	-3.567774	0.235072
C	-2.814312	-1.035369	0.903625	C	-2.781829	-1.242840	0.788133
C	-3.701995	-0.840427	-0.183075	C	-3.642693	-0.984605	-0.320742
C	-4.788600	0.033241	0.018695	C	-4.795715	-0.214733	-0.077121
C	-4.970713	0.685851	1.247810	C	-5.074303	0.283148	1.202922
C	-4.074082	0.470420	2.305338	C	-4.211888	0.020966	2.278866
C	-2.975666	-0.401055	2.159678	C	-3.043355	-0.749407	2.108252
C	-3.439439	-1.467849	-1.549947	C	-3.296034	-1.438021	-1.745325
H	-5.820562	1.374081	1.381748	H	-5.977088	0.893923	1.365870
C	-1.980300	-0.600828	3.300598	C	-2.071526	-0.965720	3.268570
C	1.767857	-2.242584	-0.237044	C	1.873701	-2.130439	-0.479144
C	2.775205	-2.019422	0.734790	C	2.893864	-2.034289	0.490710
C	4.107833	-1.958133	0.282350	C	4.216220	-1.897600	0.020889
C	4.415940	-2.101161	-1.078342	C	4.493218	-1.848356	-1.355811
C	3.392362	-2.262035	-2.023163	C	3.450603	-1.895092	-2.290673
C	2.041407	-2.328440	-1.624533	C	2.112067	-2.034891	-1.871594
C	2.429282	-1.734309	2.193333	C	2.543358	-1.962095	1.975002
H	5.465791	-2.056037	-1.409294	H	5.534627	-1.745183	-1.700727
C	0.925520	-2.393284	-2.664862	C	0.962007	-2.017842	-2.876972
H	-2.368573	-3.836482	1.213956	H	-2.160512	-4.022197	0.877122
H	0.295759	-4.508591	0.561375	H	0.522458	-4.494094	0.151421
H	-5.490998	0.222373	-0.807430	H	-5.476351	0.016273	-0.912544
H	-4.224809	0.994388	3.262049	H	-4.445008	0.436966	3.271036
H	-2.721471	-2.303142	-1.404001	H	-2.457581	-2.159449	-1.674245
H	-1.313590	-1.443768	3.020581	H	-1.318137	-1.708607	2.932652
H	4.916622	-1.776094	1.005927	H	5.039871	-1.806633	0.741749
H	3.643711	-2.327558	-3.093456	H	3.676243	-1.821035	-3.366030
H	1.393990	-2.095504	2.373120	H	1.550364	-2.449277	2.107176
H	-0.028231	-2.589088	-2.130935	H	0.037015	-2.314747	-2.337567
C	0.783512	-1.018271	-3.352836	C	0.732066	-0.578205	-3.394421
H	1.721467	-0.735115	-3.876299	H	1.638067	-0.181673	-3.898095
H	-0.037821	-1.033179	-4.098915	H	-0.108371	-0.548993	-4.120446
H	0.548481	-0.230742	-2.602617	H	0.473383	0.099322	-2.547397
C	1.127432	-3.528367	-3.686395	C	1.167183	-3.021322	-4.027339
H	1.240148	-4.511778	-3.184654	H	1.342447	-4.049079	-3.646940
H	0.257676	-3.588080	-4.373406	H	0.270969	-3.043160	-4.681162
H	2.028981	-3.363475	-4.313601	H	2.033225	-2.746619	-4.667106
C	2.427495	-0.206116	2.417926	C	2.394747	-0.476437	2.393039
H	2.149145	0.043552	3.462406	H	2.104635	-0.390470	3.460171
H	3.424449	0.233089	2.202835	H	3.343738	0.074856	2.242534

H	1.694481	0.286084	1.741062
C	3.352668	-2.458153	3.189986
H	4.392204	-2.070096	3.145452
H	2.994093	-2.300077	4.228257
H	3.388925	-3.550832	2.998163
C	-2.758495	-0.437966	-2.475917
H	-2.492509	-0.900069	-3.449700
H	-3.427185	0.425341	-2.671817
H	-1.831295	-0.044450	-2.003177
C	-4.707007	-2.060538	-2.192521
H	-5.440380	-1.271285	-2.462122
H	-4.448227	-2.594246	-3.130742
H	-5.214072	-2.777878	-1.514159
C	-1.086129	0.644455	3.468024
H	-1.688289	1.544486	3.714348
H	-0.346809	0.494435	4.281949
H	-0.528424	0.851356	2.529352
C	-2.678652	-0.986270	4.619597
H	-1.924707	-1.217378	5.400939
H	-3.307994	-0.158111	5.008751
H	-3.330530	-1.875724	4.493429
C	2.611938	2.603115	0.240780
C	2.961135	1.648367	-0.742672
C	3.640781	3.221501	0.986819
C	4.308029	1.334700	-0.983409
C	4.986402	2.914276	0.739825
C	5.324312	1.969822	-0.248691
H	2.169764	1.102237	-1.283701
H	3.353342	3.935954	1.773361
H	4.557284	0.574231	-1.738048
H	5.778857	3.408841	1.324211
H	6.381188	1.722870	-0.439546
C	1.186176	2.918459	0.637553
O	0.943604	3.280104	1.797371
F	-3.261580	2.962308	-2.889598

Zero-point correction= 0.732894 (Hartree/Particle)
Thermal correction to Energy= 0.778502
Thermal correction to Enthalpy= 0.779446
Thermal correction to Gibbs Free Energy= 0.653590
Sum of electronic and zero-point Energies= -1962.066865
Sum of electronic and thermal Energies= -1962.021257
Sum of electronic and thermal Enthalpies= -1962.020313
Sum of electronic and thermal Free Energies= -1962.146169

H	1.619075	0.039672	1.784939
C	3.544157	-2.696964	2.883041
H	4.532787	-2.192490	2.900527
H	3.171409	-2.707263	3.927799
H	3.702434	-3.747260	2.559951
C	-2.793934	-0.251711	-2.593093
H	-2.488991	-0.591056	-3.605264
H	-3.586834	0.512647	-2.708160
H	-1.915497	0.243570	-2.103710
C	-4.477170	-2.157032	-2.426377
H	-5.331708	-1.468884	-2.600431
H	-4.170736	-2.551892	-3.417909
H	-4.846581	-3.006800	-1.815147
C	-1.314818	0.338409	3.593148
H	-2.017459	1.135311	3.916815
H	-0.581135	0.179178	4.409237
H	-0.763448	0.715032	2.706792
C	-2.758864	-1.539916	4.519690
H	-2.005474	-1.766070	5.303251
H	-3.481820	-0.822118	4.962503
H	-3.310312	-2.475139	4.288651
C	2.570086	2.532057	0.573843
C	2.886378	1.787139	-0.584858
C	3.617193	2.965950	1.418040
C	4.224946	1.494747	-0.897059
C	4.953454	2.679934	1.101306
C	5.261279	1.943886	-0.058137
H	2.072266	1.388094	-1.217753
H	3.351835	3.516419	2.334113
H	4.453444	0.897945	-1.790276
H	5.762222	3.027981	1.764047
H	6.311017	1.713979	-0.303825
C	1.154118	2.795311	1.024600
O	0.926753	2.958961	2.222092
C	-3.403616	3.520830	-2.636711
H	-3.483837	4.584424	-2.921827
H	-3.294523	2.949809	-3.577899
H	-4.361170	3.223976	-2.175918

Zero-point correction= 0.767181 (Hartree/Particle)
Thermal correction to Energy= 0.812879
Thermal correction to Enthalpy= 0.813823
Thermal correction to Gibbs Free Energy= 0.688856
Sum of electronic and zero-point Energies= -1902.158195
Sum of electronic and thermal Energies= -1902.112496
Sum of electronic and thermal Enthalpies= -1902.111552
Sum of electronic and thermal Free Energies= -1902.236520

Ph(pOMe)+B-Ph(pMe)-IPr-V			
95			
IPrV-OMe SCF Done: -2053.23472198 A.U.			
C	-1.178018	0.913288	-2.487379
O	-0.720796	0.617289	-3.570270
Pd	0.594928	0.665778	-0.502249
O	-0.539184	2.023678	-1.775993
C	-4.637975	-0.986976	-0.755111
C	-4.263234	-1.227349	-2.095920
H	-4.193544	0.093288	1.070105
C	-3.891782	-0.071595	0.027831
C	-3.141762	-0.569769	-2.624884
C	-2.378846	0.324278	-1.843741
C	-2.774589	0.564758	-0.501801
H	-2.827708	-0.757383	-3.662525

Ph(pMe)+B-Ph(pMe)-IPR-V			
94			
IPrV-Me SCF Done: -1978.07785009 A.U.			
C	-1.261662	0.967839	-2.432189
O	-0.739156	0.790145	-3.512101
Pd	0.424694	0.714871	-0.455643
O	-0.773017	2.098573	-1.633629
C	-4.663447	-1.321134	-1.031707
C	-4.205084	-1.393827	-2.363087
H	-4.332044	-0.366760	0.899320
C	-3.999672	-0.437693	-0.146715
C	-3.112981	-0.624716	-2.793879
C	-2.445528	0.237507	-1.897079
C	-2.906293	0.323986	-0.560990
H	-2.747073	-0.692338	-3.829168

H	-2.177352	1.223073	0.145294	H	-2.383182	0.962188	0.165733
H	-4.822805	-1.929009	-2.729520	H	-4.703914	-2.073160	-3.073586
N	0.799212	-1.365738	1.704261	N	0.726376	-1.571979	1.489809
N	2.653595	-1.210736	0.599075	N	2.610000	-1.053426	0.559087
C	1.370421	-0.706532	0.632754	C	1.273188	-0.715005	0.554628
C	1.700629	-2.250605	2.306275	C	1.695602	-2.413758	2.047089
C	2.874193	-2.151327	1.605899	C	2.887560	-2.083893	1.457612
C	-0.555725	-1.179971	2.160462	C	-0.660575	-1.603307	1.881871
C	-1.491620	-2.212140	1.893324	C	-1.448594	-2.698754	1.445306
C	-2.776911	-2.085872	2.456649	C	-2.754335	-2.806920	1.964448
C	-3.112055	-0.970978	3.238080	C	-3.255569	-1.848221	2.856333
C	-2.189336	0.069999	3.423217	C	-2.480571	-0.731982	3.207117
C	-0.888904	-0.002815	2.882774	C	-1.163743	-0.578649	2.727183
C	-1.136910	-3.351931	0.938367	C	-0.924659	-3.652023	0.371743
H	-4.119342	-0.894918	3.678061	H	-4.275640	-1.955096	3.259024
C	0.112855	1.142815	3.021739	C	-0.311046	0.639754	3.078290
C	3.645973	-0.750547	-0.336193	C	3.590654	-0.357888	-0.232512
C	4.448691	0.357265	0.033173	C	4.213070	0.785106	0.328331
C	5.411365	0.794980	-0.897864	C	5.164753	1.455471	-0.465216
C	5.553340	0.158645	-2.140775	C	5.469799	1.005144	-1.759222
C	4.726309	-0.921105	-2.485233	C	4.820752	-0.118693	-2.292357
C	3.748845	-1.400384	-1.590027	C	3.862195	-0.827177	-1.540296
C	4.207214	1.113501	1.338327	C	3.793815	1.330092	1.692661
H	6.309888	0.518443	-2.856371	H	6.214557	1.545479	-2.365190
C	2.767532	-2.495828	-1.999175	C	3.072943	-1.983592	-2.148206
H	1.422639	-2.857214	3.173677	H	1.444168	-3.157212	2.809734
H	3.839809	-2.650030	1.731640	H	3.899350	-2.476762	1.595019
H	-3.537630	-2.855651	2.262912	H	-3.392761	-3.649537	1.660734
H	-2.488389	0.956999	4.000474	H	-2.907286	0.032998	3.872188
H	-0.073323	-3.623787	1.114104	H	0.157366	-3.821007	0.564143
H	0.585599	1.232147	2.012018	H	0.229962	0.899531	2.136965
H	6.050729	1.657402	-0.652968	H	5.665632	2.352740	-0.069682
H	4.830707	-1.391897	-3.475057	H	5.050911	-0.443771	-3.318842
H	3.605875	0.458644	2.003675	H	3.241342	0.526240	2.223434
H	2.272264	-2.864122	-1.075225	H	2.570158	-2.519918	-1.315229
C	1.664632	-1.888167	-2.893093	C	1.961915	-1.426078	-3.064253
H	2.089637	-1.502763	-3.843630	H	2.395078	-0.881773	-3.929723
H	0.890094	-2.644766	-3.137844	H	1.321538	-2.245287	-3.452990
H	1.167939	-1.037509	-2.372343	H	1.314673	-0.713699	-2.505483
C	3.452469	-3.700333	-2.669919	C	3.965812	-3.001913	-2.880621
H	2.711330	-4.503390	-2.864942	H	3.360052	-3.865798	-3.225635
H	3.899034	-3.427556	-3.649585	H	4.442036	-2.560586	-3.781727
H	4.260014	-4.120122	-2.034266	H	4.774562	-3.386025	-2.224264
C	5.506023	1.459455	2.088539	C	4.987908	1.728344	2.579097
H	6.128178	2.186661	1.525084	H	5.544778	2.591676	2.157548
H	5.271648	1.923935	3.069223	H	4.634809	2.030168	3.587410
H	6.124047	0.555998	2.271851	H	5.704230	0.889273	2.699941
C	3.355385	2.371187	1.057971	C	2.807770	2.503142	1.502007
H	3.082076	2.883628	2.005025	H	2.412350	2.852674	2.479607
H	3.907035	3.090531	0.416207	H	3.300526	3.359657	0.994975
H	2.414057	2.085221	0.526826	H	1.945559	2.177291	0.868307
C	1.224878	0.835758	4.045957	C	0.742206	0.320291	4.159375
H	1.972482	1.656801	4.058745	H	1.394948	1.201599	4.334795
H	0.805085	0.738037	5.070406	H	0.256070	0.055622	5.123128
H	1.765380	-0.102210	3.808733	H	1.395807	-0.525008	3.864079
C	-0.543327	2.499472	3.317097	C	-1.136802	1.877931	3.457863
H	-0.973521	2.548967	4.340854	H	-1.652756	1.762380	4.435559
H	0.216261	3.305902	3.244620	H	-0.468640	2.760129	3.545407
H	-1.348744	2.730530	2.589809	H	-1.900401	2.110271	2.686864
C	-1.972517	-4.624608	1.150681	C	-1.608061	-5.028949	0.372446
H	-3.035351	-4.467833	0.867639	H	-2.670556	-4.958695	0.055720
H	-1.586737	-5.444535	0.510315	H	-1.102945	-5.704169	-0.348506
H	-1.947119	-4.969146	2.205682	H	-1.579079	-5.509097	1.372983

C	-1.250209	-2.854076	-0.521299
H	-0.911585	-3.637961	-1.231121
H	-2.303349	-2.600737	-0.759496
H	-0.645182	-1.939060	-0.695920
C	-1.267137	3.122937	-1.330904
C	-0.843519	3.749866	-0.146166
C	-2.365656	3.608300	-2.061033
C	-1.542749	4.873892	0.320452
H	0.019577	3.326193	0.392526
C	-3.060178	4.729450	-1.575723
H	-2.672832	3.106135	-2.990386
C	-2.656213	5.364685	-0.387276
H	-1.216719	5.362729	1.252050
H	-3.927238	5.110124	-2.138320
H	-3.207030	6.241912	-0.014355
O	-5.678104	-1.593002	-0.118567
C	-6.456225	-2.542647	-0.835303
H	-6.959163	-2.085793	-1.718207
H	-5.842345	-3.406431	-1.179778
H	-7.228175	-2.907509	-0.131434

Zero-point correction= 0.775600 (Hartree/Particle)
Thermal correction to Energy= 0.824159
Thermal correction to Enthalpy= 0.825103
Thermal correction to Gibbs Free Energy= 0.691408
Sum of electronic and zero-point Energies= -2052.459122
Sum of electronic and thermal Energies= -2052.410563
Sum of electronic and thermal Enthalpies= -2052.409619
Sum of electronic and thermal Free Energies= -2052.543314

C	-1.048868	-2.973066	-1.012283
H	-0.615992	-3.617305	-1.806228
H	-2.115552	-2.788881	-1.254499
H	-0.531814	-1.990666	-1.039073
C	-1.635166	3.057706	-1.109566
C	-1.331042	3.592132	0.154454
C	-2.752820	3.497615	-1.839080
C	-2.171145	4.575006	0.701007
H	-0.449011	3.205198	0.689892
C	-3.588620	4.475694	-1.274222
H	-2.965298	3.068660	-2.829588
C	-3.304908	5.016434	-0.006839
H	-1.939726	4.990702	1.694383
H	-4.471426	4.819120	-1.836253
H	-3.965481	5.782498	0.427718
C	-5.803033	-2.175357	-0.531969
H	-5.442920	-2.888076	0.242187
H	-6.591737	-1.557567	-0.052164
H	-6.272709	-2.763460	-1.345275

Zero-point correction= 0.770644 (Hartree/Particle)
Thermal correction to Energy= 0.818459
Thermal correction to Enthalpy= 0.819403
Thermal correction to Gibbs Free Energy= 0.687318
Sum of electronic and zero-point Energies= -1977.307206
Sum of electronic and thermal Energies= -1977.259391
Sum of electronic and thermal Enthalpies= -1977.258447
Sum of electronic and thermal Free Energies= -1977.390532

Ph(pOMe)+B-Ph(pMe)-IPr-V-VI			
95			
IPrV-VI-OMe SCF Done: -2053.23533228 A.U.			
C	-1.255008	0.500892	-1.797931
O	-1.278197	-0.244412	-2.761368
Pd	0.639900	0.514934	-0.711393
O	-0.355206	1.855153	-2.038029
C	-4.570359	0.728102	0.976800
C	-4.491971	-0.275304	-0.013903
H	-3.598755	2.446485	1.871273
C	-3.530176	1.684245	1.081274
C	-3.399959	-0.294197	-0.894645
C	-2.363473	0.657572	-0.803840
C	-2.436582	1.637382	0.218123
H	-3.324794	-1.074846	-1.665124
H	-1.629813	2.369902	0.343673
H	-5.266443	-1.048761	-0.108638
N	2.350415	-0.976590	1.193348
C	4.452820	-0.759679	-0.786142
H	3.847906	-1.653059	-0.524546
C	4.269096	0.273790	0.323724
C	3.213338	0.173091	1.264804
C	1.221475	-0.996612	0.404877
C	2.937745	1.169998	2.233239
C	1.711362	1.084240	3.138180
H	1.323518	0.045155	3.080757
C	5.089741	1.417099	0.396923
H	5.916861	1.537562	-0.319911
C	4.857153	2.411878	1.359068
H	5.509761	3.298693	1.397550
C	3.789067	2.292886	2.261610
H	3.604737	3.094150	2.994264
C	2.572797	-2.204859	1.816397

Ph(pMe)+B-Ph(pMe)-IPR-V-VI			
94			
IPrV-VI-Me SCF Done: -1978.07866829 A.U.			
C	-1.522113	0.407505	-1.675490
O	-1.590093	-0.352000	-2.625121
Pd	0.435663	0.505502	-0.723466
O	-0.691032	1.789026	-1.998183
C	-4.682333	0.611087	1.305795
C	-4.625718	-0.395656	0.319505
H	-3.657474	2.366970	2.091130
C	-3.647545	1.576524	1.322997
C	-3.592250	-0.425959	-0.628232
C	-2.569775	0.546866	-0.609240
C	-2.599548	1.540444	0.397001
H	-3.550032	-1.214035	-1.393559
H	-1.801296	2.290147	0.461118
H	-5.405905	-1.174179	0.291501
N	2.307614	-0.879987	1.111620
C	4.260885	-0.649286	-1.013322
H	3.670903	-1.538254	-0.707595
C	4.118728	0.406925	0.080889
C	3.138102	0.295405	1.098699
C	1.138013	-0.956453	0.389454
C	2.904646	1.303420	2.066455
C	1.749234	1.201405	3.059385
H	1.405186	0.145246	3.067568
C	4.905092	1.576521	0.069722
H	5.671152	1.706579	-0.710656
C	4.713959	2.583675	1.027947
H	5.339104	3.490446	1.000590
C	3.720741	2.451098	2.010800
H	3.567372	3.260690	2.741260
C	2.607156	-2.085520	1.746999

C	0.599740	2.008926	2.595931
H	-0.335168	1.892171	3.182569
H	0.910741	3.074542	2.637699
H	0.376603	1.752652	1.533247
C	2.032767	1.378212	4.614918
H	1.130461	1.223558	5.242590
H	2.837840	0.716924	4.997654
H	2.357886	2.429487	4.765659
C	3.888058	-0.208497	-2.113338
H	4.461966	0.679468	-2.453469
H	3.931505	-0.979811	-2.910817
H	2.822242	0.097348	-1.985175
C	5.913150	-1.225268	-0.935626
H	6.318942	-1.611118	0.022664
H	5.982298	-2.035229	-1.691384
H	6.576453	-0.403127	-1.278126
C	1.554146	-3.028054	1.414111
H	1.339432	-4.076857	1.640617
H	3.432338	-2.376644	2.470890
N	0.741883	-2.277686	0.557210
C	-0.457501	-2.778273	-0.069697
C	-0.440619	-3.051005	-1.462772
C	-1.596469	-2.980057	0.753922
C	-1.628302	-3.564768	-2.022423
C	-2.750082	-3.504376	0.139378
C	-2.762420	-3.798544	-1.232133
H	-1.669835	-3.777999	-3.099390
H	-3.657675	-3.673033	0.736257
H	-3.676432	-4.202994	-1.695974
C	0.804821	-2.785262	-2.311074
H	1.154852	-1.768466	-2.017616
C	-1.573933	-2.582482	2.232366
H	-0.593643	-2.902036	2.648405
C	1.939453	-3.787264	-2.002998
H	2.845299	-3.529798	-2.591590
H	2.229653	-3.789999	-0.933717
H	1.638246	-4.821346	-2.276663
C	0.529949	-2.734659	-3.820618
H	1.447660	-2.408827	-4.352835
H	0.253121	-3.730913	-4.229756
H	-0.271899	-2.007753	-4.051026
C	-2.661545	-3.266452	3.076254
H	-2.516125	-3.026893	4.149797
H	-3.675922	-2.906574	2.800729
H	-2.646253	-4.370636	2.964349
C	-1.657506	-1.047953	2.385018
H	-0.914965	-0.521165	1.753456
H	-2.656974	-0.688310	2.073521
H	-1.495573	-0.747971	3.441838
C	-0.783975	3.140708	-1.823190
C	-1.977218	3.596949	-2.419903
C	-0.004992	4.010393	-1.030946
C	-2.392990	4.920800	-2.206859
H	-2.567769	2.899297	-3.032161
C	-0.426899	5.335200	-0.835954
H	0.916162	3.619780	-0.569073
C	-1.623976	5.795654	-1.416482
H	-3.330746	5.273011	-2.665800
H	0.183253	6.012780	-0.217138
H	-1.956183	6.832751	-1.253825
O	-5.578567	0.844631	1.887134
C	-6.624940	-0.114659	1.865680
H	-7.180462	-0.105260	0.899589

C	0.563845	2.056563	2.561089
H	-0.324311	1.925062	3.213636
H	0.830786	3.134680	2.541348
H	0.282548	1.749846	1.526163
C	2.156455	1.568030	4.498051
H	1.309399	1.392609	5.193530
H	3.020169	0.963611	4.845164
H	2.434403	2.639456	4.588443
C	3.642039	-0.133235	-2.330092
H	4.195048	0.749780	-2.714740
H	3.661933	-0.923582	-3.109617
H	2.580008	0.166547	-2.169075
C	5.717247	-1.111829	-1.206952
H	6.157548	-1.480615	-0.257247
H	5.763823	-1.933853	-1.951388
H	6.364433	-0.292012	-1.584312
C	1.596201	-2.951093	1.421145
H	1.430362	-4.000622	1.682427
H	3.507951	-2.213608	2.354320
N	0.711747	-2.248109	0.596837
C	-0.503540	-2.801031	0.049712
C	-0.556692	-3.099068	-1.337214
C	-1.586789	-3.022329	0.940419
C	-1.757073	-3.658883	-1.819709
C	-2.756185	-3.592846	0.401417
C	-2.836956	-3.911950	-0.962253
H	-1.852415	-3.892281	-2.889021
H	-3.623727	-3.776763	1.050960
H	-3.763133	-4.351198	-1.366290
C	0.629337	-2.809878	-2.259685
H	0.964030	-1.777852	-2.003263
C	-1.494473	-2.596110	2.408037
H	-0.479974	-2.868954	2.771850
C	1.811074	-3.770781	-2.001904
H	2.674164	-3.494531	-2.643949
H	2.159939	-3.747248	-0.950484
H	1.528481	-4.818009	-2.243582
C	0.267663	-2.792450	-3.751553
H	1.143450	-2.448957	-4.340321
H	-0.001812	-3.802947	-4.129332
H	-0.567827	-2.093386	-3.946121
C	-2.503174	-3.306163	3.325430
H	-2.303424	-3.042757	4.384671
H	-3.545517	-2.991016	3.105903
H	-2.450437	-4.410694	3.229582
C	-1.632481	-1.063439	2.538292
H	-0.944042	-0.518452	1.862235
H	-2.660007	-0.750958	2.269329
H	-1.430784	-0.737625	3.580692
C	-1.145222	3.063111	-1.766613
C	-2.397997	3.469692	-2.269820
C	-0.335262	3.969523	-1.050623
C	-2.840543	4.781953	-2.039938
H	-3.013047	2.742395	-2.820403
C	-0.785225	5.282345	-0.838447
H	0.632102	3.615412	-0.659294
C	-2.040605	5.693598	-1.325350
H	-3.824250	5.095545	-2.424657
H	-0.150723	5.989316	-0.279974
C	-5.776878	0.639690	2.346664
H	-5.385524	0.327502	3.340194
H	-6.191951	1.661734	2.472472
H	-6.611848	-0.041751	2.087706

H -6.245138 -1.146900 2.048534 H -7.319574 0.161865 2.681702	H -2.394113 6.721408 -1.149068
Zero-point correction= 0.774937 (Hartree/Particle) Thermal correction to Energy= 0.822870 Thermal correction to Enthalpy= 0.823814 Thermal correction to Gibbs Free Energy= 0.692175 Sum of electronic and zero-point Energies= -2052.460396 Sum of electronic and thermal Energies= -2052.412463 Sum of electronic and thermal Enthalpies= -2052.411519 Sum of electronic and thermal Free Energies= -2052.543157	Zero-point correction= 0.769849 (Hartree/Particle) Thermal correction to Energy= 0.817101 Thermal correction to Enthalpy= 0.818045 Thermal correction to Gibbs Free Energy= 0.687415 Sum of electronic and zero-point Energies= -1977.308819 Sum of electronic and thermal Energies= -1977.261567 Sum of electronic and thermal Enthalpies= -1977.260623 Sum of electronic and thermal Free Energies= -1977.391253

Ph(pOMe)+B-Ph(pMe)-IPr-VI	**Ph(pMe)+B-Ph(pMe)-IPR-VI**
95	94
IPrVI-OMe SCF Done: -2053.26068666 A.U.	IPrVI-Me SCF Done: -1978.10435609 A.U.
Pd -0.473719 -0.797058 -0.516839	Pd -0.322070 -0.804707 -0.503099
N -2.872245 0.791754 0.212634	N -2.721222 0.765831 0.272114
C -3.369889 0.856785 -2.664131	C -3.286763 0.781024 -2.590767
H -2.653005 1.454589 -2.064327	H -2.536441 1.372519 -2.026922
C -3.982928 -0.196521 -1.747432	C -3.867844 -0.264042 -1.644326
C -3.699225 -0.238978 -0.362551	C -3.553092 -0.281110 -0.265672
C -1.505638 0.685776 0.284320	C -1.352938 0.673334 0.310410
C -4.152934 -1.274099 0.494739	C -3.977352 -1.305636 0.618758
C -3.668431 -1.384347 1.939518	C -3.455414 -1.387799 2.052343
H -3.205156 -0.416065 2.222690	H -2.997604 -0.409525 2.308827
C -4.825226 -1.204340 -2.260353	C -4.714321 -1.286129 -2.120591
H -5.075425 -1.203407 -3.332747	H -4.989635 -1.304516 -3.186594
C -5.328930 -2.217237 -1.431453	C -5.190616 -2.288958 -1.263568
H -5.981569 -2.997252 -1.854659	H -5.846954 -3.080555 -1.658572
C -4.982705 -2.261160 -0.071786	C -4.811881 -2.308451 0.088016
H -5.351871 -3.086287 0.556991	H -5.158861 -3.126418 0.738357
C -3.337987 1.920018 0.885402	C -3.179123 1.905694 0.930476
C -2.563398 -2.459246 2.035864	C -2.334048 -2.446825 2.136378
H -2.129938 -2.490816 3.057560	H -1.873251 -2.456570 3.146498
H -2.961486 -3.467013 1.793986	H -2.725092 -3.463308 1.920955
H -1.734906 -2.253027 1.321479	H -1.527452 -2.241916 1.397113
C -4.805586 -1.652157 2.942010	C -4.562865 -1.655517 3.087452
H -4.413953 -1.641414 3.980648	H -4.145052 -1.623763 4.115353
H -5.602802 -0.884264 2.865525	H -5.372317 -0.899743 3.019808
H -5.274807 -2.645404 2.780085	H -5.022060 -2.657383 2.952234
C -2.550178 0.195590 -3.789858	C -2.524640 0.113520 -3.752226
H -3.197398 -0.379255 -4.485942	H -3.206342 -0.451636 -4.422960
H -2.014403 0.968580 -4.377133	H -2.005602 0.882554 -4.359288
H -1.788538 -0.490492 -3.367176	H -1.754011 -0.583047 -3.364474
C -4.444220 1.816001 -3.214449	C -4.377326 1.748836 -3.092183
H -4.995763 2.321273 -2.393917	H -4.885216 2.260154 -2.247574
H -3.979834 2.598068 -3.851083	H -3.936788 2.526106 -3.751328
H -5.188837 1.274111 -3.836052	H -5.154831 1.211571 -3.676589
C -2.232409 2.543769 1.402575	C -2.065964 2.550260 1.404273
H -2.129270 3.445633 2.012064	H -1.955016 3.466800 1.989953
H -4.403342 2.162455 0.939717	H -4.244791 2.140622 1.007105
N -1.123835 1.779860 1.026475	N -0.961049 1.786579 1.017467
C 0.227936 2.045235 1.458068	C 0.400464 2.074483 1.400912
C 0.965763 3.056450 0.795724	C 1.103540 3.086363 0.702386
C 0.759986 1.269941 2.524961	C 0.977986 1.317249 2.457493
C 2.266580 3.324161 1.270789	C 2.417541 3.372325 1.127961
C 2.060662 1.586105 2.960110	C 2.290127 1.651693 2.842138
C 2.803210 2.606835 2.346305	C 2.999943 2.672772 2.191020
H 2.872210 4.099219 0.777872	H 2.996823 4.147875 0.605130
H 2.513463 1.006120 3.776953	H 2.777197 1.087840 3.650498
H 3.823663 2.826493 2.697413	H 4.029338 2.907996 2.503967
C 0.383075 3.841851 -0.377495	C 0.473869 3.855816 -0.457115
H -0.448629 3.238523 -0.798043	H -0.370505 3.245168 -0.840309

C	-0.030138	0.112665	3.137900
H	-0.584417	-0.360069	2.299167
C	-0.189070	5.194198	0.101350
H	-0.969303	5.066713	0.878507
H	0.615095	5.825670	0.536084
H	-0.641007	5.751398	-0.746050
C	1.401764	4.057824	-1.512444
H	0.892232	4.482696	-2.401323
H	2.202088	4.769845	-1.219251
H	1.873067	3.103737	-1.815606
C	-1.069774	0.606702	4.165828
H	-1.674106	-0.244396	4.545194
H	-0.570439	1.087597	5.033845
H	-1.770092	1.343069	3.723006
C	0.859681	-0.989141	3.736308
H	1.616521	-1.347587	3.008130
H	1.387576	-0.652601	4.654054
H	0.235185	-1.860752	4.022086
C	0.686696	0.467216	-1.522605
O	0.242020	1.180150	-2.403498
O	0.345290	-2.531465	-1.190782
C	4.878469	-0.053903	-0.674310
C	4.454594	0.419166	-1.940301
H	4.269182	-0.709548	1.300260
C	3.922529	-0.322594	0.332214
C	3.088669	0.611521	-2.185745
C	2.128021	0.322053	-1.191366
C	2.568440	-0.157473	0.064137
H	2.745484	0.971201	-3.168148
H	1.816937	-0.399787	0.826769
H	5.178891	0.629265	-2.739506
C	1.513820	-2.933490	-0.690192
C	1.678208	-3.237850	0.694618
C	2.654820	-3.059478	-1.533038
C	2.927982	-3.609045	1.211203
H	0.793679	-3.152203	1.347320
C	3.900532	-3.425880	-1.005454
H	2.533827	-2.814608	-2.599408
C	4.053554	-3.697882	0.368731
H	3.027274	-3.827708	2.287993
H	4.775475	-3.484908	-1.674264
O	6.174988	-0.289591	-0.336226
C	7.184408	-0.107623	-1.319077
H	7.023812	-0.765410	-2.203765
H	7.245636	0.950169	-1.664661
H	8.141726	-0.382173	-0.836451
H	5.038143	-3.973900	0.777194
Zero-point correction=			0.775603 (Hartree/Particle)
Thermal correction to Energy=			0.824351
Thermal correction to Enthalpy=			0.825295
Thermal correction to Gibbs Free Energy=			0.691470
Sum of electronic and zero-point Energies=			-2052.485083
Sum of electronic and thermal Energies=			-2052.436335
Sum of electronic and thermal Enthalpies=			-2052.435391
Sum of electronic and thermal Free Energies=			-2052.569216

C	0.222758	0.159426	3.112185
H	-0.339767	-0.341795	2.295486
C	-0.085061	5.211486	0.027977
H	-0.835979	5.090105	0.834459
H	0.732012	5.849990	0.426798
H	-0.569128	5.758263	-0.808341
C	1.450176	4.062953	-1.630701
H	0.906966	4.475430	-2.505330
H	2.257489	4.781598	-1.374800
H	1.915625	3.108061	-1.940592
C	-0.804041	0.655476	4.152144
H	-1.379377	-0.199403	4.566298
H	-0.295741	1.168528	4.996186
H	-1.532004	1.364658	3.709525
C	1.146091	-0.912034	3.714250
H	1.895325	-1.268030	2.977209
H	1.685117	-0.546128	4.614133
H	0.545133	-1.789901	4.029648
C	0.755056	0.473324	-1.573498
O	0.255297	1.189687	-2.420013
O	0.511338	-2.528522	-1.189140
C	5.009778	-0.072865	-1.003618
C	4.483057	0.359320	-2.241944
H	4.497280	-0.624631	1.041808
C	4.115785	-0.273991	0.070454
C	3.108038	0.569576	-2.411786
C	2.220710	0.330248	-1.337857
C	2.741251	-0.097244	-0.098529
H	2.699029	0.897172	-3.379955
H	2.047059	-0.293563	0.728632
H	5.165808	0.520462	-3.092502
C	1.697359	-2.913128	-0.718668
C	1.918616	-3.154538	0.671042
C	2.801788	-3.085437	-1.601117
C	3.185558	-3.514217	1.151861
H	1.062700	-3.032213	1.355382
C	4.065136	-3.442013	-1.110090
H	2.638615	-2.888855	-2.671782
C	4.273659	-3.654754	0.267547
H	3.327713	-3.686017	2.232339
H	4.909015	-3.542434	-1.813032
H	5.269993	-3.932387	0.646340
C	6.478820	-0.373562	-0.831509
H	6.889452	0.110091	0.079816
H	6.627285	-1.468816	-0.708829
H	7.079951	-0.042253	-1.701652
Zero-point correction=			0.770797 (Hartree/Particle)
Thermal correction to Energy=			0.818677
Thermal correction to Enthalpy=			0.819621
Thermal correction to Gibbs Free Energy=			0.688387
Sum of electronic and zero-point Energies=			-1977.333559
Sum of electronic and thermal Energies=			-1977.285679
Sum of electronic and thermal Enthalpies=			-1977.284735
Sum of electronic and thermal Free Energies=			-1977.415969

Ph(pMe)+B-Ph(pMe)-IPr-VII			
101			
IPrVII-OMe SCF Done: -3517.08652024 A.U.			
Pd	0.236043	0.165171	-0.439671
N	2.402172	-1.801473	0.138810
C	2.431960	-2.044813	-2.774468

Ph(pOMe)+B-Ph(pMe)-IPR-VII			
100			
IPrVII-Me SCF Done: -3441.93054473 A.U.			
Pd	0.121646	0.179740	-0.446130
N	2.419570	-1.615223	0.164231
C	2.597526	-1.743871	-2.751428

H	1.627472	-2.354692	-2.078754	H	1.799913	-2.157812	-2.103584
C	3.422657	-1.173794	-2.009424	C	3.473878	-0.821292	-1.911106
C	3.384816	-1.043369	-0.599683	C	3.360916	-0.745943	-0.501731
C	1.096492	-1.419993	0.340520	C	1.080935	-1.349455	0.328932
C	4.256009	-0.183902	0.123693	C	4.117226	0.161037	0.289876
C	4.118872	0.016283	1.630836	C	3.893171	0.294742	1.794324
H	3.044885	-0.132617	1.862935	H	2.825390	0.051159	1.966831
C	4.426030	-0.457287	-2.701258	C	4.439335	0.004666	-2.530777
H	4.498327	-0.553780	-3.796221	H	4.568830	-0.045953	-3.623556
C	5.333092	0.362902	-2.011569	C	5.237739	0.875576	-1.772316
H	6.117635	0.903318	-2.566428	H	5.995747	1.502050	-2.270677
C	5.239586	0.504210	-0.616609	C	5.067810	0.958617	-0.379766
H	5.934427	1.177789	-0.093499	H	5.673793	1.671532	0.198555
C	2.676443	-3.012304	0.777618	C	2.769937	-2.825250	0.766304
C	4.471604	1.446773	2.077670	C	4.104530	1.732176	2.303292
H	4.113753	1.610725	3.114415	H	3.708091	1.823343	3.335184
H	5.569358	1.624378	2.076066	H	5.181552	2.006616	2.339700
H	3.986330	2.203304	1.431540	H	3.568849	2.465761	1.670438
C	4.955389	-1.009580	2.426332	C	4.772403	-0.689344	2.596354
H	4.812400	-0.854944	3.516500	H	4.572234	-0.581553	3.683149
H	4.672047	-2.055909	2.199556	H	4.579103	-1.746104	2.327015
H	6.038064	-0.893829	2.203561	H	5.851387	-0.485084	2.425211
C	1.726276	-1.257569	-3.894511	C	1.863264	-0.970943	-3.863228
H	2.434715	-0.899044	-4.672482	H	2.563143	-0.516702	-4.597893
H	0.967398	-1.897221	-4.386777	H	1.180655	-1.650564	-4.410700
H	1.176396	-0.392917	-3.468406	H	1.226556	-0.176860	-3.420963
C	3.121038	-3.317122	-3.308975	C	3.419742	-2.922124	-3.311653
H	3.586340	-3.898625	-2.485699	H	3.908232	-3.495009	-2.495737
H	2.384862	-3.972679	-3.819511	H	2.765760	-3.618844	-3.876588
H	3.921285	-3.069038	-4.039369	H	4.218246	-2.570075	-4.000177
C	1.529272	-3.383474	1.424928	C	1.634747	-3.313685	1.354628
H	1.304761	-4.237887	2.068382	H	1.457925	-4.208035	1.957416
H	3.656042	-3.492464	0.705023	H	3.787740	-3.221205	0.714033
N	0.577795	-2.397289	1.149440	N	0.616015	-2.396463	1.080968
C	-0.748517	-2.375103	1.718381	C	-0.723351	-2.500773	1.607829
C	-1.703514	-3.298100	1.224937	C	-1.586989	-3.476869	1.051996
C	-1.034151	-1.431738	2.747614	C	-1.112094	-1.622985	2.661588
C	-2.972350	-3.311696	1.840806	C	-2.865648	-3.618258	1.630829
C	-2.318088	-1.501689	3.326194	C	-2.401877	-1.817957	3.197769
C	-3.271070	-2.435512	2.889448	C	-3.262598	-2.810276	2.701628
H	-3.739906	-4.012367	1.479203	H	-3.563155	-4.363846	1.220665
H	-2.585284	-0.799010	4.127566	H	-2.747749	-1.171597	4.016357
H	-4.267451	-2.460053	3.358554	H	-4.264535	-2.935178	3.142259
C	-1.393430	-4.253990	0.073986	C	-1.177510	-4.350439	-0.132629
H	-0.493032	-3.867397	-0.447191	H	-0.300526	-3.870210	-0.614409
C	-0.031125	-0.353932	3.169098	C	-0.207502	-0.493007	3.160620
H	0.372008	0.107029	2.237548	H	0.184471	0.042449	2.264910
C	-1.084567	-5.671023	0.605278	C	-0.767365	-5.762864	0.338567
H	-0.240757	-5.675305	1.324630	H	0.064822	-5.736222	1.070922
H	-1.968753	-6.092741	1.129618	H	-1.622782	-6.276794	0.827129
H	-0.824475	-6.355606	-0.229407	H	-0.442889	-6.384279	-0.522534
C	-2.525641	-4.305589	-0.970351	C	-2.282594	-4.438916	-1.204029
H	-2.196770	-4.891362	-1.853353	H	-1.890700	-4.949810	-2.107349
H	-3.436730	-4.797233	-0.567388	H	-3.157698	-5.022271	-0.845907
H	-2.797462	-3.291728	-1.319543	H	-2.631670	-3.434143	-1.509036
C	1.167485	-0.931744	3.952588	C	1.005978	-1.018480	3.958963
H	1.884274	-0.118728	4.190151	H	1.652726	-0.168306	4.259360
H	0.833286	-1.390637	4.908324	H	0.675736	-1.544593	4.880832
H	1.721328	-1.702778	3.380744	H	1.634444	-1.719202	3.374219
C	-0.665897	0.806326	3.949222	C	-0.951087	0.578254	3.971268
H	-1.532564	1.233970	3.402962	H	-1.829297	0.966635	3.415212
H	-1.004264	0.500854	4.963930	H	-1.293382	0.201401	4.960348
H	0.081966	1.616380	4.042052	H	-0.270702	1.436850	4.125511

C	-1.081247	-0.974508	-1.396918
O	-0.759555	-1.842468	-2.210363
O	-0.464804	1.876481	-1.488707
C	-5.297808	-0.127124	-0.863128
C	-4.796232	-0.506329	-2.131364
H	-4.823138	0.256690	1.216438
C	-4.412992	-0.020476	0.234124
C	-3.427987	-0.777957	-2.280235
C	-2.533948	-0.644250	-1.196611
C	-3.049958	-0.258094	0.058761
H	-3.028932	-1.099826	-3.254913
H	-2.365288	-0.179433	0.914113
H	-5.461786	-0.595606	-3.001586
K	2.158448	2.373344	-1.986277
K	0.120694	4.972481	1.385169
C	1.566816	2.603391	0.901809
O	1.968513	3.662843	0.242910
O	0.957839	2.685954	2.019775
O	1.815688	1.423325	0.342940
C	-1.285939	2.776562	-0.984977
C	-1.831442	2.695330	0.336986
C	-1.653515	3.923759	-1.762066
C	-2.719222	3.667622	0.822362
H	-1.510144	1.858634	0.973764
C	-2.520996	4.904151	-1.255520
H	-1.246887	4.005785	-2.783521
C	-3.073870	4.789791	0.040128
H	-3.142659	3.545318	1.834498
H	-2.787194	5.767024	-1.889582
O	-6.608886	0.148042	-0.600029
C	-7.547592	0.069610	-1.660827
H	-7.311076	0.785536	-2.481889
H	-7.609049	-0.957261	-2.090939
H	-8.531397	0.334775	-1.227907
H	-3.782594	5.542667	0.419323

Zero-point correction= 0.793667 (Hartree/Particle)
Thermal correction to Energy= 0.849349
Thermal correction to Enthalpy= 0.850293
Thermal correction to Gibbs Free Energy= 0.703294
Sum of electronic and zero-point Energies= -3516.292853
Sum of electronic and thermal Energies= -3516.237171
Sum of electronic and thermal Enthalpies= -3516.236227
Sum of electronic and thermal Free Energies= -3516.383226

C	-1.037028	-1.035570	-1.500950
O	-0.611976	-1.873459	-2.296693
O	-0.672981	1.857591	-1.484479
C	-5.334978	-0.398410	-1.276551
C	-4.678859	-0.564480	-2.518615
H	-5.040377	-0.343168	0.881564
C	-4.554192	-0.448642	-0.102301
C	-3.295328	-0.776771	-2.583361
C	-2.520022	-0.787900	-1.402757
C	-3.164779	-0.619256	-0.163339
H	-2.791409	-0.932946	-3.549931
H	-2.570151	-0.651753	0.760214
H	-5.269804	-0.532950	-3.449600
K	1.909676	2.621116	-1.825618
K	-0.626932	4.843087	1.463395
C	1.119369	2.675361	1.019504
O	1.453690	3.798699	0.435324
O	0.411442	2.640706	2.080185
O	1.540555	1.553030	0.442052
C	-1.635690	2.629544	-1.019890
C	-2.271121	2.417240	0.245917
C	-2.072759	3.764464	-1.778016
C	-3.300458	3.257762	0.696074
H	-1.908101	1.584617	0.865827
C	-3.086391	4.613278	-1.305270
H	-1.599013	3.944427	-2.757033
C	-3.720619	4.371571	-0.065776
H	-3.784345	3.037571	1.663395
H	-3.401901	5.471503	-1.922765
C	-6.822741	-0.137739	-1.214151
H	-7.364889	-0.645933	-2.038194
H	-7.259399	-0.475844	-0.252118
H	-7.035386	0.950625	-1.306005
H	-4.537833	5.020913	0.285468

Zero-point correction= 0.789157 (Hartree/Particle)
Thermal correction to Energy= 0.844873
Thermal correction to Enthalpy= 0.845818
Thermal correction to Gibbs Free Energy= 0.697548
Sum of electronic and zero-point Energies= -3441.141390
Sum of electronic and thermal Energies= -3441.085674
Sum of electronic and thermal Enthalpies= -3441.084730
Sum of electronic and thermal Free Energies= -3441.232999

Ph(pOMe)+B-Ph(pMe)-IPr-VII-VIII			
101			
IPrVII-VIII-OMe SCF Done: -3517.06242862 A.U.			
Pd	0.707868	0.670314	0.005053
N	2.291731	-1.733277	0.475314
C	1.418513	-3.016838	-1.968079
H	0.653967	-2.585454	-1.284625
C	2.613072	-2.060227	-1.936098
C	3.041221	-1.445475	-0.726753
C	1.104146	-1.099662	0.760388
C	4.108851	-0.514679	-0.658175
C	4.515497	0.133673	0.661738
H	3.601687	0.206462	1.289310
C	3.324330	-1.728931	-3.106713
H	3.023214	-2.172277	-4.066506
C	4.397855	-0.824724	-3.071532
H	4.941104	-0.585657	-4.000684
C	4.782974	-0.222086	-1.862917

Ph(pMe)+B-Ph(pMe)-IPR-VII-VIII			
100			
IPrVII-VIII-Me SCF Done: -3441.90586299 A.U.			
Pd	-0.489567	-0.703725	0.058513
N	-2.387467	1.479981	0.507275
C	-1.899327	2.708610	-2.065145
H	-1.032856	2.431461	-1.424639
C	-2.938228	1.599943	-1.881163
C	-3.175651	1.009677	-0.609170
C	-1.104184	1.039780	0.728698
C	-4.087105	-0.055508	-0.398200
C	-4.281339	-0.670478	0.983831
H	-3.319184	-0.562729	1.527757
C	-3.684453	1.097874	-2.966176
H	-3.528090	1.516318	-3.970702
C	-4.609422	0.056153	-2.789235
H	-5.184237	-0.315948	-3.653306
C	-4.805013	-0.516854	-1.522066

H	5.620217	0.491746	-1.851129	H	-5.525200	-1.339651	-1.399146
C	2.569740	-2.730662	1.410589	C	-2.736362	2.490491	1.404439
C	5.039077	1.570792	0.496109	C	-4.581187	-2.178456	0.938129
H	5.143213	2.047117	1.491626	H	-4.526218	-2.601563	1.961245
H	6.037622	1.601347	0.007572	H	-5.597677	-2.394874	0.542526
H	4.326572	2.185788	-0.088428	H	-3.826820	-2.709746	0.324479
C	5.555332	-0.742780	1.395106	C	-5.381157	0.083121	1.764222
H	5.819300	-0.291738	2.374444	H	-5.491269	-0.342429	2.783550
H	5.179991	-1.768244	1.586267	H	-5.152877	1.162642	1.872658
H	6.486837	-0.832544	0.795421	H	-6.361710	-0.003288	1.247965
C	0.752229	-3.143651	-3.347822	C	-1.362204	2.832608	-3.499885
H	1.398302	-3.684129	-4.072894	H	-2.132971	3.221563	-4.199639
H	-0.187222	-3.726216	-3.251376	H	-0.515496	3.549694	-3.516166
H	0.495981	-2.148183	-3.758921	H	-0.991546	1.857566	-3.870025
C	1.789713	-4.419425	-1.435919	C	-2.425142	4.078889	-1.581816
H	2.185546	-4.389936	-0.402925	H	-2.736068	4.062738	-0.519984
H	0.893627	-5.075491	-1.427204	H	-1.632381	4.850033	-1.682688
H	2.555613	-4.893239	-2.086050	H	-3.296089	4.400216	-2.191760
C	1.517281	-2.746997	2.287238	C	-1.635047	2.713318	2.188579
H	1.309634	-3.373047	3.159371	H	-1.458269	3.416511	3.007057
H	3.480207	-3.334169	1.363811	H	-3.725955	2.955427	1.400682
N	0.621382	-1.760878	1.864562	N	-0.641395	1.834436	1.750325
C	-0.740477	-1.662782	2.336198	C	0.752096	1.945220	2.112605
C	-1.670712	-2.605073	1.826386	C	1.515458	2.946331	1.456404
C	-1.094463	-0.629900	3.238423	C	1.300263	1.039917	3.052189
C	-3.000873	-2.508822	2.279907	C	2.879574	3.040648	1.794055
C	-2.445357	-0.566665	3.638839	C	2.676456	1.166509	3.335076
C	-3.385238	-1.498981	3.172883	C	3.455142	2.157644	2.719062
H	-3.753544	-3.216733	1.900761	H	3.507191	3.797576	1.299646
H	-2.764069	0.227498	4.330178	H	3.142281	0.475961	4.054179
H	-4.434940	-1.428594	3.500033	H	4.528430	2.236333	2.955399
C	-1.264962	-3.691636	0.830264	C	0.895089	3.898690	0.435057
H	-0.269176	-3.422578	0.423395	H	-0.076286	3.466287	0.119945
C	-0.048805	0.335397	3.777616	C	0.431104	0.009303	3.759385
H	0.732267	0.467057	3.003807	H	-0.445678	-0.204614	3.118708
C	-1.118629	-5.054402	1.539540	C	0.601103	5.270293	1.079532
H	-0.385803	-5.005652	2.370468	H	-0.054372	5.173756	1.968664
H	-2.090244	-5.383282	1.966169	H	1.542695	5.760243	1.407392
H	-0.776581	-5.833331	0.825603	H	0.098174	5.944242	0.354163
C	-2.216777	-3.794425	-0.376274	C	1.740395	4.060028	-0.842057
H	-1.814825	-4.524503	-1.110267	H	1.183142	4.666693	-1.586725
H	-3.227291	-4.147487	-0.081369	H	2.698076	4.585391	-0.643437
H	-2.330319	-2.819432	-0.887052	H	1.975423	3.081052	-1.301026
C	0.626661	-0.259479	5.032288	C	-0.087033	0.585220	5.094849
H	1.423373	0.420884	5.399188	H	-0.751499	-0.147249	5.599150
H	-0.108324	-0.409434	5.852925	H	0.751958	0.824231	5.784060
H	1.095277	-1.242049	4.814266	H	-0.667697	1.518271	4.934678
C	-0.593518	1.746199	4.049145	C	1.131949	-1.344198	3.957801
H	-1.173104	2.119069	3.180442	H	1.597593	-1.682227	3.010521
H	-1.248132	1.789548	4.946966	H	1.919527	-1.308923	4.741695
H	0.253845	2.443932	4.202622	H	0.384387	-2.110790	4.242541
C	-0.259409	-0.027819	-1.590693	C	0.237577	0.008124	-1.651183
O	0.320627	-0.116685	-2.690526	O	-0.435078	-0.048298	-2.697931
O	-0.606278	2.693648	-1.421498	O	1.000071	-2.601411	-1.331188
C	-4.515856	-0.713634	-1.395000	C	4.410174	1.151356	-1.879438
C	-3.816752	-0.897196	-2.613987	C	3.581957	1.174327	-3.026489
H	-4.368039	-0.200606	0.705498	H	4.447095	0.787699	0.268059
C	-3.809132	-0.345984	-0.228430	C	3.826099	0.817485	-0.639820
C	-2.432099	-0.690744	-2.649530	C	2.226442	0.836282	-2.941243
C	-1.714601	-0.323310	-1.489055	C	1.651995	0.484321	-1.697812
C	-2.429270	-0.161420	-0.277593	C	2.468095	0.495305	-0.545876
H	-1.873968	-0.806391	-3.591493	H	1.585309	0.821560	-3.836226
H	-1.881369	0.120092	0.632592	H	2.024968	0.236333	0.426861

H	-4.345217	-1.186459	-3.533279
K	1.702465	2.058175	-2.661601
K	0.261996	4.760101	0.084395
C	1.996716	2.820107	1.022803
O	1.990022	2.768728	-0.303294
O	2.157889	3.909665	1.639883
O	1.713861	1.685909	1.629271
C	-1.832552	2.814246	-0.963084
C	-2.100889	2.847227	0.449424
C	-2.972166	2.908775	-1.825690
C	-3.404707	2.963837	0.956294
H	-1.253701	2.668684	1.137312
C	-4.269096	3.013466	-1.307843
H	-2.796340	2.853503	-2.912034
C	-4.504667	3.048342	0.084121
H	-3.560783	2.951761	2.048511
H	-5.124545	3.056576	-2.003435
H	-5.530724	3.120043	0.476636
O	-5.861348	-0.872684	-1.247832
C	-6.638526	-1.213681	-2.385632
H	-6.567238	-0.440812	-3.185299
H	-6.342423	-2.199247	-2.814195
H	-7.688162	-1.275282	-2.039613

Zero-point correction= 0.793297 (Hartree/Particle)
Thermal correction to Energy= 0.849293
Thermal correction to Enthalpy= 0.850237
Thermal correction to Gibbs Free Energy= 0.702637
Sum of electronic and zero-point Energies= -3516.269132
Sum of electronic and thermal Energies= -3516.213136
Sum of electronic and thermal Enthalpies= -3516.212191
Sum of electronic and thermal Free Energies= -3516.359792

H	4.019558	1.441766	-4.002911
K	-1.470140	-2.397976	-2.418921
K	0.564508	-4.654516	0.376031
C	-1.379740	-2.929080	1.315747
O	-1.466729	-2.993178	-0.007684
O	-1.327054	-3.973660	2.023166
O	-1.240902	-1.717872	1.814015
C	2.277493	-2.536103	-1.028187
C	2.716155	-2.459043	0.338715
C	3.306177	-2.525822	-2.024750
C	4.075419	-2.386316	0.680703
H	1.941205	-2.352351	1.119608
C	4.658385	-2.436879	-1.672598
H	2.994567	-2.547478	-3.081225
C	5.063149	-2.374156	-0.320918
H	4.360303	-2.301649	1.743150
H	5.420457	-2.403743	-2.469851
H	6.129992	-2.301091	-0.058308
C	5.893239	1.417306	-1.974776
H	6.247756	2.062255	-1.143810
H	6.454363	0.459437	-1.900598
H	6.172297	1.898952	-2.933546

Zero-point correction= 0.787969 (Hartree/Particle)
Thermal correction to Energy= 0.843300
Thermal correction to Enthalpy= 0.844244
Thermal correction to Gibbs Free Energy= 0.698016
Sum of electronic and zero-point Energies= -3441.117894
Sum of electronic and thermal Energies= -3441.062563
Sum of electronic and thermal Enthalpies= -3441.061619
Sum of electronic and thermal Free Energies= -3441.207847

Ph(pOMe)+B-Ph(pMe)-IPr-VIIIpost

101
IPrVIII-OMe SCF Done: -3517.08777463 A.U.

Pd	-0.257573	0.556165	0.658065
N	1.142505	2.545089	-0.996697
C	0.998954	0.889303	-3.361240
H	1.349945	0.448702	-2.402511
C	-0.107678	1.882576	-3.000176
C	-0.027107	2.687956	-1.829979
C	1.291823	1.495922	-0.120901
C	-1.052126	3.577207	-1.422276
C	-0.949958	4.369906	-0.121743
H	-0.219068	3.850211	0.531923
C	-1.254876	2.037847	-3.804328
H	-1.363280	1.430418	-4.714227
C	-2.266758	2.949618	-3.456984
H	-3.146320	3.065131	-4.111111
C	-2.170104	3.705296	-2.276445
H	-2.977661	4.403293	-2.006446
C	2.294987	3.330113	-1.053096
C	-2.273699	4.404304	0.662119
H	-2.120267	4.905102	1.638571
H	-3.073118	4.955607	0.122168
H	-2.625925	3.380315	0.895045
C	-0.426953	5.795491	-0.403315
H	-0.304649	6.361093	0.543867
H	0.555639	5.777693	-0.918688
H	-1.134225	6.358077	-1.050061
C	0.527007	-0.282345	-4.237674
H	0.274199	0.043922	-5.269325

Ph(pMe)+B-Ph(pMe)-IPR-VIIIpost

100
IPrVIII-Me SCF Done: -3441.92461726 A.U.

Pd	-0.379859	-0.914314	0.008288
N	-3.054113	0.170956	0.557873
C	-3.135981	1.467659	-2.018532
H	-2.234271	1.565142	-1.374929
C	-3.673776	0.050694	-1.810423
C	-3.605435	-0.585432	-0.541678
C	-1.705799	0.367609	0.721208
C	-4.017906	-1.918367	-0.314056
C	-3.836041	-2.592647	1.042077
H	-3.087477	-2.004758	1.611906
C	-4.250333	-0.686264	-2.862064
H	-4.324352	-0.236618	-3.862896
C	-4.722635	-1.992763	-2.656422
H	-5.176160	-2.547124	-3.493710
C	-4.597368	-2.604581	-1.401796
H	-4.940904	-3.641030	-1.262677
C	-3.791654	0.875641	1.508401
C	-3.254167	-4.011750	0.911301
H	-2.993436	-4.407596	1.913268
H	-3.973225	-4.718024	0.443415
H	-2.321377	-3.996561	0.314618
C	-5.159843	-2.593906	1.835457
H	-5.017040	-3.057303	2.834230
H	-5.547912	-1.565300	1.988583
H	-5.944314	-3.170594	1.299600
C	-2.676136	1.743651	-3.458685
H	-3.531927	1.809702	-4.164024

H	1.342982	-1.029480	-4.323693	H	-2.140904	2.714759	-3.498843
H	-0.350909	-0.787263	-3.789947	H	-1.985016	0.952041	-3.810647
C	2.201122	1.600001	-4.023502	C	-4.156001	2.532207	-1.557898
H	2.617861	2.404892	-3.387609	H	-4.444082	2.400368	-0.496022
H	3.016435	0.872051	-4.218380	H	-3.729676	3.551536	-1.667071
H	1.902291	2.049074	-4.994428	H	-5.080385	2.478114	-2.171427
C	3.206365	2.741577	-0.215146	C	-2.884645	1.560036	2.274705
H	4.239867	3.001521	0.031328	H	-3.016136	2.248754	3.114194
H	2.360106	4.222421	-1.682117	H	-4.883651	0.827258	1.544743
N	2.584275	1.615382	0.329494	N	-1.617675	1.254228	1.770332
C	3.282547	0.575142	1.045228	C	-0.424932	1.990289	2.114580
C	4.093687	-0.301951	0.278445	C	-0.312587	3.310454	1.602757
C	3.108676	0.445198	2.444121	C	0.580848	1.379994	2.902968
C	4.788197	-1.312452	0.971258	C	0.844506	4.039026	1.940076
C	3.820910	-0.591900	3.083442	C	1.731458	2.147579	3.183877
C	4.658719	-1.453475	2.360492	C	1.858979	3.464450	2.718850
H	5.420808	-2.016396	0.408493	H	0.965164	5.065574	1.559776
H	3.713164	-0.723355	4.171108	H	2.538067	1.703173	3.787015
H	5.204986	-2.254613	2.883483	H	2.764375	4.045142	2.957120
C	4.210757	-0.192472	-1.241931	C	-1.387747	3.947365	0.720597
H	3.528283	0.611206	-1.583605	H	-2.156685	3.179755	0.502380
C	2.204653	1.374878	3.245847	C	0.439065	-0.029779	3.462703
H	1.581189	1.953164	2.536043	H	-0.410888	-0.525501	2.955983
C	5.636252	0.217609	-1.663424	C	-2.093809	5.099631	1.464962
H	5.941066	1.171284	-1.184617	H	-2.517036	4.760341	2.433166
H	6.380549	-0.555162	-1.375679	H	-1.388192	5.929856	1.680923
H	5.695330	0.350247	-2.764288	H	-2.922801	5.510911	0.851529
C	3.756189	-1.484420	-1.948898	C	-0.835333	4.408045	-0.641670
H	3.801184	-1.354220	-3.050835	H	-1.646083	4.865860	-1.246583
H	4.401260	-2.348781	-1.686401	H	-0.030916	5.165250	-0.533239
H	2.716046	-1.745824	-1.674271	H	-0.418944	3.556902	-1.212856
C	3.045457	2.377574	4.062681	C	0.125446	0.018349	4.972405
H	2.382984	3.074430	4.617136	H	-0.021758	-1.008334	5.367849
H	3.689750	1.855190	4.802492	H	0.953730	0.491432	5.543106
H	3.707704	2.980060	3.405809	H	-0.797902	0.600854	5.174400
C	1.220437	0.592405	4.136068	C	1.674734	-0.898946	3.162554
H	0.662808	-0.157363	3.537614	H	1.917745	-0.856570	2.081486
H	1.734577	0.068139	4.970013	H	2.571821	-0.572227	3.730566
H	0.470618	1.285645	4.565479	H	1.456673	-1.955265	3.419199
C	-0.330860	-0.927852	-0.661291	C	0.025004	0.017175	-1.695030
O	-1.132269	-0.851258	-1.607208	O	-0.306103	-0.546469	-2.755261
O	-5.090165	-0.716638	0.466691	O	3.846662	-2.628560	-1.720499
C	2.007983	-4.523668	-0.152828	C	2.503009	3.570972	-1.990415
C	1.130611	-4.390714	-1.257935	C	1.749233	3.113205	-3.096590
H	2.784084	-3.607479	1.653397	H	2.994968	3.183421	0.095203
C	2.096225	-3.484578	0.804835	C	2.406198	2.858342	-0.775700
C	0.368113	-3.224007	-1.394401	C	0.943894	1.971987	-2.995460
C	0.469785	-2.170307	-0.457302	C	0.834238	1.278791	-1.766481
C	1.338203	-2.325271	0.649749	C	1.569858	1.743150	-0.656778
H	-0.327784	-3.103839	-2.239014	H	0.382984	1.595205	-3.863828
H	1.417796	-1.507219	1.383567	H	1.486412	1.204126	0.298565
H	1.036780	-5.189514	-2.006803	H	1.809506	3.657357	-4.053730
K	-3.305594	0.551292	-0.834024	K	1.518273	-2.613372	-2.662099
K	-4.235565	-0.659416	2.861361	K	3.300498	-3.605499	0.677607
C	-1.897035	1.247614	2.500210	C	0.382173	-3.152668	1.005872
O	-1.999459	0.127953	1.730378	O	0.824376	-2.650266	-0.177772
O	-2.770601	1.498838	3.358739	O	0.907344	-4.182907	1.486788
O	-0.849485	1.973496	2.218860	O	-0.551606	-2.434333	1.562300
C	-4.814690	-1.943309	0.067786	C	4.479620	-1.662891	-1.091666
C	-3.502551	-2.519845	0.230752	C	3.790448	-0.767951	-0.196430
C	-5.793123	-2.779253	-0.570141	C	5.901579	-1.477321	-1.189122
C	-3.199888	-3.814013	-0.225353	C	4.469299	0.209358	0.549699
H	-2.710566	-1.911936	0.701396	H	2.692842	-0.859146	-0.123120

C	-5.477504	-4.070694	-1.012658	C	6.564534	-0.491207	-0.445021
H	-6.805783	-2.363760	-0.703310	H	6.455748	-2.141145	-1.873261
C	-4.180166	-4.605540	-0.850540	C	5.863830	0.359432	0.438545
H	-2.173497	-4.198575	-0.094551	H	3.891914	0.863338	1.226460
H	-6.259312	-4.679291	-1.499620	H	7.657866	-0.382137	-0.550564
H	-3.943433	-5.620611	-1.206668	C	3.397160	4.784106	-2.090211
O	2.804054	-5.603830	0.073036	H	3.123420	5.545964	-1.328937
C	2.750482	-6.698968	-0.832381	H	4.457172	4.509386	-1.901264
H	1.733497	-7.151262	-0.876613	H	3.341303	5.262505	-3.088189
H	3.057032	-6.402982	-1.861912	H	6.397835	1.125857	1.021938
H	3.462906	-7.453975	-0.448991				
Zero-point correction= 0.793192 (Hartree/Particle)				Zero-point correction= 0.788447 (Hartree/Particle)			
Thermal correction to Energy= 0.850350				Thermal correction to Energy= 0.844658			
Thermal correction to Enthalpy= 0.851294				Thermal correction to Enthalpy= 0.845602			
Thermal correction to Gibbs Free Energy= 0.696976				Thermal correction to Gibbs Free Energy= 0.694834			
Sum of electronic and zero-point Energies= -3516.294582				Sum of electronic and zero-point Energies= -3441.136170			
Sum of electronic and thermal Energies= -3516.237425				Sum of electronic and thermal Energies= -3441.079959			
Sum of electronic and thermal Enthalpies= -3516.236480				Sum of electronic and thermal Enthalpies= -3441.079015			
Sum of electronic and thermal Free Energies= -3516.390799				Sum of electronic and thermal Free Energies= -3441.229784			

Ph(pOMe)+B-Ph(pMe)-IPr-VIII				**Ph(pMe)+B-Ph(pMe)-IPR-VIII**			
88				87			
IPrVIIImenysKOPh-OMe SCF Done: -2610.31388768 A.U.				IPrVIIImenysKOPh-Me SCF Done: -2535.14666787 A.U.			
Pd	-0.731542	-0.243465	-1.133387	Pd	-0.846990	-0.730496	-0.480858
N	-1.363186	-0.287948	1.733388	N	-0.846454	1.461787	1.473184
C	-0.321939	2.397930	1.929845	C	0.297884	3.414686	-0.327350
H	0.273479	1.646387	1.366190	H	0.742878	2.401088	-0.221462
C	-1.792820	2.122663	1.606831	C	-1.213711	3.247486	-0.166166
C	-2.295755	0.793015	1.522007	C	-1.762992	2.244485	0.677094
C	-0.435812	-0.652943	0.781821	C	-0.140448	0.390362	0.980614
C	-3.645937	0.486910	1.210807	C	-3.148332	1.978030	0.759978
C	-4.146669	-0.953241	1.132015	C	-3.692399	0.778195	1.527581
H	-3.272649	-1.588667	0.876865	H	-2.837018	0.123813	1.791475
C	-2.710026	3.169422	1.383368	C	-2.122764	4.065199	-0.863532
H	-2.365894	4.212308	1.435203	H	-1.740970	4.854636	-1.527382
C	-4.060385	2.901897	1.096019	C	-3.508569	3.878375	-0.738640
H	-4.762492	3.738072	0.942679	H	-4.200456	4.537784	-1.287010
C	-4.521211	1.577716	1.008761	C	-4.013825	2.834894	0.048396
H	-5.579100	1.379827	0.778389	H	-5.100746	2.665673	0.100968
C	-1.196762	-1.012327	2.914674	C	-0.448250	1.785101	2.770422
C	-5.192587	-1.182469	0.027017	C	-4.613824	-0.073287	0.630779
H	-5.443183	-2.262048	-0.019598	H	-4.803028	-1.060520	1.096155
H	-6.141443	-0.639844	0.231912	H	-5.588693	0.426878	0.442774
H	-4.810510	-0.904210	-0.976053	H	-4.119361	-0.260301	-0.344447
C	-4.707963	-1.391741	2.504780	C	-4.389650	1.204772	2.833887
H	-5.018751	-2.456832	2.473435	H	-4.763075	0.316226	3.385009
H	-3.968634	-1.278651	3.323135	H	-3.693863	1.755126	3.501741
H	-5.598537	-0.784552	2.775813	H	-5.256949	1.869961	2.630974
C	0.167042	3.781939	1.476727	C	0.707838	3.923988	-1.719151
H	-0.280541	4.600560	2.080401	H	0.439917	4.991900	-1.868707
H	1.267220	3.844883	1.605106	H	1.808194	3.841027	-1.837077
H	-0.061986	3.954286	0.406710	H	0.226803	3.318840	-2.512738
C	-0.026633	2.195452	3.433714	C	0.890115	4.312093	0.781096
H	-0.290169	1.178024	3.782616	H	0.684641	3.911907	1.793693
H	1.054702	2.346544	3.633868	H	1.991815	4.394804	0.669445
H	-0.595419	2.926608	4.046648	H	0.461719	5.335443	0.724092
C	-0.125565	-1.841765	2.713570	C	0.565026	0.920688	3.093004
H	0.364546	-2.566878	3.369731	H	1.180934	0.826373	3.991951
H	-1.841930	-0.865190	3.784744	H	-0.919998	2.595708	3.333463
N	0.335147	-1.595788	1.417834	N	0.756024	0.090962	1.984605
C	1.584119	-2.092192	0.901237	C	1.925545	-0.737063	1.810479
				C	3.148117	-0.074026	1.521240

C	2.774733	-1.528590	1.429443
C	1.576195	-3.078269	-0.115189
C	3.997447	-2.015868	0.927947
C	2.830160	-3.514200	-0.592703
C	4.026400	-2.997843	-0.073095
H	4.942715	-1.598446	1.309035
H	2.864187	-4.278849	-1.384025
H	4.993126	-3.357544	-0.460263
C	2.764634	-0.429698	2.494352
H	1.709646	-0.179282	2.726413
C	0.286080	-3.681415	-0.661846
H	-0.565958	-3.075802	-0.295398
C	3.411158	-0.924586	3.804151
H	2.915341	-1.844557	4.178077
H	4.487027	-1.160324	3.660889
H	3.339378	-0.147850	4.594381
C	3.417916	0.871368	1.989836
H	3.414618	1.639356	2.792044
H	4.470218	0.713658	1.674257
H	2.866866	1.278707	1.120701
C	0.101447	-5.119311	-0.132461
H	-0.858908	-5.542828	-0.493617
H	0.920662	-5.785758	-0.479031
H	0.094219	-5.144908	0.977661
C	0.221077	-3.623129	-2.199639
H	0.388096	-2.588366	-2.563144
H	0.967300	-4.294681	-2.676193
H	-0.789110	-3.921781	-2.542628
C	0.297410	1.445078	-1.291596
O	-0.356219	2.494513	-1.447722
C	4.618118	1.589885	-1.320786
C	3.867404	2.783819	-1.191830
H	4.552148	-0.561824	-1.570597
C	3.949973	0.351783	-1.470332
C	2.467458	2.719636	-1.206494
C	1.791367	1.483536	-1.312475
C	2.556830	0.300760	-1.447476
H	1.866304	3.637912	-1.124481
H	2.033571	-0.665559	-1.527599
H	4.364007	3.757870	-1.079528
K	-3.018351	1.973129	-2.294479
C	-2.684926	-0.833910	-2.576680
O	-1.652748	-0.053292	-2.990863
O	-3.829373	-0.670105	-3.055395
O	-2.374934	-1.623606	-1.571342
O	5.978915	1.527481	-1.296291
C	6.718184	2.733801	-1.163499
H	6.521850	3.436312	-2.005607
H	6.496767	3.254330	-0.203293
H	7.786993	2.447095	-1.177498

Zero-point correction=	0.702448 (Hartree/Particle)
Thermal correction to Energy=	0.749833
Thermal correction to Enthalpy=	0.750777
Thermal correction to Gibbs Free Energy=	0.623525
Sum of electronic and zero-point Energies=	-2609.611440
Sum of electronic and thermal Energies=	-2609.564055
Sum of electronic and thermal Enthalpies=	-2609.563110
Sum of electronic and thermal Free Energies=	-2609.690362

C	1.818740	-2.144653	1.913313
C	4.298999	-0.871192	1.369208
C	3.001611	-2.893838	1.736643
C	4.228771	-2.267454	1.477172
H	5.262645	-0.389484	1.140460
H	2.954735	-3.991286	1.810573
H	5.139062	-2.874691	1.347616
C	3.244139	1.444587	1.374248
H	2.219282	1.861372	1.427536
C	0.501514	-2.842360	2.228042
H	-0.319048	-2.107126	2.120783
C	4.043759	2.064691	2.538079
H	3.601663	1.799595	3.520913
H	5.096667	1.710453	2.537518
H	4.058196	3.171975	2.455277
C	3.814081	1.861039	0.006027
H	3.836909	2.967805	-0.079268
H	4.850942	1.493497	-0.143573
H	3.194314	1.465624	-0.820464
C	0.493897	-3.346572	3.686331
H	-0.484522	-3.811996	3.927609
H	1.286769	-4.106633	3.858309
H	0.664787	-2.515036	4.402294
C	0.191894	-3.972145	1.228459
H	0.228456	-3.591675	0.187009
H	0.900510	-4.823208	1.323273
H	-0.835670	-4.349792	1.397957
C	0.025017	0.269564	-1.952273
O	-0.621835	1.060986	-2.635272
C	4.233657	-0.423564	-2.837986
C	3.506631	0.603220	-3.485696
H	4.088471	-2.058298	-1.404446
C	3.548188	-1.248463	-1.919564
C	2.147994	0.806944	-3.212377
C	1.478814	-0.000558	-2.264119
C	2.194169	-1.035222	-1.626866
H	1.575873	1.600435	-3.717185
H	1.671775	-1.664838	-0.887457
H	4.021844	1.253884	-4.212406
K	-3.930074	-2.781976	-2.959490
C	-2.642739	-2.568558	-0.440596
O	-2.015898	-2.114267	-1.556491
O	-3.607678	-3.375664	-0.555969
O	-2.197561	-2.065235	0.667406
C	5.714501	-0.600049	-3.081115
H	6.008844	-0.276481	-4.100420
H	6.303239	0.012172	-2.361572
H	6.030838	-1.654466	-2.945374

Zero-point correction=	0.696644 (Hartree/Particle)
Thermal correction to Energy=	0.743802
Thermal correction to Enthalpy=	0.744746
Thermal correction to Gibbs Free Energy=	0.614978
Sum of electronic and zero-point Energies=	-2534.450024
Sum of electronic and thermal Energies=	-2534.402866
Sum of electronic and thermal Enthalpies=	-2534.401922
Sum of electronic and thermal Free Energies=	-2534.531690

Ph(pOMe)+B-Ph(pMe)-IPr-IX	**Ph(pMe)+B-Ph(pMe)-IPR-IX**
104	103
IPrIX-OMe SCF Done: -3018.33791272 A.U.	IPrIX-Me SCF Done: -2943.17974005 A.U.

Pd	-0.072405	0.283664	0.336427
K	2.983259	4.693787	0.406194
O	1.172773	3.980035	2.096424
H	0.837985	4.059040	3.005336
B	1.573476	2.571575	1.854012
O	2.937888	2.377570	2.358049
H	3.239081	1.469513	2.163999
C	0.469398	1.523058	2.486807
C	0.843512	0.550403	3.459768
C	-0.943485	1.666463	2.268920
C	-0.084701	-0.255786	4.128707
H	1.912812	0.427520	3.694813
C	-1.893728	0.868735	2.934771
H	-1.301933	2.462034	1.595460
C	-1.465507	-0.113064	3.848747
H	0.271799	-1.006640	4.847355
H	-2.968291	0.972874	2.723523
C	0.763852	2.942507	-0.569234
O	1.042017	3.982021	-1.211513
O	1.716215	2.463583	0.312796
O	-0.307256	2.243274	-0.691071
N	-2.033201	-0.356933	-1.800883
N	-0.100918	-1.188182	-2.338507
C	-0.764048	-0.556188	-1.321259
C	-2.152453	-0.839294	-3.104627
C	-0.933082	-1.362031	-3.446612
C	-3.115410	0.196833	-1.016030
C	-3.532509	1.525405	-1.273324
C	-4.592460	2.027977	-0.489102
C	-5.193101	1.244423	0.504135
C	-4.746383	-0.065220	0.742167
C	-3.695119	-0.624736	-0.009455
C	-2.897872	2.384300	-2.364114
H	-6.014927	1.660073	1.109036
C	-3.187954	-2.042453	0.255804
C	1.254503	-1.668388	-2.225606
C	1.448798	-2.993425	-1.759840
C	2.779900	-3.443763	-1.646546
C	3.853452	-2.607265	-1.980648
C	3.625446	-1.293032	-2.415142
C	2.317945	-0.782585	-2.531238
C	0.266048	-3.899539	-1.415687
H	4.885732	-2.975968	-1.874312
C	2.047520	0.663979	-2.940003
H	-3.093821	-0.777630	-3.656958
H	-0.581114	-1.836484	-4.366519
H	-4.942824	3.057267	-0.658619
H	-5.216282	-0.660267	1.537605
H	-1.898434	1.956009	-2.581826
H	-2.080351	-1.987144	0.252162
H	2.978808	-4.459279	-1.274048
H	4.482111	-0.639336	-2.635042
H	-0.573645	-3.243682	-1.102436
H	1.130783	0.987585	-2.403290
C	3.166730	1.636925	-2.527407
H	4.091399	1.489431	-3.126088
H	2.814812	2.677000	-2.680112
H	3.411170	1.531323	-1.451455
C	1.764658	0.772173	-4.454316
H	0.899129	0.149455	-4.757355
H	1.535638	1.822840	-4.729235
H	2.646214	0.441846	-5.044730
C	0.548246	-4.853266	-0.242663

Pd	-0.125217	0.285530	0.441080
K	2.498498	4.849610	-0.683160
O	1.094543	4.272398	1.419337
H	0.963328	4.469025	2.362158
B	1.616629	2.891402	1.284445
O	3.074305	2.922141	1.481736
H	3.443142	2.024181	1.379299
C	0.830763	1.848099	2.289586
C	1.534388	1.098179	3.279197
C	-0.597776	1.768153	2.348953
C	0.875710	0.321212	4.233797
H	2.635177	1.145689	3.291890
C	-1.264206	0.965705	3.311890
H	-1.200613	2.415604	1.690437
C	-0.540167	0.229863	4.263018
H	1.463963	-0.243485	4.977051
H	-2.366010	0.924274	3.300625
C	0.298233	2.841027	-0.936171
O	0.364067	3.781156	-1.762779
O	1.441764	2.547029	-0.213734
O	-0.720063	2.084609	-0.734414
N	-2.280068	-0.746920	-1.313573
N	-0.387042	-1.547051	-2.011341
C	-0.944128	-0.803484	-1.006495
C	-2.548520	-1.433338	-2.497175
C	-1.353873	-1.935451	-2.942062
C	-3.267368	-0.144922	-0.444524
C	-3.813762	1.114080	-0.793452
C	-4.750757	1.673798	0.100750
C	-5.111327	1.011657	1.281363
C	-4.548596	-0.235029	1.597753
C	-3.612246	-0.847292	0.742617
C	-3.445048	1.830654	-2.089516
H	-5.838289	1.473670	1.968580
C	-3.015005	-2.217664	1.061486
C	1.007563	-1.909431	-2.058697
C	1.394241	-3.138845	-1.468243
C	2.763374	-3.470516	-1.517341
C	3.689584	-2.614941	-2.128690
C	3.275351	-1.395211	-2.684547
C	1.923656	-1.001049	-2.646051
C	0.368768	-4.072768	-0.824990
H	4.755867	-2.889707	-2.148012
C	1.458573	0.348032	-3.191449
H	-3.560145	-1.504680	-2.905226
H	-1.100290	-2.522807	-3.828618
H	-5.193589	2.653888	-0.131225
H	-4.840851	-0.739298	2.530112
H	-2.451932	1.447916	-2.402012
H	-1.948188	-2.192161	0.759391
H	3.110707	-4.406649	-1.056647
H	4.023125	-0.720813	-3.126860
H	-0.468646	-3.441233	-0.458485
H	0.606171	0.678764	-2.560685
C	2.529394	1.449352	-3.098131
H	3.364097	1.283221	-3.812868
H	2.060722	2.426741	-3.330854
H	2.938821	1.520434	-2.070894
C	0.944748	0.212425	-4.641522
H	0.113533	-0.516881	-4.718281
H	0.571178	1.189825	-5.011793
H	1.759641	-0.127539	-5.316142
C	0.918601	-4.839177	0.389980

H	-0.386286	-5.375248	0.048777	H	0.091478	-5.370408	0.903812
H	1.291372	-5.633726	-0.511754	H	1.666854	-5.604619	0.092615
H	0.914433	-4.301681	0.643053	H	1.383524	-4.153759	1.122505
C	-0.191522	-4.697030	-2.657232	C	-0.200274	-5.062958	-1.866090
H	0.620673	-5.368250	-3.009231	H	0.606349	-5.715665	-2.262810
H	-1.075669	-5.322775	-2.413135	H	-0.972300	-5.712593	-1.402684
H	-0.470434	-4.033632	-3.499201	H	-0.667955	-4.543741	-2.725297
C	-2.658595	3.836615	-1.912644	C	-3.292497	3.352173	-1.912831
H	-2.047330	4.369521	-2.669079	H	-2.859850	3.795264	-2.832731
H	-3.609544	4.399162	-1.791893	H	-4.269477	3.849853	-1.729478
H	-2.090571	3.855153	-0.963968	H	-2.596302	3.575795	-1.083272
C	-3.755334	2.345129	-3.648638	C	-4.481081	1.513336	-3.191204
H	-4.763163	2.775089	-3.462642	H	-5.485861	1.893304	-2.906289
H	-3.276192	2.937795	-4.456314	H	-4.193155	1.996586	-4.148703
H	-3.902788	1.312330	-4.026234	H	-4.581987	0.424313	-3.376962
C	-3.566070	-2.585823	1.640755	C	-3.008305	-2.551467	2.558530
H	-4.653740	-2.802440	1.723477	H	-4.030047	-2.728833	2.958583
H	-3.022675	-3.535290	1.822451	H	-2.414747	-3.470997	2.733022
H	-3.283452	-1.881570	2.446802	H	-2.531795	-1.738608	3.137418
C	-3.624044	-3.032200	-0.847278	C	-3.714071	-3.330596	0.249986
H	-3.209048	-4.041040	-0.638472	H	-3.236709	-4.313002	0.451565
H	-4.731167	-3.119006	-0.886248	H	-4.787684	-3.406134	0.525982
H	-3.268951	-2.732362	-1.852936	H	-3.655112	-3.148612	-0.841945
C	1.964648	-1.560434	1.337886	C	2.212616	-1.253178	1.292304
C	2.856111	-0.637970	0.750212	C	2.915625	-0.364223	0.452756
C	2.479699	-2.602059	2.141080	C	2.936483	-2.123254	2.137054
C	4.239333	-0.760497	0.951091	C	4.318651	-0.352220	0.448254
C	3.862401	-2.723408	2.343586	C	4.339070	-2.107244	2.137062
C	4.746851	-1.803208	1.747837	C	5.035027	-1.221916	1.291319
H	2.447445	0.187067	0.142731	H	2.347884	0.332639	-0.185385
H	1.769794	-3.299282	2.612675	H	2.372748	-2.792841	2.805115
H	4.923129	-0.040333	0.473990	H	4.853319	0.336189	-0.225843
H	4.256689	-3.536794	2.973923	H	4.896521	-2.784462	2.804078
H	5.832861	-1.899329	1.907496	H	6.136839	-1.209897	1.291434
C	0.461875	-1.434565	1.168170	C	0.695797	-1.268999	1.351311
O	-0.284659	-2.303061	1.604788	O	0.109375	-2.133181	1.989297
O	-2.445933	-0.882478	4.412154	C	-1.219282	-0.654622	5.281382
C	-2.056662	-2.043648	5.134115	H	-2.316745	-0.500820	5.298085
H	-1.412614	-2.707817	4.514490	H	-1.031688	-1.725823	5.051556
H	-1.520449	-1.789390	6.077490	H	-0.829396	-0.468162	6.304682
H	-2.991680	-2.577940	5.390359				
Zero-point correction=			0.825512 (Hartree/Particle)	Zero-point correction=			0.820190 (Hartree/Particle)
Thermal correction to Energy=			0.882101	Thermal correction to Energy=			0.875117
Thermal correction to Enthalpy=			0.883045	Thermal correction to Enthalpy=			0.876061
Thermal correction to Gibbs Free Energy=			0.735162	Thermal correction to Gibbs Free Energy=			0.733018
Sum of electronic and zero-point Energies=			-3017.512401	Sum of electronic and zero-point Energies=			-2942.359550
Sum of electronic and thermal Energies=			-3017.455811	Sum of electronic and thermal Energies=			-2942.304624
Sum of electronic and thermal Enthalpies=			-3017.454867	Sum of electronic and thermal Enthalpies=			-2942.303679
Sum of electronic and thermal Free Energies=			-3017.602751	Sum of electronic and thermal Free Energies=			-2942.446722

Ph(pOMe)+B-Ph(pMe)-IPr-IX-X				**Ph(pMe)+B-Ph(pMe)-IPR-IX-X**			
104				103			
IPrIX-X-OMe SCF Done: -3018.31766681 A.U.				IPrIX-X-Me SCF Done: -2943.16102026 A.U.			
Pd	-0.159006	-0.182105	-0.046062	Pd	-0.218064	-0.262744	-0.179115
K	-2.614361	-0.848479	4.875285	K	-2.569549	-2.764228	4.142682
O	-2.995390	-1.798012	2.504301	O	-2.719844	-3.014284	1.568682
H	-3.511084	-2.319538	1.861579	H	-3.080667	-3.450710	0.775050
B	-1.615679	-1.782512	2.096282	B	-1.354661	-2.632846	1.318068
O	-1.023960	-3.032383	1.948117	O	-0.504884	-3.674310	0.956512
H	-0.100216	-2.961230	1.632588	H	0.403222	-3.356934	0.776620
C	-2.065249	-1.154637	-0.000085	C	-1.815984	-1.630278	-0.614035
C	-2.388197	-2.378292	-0.640597	C	-1.757432	-2.671810	-1.578712

C	-3.079294	-0.144958	-0.047519	C	-3.035944	-0.890261	-0.569777
C	-3.622913	-2.610947	-1.276206	C	-2.829126	-2.955800	-2.442114
H	-1.654230	-3.200245	-0.617153	H	-0.849603	-3.294397	-1.636934
C	-4.310510	-0.347712	-0.675562	C	-4.105787	-1.167004	-1.432639
H	-2.888795	0.834275	0.421728	H	-3.144346	-0.071028	0.159872
C	-4.593668	-1.584290	-1.302359	C	-4.022071	-2.200815	-2.393427
H	-3.809732	-3.583358	-1.754845	H	-2.735708	-3.772258	-3.179308
H	-5.071593	0.447155	-0.716295	H	-5.022431	-0.554750	-1.372586
C	-1.100414	0.600751	2.768619	C	-1.456826	-0.474297	2.610790
O	-1.476251	1.138228	3.840483	O	-1.986843	-0.348169	3.742331
O	-0.870932	-0.792419	2.831581	O	-0.877806	-1.738148	2.343698
O	-0.866617	1.172308	1.667124	O	-1.346303	0.405501	1.711623
N	0.754999	2.389745	-1.228447	N	0.110386	2.664962	-0.595731
N	2.541018	1.278648	-0.705164	N	2.073150	1.880896	-0.117711
C	1.174499	1.223308	-0.637212	C	0.762360	1.506652	-0.251904
C	1.837031	3.143251	-1.679571	C	0.998981	3.733340	-0.698157
C	2.969620	2.449152	-1.339936	C	2.240674	3.243265	-0.385231
C	-0.633610	2.801320	-1.224387	C	-1.332918	2.738341	-0.676981
C	-1.071152	3.646651	-0.171297	C	-2.039015	3.162885	0.478856
C	-2.438304	3.985157	-0.149100	C	-3.445539	3.156669	0.407341
C	-3.322246	3.491227	-1.119973	C	-4.108638	2.735729	-0.754959
C	-2.859660	2.644350	-2.136757	C	-3.379845	2.313747	-1.875570
C	-1.502594	2.272695	-2.209856	C	-1.970985	2.299122	-1.862467
C	-0.103460	4.194631	0.875653	C	-1.313423	3.644206	1.734363
H	-4.390301	3.758548	-1.073922	H	-5.210206	2.725170	-0.782574
C	-0.992425	1.361501	-3.320709	C	-1.176499	1.869470	-3.091810
C	3.394286	0.330568	-0.036115	C	3.088722	1.001039	0.401644
C	4.130772	-0.596056	-0.812299	C	4.077416	0.500545	-0.479200
C	4.977554	-1.488177	-0.121843	C	5.066521	-0.340627	0.071520
C	5.062668	-1.464999	1.276009	C	5.052973	-0.674724	1.431516
C	4.285294	-0.563046	2.020894	C	4.037191	-0.191929	2.272559
C	3.423966	0.353852	1.386641	C	3.022208	0.651620	1.779610
C	4.017017	-0.635059	-2.334470	C	4.086748	0.861356	-1.963144
H	5.726589	-2.174064	1.795779	H	5.832227	-1.337912	1.839709
C	2.551948	1.320083	2.189061	C	1.897810	1.163394	2.680429
H	1.702073	4.097041	-2.196694	H	0.668354	4.736166	-0.981298
H	4.029245	2.680501	-1.478239	H	3.216129	3.732297	-0.317425
H	-2.819066	4.631364	0.655683	H	-4.030270	3.469760	1.285068
H	-3.567541	2.242050	-2.876209	H	-3.911945	1.966319	-2.773372
H	0.741280	3.478181	0.945688	H	-0.310538	3.168388	1.736593
H	-0.061722	0.875201	-2.967681	H	-0.160610	1.573204	-2.763726
H	5.562274	-2.226477	-0.690946	H	5.848536	-0.754031	-0.582961
H	4.340221	-0.579272	3.119345	H	4.025813	-0.487050	3.332047
H	3.073933	-0.116235	-2.607860	H	3.066636	1.214393	-2.222936
H	1.599034	1.435192	1.632508	H	0.980383	1.217869	2.059395
C	2.150214	0.786414	3.573004	C	1.550504	0.211122	3.836084
H	3.007455	0.743342	4.279680	H	2.351685	0.163860	4.605248
H	1.381140	1.451719	4.015553	H	0.623138	0.558558	4.334846
H	1.699669	-0.224003	3.493000	H	1.351642	-0.813265	3.459490
C	3.207131	2.714112	2.285279	C	2.198129	2.589233	3.189377
H	3.407935	3.141063	1.281218	H	2.359062	3.295922	2.349507
H	2.535952	3.417643	2.821108	H	1.345836	2.969900	3.790400
H	4.170788	2.665424	2.836788	H	3.107548	2.601753	3.827914
C	3.915649	-2.069434	-2.886296	C	4.386780	-0.345593	-2.870789
H	3.688380	-2.040294	-3.971532	H	4.248149	-0.060520	-3.933746
H	4.867140	-2.629351	-2.761691	H	5.433233	-0.700951	-2.757102
H	3.106989	-2.637042	-2.388114	H	3.703652	-1.188655	-2.657121
C	5.195679	0.117790	-2.989523	C	5.085509	2.007226	-2.238161
H	6.160764	-0.373472	-2.740614	H	6.121647	1.690717	-1.991385
H	5.090695	0.125505	-4.094822	H	5.062840	2.298546	-3.309315
H	5.260970	1.170027	-2.646176	H	4.862780	2.910649	-1.635267
C	-0.709749	4.310979	2.285256	C	-2.003010	3.239110	3.049002
H	0.082842	4.601866	3.007298	H	-1.360426	3.525579	3.908755

H	-1.489947	5.101200	2.334051	H	-2.972099	3.765648	3.186729
H	-1.143150	3.348566	2.618512	H	-2.172344	2.146290	3.092606
C	0.460225	5.561102	0.423451	C	-1.117518	5.176721	1.681856
H	-0.354891	6.313762	0.362448	H	-2.101376	5.692924	1.693018
H	1.215941	5.932481	1.147833	H	-0.535756	5.528660	2.560112
H	0.940951	5.511003	-0.573808	H	-0.583676	5.502424	0.766748
C	-1.961396	0.214553	-3.653321	C	-1.768131	0.635433	-3.792269
H	-2.889175	0.573978	-4.148092	H	-2.754929	0.846401	-4.257702
H	-1.466951	-0.502196	-4.339132	H	-1.082109	0.296419	-4.594212
H	-2.245678	-0.337912	-2.736245	H	-1.889781	-0.201412	-3.077610
C	-0.642055	2.199040	-4.569344	C	-1.026371	3.064614	-4.058093
H	-0.225031	1.552777	-5.370497	H	-0.410996	2.782269	-4.938429
H	-1.543869	2.709257	-4.971806	H	-2.018024	3.406172	-4.426122
H	0.109934	2.982098	-4.334684	H	-0.537686	3.928913	-3.560114
C	1.113860	-2.743467	-0.669458	C	1.715453	-2.217256	-1.182865
C	1.789787	-2.713411	0.569507	C	2.215290	-2.361013	0.129515
C	0.944418	-3.976953	-1.335909	C	1.970860	-3.226855	-2.136463
C	2.299402	-3.897796	1.127736	C	2.976258	-3.489056	0.478769
C	1.419497	-5.164567	-0.756860	C	2.698158	-4.372022	-1.774375
C	2.103393	-5.127930	0.473149	C	3.208797	-4.502937	-0.468906
H	1.936265	-1.746382	1.075417	H	2.019323	-1.563413	0.863495
H	0.432268	-3.981704	-2.310628	H	1.585551	-3.093101	-3.159278
H	2.851943	-3.852890	2.079400	H	3.386233	-3.571438	1.497614
H	1.261619	-6.126959	-1.269987	H	2.874420	-5.167804	-2.516004
H	2.486401	-6.059312	0.919823	H	3.790346	-5.396501	-0.191227
C	0.583793	-1.479384	-1.326535	C	0.928247	-0.988041	-1.607286
O	0.634322	-1.376444	-2.548502	O	1.041811	-0.569232	-2.754506
O	-5.819994	-1.685949	-1.901345	C	-5.151547	-2.452506	-3.366077
C	-6.138156	-2.884223	-2.589243	H	-5.147081	-3.494881	-3.745944
H	-5.425720	-3.090681	-3.421545	H	-6.143004	-2.254797	-2.907850
H	-6.151909	-3.768350	-1.909278	H	-5.064797	-1.782559	-4.250850
H	-7.152051	-2.744050	-3.011775				
Zero-point correction= 0.823571 (Hartree/Particle)				Zero-point correction= 0.817972 (Hartree/Particle)			
Thermal correction to Energy= 0.880053				Thermal correction to Energy= 0.873941			
Thermal correction to Enthalpy= 0.880997				Thermal correction to Enthalpy= 0.874885			
Thermal correction to Gibbs Free Energy= 0.734061				Thermal correction to Gibbs Free Energy= 0.728196			
Sum of electronic and zero-point Energies= -3017.494096				Sum of electronic and zero-point Energies= -2942.343049			
Sum of electronic and thermal Energies= -3017.437614				Sum of electronic and thermal Energies= -2942.287079			
Sum of electronic and thermal Enthalpies= -3017.436670				Sum of electronic and thermal Enthalpies= -2942.286135			
Sum of electronic and thermal Free Energies= -3017.583605				Sum of electronic and thermal Free Energies= -2942.432824			

Ph(pOMe)+B-Ph(pMe)-IPr-X				**Ph(pMe)+B-Ph(pMe)-IPR-X**			
104				103			
IPrX-OMe SCF Done: -3018.34080876 A.U.				IPrX-Me SCF Done: -2943.18612277 A.U.			
Pd	0.193319	-0.250521	0.196284	Pd	-0.211274	0.374091	0.268609
K	3.753567	0.948638	-1.607759	K	-4.096672	0.113514	-1.505318
O	2.823326	-1.676477	-2.505979	O	-2.532367	2.455830	-2.262386
H	3.174164	-2.449522	-2.014661	H	-2.659166	3.250095	-1.700739
B	1.450104	-1.843872	-2.663514	B	-1.166069	2.279388	-2.471131
O	0.913930	-3.103270	-2.624520	O	-0.325025	3.355670	-2.373109
H	-0.051950	-3.087014	-2.477727	H	0.605290	3.086690	-2.240848
C	1.878428	-1.432695	0.464642	C	-1.579388	1.895068	0.653196
C	2.034367	-2.831493	0.276597	C	-1.419168	3.299060	0.545704
C	3.052764	-0.741821	0.857437	C	-2.878531	1.455089	1.030161
C	3.278996	-3.475613	0.378858	C	-2.496336	4.192653	0.711118
H	1.162129	-3.444115	0.001185	H	-0.434381	3.716274	0.283116
C	4.317402	-1.364693	0.995256	C	-3.956766	2.344354	1.223172
H	2.991856	0.336886	1.095636	H	-3.055583	0.376494	1.200057
C	4.438455	-2.746671	0.731392	C	-3.792524	3.735886	1.043296
H	3.378558	-4.559769	0.208914	H	-2.323942	5.276634	0.588095
H	5.180428	-0.772144	1.338768	H	-4.942752	1.953587	1.538660
C	1.253557	0.517817	-2.655214	C	-1.582869	-0.049373	-2.593704

O	1.872879	1.064506	-3.583827	O	-2.349039	-0.380211	-3.516212
O	0.653339	-0.734135	-2.893565	O	-0.693985	1.023217	-2.814861
O	1.151645	0.956284	-1.456888	O	-1.555491	-0.551117	-1.418089
N	-0.816167	2.456996	0.953705	N	0.147312	-2.541158	0.863572
N	-2.561470	1.324696	0.365415	N	2.080862	-1.839303	0.195563
C	-1.194373	1.243605	0.422464	C	0.782080	-1.430648	0.350211
C	-1.920491	3.258399	1.243535	C	1.036151	-3.599016	1.051375
C	-3.026946	2.546103	0.863352	C	2.259866	-3.159788	0.620588
C	0.569708	2.833690	1.099375	C	-1.278742	-2.578030	1.091293
C	1.159665	3.621897	0.078503	C	-2.102236	-3.160227	0.093894
C	2.528968	3.937042	0.217588	C	-3.496830	-3.130949	0.310801
C	3.271484	3.461776	1.311524	C	-4.036826	-2.529633	1.459511
C	2.657597	2.673642	2.300115	C	-3.192646	-1.959378	2.426856
C	1.288551	2.343382	2.220392	C	-1.791394	-1.972581	2.267745
C	0.337836	4.155908	-1.092470	C	-1.508177	-3.844480	-1.134907
H	4.338899	3.723228	1.405923	H	-5.128871	-2.520307	1.613545
C	0.588966	1.547082	3.318478	C	-0.860833	-1.420252	3.343574
C	-3.383639	0.323069	-0.265517	C	3.093627	-1.040725	-0.448987
C	-4.182540	-0.516236	0.548512	C	4.114299	-0.467481	0.347473
C	-4.983075	-1.476974	-0.103486	C	5.105263	0.286553	-0.315056
C	-4.973219	-1.595059	-1.498204	C	5.065765	0.465766	-1.702465
C	-4.150815	-0.765195	-2.277177	C	4.022237	-0.087791	-2.461617
C	-3.327489	0.211011	-1.683372	C	3.002118	-0.848709	-1.856891
C	-4.204508	-0.376988	2.069674	C	4.166848	-0.666410	1.861254
H	-5.600475	-2.357008	-1.987454	H	5.846184	1.062813	-2.200383
C	-2.395402	1.092642	-2.519360	C	1.829334	-1.407398	-2.668666
H	-1.819915	4.250781	1.690983	H	0.721701	-4.557983	1.471598
H	-4.090618	2.797351	0.886686	H	3.228246	-3.663797	0.561693
H	3.016040	4.570039	-0.541073	H	-4.166480	-3.594660	-0.430772
H	3.249760	2.309372	3.152595	H	-3.627550	-1.494518	3.323821
H	-0.526606	3.471820	-1.221338	H	-0.508836	-3.393538	-1.308106
H	-0.249906	0.990028	2.854241	H	0.073332	-1.086950	2.848996
H	-5.610283	-2.153333	0.496127	H	5.910279	0.753183	0.271943
H	-4.139594	-0.890583	-3.369319	H	3.994596	0.089147	-3.546222
H	-3.272819	0.149114	2.366983	H	3.149696	-0.962580	2.193638
H	-1.431112	1.140963	-1.967529	H	0.912567	-1.201143	-2.073830
C	-2.080528	0.516520	-3.908704	C	1.636539	-0.717999	-4.028351
H	-2.962899	0.547668	-4.583976	H	2.451407	-0.968023	-4.741878
H	-1.274806	1.111198	-4.385236	H	0.680819	-1.051044	-4.481207
H	-1.713002	-0.526027	-3.843909	H	1.573959	0.382621	-3.923385
C	-2.933753	2.535555	-2.646126	C	1.932033	-2.937719	-2.856447
H	-3.091718	3.015112	-1.659739	H	1.978122	-3.480523	-1.891819
H	-2.214460	3.163528	-3.212726	H	1.045778	-3.313581	-3.409411
H	-3.902167	2.547014	-3.190738	H	2.838934	-3.202296	-3.441186
C	-4.206405	-1.731908	2.799910	C	4.531234	0.621626	2.622415
H	-4.084066	-1.571245	3.890590	H	4.423740	0.456685	3.713952
H	-5.160381	-2.281649	2.651675	H	5.582184	0.929120	2.435639
H	-3.372070	-2.371830	2.458935	H	3.862861	1.456483	2.341751
C	-5.413766	0.474610	2.517051	C	5.150418	-1.801503	2.223895
H	-6.366394	-0.027905	2.244203	H	6.183356	-1.536852	1.911664
H	-5.406182	0.618807	3.617926	H	5.159093	-1.978017	3.320024
H	-5.421669	1.476392	2.042488	H	4.890008	-2.757846	1.727316
C	1.096602	4.185491	-2.430055	C	-2.325394	-3.644374	-2.422303
H	0.409795	4.506578	-3.240943	H	-1.787726	-4.099237	-3.280336
H	1.932986	4.917730	-2.416725	H	-3.315495	-4.147413	-2.367834
H	1.489590	3.187605	-2.705356	H	-2.472983	-2.572098	-2.654448
C	-0.205041	5.564867	-0.759321	C	-1.316693	-5.353984	-0.858812
H	0.632995	6.285797	-0.646794	H	-2.300237	-5.847945	-0.706659
H	-0.865594	5.931718	-1.572782	H	-0.814325	-5.847936	-1.716910
H	-0.785363	5.580087	0.184205	H	-0.707735	-5.542284	0.047175
C	1.476066	0.481166	3.977476	C	-1.412755	-0.182163	4.065518
H	2.312096	0.922447	4.562693	H	-2.296987	-0.415745	4.697420
H	0.863426	-0.126886	4.672309	H	-0.628189	0.238120	4.725361

H	1.891072	-0.209849	3.217558
C	-0.002293	2.519079	4.363991
H	-0.567745	1.957870	5.136893
H	0.801286	3.094259	4.872814
H	-0.696581	3.248803	3.897589
C	-1.308887	-2.684237	0.707126
C	-1.670787	-2.637582	-0.655618
C	-1.473169	-3.889131	1.422771
C	-2.212345	-3.767332	-1.288324
C	-1.975159	-5.033094	0.779510
C	-2.352609	-4.973865	-0.574689
H	-1.534435	-1.689179	-1.201000
H	-1.193074	-3.907600	2.487780
H	-2.539789	-3.702641	-2.339061
H	-2.078999	-5.977063	1.338591
H	-2.761329	-5.866976	-1.073903
C	-0.754995	-1.461164	1.420455
O	-0.928879	-1.330320	2.629538
O	5.606159	-3.463195	0.810328
C	6.780542	-2.788430	1.219982
H	7.063005	-1.966592	0.518210
H	6.682621	-2.356660	2.243992
H	7.592282	-3.541427	1.226911
Zero-point correction=			0.824028 (Hartree/Particle)
Thermal correction to Energy=			0.881412
Thermal correction to Enthalpy=			0.882356
Thermal correction to Gibbs Free Energy=			0.731638
Sum of electronic and zero-point Energies=			-3017.516781
Sum of electronic and thermal Energies=			-3017.459397
Sum of electronic and thermal Enthalpies=			-3017.458453
Sum of electronic and thermal Free Energies=			-3017.609171

H	-1.687102	0.607202	3.337901
C	-0.497094	-2.545658	4.337687
H	0.224461	-2.174599	5.095349
H	-1.400033	-2.913330	4.871349
H	-0.034414	-3.412896	3.821581
C	1.855072	2.369857	0.766206
C	2.190494	2.281059	-0.601891
C	2.273842	3.495092	1.507387
C	2.949881	3.289441	-1.215603
C	2.997969	4.525176	0.882909
C	3.342991	4.422841	-0.477194
H	1.868044	1.392354	-1.168486
H	2.014953	3.545312	2.576592
H	3.246577	3.183249	-2.271792
H	3.301128	5.412467	1.461914
H	3.923607	5.224023	-0.961749
C	1.063312	1.274729	1.464716
O	1.260365	1.045826	2.654601
C	-4.932302	4.705653	1.267379
H	-4.901843	5.130160	2.295555
H	-4.885495	5.563638	0.564626
H	-5.921165	4.216615	1.146207
Zero-point correction=			0.819293 (Hartree/Particle)
Thermal correction to Energy=			0.875889
Thermal correction to Enthalpy=			0.876833
Thermal correction to Gibbs Free Energy=			0.727515
Sum of electronic and zero-point Energies=			-2942.366830
Sum of electronic and thermal Energies=			-2942.310234
Sum of electronic and thermal Enthalpies=			-2942.309289
Sum of electronic and thermal Free Energies=			-2942.458607

Ph(pMe)+B-Ph(pMe)-IPr-XI			
94			
IPrXI-OMe SCF Done: -1978.05463001 A.U.			
Pd	0.527089	0.333770	-0.146171
C	2.041004	1.681355	-0.346217
C	2.075610	3.079913	-0.568022
C	3.288337	1.030399	-0.182424
C	3.282643	3.792756	-0.599337
H	1.135810	3.636500	-0.720872
C	4.515060	1.727308	-0.204430
H	3.331791	-0.066006	-0.034080
C	4.513020	3.122808	-0.414498
H	3.305785	4.880831	-0.770400
H	5.454027	1.170798	-0.067557
N	-0.001306	-2.585147	0.160578
N	-1.946267	-1.644657	0.209555
C	-0.609706	-1.355735	0.105552
C	-0.926822	-3.619457	0.287828
C	-2.162058	-3.022865	0.315985
C	1.436666	-2.696476	0.171601
C	2.104448	-2.557185	1.415901
C	3.512288	-2.620254	1.404641
C	4.215939	-2.802639	0.204807
C	3.527366	-2.910130	-1.012825
C	2.119836	-2.855894	-1.059729
C	1.347553	-2.256095	2.707205
H	5.316690	-2.840847	0.216285
C	1.378551	-2.865274	-2.392933
C	-2.971150	-0.631551	0.289987
C	-3.803536	-0.422584	-0.836539

Ph(pOMe)+B-Ph(pMe)-IPR-XI			
93			
IPrXI-Me SCF Done: -1902.89964382 A.U.			
Pd	0.580745	0.515136	-0.223238
C	1.765792	2.149822	-0.484482
C	1.511148	3.495217	-0.829048
C	3.115592	1.799041	-0.214978
C	2.546204	4.448581	-0.878025
H	0.483449	3.818869	-1.065274
C	4.149469	2.751007	-0.258928
H	3.383149	0.752978	0.030972
C	3.882165	4.098511	-0.588939
H	2.310907	5.492584	-1.150207
H	5.186721	2.440360	-0.041047
N	0.671162	-2.437312	0.244483
N	-1.420937	-1.903140	0.326987
C	-0.175333	-1.361522	0.143860
C	-0.021424	-3.624805	0.474585
C	-1.350245	-3.286358	0.523325
C	2.101839	-2.253832	0.211570
C	2.751901	-1.879186	1.416100
C	4.140395	-1.644168	1.354105
C	4.838997	-1.767897	0.144294
C	4.163235	-2.121185	-1.033611
C	2.776481	-2.370606	-1.029469
C	1.982321	-1.654028	2.715774
H	5.921847	-1.568746	0.114818
C	2.020152	-2.642995	-2.325838
C	-2.626185	-1.111967	0.396877
C	-3.522501	-1.149699	-0.698585

C	-4.799921	0.568670	-0.729509	C	-4.697414	-0.376732	-0.599826
C	-4.933400	1.331819	0.436334	C	-4.944348	0.416378	0.526883
C	-4.075428	1.121513	1.526344	C	-4.024288	0.454754	1.585196
C	-3.073093	0.133701	1.485800	C	-2.842647	-0.309640	1.552384
C	-3.652245	-1.241560	-2.117219	C	-3.251170	-1.998680	-1.939293
H	-5.700060	2.120086	0.491509	H	-5.854496	1.034085	0.574632
C	-2.117516	-0.093277	2.659929	C	-1.827450	-0.271606	2.697597
H	-0.624583	-4.669139	0.349761	H	0.488260	-4.586621	0.584284
H	-3.165614	-3.445771	0.415537	H	-2.244160	-3.893774	0.690488
H	4.065992	-2.505093	2.349366	H	4.677778	-1.338864	2.265448
H	4.093723	-3.018297	-1.950606	H	4.719927	-2.184732	-1.981023
H	0.263977	-2.379296	2.503604	H	0.939741	-2.000379	2.560730
H	0.294991	-2.973392	-2.174477	H	1.016226	-3.033119	-2.053639
H	-5.464537	0.760746	-1.585342	H	-5.416889	-0.378057	-1.432618
H	-4.177683	1.756162	2.417049	H	-4.225601	1.109553	2.443984
H	-2.645131	-1.709705	-2.094185	H	-2.171589	-2.259979	-1.932900
H	-1.100609	-0.151987	2.212104	H	-0.830434	-0.155924	2.217502
C	-2.091728	1.056429	3.678392	C	-2.003117	0.920565	3.650378
H	-3.038564	1.120098	4.256685	H	-2.929956	0.834106	4.257433
H	-1.273586	0.890115	4.409295	H	-1.150557	0.960300	4.359274
H	-1.918130	2.035370	3.192232	H	-2.036761	1.883010	3.105133
C	-2.394577	-1.426627	3.389918	C	-1.816330	-1.586640	3.509232
H	-2.332261	-2.303732	2.717170	H	-1.613788	-2.475458	2.880909
H	-1.653321	-1.578441	4.202906	H	-1.028988	-1.546697	4.291450
H	-3.406439	-1.418838	3.848438	H	-2.792953	-1.742128	4.015391
C	-3.718132	-0.377020	-3.390552	C	-3.521628	-1.238060	-3.251510
H	-3.509331	-1.002360	-4.283548	H	-3.219331	-1.860692	-4.119287
H	-4.724494	0.070216	-3.535196	H	-4.599797	-1.003771	-3.379202
H	-2.963662	0.432366	-3.355036	H	-2.940272	-0.296459	-3.285317
C	-4.708424	-2.367953	-2.166304	C	-4.066348	-3.309712	-1.886665
H	-5.733335	-1.940137	-2.196492	H	-5.155772	-3.092040	-1.891153
H	-4.573831	-2.995550	-3.072322	H	-3.842327	-3.948838	-2.766549
H	-4.654217	-3.031645	-1.279386	H	-3.851781	-3.899466	-0.972086
C	1.567383	-0.784944	3.119950	C	1.914494	-0.147529	3.043621
H	0.956195	-0.530983	4.011392	H	1.298458	0.029255	3.950135
H	2.633084	-0.587458	3.360738	H	2.925350	0.275380	3.221801
H	1.279120	-0.088120	2.298406	H	1.459026	0.427441	2.203606
C	1.709663	-3.227759	3.846352	C	2.561301	-2.467744	3.888996
H	2.769700	-3.120312	4.159384	H	3.589893	-2.140451	4.149841
H	1.081392	-3.025732	4.739037	H	1.933930	-2.336722	4.795479
H	1.551062	-4.283757	3.544701	H	2.601413	-3.550629	3.650263
C	1.567387	-1.508284	-3.106039	C	1.804793	-1.317738	-3.089923
H	2.636459	-1.334590	-3.351664	H	2.777617	-0.872500	-3.387418
H	0.982228	-1.476416	-4.048081	H	1.200797	-1.485533	-4.005449
H	1.226267	-0.669433	-2.459809	H	1.272506	-0.573269	-2.456787
C	1.791503	-4.049818	-3.287311	C	2.705495	-3.706042	-3.204925
H	1.175378	-4.067443	-4.210289	H	2.072673	-3.939668	-4.086160
H	2.852724	-3.973971	-3.605711	H	3.682935	-3.350839	-3.594403
H	1.663293	-5.021848	-2.766675	H	2.884752	-4.648876	-2.647098
C	-1.489957	2.480044	-0.578733	C	-1.845356	2.195040	-0.675135
C	-1.147539	2.946751	0.706171	C	-1.563548	2.809740	0.561338
C	-2.562736	3.081783	-1.273895	C	-3.041285	2.517876	-1.354811
C	-1.859823	4.006833	1.286064	C	-2.460816	3.738145	1.109801
C	-3.283508	4.131850	-0.687078	C	-3.943684	3.436389	-0.799300
C	-2.931986	4.598983	0.592875	C	-3.655027	4.050054	0.433537
H	-0.304378	2.461133	1.226635	H	-0.619235	2.548451	1.067962
H	-2.818852	2.703439	-2.274906	H	-3.247915	2.030184	-2.319306
H	-1.575515	4.378316	2.283453	H	-2.226064	4.226133	2.069157
H	-4.125719	4.589699	-1.230141	H	-4.879204	3.675657	-1.329775
C	-0.740840	1.354817	-1.251185	H	-4.360512	4.777326	0.866785
O	-0.950052	1.041996	-2.411528	C	-0.905310	1.202783	-1.315284
O	5.638468	3.908231	-0.463103	O	-1.083178	0.783701	-2.447426
C	6.898125	3.284270	-0.304827	C	4.993987	5.125306	-0.611999

H	7.001535	2.785527	0.688388
H	7.096329	2.525418	-1.098850
H	7.659386	4.085288	-0.380818
H	-3.493014	5.429892	1.050170

Zero-point correction=	0.770650 (Hartree/Particle)
Thermal correction to Energy=	0.818623
Thermal correction to Enthalpy=	0.819568
Thermal correction to Gibbs Free Energy=	0.687811
Sum of electronic and zero-point Energies=	-1977.283980
Sum of electronic and thermal Energies=	-1977.236007
Sum of electronic and thermal Enthalpies=	-1977.235062
Sum of electronic and thermal Free Energies=	-1977.366819

H	5.310310	5.402907	0.418323
H	5.897134	4.739305	-1.130973
H	4.681323	6.058625	-1.123338

Zero-point correction=	0.765950 (Hartree/Particle)
Thermal correction to Energy=	0.813027
Thermal correction to Enthalpy=	0.813971
Thermal correction to Gibbs Free Energy=	0.684785
Sum of electronic and zero-point Energies=	-1902.133694
Sum of electronic and thermal Energies=	-1902.086617
Sum of electronic and thermal Enthalpies=	-1902.085673
Sum of electronic and thermal Free Energies=	-1902.214859

Ph(pOMe)+B-Ph(pMe)-IPr-XI-XII

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IPrXI-XII-OMe SCF Done: -1978.04890257 A.U.

Pd	0.479220	0.280781	0.083517
C	1.551064	2.083009	-0.095172
C	1.546623	3.014378	0.974377
C	2.701723	2.015656	-0.912024
C	2.676378	3.790174	1.258906
H	0.645181	3.136729	1.594724
C	3.847861	2.778206	-0.636154
H	2.681897	1.364265	-1.801602
C	3.839659	3.670140	0.462729
H	2.688279	4.510162	2.091852
H	4.728051	2.688328	-1.289056
N	0.165776	-2.718982	0.245126
N	-1.801676	-1.829637	0.296203
C	-0.471084	-1.500250	0.198585
C	-0.734931	-3.775610	0.375601
C	-1.984282	-3.211114	0.409114
C	1.585714	-2.843634	0.037935
C	2.447731	-2.768451	1.158448
C	3.832306	-2.863289	0.914516
C	4.324938	-3.018328	-0.390425
C	3.444599	-3.065810	-1.482022
C	2.051057	-2.972860	-1.294315
C	1.904393	-2.488742	2.557477
H	5.411303	-3.087752	-0.559954
C	1.098746	-2.915302	-2.486029
C	-2.871056	-0.864566	0.228280
C	-3.206956	-0.310938	-1.035941
C	-4.263270	0.621738	-1.060310
C	-4.952570	0.968720	0.109809
C	-4.588994	0.411335	1.343685
C	-3.527499	-0.510063	1.433351
C	-2.448535	-0.705888	-2.305676
H	-5.769259	1.705696	0.062197
C	-3.039063	-1.043336	2.781609
H	-0.405653	-4.817969	0.421022
H	-2.979945	-3.657284	0.493578
H	4.537009	-2.801183	1.758063
H	3.846498	-3.158686	-2.503114
H	0.816286	-2.713341	2.545138
H	0.061307	-2.990512	-2.099053
H	-4.544124	1.096910	-2.010183
H	-5.124264	0.715886	2.254999
H	-1.370265	-0.704228	-2.037450
H	-2.652405	-2.072424	2.617964
C	-1.853052	-0.192802	3.291065
H	-2.177180	0.854159	3.472495

Ph(pMe)+B-Ph(pMe)-IPR-XI-XII

93

IPrXI-XII-Me SCF Done: -1902.89264340 A.U.

Pd	0.396923	0.587477	0.058665
C	0.671381	2.667158	-0.157843
C	0.323853	3.519062	0.914390
C	1.771774	3.025616	-0.973459
C	1.099190	4.656437	1.204295
H	-0.558762	3.296592	1.533687
C	2.548850	4.151659	-0.673090
H	1.994893	2.412865	-1.862610
C	2.227842	4.986924	0.424755
H	0.819215	5.304171	2.052626
H	3.415892	4.403602	-1.307741
N	1.313784	-2.279948	0.264109
N	-0.845793	-2.255514	0.316973
C	0.240890	-1.421222	0.206153
C	0.913685	-3.607069	0.416880
C	-0.457319	-3.591801	0.451018
C	2.664589	-1.824151	0.056613
C	3.416975	-1.390267	1.174694
C	4.724138	-0.923491	0.930937
C	5.243766	-0.885464	-0.372019
C	4.461626	-1.297059	-1.461826
C	3.148536	-1.772373	-1.274422
C	2.797976	-1.324049	2.568566
H	6.267102	-0.514573	-0.542021
C	2.259364	-2.116604	-2.466575
C	-2.211694	-1.798518	0.241841
C	-2.734820	-1.428803	-1.026243
C	-4.071868	-0.984808	-1.056152
C	-4.844443	-0.928055	0.112018
C	-4.294699	-1.291402	1.349348
C	-2.957111	-1.721810	1.444900
C	-1.879330	-1.502476	-2.293078
H	-5.884035	-0.569232	0.059730
C	-2.299681	-2.006672	2.796792
H	1.633932	-4.428588	0.473863
H	-1.189028	-4.399959	0.546415
H	5.339367	-0.569664	1.772552
H	4.871963	-1.231954	-2.481684
H	1.884045	-1.955919	2.560712
H	1.340064	-2.603011	-2.079371
H	-4.515003	-0.661917	-2.008111
H	-4.909477	-1.213967	2.258120
H	-0.894407	-1.062634	-2.026307
H	-1.542267	-2.805508	2.643582
C	-1.539554	-0.754907	3.291969
H	-2.246921	0.083890	3.465363

H	-1.454903	-0.599575	4.244614
H	-1.024548	-0.166495	2.552264
C	-4.146115	-1.140127	3.845357
H	-5.026285	-1.704699	3.473705
H	-3.762683	-1.653878	4.751101
H	-4.497171	-0.137189	4.168553
C	-2.616442	0.291061	-3.461388
H	-1.926513	0.021282	-4.286311
H	-3.649143	0.280393	-3.872544
H	-2.362250	1.321267	-3.148229
C	-2.819013	-2.129944	-2.777794
H	-3.893128	-2.185178	-3.056697
H	-2.219646	-2.401656	-3.672382
H	-2.626738	-2.899799	-2.004914
C	2.056506	-0.988091	2.884956
H	1.612587	-0.747806	3.873538
H	3.124842	-0.687113	2.893584
H	1.541724	-0.353725	2.120140
C	2.548054	-3.372237	3.642138
H	3.625301	-3.139303	3.778231
H	2.053736	-3.202892	4.621360
H	2.463441	-4.450324	3.392978
C	1.217008	-1.546201	-3.189740
H	2.222826	-1.417368	-3.643994
H	0.462081	-1.455343	-3.998721
H	1.051794	-0.709665	-2.478817
C	1.303250	-4.084749	-3.467611
H	0.542147	-4.044841	-4.274683
H	2.300050	-4.044008	-3.955786
H	1.215554	-5.066949	-2.958104
C	-1.263418	2.614828	-0.704168
C	-1.763530	2.500217	0.607745
C	-1.869566	3.524336	-1.598260
C	-2.845665	3.285992	1.027690
C	-2.953757	4.310760	-1.179212
C	-3.442325	4.196150	0.136147
H	-1.300914	1.753370	1.274875
H	-1.466510	3.600394	-2.620264
H	-3.237749	3.174224	2.050752
H	-3.420872	5.021036	-1.880513
H	-4.293577	4.814018	0.464768
C	-0.114507	1.766913	-1.200887
O	0.120016	1.654912	-2.403012
O	4.888529	4.470042	0.817997
C	6.076743	4.416503	0.044774
H	6.538337	3.401674	0.055623
H	5.899928	4.714446	-1.014874
H	6.782042	5.135002	0.505175
Zero-point correction=			0.770462 (Hartree/Particle)
Thermal correction to Energy=			0.817464
Thermal correction to Enthalpy=			0.818409
Thermal correction to Gibbs Free Energy=			0.690361
Sum of electronic and zero-point Energies=			-1977.278441
Sum of electronic and thermal Energies=			-1977.231438
Sum of electronic and thermal Enthalpies=			-1977.230494
Sum of electronic and thermal Free Energies=			-1977.358541

H	-1.013655	-0.964333	4.247289
H	-0.788271	-0.414114	2.548837
C	-3.281748	-2.514268	3.866401
H	-3.875408	-3.379044	3.504014
H	-2.728882	-2.830801	4.774948
H	-3.992527	-1.721403	4.181961
C	-2.429475	-0.673918	-3.462599
H	-1.688044	-0.660107	-4.286924
H	-3.371944	-1.101145	-3.868894
H	-2.606084	0.377821	-3.168147
C	-1.640828	-2.961124	-2.743897
H	-2.599200	-3.450058	-3.021259
H	-0.977587	-2.980049	-3.634453
H	-1.158103	-3.576540	-1.959630
C	2.348107	0.121870	2.868283
H	1.827153	0.183383	3.846519
H	3.214111	0.816017	2.883833
H	1.641693	0.494865	2.084448
C	3.728506	-1.866394	3.669132
H	4.629553	-1.230134	3.796993
H	3.201989	-1.883313	4.646079
H	4.071218	-2.897228	3.442329
C	1.813360	-0.823412	-3.182417
H	2.680850	-0.297944	-3.636215
H	1.090475	-1.054025	-3.992852
H	1.318383	-0.122658	-2.477918
C	2.924271	-3.110307	-3.437600
H	2.215988	-3.388333	-4.245855
H	3.821314	-2.673467	-3.925644
H	3.239579	-4.039946	-2.919545
C	-2.128192	2.035093	-0.717676
C	-2.518935	1.751150	0.605839
C	-3.064990	2.600680	-1.609804
C	-3.821350	2.035219	1.038828
C	-4.369777	2.884226	-1.177689
C	-4.749785	2.605866	0.149049
H	-1.781471	1.269900	1.270977
H	-2.742332	2.814538	-2.640791
H	-4.119461	1.794056	2.071254
H	-5.096178	3.328382	-1.877338
H	-5.774300	2.828959	0.488137
C	-0.739623	1.718975	-1.226270
O	-0.490797	1.699863	-2.430623
C	3.054858	6.218444	0.717589
H	4.139886	5.981270	0.739501
H	2.912761	6.993062	-0.067829
H	2.784000	6.675835	1.690405
Zero-point correction=			0.765370 (Hartree/Particle)
Thermal correction to Energy=			0.811699
Thermal correction to Enthalpy=			0.812643
Thermal correction to Gibbs Free Energy=			0.685159
Sum of electronic and zero-point Energies=			-1902.127274
Sum of electronic and thermal Energies=			-1902.080944
Sum of electronic and thermal Enthalpies=			-1902.080000
Sum of electronic and thermal Free Energies=			-1902.207484

Ph(pOMe)+B-Ph(pMe)-IPr-XII			
94			
IPrXII-OMe SCF Done: -1978.08208078 A.U.			
Pd	0.143021	0.496744	-0.306767
C	0.099430	2.488705	-1.146518

Ph(pMe)+B-Ph(pMe)-IPR-XII			
93			
IPrXII-Me SCF Done: -1902.92537588 A.U.			
Pd	-0.188199	0.702502	-0.018094
C	0.037223	2.863972	0.007354

C	0.095522	3.336414	0.009579	C	0.207541	3.305505	-1.348760
C	1.377201	1.983905	-1.592638	C	-1.305501	2.612763	0.461225
C	1.283990	3.719360	0.639657	C	-0.900272	3.522301	-2.168621
H	-0.860238	3.739624	0.376079	H	1.220104	3.517077	-1.722661
C	2.571909	2.371849	-0.950209	C	-2.408693	2.830340	-0.395365
H	1.421735	1.448217	-2.552798	H	-1.476347	2.461575	1.535249
C	2.531524	3.232164	0.160923	C	-2.229236	3.286649	-1.710301
H	1.232505	4.385456	1.511410	H	-0.745438	3.885049	-3.199024
H	3.543260	1.982627	-1.287986	H	-3.420997	2.624306	-0.012819
N	1.319841	-2.232417	0.202300	N	-1.548996	-1.957106	0.519993
N	-0.715946	-2.195203	0.926195	N	0.517380	-2.322715	-0.036814
C	0.233041	-1.395917	0.332295	C	-0.387836	-1.300007	0.135152
C	1.057791	-3.509276	0.699222	C	-1.357453	-3.337815	0.588667
C	-0.234705	-3.486453	1.160162	C	-0.052978	-3.567774	0.235072
C	2.553436	-1.770900	-0.382961	C	-2.781829	-1.242840	0.788133
C	3.495700	-1.124634	0.453827	C	-3.642693	-0.984605	-0.320742
C	4.650740	-0.597734	-0.157280	C	-4.795715	-0.214733	-0.077121
C	4.851327	-0.713237	-1.540765	C	-5.074303	0.283148	1.202922
C	3.898467	-1.358677	-2.343616	C	-4.211888	0.020966	2.278866
C	2.725436	-1.902751	-1.783016	C	-3.043355	-0.749407	2.108252
C	3.236349	-0.912098	1.942947	C	-3.296034	-1.438021	-1.745325
H	5.757139	-0.286944	-2.000796	H	-5.977088	0.893923	1.365870
C	1.648106	-2.524712	-2.668446	C	-2.071526	-0.965720	3.268570
C	-2.024314	-1.723828	1.302092	C	1.873701	-2.130439	-0.479144
C	-3.096631	-1.888503	0.389313	C	2.893864	-2.034289	0.490710
C	-4.373477	-1.466137	0.808737	C	4.216220	-1.897600	0.020889
C	-4.565667	-0.895210	2.075382	C	4.493218	-1.848356	-1.355811
C	-3.476142	-0.695360	2.934894	C	3.450603	-1.895092	-2.290673
C	-2.177158	-1.101397	2.565368	C	2.112067	-2.034891	-1.871594
C	-2.857951	-2.389718	-1.031702	C	2.543358	-1.962095	1.975002
H	-5.574028	-0.576744	2.384520	H	5.534627	-1.745183	-1.700727
C	-0.983686	-0.801674	3.468730	C	0.962007	-2.017842	-2.876972
H	1.805701	-4.307621	0.677128	H	-2.160512	-4.022197	0.877122
H	-0.852480	-4.259895	1.626456	H	0.522458	-4.494094	0.151421
H	5.394439	-0.067666	0.457729	H	-5.476351	0.016273	-0.912544
H	4.060683	-1.428458	-3.430366	H	-4.445008	0.436966	3.271036
H	2.370097	-1.546205	2.227663	H	-2.457581	-2.159449	-1.674245
H	0.945901	-3.075345	-2.006837	H	-1.318137	-1.708607	2.932652
H	-5.228947	-1.568940	0.124628	H	5.039871	-1.806633	0.741749
H	-3.633793	-0.209688	3.910728	H	3.676243	-1.821035	-3.366030
H	-1.905356	-2.962596	-1.030743	H	1.550364	-2.449277	2.107176
H	-0.102206	-1.338565	3.059599	H	0.037015	-2.314747	-2.337567
C	-0.659286	0.706766	3.413929	C	0.732066	-0.578205	-3.394421
H	-1.520195	1.312808	3.768587	H	1.638067	-0.181673	-3.898095
H	0.216660	0.944722	4.052639	H	-0.108371	-0.548993	-4.120446
H	-0.417646	1.013580	2.371962	H	0.473383	0.099322	-2.547397
C	-1.193129	-1.293267	4.913511	C	1.167183	-3.021322	-4.027339
H	-1.442644	-2.374228	4.942208	H	1.342447	-4.049079	-3.646940
H	-0.271915	-1.134702	5.512346	H	0.270969	-3.043160	-4.681162
H	-2.012829	-0.743719	5.422954	H	2.033225	-2.746619	-4.667106
C	-2.662749	-1.173837	-1.964238	C	2.394747	-0.476437	2.393039
H	-2.445144	-1.497222	-3.002911	H	2.104635	-0.390470	3.460171
H	-3.566537	-0.528726	-1.976748	H	3.343738	0.074856	2.242534
H	-1.812640	-0.545609	-1.615411	H	1.619075	0.039672	1.784939
C	-3.963343	-3.329196	-1.545232	C	3.544157	-2.696964	2.883041
H	-4.925690	-2.793572	-1.687469	H	4.532787	-2.192490	2.900527
H	-3.679886	-3.747362	-2.533258	H	3.171409	-2.707263	3.927799
H	-4.143046	-4.174854	-0.848963	H	3.702434	-3.747260	2.559951
C	2.832052	0.554752	2.195023	C	-2.793934	-0.251711	-2.593093
H	2.577441	0.716651	3.263488	H	-2.488991	-0.591056	-3.605264
H	3.654140	1.247124	1.918513	H	-3.586834	0.512647	-2.708160
H	1.947191	0.816792	1.572089	H	-1.915497	0.243570	-2.103710
C	4.428557	-1.338907	2.819500	C	-4.477170	-2.157032	-2.426377

H	5.318987	-0.699565	2.641107
H	4.169676	-1.244752	3.895055
H	4.723468	-2.391107	2.625130
C	0.835210	-1.416807	-3.370598
H	1.481216	-0.813392	-4.042911
H	0.015184	-1.850860	-3.979478
H	0.384169	-0.728469	-2.622934
C	2.221206	-3.539523	-3.675903
H	1.398448	-4.036752	-4.230809
H	2.870872	-3.048361	-4.431147
H	2.822770	-4.323848	-3.170800
C	-2.500270	2.314746	-1.442285
C	-2.839069	1.989634	-0.108719
C	-3.531458	2.664161	-2.343095
C	-4.176039	2.036207	0.316738
C	-4.866057	2.717840	-1.915585
C	-5.192137	2.406222	-0.581631
H	-2.053564	1.636300	0.582064
H	-3.258334	2.876612	-3.388093
H	-4.421296	1.759513	1.352765
H	-5.659733	2.998679	-2.626537
H	-6.241091	2.442380	-0.245636
C	-1.101077	2.196458	-2.007356
O	-0.953352	1.879395	-3.196459
O	3.737717	3.526205	0.734066
C	3.759478	4.335822	1.900430
H	3.349656	5.354483	1.710559
H	3.191712	3.868667	2.738064
H	4.822300	4.428330	2.195314

Zero-point correction=	0.772260 (Hartree/Particle)
Thermal correction to Energy=	0.819669
Thermal correction to Enthalpy=	0.820614
Thermal correction to Gibbs Free Energy=	0.690713
Sum of electronic and zero-point Energies=	-1977.309821
Sum of electronic and thermal Energies=	-1977.262411
Sum of electronic and thermal Enthalpies=	-1977.261467
Sum of electronic and thermal Free Energies=	-1977.391368

H	-5.331708	-1.468884	-2.600431
H	-4.170736	-2.551892	-3.417909
H	-4.846581	-3.006800	-1.815147
C	-1.314818	0.338409	3.593148
H	-2.017459	1.135311	3.916815
H	-0.581135	0.179178	4.409237
H	-0.763448	0.715032	2.706792
C	-2.758864	-1.539916	4.519690
H	-2.005474	-1.766070	5.303251
H	-3.481820	-0.822118	4.962503
H	-3.310312	-2.475139	4.288651
C	2.570086	2.532057	0.573843
C	2.886378	1.787139	-0.584858
C	3.617193	2.965950	1.418040
C	4.224946	1.494747	-0.897059
C	4.953454	2.679934	1.101306
C	5.261279	1.943886	-0.058137
H	2.072266	1.388094	-1.217753
H	3.351835	3.516419	2.334113
H	4.453444	0.897945	-1.790276
H	5.762222	3.027981	1.764047
H	6.311017	1.713979	-0.303825
C	1.154118	2.795311	1.024600
O	0.926753	2.958961	2.222092
C	-3.403616	3.520830	-2.636711
H	-3.483837	4.584424	-2.921827
H	-3.294523	2.949809	-3.577899
H	-4.361170	3.223976	-2.175918

Zero-point correction=	0.767181 (Hartree/Particle)
Thermal correction to Energy=	0.812879
Thermal correction to Enthalpy=	0.813823
Thermal correction to Gibbs Free Energy=	0.688856
Sum of electronic and zero-point Energies=	-1902.158195
Sum of electronic and thermal Energies=	-1902.112496
Sum of electronic and thermal Enthalpies=	-1902.111552
Sum of electronic and thermal Free Energies=	-1902.236520

Ph(pF)+B-Ph(pMe)-IPr-V			
91			
IPrV-F SCF Done: -2037.95098018 A.U.			
C	-1.289951	0.785800	-2.435053
O	-0.758892	0.561312	-3.502873
Pd	0.408212	0.708206	-0.481521
O	-0.851579	1.984864	-1.710018
C	-4.674061	-1.423175	-1.006853
C	-4.255709	-1.550583	-2.338418
H	-4.367016	-0.511373	0.936404
C	-4.021976	-0.567944	-0.103962
C	-3.152330	-0.799653	-2.769892
C	-2.473452	0.065269	-1.881415
C	-2.917823	0.167952	-0.541374
H	-2.790028	-0.880099	-3.805377
H	-2.368081	0.794008	0.176854
H	-4.791055	-2.235425	-3.012198
N	0.780925	-1.471736	1.566302
N	2.641078	-0.983723	0.573734
C	1.301313	-0.658323	0.579325
C	1.768285	-2.276812	2.144857
C	2.945434	-1.966145	1.516478
C	-0.598629	-1.493122	1.984977

Ph(pCF3)+B-Ph(pMe)-IPR-V			
94			
IPrV-CF3 SCF Done: -2275.58985141 A.U.			
C	-0.619330	1.166732	-2.436382
O	-0.147972	0.845975	-3.508817
Pd	0.924924	0.737195	-0.467944
O	0.030932	2.270374	-1.720079
C	-4.306246	-0.506890	-0.956404
C	-3.870655	-0.744642	-2.272884
H	-3.910579	0.535886	0.912305
C	-3.567639	0.346065	-0.112219
C	-2.682128	-0.158685	-2.728442
C	-1.912913	0.664406	-1.873377
C	-2.377748	0.922856	-0.562555
H	-2.313159	-0.347360	-3.746994
H	-1.788695	1.542271	0.127713
H	-4.454054	-1.403429	-2.933523
N	0.803387	-1.453938	1.614554
N	2.711323	-1.410132	0.593302
C	1.474683	-0.803181	0.599708
C	1.602813	-2.433801	2.212766
C	2.810440	-2.404843	1.566187
C	-0.547033	-1.171430	2.036699

C	-1.385136	-2.615444	1.618723	C	-1.552135	-2.118484	1.711700
C	-2.684056	-2.702540	2.158356	C	-2.842625	-1.902009	2.234880
C	-3.179042	-1.699879	3.004713	C	-3.114287	-0.783555	3.035553
C	-2.406609	-0.562273	3.285656	C	-2.115152	0.168735	3.289642
C	-1.096909	-0.427098	2.781195	C	-0.805507	0.002987	2.793303
C	-0.870525	-3.619579	0.587713	C	-1.254301	-3.272435	0.753866
H	-4.193324	-1.790777	3.425574	H	-4.129726	-0.634366	3.435763
C	-0.249999	0.816163	3.051229	C	0.288983	1.042727	3.038863
C	3.602905	-0.313884	-0.262279	C	3.786774	-0.977812	-0.260980
C	4.206219	0.869696	0.231006	C	4.625925	0.065984	0.201847
C	5.137147	1.515871	-0.605993	C	5.670117	0.478506	-0.649374
C	5.442781	1.001813	-1.875776	C	5.856743	-0.122520	-1.903722
C	4.814959	-0.163561	-2.341066	C	4.996000	-1.141382	-2.339887
C	3.875864	-0.848898	-1.544355	C	3.936207	-1.592543	-1.527732
C	3.793879	1.474925	1.571783	C	4.355569	0.780775	1.524774
H	6.171565	1.523583	-2.516404	H	6.677593	0.216206	-2.555808
C	3.104774	-2.051109	-2.082446	C	2.925776	-2.619437	-2.031908
H	1.538252	-2.984795	2.946972	H	1.238284	-3.048736	3.041364
H	3.963503	-2.342744	1.652923	H	3.725601	-2.986998	1.709179
H	-3.326415	-3.556859	1.900537	H	-3.654565	-2.599523	1.989203
H	-2.829331	0.234140	3.915245	H	-2.359663	1.058324	3.888149
H	0.217971	-3.761298	0.763431	H	-0.230954	-3.644119	0.978966
H	0.252303	1.041097	2.078679	H	0.834465	1.131737	2.068073
H	5.621518	2.443600	-0.263620	H	6.341029	1.291983	-0.331656
H	5.046536	-0.540402	-3.349255	H	5.141574	-1.585122	-3.336727
H	3.247329	0.694452	2.141726	H	3.642877	0.159450	2.106853
H	2.630285	-2.559707	-1.216017	H	2.391210	-3.025679	-1.146431
C	1.965859	-1.560898	-3.002799	C	1.872233	-1.914047	-2.914911
H	2.373679	-1.048383	-3.899365	H	2.339118	-1.495195	-3.831027
H	1.337137	-2.410305	-3.342766	H	1.075157	-2.622723	-3.222655
H	1.313220	-0.836198	-2.467840	H	1.396787	-1.071298	-2.366326
C	4.007641	-3.081720	-2.784653	C	3.579377	-3.806444	-2.762168
H	3.416758	-3.975657	-3.074415	H	2.813108	-4.567475	-3.018062
H	4.452989	-2.673214	-3.716552	H	4.053250	-3.492874	-3.716221
H	4.839543	-3.414257	-2.129099	H	4.358470	-4.294258	-2.139871
C	4.994357	1.912020	2.431116	C	5.620129	0.952545	2.386287
H	5.548373	2.755946	1.968367	H	6.355492	1.635438	1.910664
H	4.648691	2.257195	3.428072	H	5.358104	1.391231	3.371873
H	5.711570	1.078847	2.583330	H	6.126459	-0.018823	2.564060
C	2.804122	2.636651	1.338755	C	3.657166	2.131062	1.256954
H	2.423580	3.033274	2.304160	H	3.365830	2.623436	2.209098
H	3.286896	3.468414	0.783327	H	4.318965	2.820957	0.691920
H	1.932802	2.279924	0.735914	H	2.732487	1.966686	0.648321
C	0.844793	0.559151	4.107449	C	1.299009	0.584899	4.111164
H	1.490458	1.455691	4.219730	H	2.116933	1.329182	4.213996
H	0.395025	0.333554	5.098338	H	0.805560	0.478080	5.101119
H	1.499833	-0.290615	3.829722	H	1.764484	-0.387856	3.855896
C	-1.079451	2.058336	3.409141	C	-0.254406	2.443207	3.359488
H	-1.556203	1.977208	4.409944	H	-0.734836	2.492475	4.360402
H	-0.421681	2.952241	3.434171	H	0.579050	3.176523	3.362876
H	-1.875461	2.247423	2.659532	H	-0.993863	2.778208	2.603128
C	-1.531654	-5.004404	0.680559	C	-2.217321	-4.462494	0.898111
H	-2.602101	-4.968983	0.386430	H	-3.241069	-4.197320	0.562317
H	-1.031620	-5.711490	-0.012864	H	-1.875093	-5.305892	0.263553
H	-1.471976	-5.426110	1.705672	H	-2.278780	-4.823146	1.946090
C	-1.033491	-3.018279	-0.827799	C	-1.245990	-2.749559	-0.701348
H	-0.596317	-3.691285	-1.594896	H	-0.937087	-3.551631	-1.404060
H	-2.108151	-2.874668	-1.063171	H	-2.262145	-2.412928	-0.986765
H	-0.541373	-2.026328	-0.911269	H	-0.559542	-1.887661	-0.833676
C	-1.754894	2.921568	-1.212464	C	-0.677546	3.379271	-1.263104
C	-1.465767	3.516839	0.027324	C	-0.302238	3.934589	-0.027926
C	-2.896791	3.283403	-1.947349	C	-1.709639	3.939950	-2.034156
C	-2.345163	4.480600	0.545467	C	-0.984567	5.065466	0.447569

H	-0.561682	3.193096	0.567645
C	-3.771977	4.242979	-1.410972
H	-3.097410	2.810557	-2.920210
C	-3.503640	4.842837	-0.167119
H	-2.124301	4.943596	1.520115
H	-4.673846	4.524835	-1.976909
F	-5.723641	-2.151461	-0.572846
H	-4.195448	5.593436	0.245152

Zero-point correction= 0.736402 (Hartree/Particle)
Thermal correction to Energy= 0.783148
Thermal correction to Enthalpy= 0.784092
Thermal correction to Gibbs Free Energy= 0.655143
Sum of electronic and zero-point Energies= -2037.214578
Sum of electronic and thermal Energies= -2037.167832
Sum of electronic and thermal Enthalpies= -2037.166888
Sum of electronic and thermal Free Energies= -2037.295837

H	0.506803	3.453214	0.544282
C	-2.389082	5.066381	-1.539847
H	-1.976812	3.490904	-3.002358
C	-2.033240	5.631547	-0.301704
H	-0.698033	5.499936	1.418214
H	-3.205443	5.506319	-2.133986
H	-2.571728	6.513348	0.078166
C	-5.497558	-1.260737	-0.418913
F	-5.146621	-2.535702	-0.048309
F	-6.034096	-0.674885	0.680334
F	-6.482387	-1.390661	-1.342283

Zero-point correction= 0.748757 (Hartree/Particle)
Thermal correction to Energy= 0.798349
Thermal correction to Enthalpy= 0.799293
Thermal correction to Gibbs Free Energy= 0.662739
Sum of electronic and zero-point Energies= -2274.841094
Sum of electronic and thermal Energies= -2274.791502
Sum of electronic and thermal Enthalpies= -2274.790558
Sum of electronic and thermal Free Energies= -2274.927112

Ph(pF)+B-Ph(pMe)-IPr-V-VI

91

IPrV-VI-F SCF Done: -2037.95197643 A.U.

C	-1.571291	0.377061	-1.634282
O	-1.644109	-0.394872	-2.575300
Pd	0.405290	0.504722	-0.714354
O	-0.779669	1.754328	-1.971766
C	-4.680361	0.559814	1.333413
C	-4.659462	-0.462650	0.374927
H	-3.714963	2.312738	2.166868
C	-3.674673	1.538392	1.387274
C	-3.624112	-0.480424	-0.570389
C	-2.607940	0.501758	-0.553903
C	-2.632950	1.495719	0.452583
H	-3.576815	-1.268130	-1.335728
H	-1.834366	2.245444	0.513192
H	-5.450027	-1.227283	0.379828
N	2.343469	-0.832923	1.090982
C	4.240618	-0.577310	-1.079996
H	3.659824	-1.468647	-0.764043
C	4.104447	0.482048	0.011947
C	3.151852	0.357396	1.054425
C	1.164157	-0.935295	0.389101
C	2.925072	1.364441	2.024693
C	1.796540	1.244832	3.046324
H	1.481257	0.179992	3.075612
C	4.869945	1.665012	-0.022594
H	5.614125	1.804995	-0.822220
C	4.685673	2.671840	0.937305
H	5.294676	3.588806	0.892094
C	3.719599	2.525733	1.945123
H	3.571243	3.334643	2.677274
C	2.679802	-2.031965	1.720498
C	0.577314	2.061806	2.565425
H	-0.291260	1.916148	3.241001
H	0.815492	3.146066	2.525689
H	0.280661	1.734273	1.541031
C	2.226109	1.640988	4.470539
H	1.400978	1.449656	5.187739
H	3.115028	1.066340	4.804163
H	2.474165	2.721112	4.541942
C	3.604559	-0.072438	-2.392760

Ph(pCF3)+B-Ph(pMe)-IPR-V-VI

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IPrV-VI-CF3 SCF Done: -2275.59017326 A.U.

C	-0.727368	0.422721	-2.042683
O	-0.609361	-0.307169	-3.009883
Pd	0.954783	0.530070	-0.728546
O	0.131637	1.851163	-2.185282
C	-4.350172	0.459733	0.310944
C	-4.103938	-0.527864	-0.659648
H	-3.601412	2.256529	1.284348
C	-3.409676	1.487989	0.521711
C	-2.928714	-0.482368	-1.417635
C	-1.970575	0.533045	-1.202175
C	-2.220871	1.515455	-0.216364
H	-2.718117	-1.249516	-2.175421
H	-1.486127	2.304072	-0.013138
H	-4.830715	-1.338507	-0.817525
N	2.446789	-0.900192	1.372286
C	4.739185	-0.772447	-0.388041
H	4.107069	-1.650373	-0.138584
C	4.427496	0.329757	0.622600
C	3.289857	0.263661	1.466243
C	1.405521	-0.966460	0.474998
C	2.909768	1.309136	2.344616
C	1.614440	1.245013	3.150263
H	1.249400	0.196742	3.118012
C	5.216476	1.495169	0.697070
H	6.104846	1.589935	0.053394
C	4.875577	2.542613	1.566523
H	5.503953	3.446619	1.606267
C	3.732922	2.452761	2.376416
H	3.467749	3.291754	3.038524
C	2.603965	-2.093522	2.076296
C	0.535020	2.116304	2.472626
H	-0.443012	2.008623	2.986052
H	0.820917	3.189565	2.481078
H	0.406554	1.800747	1.410183
C	1.810047	1.621065	4.630561
H	0.861606	1.482027	5.190034
H	2.590218	0.995136	5.111318
H	2.106737	2.684456	4.751372
C	4.337022	-0.319370	-1.808171

H	4.146593	0.812410	-2.788696
H	3.622838	-0.866897	-3.168133
H	2.542139	0.219709	-2.223154
C	5.698154	-1.031051	-1.286070
H	6.148879	-1.395471	-0.339606
H	5.743489	-1.854121	-2.029444
H	6.336685	-0.207441	-1.669847
C	1.682450	-2.919500	1.411450
H	1.543031	-3.971966	1.676400
H	3.593348	-2.140542	2.312393
N	0.769464	-2.235844	0.602384
C	-0.441827	-2.811644	0.070245
C	-0.507014	-3.107502	-1.316686
C	-1.510868	-3.050411	0.973191
C	-1.705260	-3.682305	-1.786481
C	-2.679013	-3.635265	0.446629
C	-2.771735	-3.951450	-0.917114
H	-1.810029	-3.914215	-2.855238
H	-3.535448	-3.834280	1.106588
H	-3.696339	-4.402819	-1.311341
C	0.663291	-2.797687	-2.252215
H	0.987530	-1.762712	-1.994255
C	-1.407626	-2.626735	2.440770
H	-0.380944	-2.873073	2.788765
C	1.860880	-3.744036	-2.014726
H	2.712260	-3.452231	-2.665469
H	2.222212	-3.722044	-0.967453
H	1.589468	-4.793468	-2.259480
C	0.282659	-2.775724	-3.739348
H	1.146365	-2.416665	-4.336636
H	0.022420	-3.787341	-4.120438
H	-0.564992	-2.087185	-3.918654
C	-2.383671	-3.366518	3.370094
H	-2.174055	-3.104038	4.427554
H	-3.437207	-3.077298	3.169761
H	-2.303839	-4.468684	3.266542
C	-1.583028	-1.098459	2.577126
H	-0.908702	-0.534477	1.902469
H	-2.618977	-0.811497	2.312463
H	-1.389301	-0.771412	3.620482
C	-1.254365	3.023285	-1.740003
C	-2.524318	3.402469	-2.219300
C	-0.444704	3.947348	-1.047875
C	-2.985091	4.708429	-1.988400
H	-3.137674	2.661045	-2.752651
C	-0.913358	5.253540	-0.834879
H	0.536882	3.612211	-0.675643
C	-2.186117	5.638705	-1.297353
H	-3.982040	5.002117	-2.354006
H	-0.279795	5.975556	-0.295053
H	-2.554109	6.661189	-1.120140
F	-5.678929	0.593838	2.240944

H	4.945867	0.548511	-2.139205
H	4.479786	-1.143322	-2.538421
H	3.264357	-0.016432	-1.833535
C	6.207508	-1.234101	-0.329595
H	6.494794	-1.551412	0.694326
H	6.368057	-2.091987	-1.015247
H	6.906182	-0.430022	-0.643291
C	1.632427	-2.940934	1.612138
H	1.397172	-3.979158	1.865087
H	3.391365	-2.227536	2.823761
N	0.911626	-2.239197	0.640213
C	-0.212712	-2.786366	-0.081329
C	-0.046202	-3.120853	-1.451338
C	-1.425496	-2.981606	0.632616
C	-1.159539	-3.688656	-2.104731
C	-2.499027	-3.559548	-0.073171
C	-2.364372	-3.914215	-1.423691
H	-1.084113	-3.954818	-3.168086
H	-3.458973	-3.725692	0.435578
H	-3.217622	-4.361585	-1.958254
C	1.279585	-2.877457	-2.176468
H	1.589471	-1.843553	-1.901126
C	-1.556275	-2.548293	2.096410
H	-0.636423	-2.887393	2.621441
C	2.384469	-3.848347	-1.702234
H	3.342592	-3.611502	-2.211263
H	2.567587	-3.792823	-0.611086
H	2.118453	-4.898370	-1.949774
C	1.166696	-2.912225	-3.707411
H	2.130885	-2.595095	-4.155829
H	0.952085	-3.935272	-4.086243
H	0.383340	-2.217548	-4.064837
C	-2.752306	-3.181709	2.826132
H	-2.718494	-2.920243	3.903732
H	-3.715769	-2.794658	2.433380
H	-2.757134	-4.288339	2.742178
C	-1.612944	-1.009382	2.225450
H	-0.821426	-0.502468	1.639342
H	-2.586796	-0.635103	1.859501
H	-1.510724	-0.704436	3.288131
C	-0.371833	3.113713	-2.007361
C	-1.508584	3.529199	-2.731930
C	0.272145	4.005001	-1.122033
C	-2.005926	4.829646	-2.552151
H	-1.993303	2.817301	-3.416711
C	-0.228893	5.306711	-0.961427
H	1.154486	3.651437	-0.564538
C	-1.372618	5.723744	-1.668544
H	-2.900206	5.148320	-3.111310
H	0.276642	6.000496	-0.270484
H	-1.767908	6.742314	-1.532548
C	-5.555459	0.328565	1.208708
F	-5.305593	-0.549510	2.231702
F	-5.908164	1.504573	1.782884
F	-6.639661	-0.150457	0.547773

Zero-point correction=	0.735506 (Hartree/Particle)
Thermal correction to Energy=	0.781756
Thermal correction to Enthalpy=	0.782700
Thermal correction to Gibbs Free Energy=	0.654512
Sum of electronic and zero-point Energies=	-2037.216470
Sum of electronic and thermal Energies=	-2037.170220
Sum of electronic and thermal Enthalpies=	-2037.169276
Sum of electronic and thermal Free Energies=	-2037.297465

Zero-point correction=	0.748589 (Hartree/Particle)
Thermal correction to Energy=	0.797450
Thermal correction to Enthalpy=	0.798394
Thermal correction to Gibbs Free Energy=	0.664375
Sum of electronic and zero-point Energies=	-2274.841584
Sum of electronic and thermal Energies=	-2274.792723
Sum of electronic and thermal Enthalpies=	-2274.791779
Sum of electronic and thermal Free Energies=	-2274.925798

Ph(pF)+B-Ph(pMe)-IPr-VI				**Ph(pCF3)+B-Ph(pMe)-IPR-VI**			
91				94			
IPrVI-F SCF Done: -2037.97757759 A.U.				IPrVI-CF3 SCF Done: -2275.61387006 A.U.			
Pd	-0.338457	-0.787898	-0.559786	Pd	-0.673417	-0.860102	-0.311566
N	-2.695212	0.792580	0.332215	N	-3.185296	0.712535	-0.038075
C	-3.350227	0.962445	-2.510145	C	-3.428183	0.179064	-2.901286
H	-2.624886	1.561559	-1.921555	H	-2.740196	0.878411	-2.383843
C	-3.922233	-0.116311	-1.596295	C	-4.101317	-0.688605	-1.843250
C	-3.561476	-0.211657	-0.232354	C	-3.942124	-0.440542	-0.459946
C	-1.328561	0.672611	0.336830	C	-1.828667	0.675951	0.157269
C	-3.975473	-1.273694	0.612191	C	-4.452619	-1.296083	0.549630
C	-3.420934	-1.432033	2.027008	C	-4.099998	-1.095426	2.022958
H	-2.938723	-0.475068	2.317034	H	-3.683553	-0.073245	2.142821
C	-4.796706	-1.102352	-2.097963	C	-4.879887	-1.806282	-2.207379
H	-5.105829	-1.061845	-3.154145	H	-5.034731	-2.029017	-3.274501
C	-5.258373	-2.143556	-1.279840	C	-5.438759	-2.647760	-1.234592
H	-5.936686	-2.906023	-1.694496	H	-6.039312	-3.518157	-1.542954
C	-4.839276	-2.237397	0.056650	C	-5.212639	-2.405155	0.129411
H	-5.178961	-3.082928	0.674829	H	-5.621474	-3.098518	0.880603
C	-3.117147	1.907730	1.053940	C	-3.729192	1.929687	0.368972
C	-2.319580	-2.514797	2.037395	C	-2.989847	-2.087949	2.434023
H	-1.836837	-2.579787	3.035134	H	-2.660412	-1.901382	3.477714
H	-2.734967	-3.512855	1.784885	H	-3.345630	-3.137216	2.363998
H	-1.524985	-2.291080	1.290511	H	-2.098409	-1.998025	1.774909
C	-4.510206	-1.725392	3.074685	C	-5.320796	-1.198947	2.955541
H	-4.068952	-1.747297	4.092983	H	-5.028348	-0.966373	4.000751
H	-5.305949	-0.952453	3.059068	H	-6.121697	-0.492448	2.655030
H	-4.991864	-2.711453	2.905923	H	-5.753790	-2.221329	2.957055
C	-2.552988	0.325968	-3.666350	C	-2.546096	-0.672335	-3.835763
H	-3.212540	-0.249296	-4.350315	H	-3.149846	-1.362304	-4.463119
H	-2.042098	1.111886	-4.258533	H	-1.963954	-0.014055	-4.511668
H	-1.773048	-0.356505	-3.272055	H	-1.823327	-1.274652	-3.248301
C	-4.449600	1.915947	-3.018672	C	-4.462971	1.014313	-3.681398
H	-4.987932	2.400909	-2.177480	H	-5.056300	1.662010	-3.002371
H	-4.009908	2.713782	-3.653215	H	-3.957907	1.665353	-4.425371
H	-5.201798	1.375911	-3.632539	H	-5.174898	0.361764	-4.230910
C	-1.982271	2.508453	1.533238	C	-2.684409	2.682112	0.839880
H	-1.842034	3.394886	2.157757	H	-2.653145	3.687571	1.268296
H	-4.176270	2.158377	1.163952	H	-4.800902	2.136743	0.296432
N	-0.900659	1.743982	1.087163	N	-1.531880	1.904570	0.700388
C	0.473229	1.988121	1.457538	C	-0.219921	2.288911	1.162578
C	1.182841	3.020117	0.795672	C	0.541984	3.194758	0.384070
C	1.053777	1.173544	2.468716	C	0.255112	1.721286	2.377453
C	2.510994	3.258502	1.206772	C	1.810569	3.563349	0.879177
C	2.379721	1.462923	2.842036	C	1.524689	2.133146	2.825524
C	3.099395	2.496884	2.222931	C	2.292752	3.047839	2.088013
H	3.095439	4.048260	0.711613	H	2.435125	4.258077	0.298219
H	2.869152	0.853372	3.615053	H	1.932229	1.717613	3.758475
H	4.139765	2.695326	2.524748	H	3.287955	3.346100	2.453359
C	0.543019	3.866754	-0.302946	C	0.019239	3.776710	-0.927649
H	-0.325125	3.298364	-0.697915	H	-0.784912	3.104485	-1.293988
C	0.284635	0.006825	3.090151	C	-0.566086	0.687406	3.147820
H	-0.313028	-0.441405	2.267881	H	-1.095496	0.077614	2.386045
C	0.028175	5.204561	0.273097	C	-0.587788	5.178071	-0.694421
H	-0.702128	5.053912	1.093366	H	-1.409522	5.158847	0.049417
H	0.870035	5.802594	0.682887	H	0.185396	5.881327	-0.318000
H	-0.466468	5.807232	-0.517315	H	-0.994832	5.591300	-1.641020
C	1.493042	4.121526	-1.488439	C	1.097009	3.831818	-2.027092
H	0.937806	4.601794	-2.319942	H	0.633075	4.108311	-2.995793
H	2.326246	4.801942	-1.212564	H	1.875463	4.592396	-1.805723
H	1.922272	3.176148	-1.870439	H	1.593413	2.851386	-2.157650

C	-0.699941	0.482612	4.179507
H	-1.293556	-0.373167	4.565186
H	-0.153286	0.934322	5.034563
H	-1.414052	1.237350	3.793022
C	1.192680	-1.114894	3.619381
H	1.913446	-1.456959	2.848418
H	1.763773	-0.805584	4.520637
H	0.575945	-1.990293	3.910143
C	0.772447	0.515955	-1.560842
O	0.291249	1.281227	-2.375034
O	0.456704	-2.490396	-1.336278
C	4.980400	-0.026513	-0.990916
C	4.507729	0.493134	-2.208182
H	4.524230	-0.781950	0.990514
C	4.118467	-0.354643	0.063566
C	3.130854	0.686654	-2.369948
C	2.236665	0.350495	-1.325576
C	2.744144	-0.178906	-0.120137
H	2.725432	1.086075	-3.312070
H	2.039095	-0.448911	0.676532
H	5.226342	0.728220	-3.007200
C	1.628140	-2.925265	-0.871394
C	1.823936	-3.243278	0.506488
C	2.740656	-3.076021	-1.747389
C	3.076632	-3.653758	0.984784
H	0.960683	-3.138709	1.184331
C	3.989556	-3.483936	-1.258934
H	2.595960	-2.822610	-2.808856
C	4.173868	-3.770656	0.108692
H	3.199665	-3.885496	2.056353
H	4.841851	-3.566612	-1.953572
H	5.159719	-4.084975	0.485328
F	6.305721	-0.219828	-0.839239

C	-1.637564	1.358589	4.032799
H	-2.264722	0.590472	4.532997
H	-1.164720	1.982952	4.820544
H	-2.312296	2.009201	3.440110
C	0.296224	-0.294212	3.956758
H	1.084804	-0.752936	3.325476
H	0.785269	0.190884	4.828077
H	-0.337840	-1.113551	4.353741
C	0.393571	0.293878	-1.513443
O	-0.076452	0.879331	-2.470268
O	0.256131	-2.634821	-0.634024
C	4.607279	-0.045229	-0.722512
C	4.141012	0.123006	-2.043383
H	4.073217	-0.195013	1.379074
C	3.707167	-0.047306	0.354636
C	2.771203	0.271346	-2.284086
C	1.857023	0.233982	-1.204924
C	2.334854	0.071714	0.110443
H	2.385477	0.394380	-3.307374
H	1.618487	0.036691	0.941867
H	4.855393	0.121125	-2.880796
C	1.457945	-2.869338	-0.104368
C	1.670803	-2.887652	1.306439
C	2.583221	-3.101627	-0.945314
C	2.950523	-3.095824	1.842504
H	0.797372	-2.725420	1.959147
C	3.859052	-3.298692	-0.400493
H	2.423812	-3.078685	-2.034283
C	4.058211	-3.292792	0.994970
H	3.087032	-3.098353	2.937137
H	4.722108	-3.428753	-1.072303
H	5.067064	-3.431570	1.413152
C	6.085185	-0.273572	-0.500712
F	6.827491	0.758247	-0.988779
F	6.400508	-0.415473	0.809653
F	6.513658	-1.395527	-1.143921

Zero-point correction=	0.736572 (Hartree/Particle)
Thermal correction to Energy=	0.783434
Thermal correction to Enthalpy=	0.784378
Thermal correction to Gibbs Free Energy=	0.655529
Sum of electronic and zero-point Energies=	-2037.241006
Sum of electronic and thermal Energies=	-2037.194144
Sum of electronic and thermal Enthalpies=	-2037.193199
Sum of electronic and thermal Free Energies=	-2037.322049

Zero-point correction=	0.749155 (Hartree/Particle)
Thermal correction to Energy=	0.798804
Thermal correction to Enthalpy=	0.799748
Thermal correction to Gibbs Free Energy=	0.664662
Sum of electronic and zero-point Energies=	-2274.864715
Sum of electronic and thermal Energies=	-2274.815066
Sum of electronic and thermal Enthalpies=	-2274.814122
Sum of electronic and thermal Free Energies=	-2274.949208

Ph(pF)+B-Ph(pMe)-IPr-VII			
97			
IPrVII-F SCF Done: -3501.80498647 A.U.			
Pd	0.120660	0.180347	-0.448165
N	2.383426	-1.651827	0.181229
C	2.570664	-1.798219	-2.731867
H	1.758643	-2.188160	-2.086855
C	3.458773	-0.885406	-1.893178
C	3.342537	-0.802072	-0.484516
C	1.048037	-1.364414	0.335582
C	4.111427	0.094957	0.306160
C	3.884320	0.239274	1.809214
H	2.812515	0.012169	1.979767
C	4.440602	-0.078978	-2.512870
H	4.573198	-0.136390	-3.604910
C	5.251573	0.780843	-1.755021
H	6.022282	1.391694	-2.253280

Ph(pCF3)+B-Ph(pMe)-IPR-VII			
100			
IPrVII-CF3 SCF Done: -3739.44326356 A.U.			
Pd	0.435865	0.215175	-0.371167
N	3.126665	-0.993902	-0.101624
C	3.017837	-0.694796	-3.014281
H	2.438818	-1.396688	-2.382129
C	3.741672	0.294839	-2.106722
C	3.756758	0.161488	-0.696387
C	1.783129	-1.112058	0.163351
C	4.352208	1.120500	0.167035
C	4.257906	1.002434	1.685767
H	3.329734	0.433798	1.895497
C	4.418025	1.405999	-2.660799
H	4.442358	1.529945	-3.755303
C	5.063705	2.342789	-1.837491
H	5.600931	3.193507	-2.288158

C	5.078493	0.872657	-0.363399	C	5.018964	2.205328	-0.439376
H	5.695298	1.577100	0.213953	H	5.497846	2.964844	0.196578
C	2.710985	-2.863652	0.792187	C	3.823989	-2.128672	0.316197
C	4.115864	1.676086	2.311292	C	4.104618	2.367390	2.381303
H	3.716204	1.779278	3.340807	H	3.832840	2.213484	3.445883
H	5.196898	1.933524	2.351430	H	5.050587	2.951331	2.368095
H	3.595270	2.414727	1.671728	H	3.301987	2.966282	1.909487
C	4.746532	-0.753582	2.618944	C	5.462452	0.233709	2.271441
H	4.544130	-0.637867	3.704500	H	5.355090	0.133275	3.371923
H	4.539360	-1.808765	2.353724	H	5.557587	-0.786715	1.851027
H	5.828869	-0.565373	2.450786	H	6.411926	0.774569	2.068620
C	1.863335	-1.023529	-3.859757	C	1.979713	0.016793	-3.904218
H	2.579184	-0.595155	-4.594395	H	2.453423	0.728789	-4.613952
H	1.170122	-1.694895	-4.404006	H	1.408578	-0.729191	-4.492004
H	1.241249	-0.209187	-3.433832	H	1.241571	0.560891	-3.277697
C	3.373526	-2.999833	-3.270407	C	4.020066	-1.520719	-3.845859
H	3.843015	-3.572492	-2.443271	H	4.732558	-2.065300	-3.191626
H	2.710640	-3.689962	-3.833039	H	3.483851	-2.267841	-4.467369
H	4.184974	-2.671924	-3.955571	H	4.615284	-0.875476	-4.527472
C	1.564545	-3.331413	1.375449	C	2.903262	-2.966619	0.883688
H	1.369818	-4.219880	1.981421	H	3.009237	-3.941281	1.366586
H	3.722942	-3.275359	0.748844	H	4.902086	-2.230733	0.165458
N	0.562098	-2.400000	1.089862	N	1.663217	-2.327949	0.783544
C	-0.782855	-2.480409	1.605847	C	0.449182	-2.871256	1.343905
C	-1.659610	-3.440356	1.042414	C	-0.118271	-4.013128	0.723431
C	-1.163923	-1.595525	2.656380	C	-0.102845	-2.259812	2.507716
C	-2.945655	-3.557586	1.610278	C	-1.240540	-4.600698	1.345645
C	-2.461470	-1.766605	3.182171	C	-1.233016	-2.887934	3.071057
C	-3.336327	-2.742688	2.678355	C	-1.784387	-4.052407	2.512460
H	-3.653414	-4.290474	1.194852	H	-1.704995	-5.489734	0.892806
H	-2.801890	-1.114290	3.998349	H	-1.697063	-2.456161	3.968520
H	-4.343887	-2.849500	3.110773	H	-2.662849	-4.521810	2.983135
C	-1.253574	-4.323897	-0.136054	C	0.417541	-4.590829	-0.585397
H	-0.365441	-3.858431	-0.612080	H	1.090493	-3.832086	-1.036113
C	-0.242559	-0.481423	3.160933	C	0.469515	-0.973600	3.107636
H	0.168620	0.043438	2.267528	H	0.610925	-0.246927	2.274654
C	-0.868152	-5.740251	0.344433	C	1.224383	-5.883553	-0.339721
H	-0.043008	-5.722366	1.084848	H	2.082029	-5.719146	0.343783
H	-1.735643	-6.239782	0.826474	H	0.582967	-6.668256	0.115535
H	-0.544122	-6.369624	-0.510987	H	1.624000	-6.283350	-1.295360
C	-2.350283	-4.401246	-1.216550	C	-0.713577	-4.840209	-1.603918
H	-1.959262	-4.925249	-2.112696	H	-0.281121	-5.098467	-2.592226
H	-3.238640	-4.966798	-0.862746	H	-1.368796	-5.683044	-1.296760
H	-2.678350	-3.392760	-1.532094	H	-1.338235	-3.936182	-1.737834
C	0.952804	-1.027485	3.972694	C	1.846962	-1.198215	3.770533
H	1.612581	-0.188877	4.277244	H	2.243400	-0.230934	4.142151
H	0.603809	-1.544778	4.892575	H	1.762892	-1.892597	4.634462
H	1.573640	-1.741389	3.395813	H	2.598705	-1.616752	3.072265
C	-0.973990	0.606241	3.960698	C	-0.482039	-0.276991	4.090593
H	-1.839622	1.008675	3.394933	H	-1.477456	-0.102223	3.632846
H	-1.332605	0.239342	4.947665	H	-0.616211	-0.854527	5.031761
H	-0.279629	1.452842	4.118810	H	-0.068794	0.719791	4.334539
C	-1.061425	-1.007310	-1.507347	C	-0.462129	-1.126103	-1.512207
O	-0.654520	-1.842406	-2.315523	O	0.059402	-1.874458	-2.333520
O	-0.637680	1.868413	-1.494908	O	-0.741085	1.797248	-1.189535
C	-5.305391	-0.337054	-1.265535	C	-4.706952	-0.610931	-0.918745
C	-4.703452	-0.509656	-2.522582	C	-4.094931	-0.135182	-2.092392
H	-5.071812	-0.247720	0.887865	H	-4.434780	-1.709527	0.941957
C	-4.561685	-0.371208	-0.078464	C	-3.956104	-1.342028	0.021791
C	-3.320896	-0.733456	-2.581942	C	-2.731674	-0.374892	-2.317106
C	-2.542005	-0.741270	-1.402572	C	-1.962090	-1.047719	-1.346288
C	-3.174520	-0.553359	-0.158109	C	-2.585129	-1.536245	-0.178818
H	-2.821117	-0.901030	-3.548424	H	-2.238473	0.022619	-3.216636

H	-2.572272	-0.580616	0.760571
H	-5.328258	-0.472170	-3.427559
K	1.960358	2.588581	-1.826518
K	-0.546161	4.866751	1.447728
C	1.153081	2.656784	1.013274
O	1.515560	3.773224	0.433454
O	0.432849	2.634388	2.065688
O	1.559412	1.526745	0.439066
C	-1.588075	2.660289	-1.036634
C	-2.226827	2.468541	0.230538
C	-2.006101	3.795743	-1.804149
C	-3.244064	3.328057	0.672781
H	-1.872767	1.639576	0.860525
C	-3.007099	4.663623	-1.339272
H	-1.528910	3.960307	-2.784204
C	-3.646429	4.441317	-0.098881
H	-3.732295	3.123573	1.641326
H	-3.309205	5.521220	-1.964154
H	-4.455309	5.104705	0.245091
F	-6.640434	-0.137054	-1.200940

Zero-point correction=	0.754827 (Hartree/Particle)
Thermal correction to Energy=	0.809484
Thermal correction to Enthalpy=	0.810428
Thermal correction to Gibbs Free Energy=	0.664913
Sum of electronic and zero-point Energies=	-3501.050159
Sum of electronic and thermal Energies=	-3500.995503
Sum of electronic and thermal Enthalpies=	-3500.994558
Sum of electronic and thermal Free Energies=	-3501.140073

H	-1.982458	-2.036150	0.589836
H	-4.682525	0.450962	-2.813610
K	1.499657	3.250802	-1.370617
K	-1.546228	4.156677	2.031328
C	0.756477	2.633807	1.406340
O	0.794536	3.885673	1.029304
O	0.037404	2.233824	2.380831
O	1.489587	1.771957	0.700227
C	-1.910148	2.186318	-0.709794
C	-2.484938	1.643727	0.482083
C	-2.662716	3.195032	-1.391519
C	-3.762103	2.032393	0.914377
H	-1.900920	0.896711	1.040903
C	-3.925993	3.599017	-0.929612
H	-2.237283	3.622226	-2.314603
C	-4.499892	3.015715	0.220402
H	-4.201204	1.539859	1.797770
H	-4.486714	4.363838	-1.493086
H	-5.512670	3.294202	0.548608
C	-6.167316	-0.343341	-0.651447
F	-6.951495	-1.410435	-0.976307
F	-6.397920	-0.086779	0.668488
F	-6.636309	0.718653	-1.355782

Zero-point correction=	0.767097 (Hartree/Particle)
Thermal correction to Energy=	0.824621
Thermal correction to Enthalpy=	0.825566
Thermal correction to Gibbs Free Energy=	0.672635
Sum of electronic and zero-point Energies=	-3738.676166
Sum of electronic and thermal Energies=	-3738.618642
Sum of electronic and thermal Enthalpies=	-3738.617698
Sum of electronic and thermal Free Energies=	-3738.770629

Ph(pF)+B-Ph(pMe)-IPr-VII-VIII			
97			
IPrVII-VIII-F SCF Done: -3501.77995833 A.U.			
Pd	-0.525603	-0.719855	0.021414
N	-2.284269	1.530290	0.633284
C	-1.796685	2.851294	-1.894892
H	-0.934110	2.511658	-1.279876
C	-2.886626	1.789360	-1.731909
C	-3.122885	1.153287	-0.482363
C	-1.020068	1.016225	0.801516
C	-4.081429	0.125523	-0.296687
C	-4.265590	-0.550595	1.058001
H	-3.285047	-0.513349	1.577950
C	-3.685945	1.379500	-2.817468
H	-3.533169	1.837282	-3.805251
C	-4.659996	0.380077	-2.663449
H	-5.276193	0.080541	-3.527171
C	-4.851867	-0.243076	-1.419791
H	-5.610778	-1.033140	-1.315968
C	-2.559671	2.515914	1.581674
C	-4.633732	-2.039825	0.943873
H	-4.567253	-2.518625	1.941479
H	-5.669959	-2.191536	0.570256
H	-3.922823	-2.570900	0.280018
C	-5.308143	0.208770	1.907895
H	-5.414099	-0.267350	2.905049
H	-5.024618	1.268585	2.068752
H	-6.303838	0.197777	1.414052
C	-1.278608	3.001014	-3.334488
H	-2.038038	3.460449	-4.003160

Ph(pCF3)+B-Ph(pMe)-IPR-VII-VIII			
100			
IPrVII-VIII-CF3 SCF Done: -3739.41689414 A.U.			
Pd	0.945123	0.664702	-0.009968
N	2.520483	-1.751569	0.443442
C	1.599180	-3.042593	-1.979757
H	0.847703	-2.605263	-1.285536
C	2.797181	-2.089467	-1.972451
C	3.250325	-1.472783	-0.773104
C	1.346402	-1.104545	0.749552
C	4.323106	-0.546611	-0.726624
C	4.756916	0.102389	0.584221
H	3.854920	0.181567	1.227664
C	3.487350	-1.763291	-3.157135
H	3.167387	-2.208317	-4.110020
C	4.565100	-0.863286	-3.144237
H	5.092005	-0.629110	-4.083936
C	4.975807	-0.259734	-1.944505
H	5.816493	0.450047	-1.950049
C	2.803220	-2.751371	1.374656
C	5.286306	1.535908	0.406292
H	5.410674	2.013753	1.398717
H	6.276537	1.559211	-0.099084
H	4.568562	2.154435	-0.168071
C	5.803628	-0.779539	1.301246
H	6.087587	-0.328399	2.274867
H	5.424773	-1.802107	1.500936
H	6.723864	-0.876723	0.685696
C	0.910081	-3.176242	-3.347773
H	1.544562	-3.720324	-4.080137

H	-0.391377	3.667370	-3.341026	H	-0.026617	-3.759895	-3.233181
H	-0.974774	2.021169	-3.750554	H	0.645438	-2.184395	-3.761982
C	-2.249628	4.226267	-1.354014	C	1.973670	-4.443907	-1.446433
H	-2.548236	4.184547	-0.289136	H	2.385266	-4.411225	-0.419888
H	-1.422807	4.962803	-1.438069	H	1.075310	-5.096288	-1.420752
H	-3.112259	4.610154	-1.938957	H	2.727394	-4.923647	-2.106197
C	-1.429974	2.648675	2.344995	C	1.765948	-2.754898	2.269607
H	-1.194967	3.312747	3.181505	H	1.567074	-3.377923	3.145926
H	-3.523891	3.029803	1.622149	H	3.706012	-3.364986	1.313097
N	-0.492355	1.740316	1.844941	N	0.874585	-1.758456	1.862350
C	0.917939	1.795812	2.155780	C	-0.477104	-1.637825	2.358997
C	1.673556	2.828149	1.541257	C	-1.434586	-2.559033	1.860126
C	1.486796	0.816083	3.007033	C	-0.795983	-0.599517	3.268313
C	3.052379	2.876574	1.827861	C	-2.756831	-2.433427	2.330194
C	2.876295	0.897138	3.234195	C	-2.140045	-0.507175	3.686123
C	3.648505	1.918542	2.659365	C	-3.106549	-1.416921	3.230117
H	3.672651	3.659669	1.365413	H	-3.532061	-3.119924	1.957510
H	3.360409	0.148180	3.878031	H	-2.432826	0.292044	4.382874
H	4.731989	1.961531	2.854612	H	-4.150580	-1.323226	3.569130
C	1.038033	3.864620	0.614253	C	-1.065164	-3.651927	0.857025
H	0.015746	3.516443	0.364897	H	-0.077012	-3.393402	0.424817
C	0.619660	-0.241457	3.675313	C	0.278085	0.342044	3.794435
H	-0.201242	-0.506538	2.980079	H	1.038186	0.476675	3.000196
C	0.895444	5.221794	1.335115	C	-0.914399	-5.014324	1.566494
H	0.318122	5.124699	2.277266	H	-0.159331	-4.971702	2.377438
H	1.891660	5.640065	1.593473	H	-1.878029	-5.330909	2.019405
H	0.373646	5.957156	0.686848	H	-0.599995	-5.798710	0.845988
C	1.784893	4.022047	-0.723684	C	-2.049409	-3.751125	-0.323660
H	1.238710	4.733603	-1.378242	H	-1.667273	-4.477883	-1.071133
H	2.810436	4.423440	-0.584813	H	-3.050888	-4.107024	-0.003371
H	1.865304	3.056886	-1.258996	H	-2.179356	-2.775231	-0.828829
C	-0.017956	0.330515	4.960508	C	0.979709	-0.283998	5.019541
H	-0.687789	-0.422996	5.424755	H	1.794682	0.379666	5.376643
H	0.759795	0.610745	5.703878	H	0.264967	-0.438479	5.856840
H	-0.625198	1.234838	4.747521	H	1.429659	-1.268314	4.772766
C	1.354229	-1.560072	3.961161	C	-0.238432	1.754686	4.107762
H	1.901570	-1.913655	3.063945	H	-0.835090	2.154110	3.262923
H	2.081957	-1.475853	4.797670	H	-0.867745	1.789281	5.023721
H	0.614217	-2.341765	4.226015	H	0.622463	2.437259	4.253264
C	0.171877	0.029950	-1.684971	C	-0.061553	-0.028035	-1.576871
O	-0.530866	0.015248	-2.713808	O	0.473544	-0.148406	-2.693814
O	0.888796	-2.596732	-1.441755	O	-0.410341	2.651712	-1.384260
C	4.287383	1.185322	-2.009923	C	-4.327110	-0.558870	-1.246552
C	3.464190	1.244385	-3.148526	C	-3.684750	-0.761069	-2.486064
H	4.472332	0.756553	0.107821	H	-4.080205	-0.066004	0.859632
C	3.797198	0.801105	-0.756463	C	-3.579706	-0.229840	-0.103601
C	2.118011	0.885758	-3.020072	C	-2.296021	-0.613041	-2.577197
C	1.589818	0.494121	-1.766223	C	-1.534519	-0.278926	-1.433957
C	2.443075	0.464729	-0.641135	C	-2.189238	-0.101788	-0.197783
H	1.445192	0.893406	-3.891203	H	-1.770743	-0.744947	-3.535304
H	2.030303	0.171069	0.333879	H	-1.594869	0.146854	0.691690
H	3.899416	1.554650	-4.110270	H	-4.281416	-1.026618	-3.371432
K	-1.601167	-2.315899	-2.501749	K	1.894162	2.016256	-2.706958
K	0.433529	-4.696773	0.204849	K	0.518371	4.767262	0.054750
C	-1.466552	-2.961995	1.208378	C	2.258891	2.813875	0.962069
O	-1.578151	-2.961463	-0.113819	O	2.224574	2.750686	-0.363027
O	-1.447803	-4.036808	1.869199	O	2.441760	3.905803	1.566891
O	-1.264501	-1.779792	1.754447	O	1.977998	1.686588	1.583593
C	2.160326	-2.559156	-1.108661	C	-1.611871	2.808845	-0.870271
C	2.567495	-2.491496	0.268624	C	-1.813924	2.856427	0.552446
C	3.211717	-2.571763	-2.081019	C	-2.786454	2.921233	-1.682201
C	3.919887	-2.441951	0.641844	C	-3.092990	2.992407	1.116148
H	1.775606	-2.373040	1.031171	H	-0.938620	2.672271	1.202758

C 4.557060 -2.510231 -1.697196 H 2.924299 -2.591380 -3.144511 C 4.930545 -2.450481 -0.336389 H 4.181314 -2.360226 1.710693 H 5.338967 -2.494434 -2.475163 H 5.992009 -2.394932 -0.049535 F 5.591170 1.512825 -2.134311	C -4.058042 3.040191 -1.108179 H -2.660507 2.858822 -2.775028 C -4.229516 3.082281 0.293048 H -3.200323 2.988657 2.214219 H -4.944852 3.075405 -1.761816 H -5.237397 3.158935 0.728597 C -5.832961 -0.623474 -1.145769 F -6.395802 0.613260 -1.243480 F -6.383454 -1.385157 -2.127525 F -6.237170 -1.142796 0.045185
Zero-point correction= 0.753783 (Hartree/Particle) Thermal correction to Energy= 0.808037 Thermal correction to Enthalpy= 0.808981 Thermal correction to Gibbs Free Energy= 0.665077 Sum of electronic and zero-point Energies= -3501.026175 Sum of electronic and thermal Energies= -3500.971922 Sum of electronic and thermal Enthalpies= -3500.970978 Sum of electronic and thermal Free Energies= -3501.114881	Zero-point correction= 0.766388 (Hartree/Particle) Thermal correction to Energy= 0.823483 Thermal correction to Enthalpy= 0.824427 Thermal correction to Gibbs Free Energy= 0.673023 Sum of electronic and zero-point Energies= -3738.650506 Sum of electronic and thermal Energies= -3738.593411 Sum of electronic and thermal Enthalpies= -3738.592467 Sum of electronic and thermal Free Energies= -3738.743871

Ph(pF)+B-Ph(pMe)-IPr-VIIIpost	**Ph(pCF3)+B-Ph(pMe)-IPR-VIIIpost**
97 IPrVIII-F SCF Done: -3501.79826244 A.U. Pd -0.339244 -0.912006 0.029775 N -3.043542 0.101218 0.543112 C -3.136719 1.332523 -2.063609 H -2.244243 1.475560 -1.415305 C -3.627605 -0.097323 -1.828459 C -3.558119 -0.699215 -0.543143 C -1.704103 0.349184 0.709607 C -3.931873 -2.038626 -0.287061 C -3.755377 -2.670294 1.090224 H -3.027066 -2.050724 1.652700 C -4.160434 -0.879963 -2.870128 H -4.233172 -0.458591 -3.883224 C -4.590666 -2.196595 -2.638713 H -5.009819 -2.787399 -3.468949 C -4.468115 -2.771580 -1.366470 H -4.779676 -3.815085 -1.206657 C -3.811680 0.799011 1.473998 C -3.144445 -4.081034 1.011506 H -2.887870 -4.438786 2.028755 H -3.844684 -4.816423 0.560349 H -2.205443 -4.068713 0.424735 C -5.090719 -2.676783 1.864294 H -4.953241 -3.108149 2.878051 H -5.503288 -1.653196 1.981870 H -5.854362 -3.285541 1.333936 C -2.675474 1.593540 -3.506016 H -3.526729 1.611604 -4.219588 H -2.177710 2.583510 -3.564133 H -1.952411 0.820841 -3.835315 C -4.196503 2.370888 -1.633698 H -4.483323 2.256445 -0.569478 H -3.806932 3.401717 -1.768191 H -5.116131 2.267825 -2.247988 C -2.934174 1.530991 2.230721 H -3.094902 2.232103 3.054810 H -4.901603 0.714059 1.504577 N -1.653752 1.259716 1.740367 C -0.490726 2.043675 2.080572 C -0.426179 3.362229 1.556023 C 0.533825 1.479839 2.879808	100 IPrVIII-CF3 SCF Done: -3739.44315564 A.U. Pd 0.324137 -0.106362 0.523339 N -0.599021 -2.745194 -0.353190 C -1.265540 -1.730792 -2.970781 H -1.590406 -1.175227 -2.063659 C 0.115658 -2.309438 -2.657386 C 0.437517 -2.787364 -1.356373 C -0.975003 -1.585531 0.282466 C 1.718020 -3.278501 -1.001374 C 2.051446 -3.689776 0.429656 H 1.289566 -3.234537 1.094891 C 1.124303 -2.395124 -3.638326 H 0.920564 -2.037098 -4.657875 C 2.387792 -2.933337 -3.334797 H 3.153950 -3.007981 -4.123371 C 2.683626 -3.361481 -2.030386 H 3.684275 -3.758767 -1.799935 C -1.420030 -3.814418 0.006333 C 3.410256 -3.136201 0.896407 H 3.553435 -3.345590 1.974842 H 4.263635 -3.586005 0.345690 H 3.453885 -2.034497 0.789210 C 1.987883 -5.224450 0.584131 H 2.191223 -5.518802 1.634689 H 0.991420 -5.625210 0.305050 H 2.742062 -5.721923 -0.062810 C -1.264060 -0.722684 -4.130797 H -1.084685 -1.213768 -5.111115 H -2.254502 -0.226124 -4.190765 H -0.495991 0.060984 -3.977131 C -2.298003 -2.851282 -3.228080 H -2.382335 -3.547291 -2.370542 H -3.302218 -2.413893 -3.405594 H -2.017336 -3.443661 -4.124652 C -2.357817 -3.308568 0.867761 H -3.205578 -3.777867 1.375413 H -1.266423 -4.822401 -0.389245 N -2.084534 -1.945711 1.009584 C -3.001901 -1.014457 1.624413 C -4.182916 -0.700724 0.901203 C -2.695990 -0.454090 2.888277

C	0.702768	4.136517	1.888488
C	1.655470	2.291463	3.153576
C	1.736377	3.606969	2.674274
H	0.787159	5.162998	1.498246
H	2.475352	1.883395	3.764562
H	2.619239	4.223119	2.907977
C	-1.518767	3.949763	0.660812
H	-2.274852	3.161844	0.470784
C	0.441166	0.073970	3.459732
H	-0.397682	-0.455391	2.968822
C	-2.243511	5.112210	1.369820
H	-2.657267	4.795906	2.349885
H	-1.554068	5.962694	1.556657
H	-3.081884	5.487864	0.746452
C	-0.979186	4.373665	-0.718593
H	-1.800165	4.793374	-1.337017
H	-0.189754	5.149927	-0.639990
H	-0.549646	3.509180	-1.259748
C	0.140471	0.133179	4.971741
H	0.025924	-0.892083	5.381396
H	0.959999	0.636476	5.529031
H	-0.797188	0.691856	5.174913
C	1.701417	-0.759482	3.160054
H	1.924778	-0.737854	2.073997
H	2.595810	-0.387489	3.703854
H	1.524972	-1.815547	3.448015
C	0.065475	-0.007435	-1.687487
O	-0.225467	-0.604024	-2.741658
O	3.890025	-2.588910	-1.670568
C	2.353755	3.610788	-2.024962
C	1.660369	3.130860	-3.150195
H	2.878780	3.353515	0.060703
C	2.308439	2.954774	-0.788367
C	0.913796	1.954284	-3.023076
C	0.822802	1.285379	-1.777017
C	1.523495	1.801765	-0.667175
H	0.382000	1.529236	-3.887120
H	1.453801	1.277008	0.297034
H	1.729947	3.681421	-4.100194
K	1.564674	-2.685535	-2.604115
K	3.388471	-3.491504	0.767272
C	0.459145	-3.109320	1.082533
O	0.895317	-2.627691	-0.111884
O	1.003925	-4.114839	1.591599
O	-0.491818	-2.395514	1.616431
C	4.509862	-1.591270	-1.079538
C	3.810145	-0.675758	-0.213509
C	5.928427	-1.388014	-1.188780
C	4.477018	0.336967	0.495628
H	2.714792	-0.782998	-0.130767
C	6.578813	-0.366492	-0.482262
H	6.490323	-2.066845	-1.851531
C	5.868578	0.504039	0.373662
H	3.892912	1.005460	1.152213
H	7.669791	-0.244146	-0.596495
H	6.392704	1.299486	0.926110
F	3.078229	4.742014	-2.140775

Zero-point correction=	0.754226 (Hartree/Particle)
Thermal correction to Energy=	0.809309
Thermal correction to Enthalpy=	0.810254
Thermal correction to Gibbs Free Energy=	0.662449

C	-5.086221	0.201817	1.496160
C	-3.635155	0.447798	3.433094
C	-4.817743	0.768364	2.750798
H	-5.998890	0.492098	0.953332
H	-3.432593	0.900765	4.415955
H	-5.534398	1.476718	3.196322
C	-4.495234	-1.294264	-0.473552
H	-3.669159	-1.977179	-0.757381
C	-1.435356	-0.819040	3.662264
H	-0.762278	-1.386371	2.991144
C	-5.784546	-2.139567	-0.432369
H	-5.725799	-2.932022	0.342517
H	-6.672522	-1.512962	-0.204821
H	-5.961217	-2.628045	-1.413576
C	-4.560451	-0.206828	-1.562340
H	-4.817830	-0.656849	-2.544274
H	-5.318666	0.569868	-1.336085
H	-3.584617	0.304124	-1.666740
C	-1.781666	-1.732002	4.857191
H	-0.856301	-2.034370	5.390084
H	-2.443423	-1.215203	5.585292
H	-2.303710	-2.653455	4.523565
C	-0.644626	0.426303	4.105536
H	-0.438537	1.091119	3.241167
H	-1.184039	1.013023	4.879654
H	0.336859	0.120167	4.518687
C	-0.217412	1.004705	-1.026485
O	0.505868	1.074942	-2.033316
O	5.071497	1.292135	-0.771365
C	-3.921067	3.221790	-0.938709
C	-3.230882	3.057362	-2.155647
H	-3.908805	2.882379	1.211483
C	-3.375674	2.731530	0.262899
C	-2.006869	2.375486	-2.168710
C	-1.485523	1.820767	-0.977429
C	-2.172696	2.016852	0.238724
H	-1.444025	2.234909	-3.103565
H	-1.758469	1.587249	1.164716
H	-3.662765	3.456927	-3.085043
K	3.050923	0.170555	-1.486512
K	4.438101	2.087206	1.668368
C	2.282007	0.017033	2.153268
O	2.036506	0.926513	1.170076
O	3.260642	0.149825	2.916903
O	1.420766	-0.966956	2.175710
C	6.250096	1.848525	-0.608322
C	6.508767	3.208451	-0.996675
C	7.331655	1.157727	0.040458
C	7.743174	3.824654	-0.737516
H	5.701226	3.753768	-1.514713
C	8.559911	1.789068	0.293682
H	7.165788	0.106208	0.331538
C	8.781436	3.127767	-0.086858
H	7.900565	4.870661	-1.052535
H	9.363214	1.223058	0.796017
C	-5.303108	3.831879	-0.910204
H	9.747690	3.616529	0.113023
F	-6.260300	2.854600	-0.804556
F	-5.586516	4.538392	-2.029979
F	-5.476438	4.653528	0.154958

Zero-point correction=	0.766537 (Hartree/Particle)
Thermal correction to Energy=	0.824674
Thermal correction to Enthalpy=	0.825618
Thermal correction to Gibbs Free Energy=	0.668853

Sum of electronic and zero-point Energies= -3501.044036 Sum of electronic and thermal Energies= -3500.988953 Sum of electronic and thermal Enthalpies= -3500.988009 Sum of electronic and thermal Free Energies= -3501.135813	Sum of electronic and zero-point Energies= -3738.676618 Sum of electronic and thermal Energies= -3738.618482 Sum of electronic and thermal Enthalpies= -3738.617538 Sum of electronic and thermal Free Energies= -3738.774303

Ph(pF)+B-Ph(pMe)-IPr-VIII				**Ph(pCF3)+B-Ph(pMe)-IPR-VIII**			
84				87			
IPrVIIImenysKOPh-F SCF Done: -2595.02094141 A.U.				IPrVIIImenysKOPh-CF3 SCF Done: -2832.65861456 A.U.			
Pd	-0.837767	-0.731125	-0.462059	Pd	-1.140726	-0.765688	-0.472473
N	-0.838232	1.497510	1.450358	N	-1.543294	1.538937	1.305104
C	0.304059	3.419887	-0.384174	C	-0.185705	3.422337	-0.409048
H	0.752081	2.410287	-0.256390	H	0.270932	2.445072	-0.138819
C	-1.207372	3.251204	-0.223028	C	-1.694695	3.190078	-0.497617
C	-1.755606	2.263677	0.639048	C	-2.343588	2.224188	0.316851
C	-0.132177	0.417524	0.978398	C	-0.720178	0.480208	1.004097
C	-3.140476	1.996726	0.726903	C	-3.711749	1.894864	0.187721
C	-3.684366	0.816205	1.524205	C	-4.333273	0.737217	0.961319
H	-2.829360	0.167729	1.803359	H	-3.507669	0.126816	1.379733
C	-2.117275	4.053001	-0.937446	C	-2.498978	3.906983	-1.403630
H	-1.736488	4.830504	-1.615752	H	-2.038548	4.665251	-2.053742
C	-3.502801	3.865238	-0.810861	C	-3.876982	3.657101	-1.502266
H	-4.195492	4.511881	-1.373190	H	-4.487599	4.236710	-2.213114
C	-4.006731	2.836929	-0.003328	C	-4.471706	2.650628	-0.729378
H	-5.093367	2.667050	0.052025	H	-5.544072	2.430959	-0.848852
C	-0.439152	1.845379	2.740997	C	-1.372684	1.960727	2.623237
C	-4.609763	-0.056154	0.652084	C	-5.117598	-0.203098	0.024961
H	-4.802478	-1.029011	1.145535	H	-5.355235	-1.152613	0.543700
H	-5.583344	0.441843	0.452171	H	-6.066937	0.255360	-0.327444
H	-4.118751	-0.272923	-0.318629	H	-4.500292	-0.459617	-0.859972
C	-4.377818	1.277503	2.820869	C	-5.203240	1.241425	2.129674
H	-4.751667	0.404258	3.395624	H	-5.633654	0.387393	2.693627
H	-3.679456	1.843605	3.472669	H	-4.611982	1.857557	2.839306
H	-5.244117	1.939079	2.602682	H	-6.044412	1.867847	1.761453
C	0.716250	3.902228	-1.784986	C	0.443564	3.843120	-1.747589
H	0.444663	4.965714	-1.957066	H	0.168924	4.882047	-2.030031
H	1.817393	3.821903	-1.897933	H	1.549830	3.807197	-1.667548
H	0.239417	3.279433	-2.567404	H	0.129762	3.158837	-2.560551
C	0.890506	4.340984	0.707730	C	0.169246	4.432043	0.704007
H	0.681876	3.960637	1.727261	H	-0.203891	4.105911	1.694998
H	1.992432	4.423923	0.598653	H	1.269957	4.554403	0.782446
H	0.460113	5.361976	0.628737	H	-0.272323	5.426966	0.482243
C	0.574513	0.987372	3.079406	C	-0.388844	1.171514	3.159723
H	1.191277	0.910475	3.979445	H	0.079393	1.164758	4.148329
H	-0.910360	2.666612	3.288905	H	-1.961712	2.778904	3.047822
N	0.764710	0.136614	1.987027	N	0.013438	0.288279	2.154272
C	1.934778	-0.693242	1.825054	C	1.222911	-0.497250	2.229462
C	3.155183	-0.033817	1.518368	C	2.455398	0.199384	2.112379
C	1.830263	-2.099072	1.953114	C	1.145157	-1.900409	2.401101
C	4.306463	-0.832105	1.374374	C	3.640611	-0.558220	2.190738
C	3.013242	-2.849760	1.782733	C	2.364006	-2.609028	2.465787
C	4.238378	-2.226557	1.505965	C	3.597068	-1.948695	2.367430
H	5.268663	-0.353648	1.133178	H	4.612657	-0.054004	2.076059
H	2.968324	-3.945792	1.876353	H	2.339301	-3.701320	2.601467
H	5.148973	-2.834562	1.382500	H	4.535221	-2.524251	2.418377
C	3.248505	1.481934	1.341897	C	2.535529	1.711571	1.902253
H	2.224281	1.899736	1.399001	H	1.503947	2.110766	1.837838
C	0.515965	-2.793777	2.286457	C	-0.182167	-2.634292	2.551213
H	-0.306090	-2.060794	2.175625	H	-1.000681	-1.945479	2.266359
C	4.061024	2.124672	2.484259	C	3.211916	2.402985	3.103455
H	3.628978	1.879270	3.476662	H	2.690291	2.166956	4.054350
H	5.113782	1.770298	2.479723	H	4.269613	2.081878	3.211978

H	4.074750	3.230039	2.379313
C	3.802690	1.870560	-0.040961
H	3.822891	2.975199	-0.150285
H	4.837640	1.500619	-0.195861
H	3.171159	1.458207	-0.850482
C	0.518960	-3.279436	3.751023
H	-0.457314	-3.742656	4.004821
H	1.313586	-4.036600	3.927322
H	0.693829	-2.438764	4.455198
C	0.201563	-3.936931	1.303566
H	0.230050	-3.569807	0.257015
H	0.912849	-4.785018	1.404218
H	-0.823858	-4.314972	1.484827
C	0.033843	0.239664	-1.952040
O	-0.607333	1.025982	-2.646391
C	4.177459	-0.507217	-2.864564
C	3.495035	0.514415	-3.546641
H	4.116014	-2.098282	-1.392390
C	3.544878	-1.313762	-1.908218
C	2.142996	0.730605	-3.250576
C	1.483255	-0.048627	-2.271045
C	2.196726	-1.071472	-1.610239
H	1.568146	1.516077	-3.764582
H	1.677794	-1.671462	-0.844024
H	4.036154	1.119340	-4.289795
K	-3.888667	-2.914995	-2.898583
C	-2.625924	-2.571982	-0.376759
O	-2.005374	-2.140319	-1.505363
O	-3.580898	-3.393097	-0.468065
O	-2.182431	-2.036013	0.716687
F	5.485273	-0.711869	-3.134153

Zero-point correction= 0.662266 (Hartree/Particle)
Thermal correction to Energy= 0.708430
Thermal correction to Enthalpy= 0.709374
Thermal correction to Gibbs Free Energy= 0.582179
Sum of electronic and zero-point Energies= -2594.358676
Sum of electronic and thermal Energies= -2594.312511
Sum of electronic and thermal Enthalpies= -2594.311567
Sum of electronic and thermal Free Energies= -2594.438762

H	3.206079	3.505445	2.971245
C	3.228692	2.068195	0.574496
H	3.281393	3.170275	0.450170
H	4.261789	1.669495	0.516514
H	2.666448	1.655471	-0.283932
C	-0.403290	-3.043954	4.022531
H	-1.388626	-3.541442	4.139746
H	0.381611	-3.750931	4.368718
H	-0.380988	-2.161020	4.695610
C	-0.290914	-3.840348	1.599920
H	-0.100594	-3.530848	0.551667
H	0.420284	-4.651993	1.865846
H	-1.319293	-4.250917	1.633663
C	-0.076288	0.155167	-1.861187
O	-0.612236	0.857482	-2.714617
C	4.223766	-0.330101	-1.854274
C	3.625001	0.625663	-2.698795
H	3.899330	-1.938106	-0.422407
C	3.427547	-1.183694	-1.067207
C	2.228725	0.743562	-2.728995
C	1.425086	-0.064757	-1.893858
C	2.035311	-1.039005	-1.077898
H	1.733037	1.479878	-3.379568
H	1.397483	-1.667068	-0.434174
H	4.258765	1.278420	-3.317359
K	-3.635689	-3.218321	-3.256594
C	-2.850290	-2.675286	-0.576942
O	-2.053247	-2.284063	-1.605846
O	-3.748203	-3.538275	-0.780260
O	-2.621210	-2.059533	0.540531
C	5.724298	-0.391141	-1.699319
F	6.123387	0.249026	-0.554293
F	6.382059	0.200022	-2.726679
F	6.177016	-1.667351	-1.599796

Zero-point correction= 0.675031 (Hartree/Particle)
Thermal correction to Energy= 0.723951
Thermal correction to Enthalpy= 0.724895
Thermal correction to Gibbs Free Energy= 0.590606
Sum of electronic and zero-point Energies= -2831.983583
Sum of electronic and thermal Energies= -2831.934664
Sum of electronic and thermal Enthalpies= -2831.933720
Sum of electronic and thermal Free Energies= -2832.068009

Ph(pF)+B-Ph(pMe)-IPr-IX			
100			
IPrIX-F SCF Done: -3003.05494938 A.U.			
Pd	-0.095165	0.314827	0.382902
K	2.574088	4.804841	-0.753669
O	1.045784	4.350819	1.280884
H	0.856381	4.597914	2.201747
B	1.514638	2.944825	1.246706
O	2.943142	2.914572	1.576330
H	3.283609	2.002559	1.498388
C	0.583818	1.980728	2.212612
C	1.152959	1.267253	3.311418
C	-0.846677	1.956510	2.117687
C	0.373728	0.561493	4.234440
H	2.247417	1.280358	3.435705
C	-1.652164	1.242635	3.036935
H	-1.345332	2.568868	1.349268
C	-1.023115	0.553220	4.073455
H	0.820513	0.004162	5.071242

Ph(pCF3)+B-Ph(pMe)-IPR-IX			
103			
IPrIX-CF3 SCF Done: -3240.69205384 A.U.			
Pd	0.107554	0.080692	-0.353096
K	-3.492687	0.942292	-4.293827
O	-1.016886	0.177646	-4.506914
H	-0.426461	-0.328970	-5.090371
B	-1.239684	-0.590488	-3.258992
O	-2.239953	-1.634334	-3.523602
H	-2.416640	-2.142545	-2.709098
C	0.182376	-1.172345	-2.659018
C	0.395516	-2.571323	-2.480941
C	1.314681	-0.325058	-2.442815
C	1.634769	-3.093754	-2.108043
H	-0.445343	-3.259989	-2.658746
C	2.573293	-0.846020	-2.044126
H	1.241071	0.745573	-2.693901
C	2.729935	-2.226641	-1.880459
H	1.768142	-4.180058	-1.987217

H	-2.746726	1.215329	2.936489	H	3.419420	-0.164059	-1.875403
C	0.371788	2.801014	-1.072828	C	-1.556238	1.714935	-2.142248
O	0.492493	3.720933	-1.914175	O	-2.293406	2.590396	-2.652247
O	1.455417	2.541405	-0.248897	O	-1.938414	0.391929	-2.300775
O	-0.645782	2.029252	-0.934259	O	-0.506145	1.929659	-1.435808
N	-2.203026	-0.881478	-1.336183	N	0.808979	2.188594	1.612033
N	-0.273566	-1.683138	-1.925447	N	-0.909420	1.102394	2.372946
C	-0.877147	-0.890012	-0.987391	C	-0.004792	1.117323	1.346491
C	-2.419161	-1.643380	-2.484622	C	0.417550	2.832801	2.783953
C	-1.201774	-2.146864	-2.860678	C	-0.671553	2.153271	3.262791
C	-3.233604	-0.237975	-0.550922	C	1.964269	2.510517	0.802713
C	-3.781902	0.983467	-1.013304	C	1.879777	3.582023	-0.119817
C	-4.775131	1.583602	-0.210604	C	3.006228	3.806718	-0.938422
C	-5.187840	0.995021	0.991606	C	4.145035	2.995182	-0.843768
C	-4.617685	-0.212909	1.424633	C	4.197872	1.946206	0.087963
C	-3.622956	-0.860882	0.667001	C	3.108450	1.679975	0.940065
C	-3.355667	1.620028	-2.333640	C	0.651690	4.484324	-0.203521
H	-5.960875	1.485164	1.605044	H	5.005914	3.180988	-1.505950
C	-2.996253	-2.177232	1.128173	C	3.165213	0.575443	1.994249
C	1.127096	-2.025384	-1.898959	C	-1.947266	0.112027	2.527038
C	1.508257	-3.205681	-1.211817	C	-1.680284	-1.007471	3.353926
C	2.882330	-3.519805	-1.193801	C	-2.707394	-1.963702	3.491413
C	3.817977	-2.695339	-1.833489	C	-3.936105	-1.798390	2.839423
C	3.408499	-1.520151	-2.481234	C	-4.160647	-0.686968	2.012911
C	2.051724	-1.142877	-2.511678	C	-3.163333	0.288355	1.818307
C	0.472495	-4.101960	-0.531795	C	-0.352312	-1.158975	4.095582
H	4.887230	-2.957187	-1.801702	H	-4.723529	-2.559356	2.957032
C	1.590810	0.167011	-3.149114	C	-3.364324	1.471717	0.872103
H	-3.415813	-1.764026	-2.917028	H	0.950093	3.706602	3.168042
H	-0.909131	-2.783466	-3.699901	H	-1.300940	2.318555	4.141127
H	-5.224351	2.534403	-0.534617	H	2.980383	4.623982	-1.674371
H	-4.944206	-0.655572	2.376413	H	5.098777	1.318432	0.147912
H	-2.347485	1.226456	-2.576210	H	-0.213964	3.887370	0.151246
H	-1.908421	-2.108142	0.923254	H	2.154495	0.123041	2.057497
H	3.226072	-4.416812	-0.658579	H	-2.536220	-2.856084	4.111143
H	4.162664	-0.866120	-2.942970	H	-5.120179	-0.593280	1.483726
H	-0.375290	-3.452410	-0.225467	H	0.412354	-0.586847	3.527954
H	0.711933	0.521560	-2.569733	H	-2.381710	1.679317	0.397497
C	2.644153	1.287208	-3.074514	C	-4.351957	1.182148	-0.271615
H	3.503921	1.100531	-3.753467	H	-5.399868	1.104947	0.090124
H	2.172289	2.247157	-3.365787	H	-4.297592	2.009757	-1.007268
H	3.021618	1.410885	-2.039653	H	-4.082319	0.249457	-0.806319
C	1.133021	-0.055240	-4.606910	C	-3.787461	2.742033	1.641756
H	0.311391	-0.796636	-4.670870	H	-3.041982	3.027315	2.410561
H	0.764858	0.895321	-5.046082	H	-3.892395	3.597369	0.942358
H	1.974891	-0.424451	-5.231118	H	-4.762541	2.586546	2.151236
C	0.998837	-4.781536	0.743598	C	0.140771	-2.614430	4.172922
H	0.162970	-5.279665	1.275789	H	1.168137	-2.640185	4.589929
H	1.755438	-5.561907	0.514177	H	-0.499469	-3.234700	4.835600
H	1.446300	-4.045064	1.436639	H	0.174506	-3.081255	3.171387
C	-0.069717	-5.161679	-1.516789	C	-0.454000	-0.551624	5.512735
H	0.747254	-5.836816	-1.849684	H	-1.213991	-1.094913	6.113833
H	-0.851347	-5.780983	-1.028766	H	0.519978	-0.626978	6.040233
H	-0.518644	-4.702687	-2.419150	H	-0.745648	0.516800	5.489502
C	-3.217435	3.150717	-2.245019	C	0.320912	4.932085	-1.637769
H	-2.747032	3.538661	-3.171448	H	-0.659223	5.450928	-1.652187
H	-4.202869	3.653046	-2.136151	H	1.077306	5.642260	-2.036537
H	-2.558617	3.431650	-1.402369	H	0.239183	4.055695	-2.307205
C	-4.337060	1.228212	-3.461000	C	0.830234	5.711697	0.718883
H	-5.356461	1.614696	-3.245740	H	1.685834	6.334784	0.380294
H	-4.008219	1.656591	-4.431346	H	-0.080400	6.347265	0.706223
H	-4.421894	0.129286	-3.585758	H	1.030224	5.424894	1.771362
C	-3.117214	-2.428027	2.637711	C	4.110843	-0.574439	1.630274

H	-4.166333	-2.626843	2.947352
H	-2.515330	-3.317512	2.912364
H	-2.728748	-1.577521	3.229095
C	-3.556048	-3.378563	0.333832
H	-3.054980	-4.316179	0.655056
H	-4.647007	-3.495119	0.509449
H	-3.394884	-3.274587	-0.757652
C	2.210351	-1.130238	1.451898
C	2.945047	-0.303823	0.575950
C	2.900352	-1.923959	2.395178
C	4.347129	-0.279921	0.631873
C	4.301475	-1.897191	2.453101
C	5.029437	-1.075765	1.570284
H	2.402521	0.329613	-0.144965
H	2.310453	-2.544223	3.087797
H	4.907243	0.359268	-0.069151
H	4.832838	-2.515797	3.194155
H	6.130107	-1.055530	1.616690
C	0.693365	-1.160640	1.440481
O	0.084732	-1.978882	2.116532
F	-1.777766	-0.149483	4.953498

Zero-point correction=	0.785996 (Hartree/Particle)
Thermal correction to Energy=	0.840825
Thermal correction to Enthalpy=	0.841769
Thermal correction to Gibbs Free Energy=	0.698124
Sum of electronic and zero-point Energies=	-3002.268954
Sum of electronic and thermal Energies=	-3002.214125
Sum of electronic and thermal Enthalpies=	-3002.213181
Sum of electronic and thermal Free Energies=	-3002.356825

H	5.178856	-0.269087	1.651795
H	3.984030	-1.407818	2.349083
H	3.876046	-0.972746	0.627978
C	3.514630	1.166440	3.378067
H	3.512531	0.369065	4.151018
H	4.524750	1.628767	3.363589
H	2.789732	1.943917	3.694211
C	-0.836906	-2.579996	0.405924
C	-2.067395	-2.132842	-0.118597
C	-0.667247	-3.949833	0.706380
C	-3.119369	-3.037547	-0.326173
C	-1.715562	-4.855856	0.487519
C	-2.945337	-4.401815	-0.027327
H	-2.184115	-1.068026	-0.377433
H	0.308284	-4.285268	1.091510
H	-4.083004	-2.671322	-0.715339
H	-1.574728	-5.924768	0.714748
H	-3.768768	-5.114128	-0.196570
C	0.335138	-1.638777	0.605423
O	1.324892	-1.994578	1.228178
C	4.051985	-2.829298	-1.472196
F	5.045191	-1.903655	-1.393676
F	3.977137	-3.439194	-0.257018
F	4.459364	-3.782209	-2.356305

Zero-point correction=	0.798236 (Hartree/Particle)
Thermal correction to Energy=	0.856131
Thermal correction to Enthalpy=	0.857075
Thermal correction to Gibbs Free Energy=	0.704503
Sum of electronic and zero-point Energies=	-3239.893818
Sum of electronic and thermal Energies=	-3239.835923
Sum of electronic and thermal Enthalpies=	-3239.834978
Sum of electronic and thermal Free Energies=	-3239.987551

Ph(pF)+B-Ph(pMe)-IPr-IX-X			
100			
IPrIX-X-F SCF Done: -3003.03625502 A.U.			
Pd	-0.216653	-0.254824	-0.200274
K	-2.639013	-2.874600	4.020070
O	-2.745296	-3.070918	1.434698
H	-3.080491	-3.522241	0.638374
B	-1.379096	-2.673595	1.215844
O	-0.515537	-3.702397	0.849126
H	0.395443	-3.377207	0.700007
C	-1.797291	-1.631359	-0.696695
C	-1.702040	-2.649880	-1.684803
C	-3.023917	-0.899795	-0.663132
C	-2.746706	-2.936757	-2.580762
H	-0.783962	-3.257177	-1.738296
C	-4.081123	-1.162705	-1.547570
H	-3.152640	-0.094524	0.078420
C	-3.925235	-2.180760	-2.500055
H	-2.662982	-3.724820	-3.344997
H	-5.015874	-0.581774	-1.523336
C	-1.521886	-0.541653	2.549272
O	-2.079016	-0.446395	3.670402
O	-0.927598	-1.794951	2.265159
O	-1.395822	0.360296	1.674340
N	0.099297	2.683897	-0.528481
N	2.058580	1.899123	-0.037656
C	0.753414	1.520376	-0.208003
C	0.981455	3.761089	-0.581323
C	2.220628	3.270306	-0.259494

Ph(pCF3)+B-Ph(pMe)-IPR-IX-X			
103			
IPrIX-X-CF3 SCF Done: -3240.67441959 A.U.			
Pd	0.071106	-0.175822	0.109375
K	-1.315150	-0.962927	5.392997
O	-2.215325	-1.805832	3.111608
H	-2.849908	-2.350793	2.611059
B	-0.949679	-1.797441	2.422402
O	-0.427065	-3.055181	2.132570
H	0.421770	-2.988959	1.649804
C	-1.824754	-1.132675	0.514974
C	-2.262398	-2.308013	-0.153672
C	-2.782530	-0.080194	0.641893
C	-3.548202	-2.420631	-0.709126
H	-1.567474	-3.159069	-0.239915
C	-4.067381	-0.179084	0.096634
H	-2.501093	0.850286	1.161947
C	-4.449021	-1.344875	-0.599258
H	-3.849635	-3.330899	-1.249363
H	-4.770822	0.663610	0.182419
C	-0.275148	0.553477	3.053443
O	-0.424322	1.060385	4.191609
O	-0.051253	-0.842650	3.026816
O	-0.262081	1.156563	1.941931
N	0.687360	2.380486	-1.278378
N	2.557362	1.300452	-1.089837
C	1.228960	1.228583	-0.766686
C	1.652996	3.142640	-1.932657
C	2.839949	2.468542	-1.804801

C	-1.341891	2.747038	-0.644947	C	-0.684139	2.774529	-1.030807
C	-2.082599	3.136056	0.501709	C	-0.941837	3.607438	0.089995
C	-3.486630	3.119125	0.391220	C	-2.287926	3.932887	0.346662
C	-4.113880	2.722094	-0.799174	C	-3.319466	3.447219	-0.471565
C	-3.351239	2.335333	-1.910062	C	-3.029864	2.619409	-1.564740
C	-1.943085	2.333007	-1.858441	C	-1.701991	2.255800	-1.866854
C	-1.395606	3.591335	1.788217	C	0.186907	4.166201	0.955753
H	-5.214156	2.704006	-0.857575	H	-4.365874	3.707875	-0.244717
C	-1.111096	1.943299	-3.076194	C	-1.386219	1.364439	-3.062901
C	3.069429	1.012603	0.479265	C	3.536250	0.365761	-0.596240
C	4.077624	0.538515	-0.394141	C	4.119506	-0.555580	-1.498555
C	5.060896	-0.309953	0.155834	C	5.087895	-1.441320	-0.980996
C	5.024234	-0.674716	1.507573	C	5.436939	-1.416053	0.375008
C	3.990050	-0.217145	2.340178	C	4.813028	-0.514775	1.252850
C	2.978864	0.630834	1.847105	C	3.841027	0.396080	0.793692
C	4.112687	0.934313	-1.868682	C	3.732056	-0.592791	-2.975067
H	5.799823	-1.342520	1.915178	H	6.191689	-2.120525	0.759342
C	1.832190	1.111541	2.737239	C	3.143214	1.367670	1.745572
H	0.648627	4.769545	-0.840994	H	1.406438	4.085927	-2.427149
H	3.190841	3.763820	-0.157367	H	3.851173	2.710730	-2.142510
H	-4.098363	3.405263	1.259707	H	-2.532356	4.568360	1.210671
H	-3.855655	2.008273	-2.831274	H	-3.849382	2.220559	-2.181120
H	-0.389865	3.121602	1.807281	H	1.036145	3.454481	0.887403
H	-0.100228	1.652033	-2.728508	H	-0.368201	0.948103	-2.923521
H	5.857518	-0.704031	-0.492890	H	5.561568	-2.174383	-1.651152
H	3.960446	-0.536611	3.392253	H	5.079432	-0.525861	2.319908
H	3.095128	1.286432	-2.139660	H	2.756184	-0.073184	-3.074839
H	0.929600	1.186172	2.096907	H	2.099827	1.484346	1.388415
C	1.458738	0.119708	3.850783	C	3.020757	0.840141	3.183755
H	2.241195	0.045291	4.636878	H	4.000211	0.795083	3.707500
H	0.519626	0.449322	4.339688	H	2.355980	1.508053	3.768005
H	1.269788	-0.891039	3.434221	H	2.560859	-0.169407	3.196432
C	2.117311	2.519641	3.301053	C	3.805382	2.761050	1.702153
H	2.299372	3.254097	2.489737	H	3.805276	3.180018	0.674923
H	1.249184	2.879774	3.892066	H	3.252259	3.469343	2.353950
H	3.009610	2.511161	3.963432	H	4.858334	2.714183	2.054041
C	4.439360	-0.248472	-2.798729	C	3.533780	-2.026199	-3.502645
H	4.319636	0.061012	-3.857148	H	3.117372	-1.995164	-4.530184
H	5.485946	-0.599276	-2.672866	H	4.491801	-2.586183	-3.550420
H	3.758286	-1.101195	-2.619063	H	2.826934	-2.594716	-2.869535
C	5.107755	2.093635	-2.096402	C	4.775603	0.160538	-3.829055
H	6.141052	1.778790	-1.836065	H	5.769239	-0.331309	-3.755720
H	5.104405	2.409966	-3.160635	H	4.475949	0.168678	-4.898037
H	4.865592	2.980712	-1.477011	H	4.902272	1.212775	-3.502660
C	-2.119467	3.150934	3.072763	C	-0.172098	4.291039	2.446575
H	-1.504943	3.423795	3.957074	H	0.728615	4.596970	3.020005
H	-3.096972	3.665899	3.193293	H	-0.942387	5.072709	2.622164
H	-2.280043	2.056038	3.087747	H	-0.525713	3.325673	2.855714
C	-1.208661	5.125880	1.778039	C	0.657691	5.531905	0.404883
H	-2.195759	5.635889	1.772748	H	-0.161575	6.279524	0.470025
H	-0.655146	5.459870	2.681161	H	1.518811	5.914545	0.992687
H	-0.650416	5.476894	0.887205	H	0.970265	5.473895	-0.656514
C	-1.667884	0.719078	-3.821137	C	-2.326671	0.152568	-3.163022
H	-2.646768	0.925951	-4.304022	H	-3.382789	0.438628	-3.348649
H	-0.958330	0.409238	-4.614227	H	-2.001292	-0.508164	-3.991506
H	-1.791315	-0.137074	-3.129742	H	-2.292270	-0.440312	-2.230248
C	-0.951161	3.163608	-4.008813	C	-1.386245	2.202967	-4.358991
H	-0.307739	2.911514	-4.878163	H	-1.110823	1.573724	-5.231518
H	-1.936751	3.501133	-4.396065	H	-2.391472	2.635657	-4.552026
H	-0.488560	4.021499	-3.476051	H	-0.664066	3.044828	-4.299836
C	1.754125	-2.176218	-1.188734	C	1.216582	-2.721627	-0.772919
C	2.214114	-2.342054	0.135516	C	2.112222	-2.692324	0.318401
C	2.046701	-3.165214	-2.153319	C	0.935350	-3.951080	-1.408502

C	2.972129	-3.471416	0.486664
C	2.770575	-4.312413	-1.790656
C	3.240985	-4.465317	-0.472543
H	1.989883	-1.559466	0.877410
H	1.692987	-3.014046	-3.185127
H	3.351149	-3.570630	1.515913
H	2.976027	-5.092225	-2.541624
H	3.820046	-5.360209	-0.194034
C	0.967952	-0.946280	-1.613142
O	1.101044	-0.510432	-2.751480
F	-4.936412	-2.438652	-3.363977

Zero-point correction= 0.783807 (Hartree/Particle)
Thermal correction to Energy= 0.838702
Thermal correction to Enthalpy= 0.839646
Thermal correction to Gibbs Free Energy= 0.695882
Sum of electronic and zero-point Energies= -3002.252448
Sum of electronic and thermal Energies= -3002.197553
Sum of electronic and thermal Enthalpies= -3002.196609
Sum of electronic and thermal Free Energies= -3002.340373

C	2.732457	-3.874543	0.756061
C	1.526879	-5.136386	-0.943779
C	2.432093	-5.100276	0.134135
H	2.338265	-1.728755	0.801125
H	0.247397	-3.954321	-2.268164
H	3.452834	-3.831490	1.587893
H	1.286416	-6.096280	-1.428350
H	2.904729	-6.030194	0.488280
C	0.567738	-1.457387	-1.308268
O	0.385137	-1.339305	-2.513913
C	-5.790431	-1.371006	-1.283383
F	-5.817419	-0.519907	-2.355324
F	-6.123864	-2.601409	-1.749232
F	-6.794605	-0.965434	-0.455599

Zero-point correction= 0.795971 (Hartree/Particle)
Thermal correction to Energy= 0.853898
Thermal correction to Enthalpy= 0.854842
Thermal correction to Gibbs Free Energy= 0.702574
Sum of electronic and zero-point Energies= -3239.878448
Sum of electronic and thermal Energies= -3239.820522
Sum of electronic and thermal Enthalpies= -3239.819578
Sum of electronic and thermal Free Energies= -3239.971845

Ph(pF)+B-Ph(pMe)-IPr-X

100
IPrX-F SCF Done: -3003.06063510 A.U.

Pd	-0.205944	0.382173	0.271467
K	-4.100391	0.239598	-1.520238
O	-2.459433	2.541158	-2.279039
H	-2.572133	3.362357	-1.756638
B	-1.095580	2.322035	-2.465417
O	-0.225961	3.373879	-2.355079
H	0.695981	3.080364	-2.215012
C	-1.540403	1.935104	0.658626
C	-1.347194	3.335523	0.553623
C	-2.844539	1.516579	1.045046
C	-2.397560	4.261478	0.730027
H	-0.354140	3.730509	0.288916
C	-3.911034	2.419027	1.251245
H	-3.039542	0.441978	1.217800
C	-3.674325	3.788762	1.065400
H	-2.236962	5.346176	0.625372
H	-4.908820	2.084083	1.581049
C	-1.581997	0.006834	-2.586825
O	-2.351253	-0.296621	-3.515724
O	-0.657282	1.051267	-2.796832
O	-1.579208	-0.498495	-1.412290
N	0.082203	-2.537790	0.868742
N	2.030932	-1.886392	0.193946
C	0.743610	-1.444682	0.351902
C	0.944638	-3.617143	1.056941
C	2.177989	-3.209675	0.622249
C	-1.344524	-2.539208	1.095610
C	-2.181517	-3.095064	0.094298
C	-3.575066	-3.030195	0.309867
C	-4.100311	-2.421659	1.461691
C	-3.242700	-1.879578	2.433525
C	-1.842046	-1.927818	2.275309
C	-1.602906	-3.789089	-1.136349
H	-5.191868	-2.385105	1.614969
C	-0.897036	-1.403734	3.352558
C	3.059355	-1.118443	-0.462609

Ph(pCF3)+B-Ph(pMe)-IPR-X

103
IPrX-CF3 SCF Done: -3240.70165177 A.U.

Pd	-0.068313	-0.076669	0.370433
K	3.931425	0.667413	-1.928866
O	2.970118	-1.841897	-2.231857
H	3.431279	-2.587977	-1.801964
B	1.593277	-2.080205	-2.158375
O	1.181644	-3.333469	-1.799448
H	0.247259	-3.358105	-1.499213
C	1.815685	-0.720042	0.910257
C	2.379863	-2.019239	0.890744
C	2.719124	0.360762	1.143290
C	3.773259	-2.225694	0.901003
H	1.721059	-2.895555	0.782047
C	4.108107	0.169996	1.196201
H	2.328118	1.387438	1.247981
C	4.645337	-1.124883	1.007356
H	4.190673	-3.240376	0.794231
H	4.788284	1.023552	1.361398
C	1.186682	0.270651	-2.487876
O	1.834503	0.624144	-3.491226
O	0.703739	-1.067605	-2.443800
O	0.935713	0.958540	-1.450514
N	-1.678193	2.419081	0.601891
N	-3.080305	0.903864	-0.038502
C	-1.745876	1.104816	0.200614
C	-2.939816	3.009348	0.644256
C	-3.830198	2.053279	0.231193
C	-0.424679	3.092141	0.854409
C	0.187874	3.786809	-0.221172
C	1.421917	4.415577	0.041650
C	2.012614	4.346485	1.312859
C	1.387969	3.636091	2.349428
C	0.156783	2.980225	2.141453
C	-0.476249	3.877434	-1.593333
H	2.976071	4.848978	1.497563
C	-0.526924	2.201299	3.260316
C	-3.609261	-0.297225	-0.633110

C	4.101297	-0.567982	0.322037	C	-4.331982	-1.198678	0.185455
C	5.106868	0.154868	-0.353238	C	-4.867381	-2.347551	-0.433326
C	5.060267	0.327606	-1.741296	C	-4.663629	-2.590645	-1.796903
C	3.996089	-0.202455	-2.488669	C	-3.900741	-1.702268	-2.572345
C	2.961975	-0.933755	-1.871199	C	-3.346997	-0.533020	-2.012631
C	4.159389	-0.756133	1.836902	C	-4.516521	-0.955072	1.681936
H	5.852471	0.900268	-2.249183	H	-5.084313	-3.497066	-2.260743
C	1.771825	-1.472214	-2.671208	C	-2.475405	0.416609	-2.839664
H	0.607022	-4.567304	1.479215	H	-3.087000	4.044543	0.963903
H	3.133345	-3.737818	0.561244	H	-4.913141	2.087373	0.084951
H	-4.255900	-3.472430	-0.434624	H	1.927628	4.968247	-0.764534
H	-3.666508	-1.409892	3.333325	H	1.870538	3.576227	3.336467
H	-0.592928	-3.361573	-1.306526	H	-1.105600	2.970511	-1.705929
H	0.045539	-1.094228	2.858106	H	-1.203233	1.457335	2.793531
H	5.929482	0.602297	0.224287	H	-5.431484	-3.073272	0.171216
H	3.964692	-0.032190	-3.574244	H	-3.725670	-1.929852	-3.633599
H	3.138369	-1.027346	2.178508	H	-3.715879	-0.255881	2.003273
H	0.863812	-1.245262	-2.070375	H	-1.609446	0.685126	-2.195720
C	1.583268	-0.786182	-4.033292	C	-1.894136	-0.226321	-4.108608
H	2.385713	-1.059671	-4.752196	H	-2.674634	-0.414624	-4.877350
H	0.616235	-1.099467	-4.476185	H	-1.141183	0.453036	-4.557469
H	1.547645	0.316134	-3.934501	H	-1.374031	-1.176777	-3.880436
C	1.843486	-3.005179	-2.852298	C	-3.221897	1.722486	-3.193269
H	1.882385	-3.544696	-1.885488	H	-3.565662	2.270256	-2.293814
H	0.947925	-3.365799	-3.400377	H	-2.552877	2.402591	-3.760959
H	2.742678	-3.290160	-3.439296	H	-4.109715	1.508363	-3.825973
C	4.556515	0.530445	2.584271	C	-4.351478	-2.239019	2.517403
H	4.447138	0.379562	3.677623	H	-4.315179	-1.984077	3.595892
H	5.614236	0.810431	2.392587	H	-5.200753	-2.940005	2.370047
H	3.908731	1.378898	2.295831	H	-3.413497	-2.769771	2.266274
C	5.119766	-1.909726	2.202942	C	-5.884590	-0.298765	1.968947
H	6.156068	-1.671563	1.880733	H	-6.712596	-0.967833	1.650698
H	5.132755	-2.076114	3.300584	H	-6.003050	-0.100068	3.054775
H	4.833777	-2.864457	1.717360	H	-6.007846	0.663096	1.432272
C	-2.413268	-3.565735	-2.424191	C	0.517554	3.883421	-2.767278
H	-1.885776	-4.031430	-3.282707	H	-0.037849	3.832456	-3.727082
H	-3.415388	-4.044431	-2.372337	H	1.121485	4.816165	-2.795782
H	-2.534015	-2.489661	-2.653763	H	1.192224	3.007405	-2.725688
C	-1.447359	-5.303602	-0.865199	C	-1.398693	5.115024	-1.670106
H	-2.442541	-5.775037	-0.717244	H	-0.805360	6.049187	-1.571637
H	-0.954569	-5.805911	-1.723977	H	-1.928565	5.145608	-2.645449
H	-0.845107	-5.509475	0.041434	H	-2.164199	5.117885	-0.869696
C	-1.415007	-0.152813	4.077556	C	0.460555	1.389276	4.113652
H	-2.308901	-0.361920	4.704249	H	1.124193	2.036589	4.726232
H	-0.621467	0.241239	4.742819	H	-0.100638	0.727691	4.802822
H	-1.661594	0.647655	3.352155	H	1.087116	0.739914	3.470159
C	-0.563877	-2.540928	4.343934	C	-1.383616	3.152390	4.123147
H	0.169450	-2.192211	5.100833	H	-1.917996	2.586276	4.914722
H	-1.475884	-2.883793	4.878670	H	-0.750228	3.920993	4.616436
H	-0.127181	-3.420131	3.825502	H	-2.142872	3.683687	3.511495
C	1.900602	2.331299	0.782028	C	-1.043907	-2.685866	1.181579
C	2.257015	2.237058	-0.580633	C	-1.472441	-2.953440	-0.137835
C	2.315742	3.454936	1.527870	C	-0.781827	-3.763393	2.054019
C	3.032751	3.239648	-1.183816	C	-1.667482	-4.277597	-0.565628
C	3.055493	4.479533	0.912640	C	-0.922785	-5.088751	1.606307
C	3.420822	4.372392	-0.441710	C	-1.375480	-5.349832	0.300648
H	1.940004	1.349720	-1.151952	H	-1.676715	-2.111464	-0.816587
H	2.042119	3.508623	2.593194	H	-0.467446	-3.541191	3.085607
H	3.345259	3.129290	-2.234967	H	-2.053106	-4.468533	-1.579986
H	3.355253	5.365835	1.494849	H	-0.689959	-5.924710	2.285454
H	4.013771	5.169024	-0.918666	H	-1.506492	-6.388407	-0.042173
C	1.089854	1.245115	1.472180	C	-0.889384	-1.265884	1.703845
O	1.282035	1.003742	2.660021	O	-1.248526	-1.000729	2.846402

F -4.693411 4.669186 1.233267	C 6.106516 -1.253824 0.709377 F 6.575275 -2.516519 0.782613 F 6.347267 -0.832586 -0.611488 F 6.892392 -0.463472 1.478095
Zero-point correction= 0.785201 (Hartree/Particle) Thermal correction to Energy= 0.840662 Thermal correction to Enthalpy= 0.841607 Thermal correction to Gibbs Free Energy= 0.695889 Sum of electronic and zero-point Energies= -3002.275434 Sum of electronic and thermal Energies= -3002.219973 Sum of electronic and thermal Enthalpies= -3002.219029 Sum of electronic and thermal Free Energies= -3002.364746	Zero-point correction= 0.797612 (Hartree/Particle) Thermal correction to Energy= 0.855988 Thermal correction to Enthalpy= 0.856932 Thermal correction to Gibbs Free Energy= 0.703302 Sum of electronic and zero-point Energies= -3239.904040 Sum of electronic and thermal Energies= -3239.845664 Sum of electronic and thermal Enthalpies= -3239.844719 Sum of electronic and thermal Free Energies= -3239.998350

Ph(pF)+B-Ph(pMe)-IPr-XI	**Ph(pCF3)+B-Ph(pMe)-IPR-XI**
90 IPrXI-F SCF Done: -1962.77484202 A.U. Pd 0.578430 0.535984 -0.206510 C 1.727919 2.199669 -0.465698 C 1.426318 3.538011 -0.809392 C 3.089520 1.887661 -0.206941 C 2.423468 4.530409 -0.873105 H 0.386336 3.829081 -1.032350 C 4.103268 2.863621 -0.258824 H 3.388753 0.851383 0.041572 C 3.750436 4.178489 -0.592050 H 2.190215 5.573430 -1.138450 H 5.157816 2.621509 -0.054139 N 0.736616 -2.411759 0.233180 N -1.369753 -1.934575 0.304763 C -0.137700 -1.357965 0.139301 C 0.074185 -3.620044 0.442652 C -1.263513 -3.317840 0.484334 C 2.162260 -2.190150 0.211821 C 2.794002 -1.806231 1.423347 C 4.176409 -1.534932 1.372765 C 4.886779 -1.634166 0.167532 C 4.228951 -1.998937 -1.017068 C 2.849108 -2.284270 -1.024524 C 2.010289 -1.610729 2.719521 H 5.964424 -1.407521 0.147179 C 2.110070 -2.571420 -2.327703 C -2.595538 -1.175833 0.374912 C -3.482616 -1.222273 -0.727949 C -4.675522 -0.477335 -0.629752 C -4.948990 0.297327 0.503651 C -4.038453 0.344544 1.569761 C -2.839435 -0.392420 1.537916 C -3.182228 -2.051548 -1.975337 H -5.873496 0.893344 0.551008 C -1.834949 -0.343957 2.692248 H 0.608735 -4.569106 0.544947 H -2.142047 -3.950794 0.637553 H 4.699396 -1.222277 2.289959 H 4.794167 -2.043993 -1.960377 H 0.977683 -1.981508 2.554437 H 1.116617 -2.993458 -2.064838 H -5.388792 -0.485901 -1.467818 H -4.261471 0.984586 2.434293 H -2.095637 -2.282318 -1.966624 H -0.837063 -0.195266 2.223170 C -2.050394 0.829381 3.660249 H -2.979407 0.709334 4.258117	93 IPrXI-CF3 SCF Done: -2200.41319811 A.U. Pd -0.319730 -0.040766 -0.123805 C -2.163339 -0.898527 -0.235334 C -2.598665 -2.201637 -0.572603 C -3.163074 0.052488 0.104763 C -3.960227 -2.548083 -0.563055 H -1.861020 -2.974132 -0.846475 C -4.527160 -0.281040 0.121716 H -2.882391 1.090961 0.365275 C -4.930231 -1.588404 -0.214042 H -4.278106 -3.569995 -0.823021 H -5.283717 0.470570 0.396778 N 1.052180 2.594068 0.100794 N 2.637885 1.126771 0.133123 C 1.274837 1.241468 0.056398 C 2.241454 3.314247 0.193031 C 3.248934 2.382628 0.210651 C -0.292466 3.116017 0.148540 C -0.933427 3.185430 1.412774 C -2.263514 3.651474 1.437337 C -2.921770 4.014809 0.252888 C -2.268697 3.908158 -0.984235 C -0.937391 3.453902 -1.067594 C -0.256973 2.689257 2.688631 H -3.964786 4.366398 0.292294 C -0.266072 3.233311 -2.419017 C 3.327652 -0.138703 0.218216 C 4.045714 -0.593187 -0.914281 C 4.727852 -1.821465 -0.797176 C 4.666975 -2.568838 0.384809 C 3.922212 -2.107384 1.480595 C 3.234653 -0.880140 1.430043 C 4.104642 0.209176 -2.212928 H 5.187097 -3.537112 0.449408 C 2.414268 -0.368122 2.617228 H 2.260728 4.407113 0.240414 H 4.334329 2.494044 0.284738 H -2.798152 3.711101 2.397939 H -2.809464 4.163633 -1.908408 H 0.805689 2.477383 2.450610 H 0.810944 3.036349 -2.232186 H 5.297396 -2.206154 -1.656718 H 3.863020 -2.726224 2.386147 H 3.282413 0.955301 -2.181124 H 1.447189 -0.019460 2.192516 C 2.077917 -1.446815 3.657803 H 2.978178 -1.779079 4.218370

H	-1.205055	0.882021	4.376878
H	-2.105657	1.798243	3.128213
C	-1.795453	-1.669807	3.485331
H	-1.558187	-2.543051	2.847345
H	-1.019937	-1.618029	4.278559
H	-2.773466	-1.861361	3.976103
C	-3.468835	-1.287809	-3.282294
H	-3.142164	-1.892798	-4.153663
H	-4.552989	-1.086223	-3.414678
H	-2.917079	-0.328303	-3.304742
C	-3.960423	-3.385442	-1.938200
H	-5.055478	-3.198274	-1.945039
H	-3.715337	-4.009768	-2.823075
H	-3.733282	-3.977732	-1.028366
C	1.903737	-0.109105	3.059057
H	1.275699	0.045778	3.961275
H	2.902710	0.335872	3.249876
H	1.441699	0.461735	2.219492
C	2.601317	-2.419752	3.890023
H	3.620082	-2.070093	4.160155
H	1.965237	-2.311083	4.793359
H	2.668780	-3.499380	3.642981
C	1.860023	-1.248379	-3.085074
H	2.821184	-0.772955	-3.373665
H	1.267172	-1.428103	-4.005598
H	1.302002	-0.524155	-2.450780
C	2.833288	-3.607561	-3.208395
H	2.213148	-3.856005	-4.094544
H	3.801390	-3.220039	-3.590260
H	3.038731	-4.547374	-2.654566
C	-1.887168	2.154962	-0.651250
C	-1.626509	2.761810	0.593893
C	-3.085196	2.459972	-1.335540
C	-2.546430	3.665507	1.145944
C	-4.009823	3.353892	-0.776542
C	-3.742184	3.960046	0.464678
H	-0.680639	2.515206	1.105031
H	-3.275626	1.978197	-2.306267
H	-2.328395	4.147627	2.112123
H	-4.946350	3.579566	-1.311080
C	-0.922720	1.190986	-1.297141
O	-1.085081	0.776912	-2.432812
F	4.716912	5.129493	-0.648203
H	-4.465416	4.668018	0.900541

H	1.363524	-1.037703	4.401767
H	1.612486	-2.336908	3.192872
C	3.090137	0.833925	3.314326
H	3.273279	1.680303	2.624458
H	2.447074	1.209454	4.138192
H	4.065442	0.533352	3.752894
C	3.869992	-0.663571	-3.460613
H	3.820327	-0.024564	-4.366762
H	4.694938	-1.390032	-3.619836
H	2.913835	-1.215244	-3.377857
C	5.444106	0.970981	-2.318563
H	6.295882	0.259095	-2.362180
H	5.472679	1.593183	-3.237711
H	5.615250	1.637374	-1.448560
C	-0.892563	1.358107	3.144113
H	-0.359631	0.950774	4.028702
H	-1.961689	1.489836	3.412790
H	-0.845435	0.591007	2.335706
C	-0.271521	3.742033	3.813021
H	-1.304178	3.965555	4.154558
H	0.293957	3.372547	4.693938
H	0.189517	4.695393	3.481848
C	-0.851578	1.970769	-3.089035
H	-1.930933	2.104977	-3.313177
H	-0.322084	1.747529	-4.038063
H	-0.750505	1.086326	-2.421001
C	-0.357794	4.468596	-3.335102
H	0.209330	4.293263	-4.272758
H	-1.406596	4.689416	-3.625738
H	0.055314	5.374635	-2.844605
C	0.968293	-2.704222	-0.498759
C	0.488552	-3.042900	0.782857
C	1.841861	-3.588065	-1.171572
C	0.871762	-4.251541	1.382893
C	2.235651	-4.788597	-0.563618
C	1.750718	-5.123834	0.713984
H	-0.197441	-2.340910	1.285739
H	2.209160	-3.307860	-2.169992
H	0.480215	-4.517764	2.377447
H	2.926622	-5.467699	-1.088002
C	0.575187	-1.427110	-1.196946
O	0.842273	-1.218725	-2.367903
C	-6.396262	-1.934626	-0.270359
F	-6.625838	-3.250192	-0.009226
F	-7.129596	-1.211835	0.621334
F	-6.932217	-1.685264	-1.500902
H	2.054244	-6.071022	1.188065

Zero-point correction=	0.731819 (Hartree/Particle)
Thermal correction to Energy=	0.777790
Thermal correction to Enthalpy=	0.778734
Thermal correction to Gibbs Free Energy=	0.652576
Sum of electronic and zero-point Energies=	-1962.043023
Sum of electronic and thermal Energies=	-1961.997052
Sum of electronic and thermal Enthalpies=	-1961.996108
Sum of electronic and thermal Free Energies=	-1962.122266

Zero-point correction=	0.744529 (Hartree/Particle)
Thermal correction to Energy=	0.793325
Thermal correction to Enthalpy=	0.794269
Thermal correction to Gibbs Free Energy=	0.660100
Sum of electronic and zero-point Energies=	-2199.668669
Sum of electronic and thermal Energies=	-2199.619873
Sum of electronic and thermal Enthalpies=	-2199.618929
Sum of electronic and thermal Free Energies=	-2199.753098

Ph(pF)+B-Ph(pMe)-IPr-XI-XII			
90			
IPrXI-XII-F SCF Done: -1962.76720178 A.U.			
Pd	0.386715	0.612980	0.072892
C	0.586627	2.702380	-0.131197
C	0.205470	3.536893	0.946127

Ph(pCF3)+B-Ph(pMe)-IPR-XI-XII			
93			
IPrXI-XII-CF3 SCF Done: -2200.40290996 A.U.			
Pd	-0.241072	-0.003164	-0.020045
C	-1.913233	-1.241561	-0.372319
C	-2.369889	-2.083100	0.668062

C	1.678896	3.095563	-0.942635	C	-2.862963	-0.635875	-1.230441
C	0.936698	4.697943	1.253142	C	-3.746095	-2.256493	0.892949
H	-0.674490	3.282933	1.556704	H	-1.647986	-2.607064	1.312993
C	2.428136	4.242174	-0.642909	C	-4.235413	-0.790048	-1.000216
H	1.919956	2.494895	-1.835010	H	-2.502021	-0.053601	-2.093836
C	2.045451	5.025196	0.459289	C	-4.677829	-1.599338	0.068347
H	0.661439	5.356492	2.090964	H	-4.101751	-2.896360	1.714656
H	3.289978	4.555269	-1.251745	H	-4.972709	-0.289568	-1.646789
N	1.388871	-2.227615	0.249960	N	1.158605	2.647428	0.305039
N	-0.770662	-2.269186	0.298749	N	2.647282	1.083314	0.371023
C	0.290665	-1.401289	0.199088	C	1.297055	1.282732	0.223642
C	1.028789	-3.567749	0.387507	C	2.382747	3.284024	0.507026
C	-0.341930	-3.594473	0.418735	C	3.328444	2.290947	0.547697
C	2.726931	-1.732721	0.048665	C	-0.114732	3.291018	0.101762
C	3.466297	-1.289901	1.171816	C	-0.983883	3.441182	1.209137
C	4.761437	-0.787535	0.934341	C	-2.241322	4.030272	0.967025
C	5.282335	-0.726050	-0.367245	C	-2.608951	4.438791	-0.323605
C	4.512834	-1.148734	-1.461892	C	-1.733620	4.252595	-1.404776
C	3.211734	-1.658419	-1.280922	C	-0.466120	3.665856	-1.219563
C	2.844090	-1.253774	2.565382	C	-0.621939	2.898781	2.589654
H	6.296446	-0.328535	-0.532134	H	-3.598036	4.893458	-0.492429
C	2.333736	-2.016689	-2.477313	C	0.436266	3.343779	-2.408553
C	-2.151069	-1.857432	0.221789	C	3.266065	-0.218724	0.319696
C	-2.681240	-1.494221	-1.045269	C	3.427777	-0.845203	-0.944600
C	-4.034179	-1.101295	-1.078184	C	4.027863	-2.120575	-0.949240
C	-4.814781	-1.087493	0.085723	C	4.454018	-2.726353	0.240922
C	-4.258478	-1.443962	1.322163	C	4.271877	-2.083909	1.473655
C	-2.905912	-1.823977	1.421081	C	3.659146	-0.817607	1.542457
C	-1.818699	-1.524578	-2.308969	C	2.964429	-0.165108	-2.234961
H	-5.867295	-0.768864	0.031241	H	4.912761	-3.726688	0.207813
C	-2.246274	-2.102676	2.773257	C	3.342222	-0.151739	2.882788
H	1.773697	-4.367470	0.436982	H	2.465970	4.371678	0.591008
H	-1.048816	-4.425637	0.502870	H	4.414245	2.328443	0.678845
H	5.366150	-0.425450	1.780032	H	-2.949991	4.155467	1.800293
H	4.923737	-1.066185	-2.480195	H	-2.048478	4.550061	-2.417013
H	1.948356	-1.911082	2.550430	H	0.461471	2.654469	2.582681
H	1.429770	-2.535385	-2.095787	H	1.446164	3.099711	-2.016476
H	-4.484126	-0.786418	-2.029624	H	4.151383	-2.658472	-1.899198
H	-4.881439	-1.401788	2.227544	H	4.589375	-2.587242	2.398729
H	-0.849590	-1.056845	-2.033338	H	1.961196	0.261882	-2.021529
H	-1.466263	-2.878675	2.615743	H	3.386958	0.948660	2.732503
C	-1.523338	-0.834829	3.283024	C	1.896706	-0.489565	3.312872
H	-2.254828	-0.018520	3.463605	H	1.788708	-1.582116	3.482292
H	-0.993524	-1.038882	4.237298	H	1.632045	0.032986	4.256145
H	-0.780518	-0.464897	2.545466	H	1.162937	-0.194424	2.533771
C	-3.217402	-2.647218	3.834476	C	4.346068	-0.496311	3.996095
H	-3.784369	-3.525728	3.462586	H	5.393132	-0.313044	3.677490
H	-2.659098	-2.955460	4.742490	H	4.145580	0.119998	4.896808
H	-3.951765	-1.877681	4.153656	H	4.266469	-1.558822	4.309489
C	-2.391051	-0.699979	-3.470656	C	2.788822	-1.131140	-3.415460
H	-1.646314	-0.649450	-4.290532	H	2.317791	-0.595907	-4.264658
H	-3.316035	-1.153840	-3.887949	H	3.761749	-1.532204	-3.773294
H	-2.605501	0.340983	-3.163223	H	2.123058	-1.975103	-3.153479
C	-1.530656	-2.969220	-2.776011	C	3.898727	0.998200	-2.637263
H	-2.471273	-3.486520	-3.062432	H	4.918967	0.622033	-2.865108
H	-0.864449	-2.955580	-3.664396	H	3.508668	1.501077	-3.547198
H	-1.029949	-3.577352	-1.997315	H	3.986935	1.767759	-1.845327
C	2.353251	0.176106	2.877625	C	-1.382063	1.581394	2.852699
H	1.833329	0.215139	3.857553	H	-1.084059	1.138606	3.825862
H	3.199054	0.894650	2.896558	H	-2.480064	1.744298	2.861253
H	1.634049	0.534164	2.098384	H	-1.164258	0.827086	2.055756
C	3.788315	-1.779281	3.662457	C	-0.857862	3.925412	3.713605
H	4.670095	-1.118246	3.798243	H	-1.934751	4.170992	3.828029

H	3.260878	-1.821053	4.638126
H	4.161241	-2.797424	3.426374
C	1.848367	-0.730025	-3.179209
H	2.699616	-0.172549	-3.625405
H	1.134267	-0.973622	-3.993577
H	1.330468	-0.053264	-2.467716
C	3.028185	-2.979212	-3.458973
H	2.328493	-3.269667	-4.270328
H	3.911753	-2.510949	-3.942459
H	3.371101	-3.904566	-2.950950
C	-2.183925	1.980687	-0.701582
C	-2.573246	1.657733	0.613167
C	-3.131877	2.536745	-1.587972
C	-3.885599	1.894938	1.044458
C	-4.446344	2.773815	-1.157430
C	-4.825064	2.457601	0.161204
H	-1.825802	1.181534	1.270787
H	-2.810711	2.780554	-2.612730
H	-4.182545	1.621923	2.069194
H	-5.181517	3.211462	-1.851923
H	-5.857241	2.644567	0.498750
C	-0.783861	1.717744	-1.207981
O	-0.529522	1.716555	-2.411197
F	2.753721	6.139378	0.748199

Zero-point correction=	0.730800 (Hartree/Particle)
Thermal correction to Energy=	0.776151
Thermal correction to Enthalpy=	0.777095
Thermal correction to Gibbs Free Energy=	0.652453
Sum of electronic and zero-point Energies=	-1962.036402
Sum of electronic and thermal Energies=	-1961.991051
Sum of electronic and thermal Enthalpies=	-1961.990107
Sum of electronic and thermal Free Energies=	-1962.114749

H	-0.510203	3.520115	4.686704
H	-0.314042	4.872953	3.519003
C	-0.084840	2.080651	-3.129436
H	-1.082326	2.266861	-3.581658
H	0.609028	1.773037	-3.939577
H	-0.185418	1.226922	-2.425307
C	0.598765	4.528986	-3.378409
H	1.328081	4.274956	-4.175554
H	-0.357144	4.784445	-3.882836
H	0.960141	5.439233	-2.856158
C	0.485846	-2.829342	-0.774582
C	0.884866	-2.928483	0.573277
C	0.780443	-3.886980	-1.662926
C	1.562368	-4.066505	1.032521
C	1.457770	-5.026830	-1.203600
C	1.847485	-5.120761	0.145900
H	0.679675	-2.075267	1.242031
H	0.461591	-3.793600	-2.712753
H	1.884758	-4.123695	2.083943
H	1.681949	-5.850373	-1.900510
H	2.379278	-6.016241	0.505680
C	-0.217452	-1.605958	-1.314676
O	-0.298976	-1.396800	-2.524380
C	-6.160058	-1.813466	0.270636
F	-6.649980	-2.766260	-0.570233
F	-6.454089	-2.214459	1.535246
F	-6.870595	-0.678672	0.028855

Zero-point correction=	0.743311 (Hartree/Particle)
Thermal correction to Energy=	0.791607
Thermal correction to Enthalpy=	0.792551
Thermal correction to Gibbs Free Energy=	0.659164
Sum of electronic and zero-point Energies=	-2199.659599
Sum of electronic and thermal Energies=	-2199.611303
Sum of electronic and thermal Enthalpies=	-2199.610359
Sum of electronic and thermal Free Energies=	-2199.743746

Ph(pF)+B-Ph(pMe)-IPr-XII

90

IPrXII-F SCF Done: -1962.79975881 A.U.

Pd	-0.136980	0.666080	-0.071276
C	0.067765	2.797860	-0.365838
C	0.214114	2.986596	-1.783467
C	-1.267539	2.616778	0.157701
C	-0.902186	3.062442	-2.617734
H	1.220147	3.124151	-2.206844
C	-2.396552	2.693595	-0.700362
H	-1.414900	2.645837	1.247733
C	-2.192049	2.914509	-2.058319
H	-0.803656	3.228075	-3.700421
H	-3.413820	2.556087	-0.307861
N	-1.640175	-1.844707	0.693460
N	0.399530	-2.357597	0.199315
C	-0.455507	-1.284571	0.273537
C	-1.527254	-3.223132	0.877481
C	-0.231798	-3.550011	0.561749
C	-2.814312	-1.035369	0.903625
C	-3.701995	-0.840427	-0.183075
C	-4.788600	0.033241	0.018695
C	-4.970713	0.685851	1.247810
C	-4.074082	0.470420	2.305338
C	-2.975666	-0.401055	2.159678
C	-3.439439	-1.467849	-1.549947

Ph(pCF3)+B-Ph(pMe)-IPR-XII

93

IPrXII-CF3 SCF Done: -2200.43852643 A.U.

Pd	-0.025855	-0.362394	-0.330412
C	-0.339188	-2.274211	-1.286882
C	-0.548709	-3.234682	-0.237157
C	-1.452445	-1.441617	-1.677647
C	-1.802639	-3.389408	0.349292
H	0.283409	-3.885068	0.070715
C	-2.718986	-1.606173	-1.055292
H	-1.373633	-0.848310	-2.600896
C	-2.891172	-2.570223	-0.059961
H	-1.954115	-4.141758	1.137584
H	-3.557021	-0.963965	-1.359597
N	-0.625846	2.548805	0.230266
N	1.310334	2.059594	1.052794
C	0.248370	1.499329	0.386106
C	-0.128103	3.727576	0.784230
C	1.102430	3.417546	1.308201
C	-1.897538	2.359243	-0.420371
C	-2.993259	1.931680	0.367989
C	-4.196785	1.637694	-0.303000
C	-4.292364	1.763399	-1.697565
C	-3.187653	2.190944	-2.450248
C	-1.961471	2.500732	-1.827743
C	-2.859676	1.711180	1.872765

H	-5.820562	1.374081	1.381748	H	-5.238251	1.515842	-2.205232
C	-1.980300	-0.600828	3.300598	C	-0.746776	2.918198	-2.654181
C	1.767857	-2.242584	-0.237044	C	2.472323	1.310791	1.458379
C	2.775205	-2.019422	0.734790	C	3.610108	1.312981	0.612043
C	4.107833	-1.958133	0.282350	C	4.749694	0.616586	1.059328
C	4.415940	-2.101161	-1.078342	C	4.746302	-0.059110	2.288890
C	3.392362	-2.262035	-2.023163	C	3.587808	-0.089147	3.077757
C	2.041407	-2.328440	-1.624533	C	2.418956	0.591308	2.677008
C	2.429282	-1.734309	2.193333	C	3.562466	1.942111	-0.778063
H	5.465791	-2.056037	-1.409294	H	5.651146	-0.591516	2.622822
C	0.925520	-2.393284	-2.664862	C	1.136742	0.482122	3.498906
H	-2.368573	-3.836482	1.213956	H	-0.688329	4.666952	0.755333
H	0.295759	-4.508591	0.561375	H	1.843333	4.028408	1.832764
H	-5.490998	0.222373	-0.807430	H	-5.062117	1.272897	0.271142
H	-4.224809	0.994388	3.262049	H	-3.273933	2.275745	-3.544905
H	-2.721471	-2.303142	-1.404001	H	-1.892479	2.152206	2.193993
H	-1.313590	-1.443768	3.020581	H	0.050008	3.232328	-1.947049
H	4.916622	-1.776094	1.005927	H	5.649373	0.587543	0.426925
H	3.643711	-2.327558	-3.093456	H	3.586002	-0.655559	4.022254
H	1.393990	-2.095504	2.373120	H	2.761041	2.712321	-0.773975
H	-0.028231	-2.589088	-2.130935	H	0.399939	1.199287	3.080130
C	0.783512	-1.018271	-3.352836	C	0.532662	-0.928947	3.334844
H	1.721467	-0.735115	-3.876299	H	1.240015	-1.711797	3.682132
H	-0.037821	-1.033179	-4.098915	H	-0.405924	-1.027034	3.918125
H	0.548481	-0.230742	-2.602617	H	0.289845	-1.123535	2.266246
C	1.127432	-3.528367	-3.686395	C	1.348323	0.848518	4.980205
H	1.240148	-4.511778	-3.184654	H	1.789072	1.861113	5.089329
H	0.257676	-3.588080	-4.373406	H	0.380026	0.832200	5.522584
H	2.028981	-3.363475	-4.313601	H	2.022362	0.129324	5.491752
C	2.427495	-0.206116	2.417926	C	3.157474	0.862285	-1.806295
H	2.149145	0.043552	3.462406	H	3.083329	1.291308	-2.826917
H	3.424449	0.233089	2.202835	H	3.894839	0.032383	-1.824555
H	1.694481	0.286084	1.741062	H	2.169930	0.420719	-1.548596
C	3.352668	-2.458153	3.189986	C	4.872504	2.643038	-1.179215
H	4.392204	-2.070096	3.145452	H	5.701157	1.918245	-1.324527
H	2.994093	-2.300077	4.228257	H	4.739970	3.175958	-2.143410
H	3.388925	-3.550832	2.998163	H	5.195266	3.381664	-0.416136
C	-2.758495	-0.437966	-2.475917	C	-2.802726	0.202095	2.184896
H	-2.492509	-0.900069	-3.449700	H	-2.631638	0.029971	3.268001
H	-3.427185	0.425341	-2.671817	H	-3.753488	-0.293108	1.906357
H	-1.831295	-0.044450	-2.003177	H	-1.980915	-0.284443	1.615337
C	-4.707007	-2.060538	-2.192521	C	-3.973468	2.417412	2.669095
H	-5.440380	-1.271285	-2.462122	H	-4.971870	1.984565	2.448323
H	-4.448227	-2.594246	-3.130742	H	-3.801207	2.302002	3.759673
H	-5.214072	-2.777878	-1.514159	H	-4.015989	3.502144	2.437848
C	-1.086129	0.644455	3.468024	C	-0.189345	1.725264	-3.457318
H	-1.688289	1.544486	3.714348	H	-0.945636	1.324587	-4.165217
H	-0.346809	0.494435	4.281949	H	0.700351	2.028802	-4.047315
H	-0.528424	0.851356	2.529352	H	0.114706	0.900904	-2.779612
C	-2.678652	-0.986270	4.619597	C	-1.058501	4.123604	-3.563566
H	-1.924707	-1.217378	5.400939	H	-0.139955	4.460108	-4.088364
H	-3.307994	-0.158111	5.008751	H	-1.805634	3.865329	-4.343492
H	-3.330530	-1.875724	4.493429	H	-1.459730	4.980200	-2.982909
C	2.611938	2.603115	0.240780	C	2.254622	-2.552686	-1.543905
C	2.961135	1.648367	-0.742672	C	2.575228	-2.427139	-0.171944
C	3.640781	3.221501	0.986819	C	3.268675	-2.935390	-2.450893
C	4.308029	1.334700	-0.983409	C	3.876656	-2.694448	0.280657
C	4.986402	2.914276	0.739825	C	4.566097	-3.210788	-1.996614
C	5.324312	1.969822	-0.248691	C	4.873495	-3.091699	-0.627369
H	2.169764	1.102237	-1.283701	H	1.815679	-2.063017	0.540141
H	3.353342	3.935954	1.773361	H	3.012784	-2.994359	-3.519782
H	4.557284	0.574231	-1.738048	H	4.112225	-2.571710	1.347936
H	5.778857	3.408841	1.324211	H	5.345954	-3.515222	-2.712888

H 6.381188 1.722870 -0.439546 C 1.186176 2.918459 0.637553 O 0.943604 3.280104 1.797371 F -3.261580 2.962308 -2.889598	H 5.894338 -3.301532 -0.269460 C 0.911061 -2.181574 -2.127329 O 0.838483 -1.795017 -3.301039 C -4.236481 -2.776360 0.587244 F -4.846530 -3.911254 0.149802 F -4.130773 -2.893108 1.942119 F -5.095196 -1.746068 0.342699
Zero-point correction= 0.732894 (Hartree/Particle) Thermal correction to Energy= 0.778502 Thermal correction to Enthalpy= 0.779446 Thermal correction to Gibbs Free Energy= 0.653590 Sum of electronic and zero-point Energies= -1962.066865 Sum of electronic and thermal Energies= -1962.021257 Sum of electronic and thermal Enthalpies= -1962.020313 Sum of electronic and thermal Free Energies= -1962.146169	Zero-point correction= 0.745314 (Hartree/Particle) Thermal correction to Energy= 0.793912 Thermal correction to Enthalpy= 0.794856 Thermal correction to Gibbs Free Energy= 0.660953 Sum of electronic and zero-point Energies= -2199.693213 Sum of electronic and thermal Energies= -2199.644615 Sum of electronic and thermal Enthalpies= -2199.643671 Sum of electronic and thermal Free Energies= -2199.777574

Ph(oMe)+B-Ph(pMe)-IPr-V	**Ph(oMeISOMER)+B-Ph(pMe)-IPR-V**
94 IPrV-MeOrto SCF Done: -1978.10671650 A.U. C 1.433569 -2.762637 0.103824 O 2.090123 -2.903415 1.123332 Pd -0.267153 -0.694108 0.116882 O 2.027035 -2.494991 -1.135356 C -2.843240 -3.229271 -0.416334 C -2.099564 -2.597261 -1.408796 H -2.823163 -4.164608 1.551313 C -2.214110 -3.677468 0.772648 C -0.698454 -2.410939 -1.234987 C -0.046804 -2.873625 -0.027066 C -0.847073 -3.498869 1.013902 H -0.079849 -2.138555 -2.102462 H -2.579363 -2.235325 -2.330435 N -1.897126 1.856341 -0.158961 N 0.070089 2.329470 0.598563 C -0.691404 1.270369 0.160821 C -1.887110 3.231842 0.077785 C -0.638663 3.532596 0.559855 C -3.025203 1.093877 -0.631502 C -3.861457 0.467616 0.324569 C -4.923370 -0.321372 -0.160659 C -5.144652 -0.465256 -1.537759 C -4.303779 0.175088 -2.460682 C -3.222665 0.969103 -2.028400 C -3.601381 0.589726 1.823317 H -5.978542 -1.088973 -1.897389 C -2.249426 1.588082 -3.028774 C 1.436453 2.196854 1.034822 C 2.466865 2.544759 0.123535 C 3.793958 2.463781 0.586376 C 4.079210 2.013312 1.884789 C 3.042220 1.622801 2.742636 C 1.692753 1.714964 2.341721 C 2.150724 2.858535 -1.337132 H 5.124938 1.946798 2.224992 C 0.577336 1.249083 3.273815 H -2.761869 3.860648 -0.113783 H -0.190530 4.479897 0.874783 H -5.581222 -0.839072 0.554882 H -4.482654 0.045648 -3.539181 H -2.813242 1.358781 1.965470 H -1.686421 2.387354 -2.500888 H 4.619528 2.727000 -0.091046	94 IPrV-MeOrto180 SCF Done: -1978.08742360 A.U. C 0.584397 -3.156427 0.600955 O -0.075713 -4.012749 0.044839 Pd -0.128415 -0.267549 0.496879 O -0.027286 -2.249718 1.511683 C 4.834337 -2.904048 -0.095653 C 4.006265 -3.809987 -0.784406 H 4.920582 -1.310601 1.369735 C 4.273191 -2.032588 0.847201 C 2.638053 -3.827367 -0.506587 C 2.055223 -2.954038 0.451907 C 2.892209 -2.023250 1.154299 H 1.969001 -4.527024 -1.028568 H 4.426652 -4.497689 -1.534534 N 0.741319 2.313471 -0.768850 N -1.260630 1.748918 -1.374207 C -0.206552 1.325717 -0.592840 C 0.289009 3.316245 -1.629881 C -0.979578 2.958080 -2.013744 C 2.034967 2.234476 -0.140419 C 3.081062 1.578593 -0.836884 C 4.310894 1.427474 -0.165623 C 4.489066 1.922675 1.134667 C 3.436729 2.573684 1.795402 C 2.182503 2.739713 1.174437 C 2.863991 0.978669 -2.223554 H 5.457724 1.791552 1.643238 C 1.010179 3.357282 1.932554 C -2.472082 0.979963 -1.502072 C -3.532016 1.226372 -0.593887 C -4.711933 0.473651 -0.752951 C -4.819822 -0.496460 -1.760732 C -3.732809 -0.758661 -2.607413 C -2.530717 -0.030476 -2.493496 C -3.359211 2.167852 0.594782 H -5.752568 -1.072662 -1.871015 C -1.318209 -0.402436 -3.343230 H 0.906258 4.181817 -1.888878 H -1.701124 3.446633 -2.675493 H 5.136888 0.898705 -0.665112 H 3.585521 2.943460 2.822044 H 1.947797 1.441270 -2.648844 H 0.201100 3.552362 1.196925 H -5.551819 0.634005 -0.059549

H	3.281935	1.238522	3.746177
H	1.121201	3.274137	-1.381677
H	-0.391568	1.545246	2.819074
C	0.581026	-0.290719	3.367541
H	1.543697	-0.675572	3.762832
H	-0.240693	-0.650041	4.020524
H	0.431264	-0.739051	2.352166
C	0.656590	1.909124	4.663806
H	-0.215555	1.609671	5.281935
H	1.569572	1.601866	5.216303
H	0.663417	3.016444	4.588917
C	3.093346	3.898192	-1.966701
H	4.126680	3.505743	-2.073770
H	2.744115	4.162473	-2.986308
H	3.141994	4.829851	-1.365272
C	2.150610	1.537469	-2.141253
H	1.835214	1.716129	-3.190499
H	3.164114	1.085392	-2.149340
H	1.459233	0.794761	-1.688448
C	-2.954257	2.239600	-4.232455
H	-2.214889	2.761853	-4.874656
H	-3.462784	1.486604	-4.871118
H	-3.716322	2.979313	-3.910080
C	-1.219011	0.528552	-3.473020
H	-1.720376	-0.308834	-4.004351
H	-0.465100	0.970187	-4.157623
H	-0.692931	0.110867	-2.590261
C	-4.847788	1.060458	2.597036
H	-5.667248	0.312337	2.550009
H	-4.602433	1.210207	3.669405
H	-5.241157	2.017476	2.195263
C	-3.042582	-0.736284	2.372192
H	-2.762246	-0.636238	3.441624
H	-3.785226	-1.556362	2.281137
H	-2.138835	-1.033847	1.792056
C	3.332489	-2.032220	-1.186333
C	3.798941	-1.006899	-0.341661
C	4.158313	-2.580496	-2.182841
C	5.118050	-0.552301	-0.497905
H	3.130727	-0.563482	0.410920
C	5.469687	-2.101396	-2.338465
H	3.754023	-3.378003	-2.824050
C	5.957246	-1.090980	-1.490584
H	5.487843	0.242139	0.166656
H	6.115126	-2.527829	-3.122831
H	6.988980	-0.722624	-1.603294
H	-3.927824	-3.368404	-0.545322
C	-0.246147	-3.961872	2.316779
H	0.592861	-4.668801	2.153716
H	0.193876	-3.111735	2.876671
H	-1.014713	-4.449930	2.948913

Zero-point correction= 0.772057 (Hartree/Particle)
Thermal correction to Energy= 0.819118
Thermal correction to Enthalpy= 0.820062
Thermal correction to Gibbs Free Energy= 0.691848
Sum of electronic and zero-point Energies= -1977.334659
Sum of electronic and thermal Energies= -1977.287598
Sum of electronic and thermal Enthalpies= -1977.286654
Sum of electronic and thermal Free Energies= -1977.414868

H	-3.812164	-1.553655	-3.365552
H	-2.464655	2.797094	0.399550
H	-0.526243	0.352099	-3.153344
C	-0.760923	-1.764747	-2.878621
H	-1.513067	-2.573173	-2.996653
H	0.140043	-2.045878	-3.461714
H	-0.469638	-1.708445	-1.806283
C	-1.626053	-0.386501	-4.852414
H	-0.704829	-0.589332	-5.437787
H	-2.368637	-1.164637	-5.129344
H	-2.030951	0.595605	-5.174145
C	-4.555894	3.114530	0.800032
H	-5.477424	2.561137	1.079557
H	-4.344322	3.828039	1.623617
H	-4.777287	3.699947	-0.116700
C	-3.061979	1.332289	1.859842
H	-2.883107	1.990965	2.735432
H	-3.903288	0.648271	2.097447
H	-2.152873	0.704821	1.700204
C	1.371564	4.702928	2.589393
H	0.470996	5.162231	3.048172
H	2.122011	4.579614	3.398976
H	1.787023	5.419155	1.850291
C	0.454573	2.346693	2.958208
H	1.225122	2.082233	3.713293
H	-0.425807	2.765896	3.488695
H	0.139211	1.411701	2.438400
C	4.022333	1.280406	-3.192380
H	4.960268	0.772840	-2.882366
H	3.776661	0.911640	-4.210111
H	4.231017	2.368629	-3.258845
C	2.599168	-0.536277	-2.105735
H	2.358341	-0.971607	-3.097873
H	3.484590	-1.067056	-1.699636
H	1.746592	-0.728467	-1.417929
C	-1.412232	-2.343371	1.793607
C	-2.380952	-2.404169	0.773459
C	-1.767087	-2.260375	3.147316
C	-3.734952	-2.366738	1.139105
H	-2.078060	-2.467289	-0.278558
C	-3.129389	-2.219113	3.493214
H	-0.972463	-2.206610	3.905579
C	-4.113932	-2.271936	2.491572
H	-4.497809	-2.395251	0.347316
H	-3.418264	-2.142576	4.553177
H	-5.180264	-2.235581	2.764092
H	5.917055	-2.872072	-0.297329
C	2.398714	-0.984842	2.115574
H	1.721553	-0.263884	1.551216
H	1.774343	-1.399812	2.929229
H	3.233957	-0.399059	2.542732

Zero-point correction= 0.771680 (Hartree/Particle)
Thermal correction to Energy= 0.818535
Thermal correction to Enthalpy= 0.819479
Thermal correction to Gibbs Free Energy= 0.692168
Sum of electronic and zero-point Energies= -1977.315744
Sum of electronic and thermal Energies= -1977.268889
Sum of electronic and thermal Enthalpies= -1977.267944
Sum of electronic and thermal Free Energies= -1977.395256

Ph(oMe)+B-Ph(pMe)-IPr-V-VI	**Ph(oMeISOMER)+B-Ph(pMe)-IPR-V-VI**
94	94

IPrV-VI-MeOrto SCF Done: -1978.07576223 A.U.				IPrV-VI-MeOrto180 SCF Done: -1978.07314355 A.U.			
C	-2.011950	0.687558	-1.235787	C	-1.673936	0.467454	-1.359801
O	-2.297228	-0.065983	-2.149868	O	-1.623223	-0.160012	-2.404813
Pd	0.265376	0.478090	-0.620445	Pd	0.275648	0.665490	-0.479381
O	-1.072674	1.835657	-1.604874	O	-1.013057	2.003640	-1.548955
C	-4.207283	1.262359	2.451083	C	-5.180503	-0.119739	1.129171
C	-4.707419	0.425472	1.443399	C	-5.027225	-0.726139	-0.127961
H	-2.561693	2.574570	3.040905	H	-4.287377	1.194892	2.601464
C	-2.978202	1.918905	2.261038	C	-4.169628	0.722328	1.612191
C	-4.021858	0.216403	0.223867	C	-3.868167	-0.478355	-0.869174
C	-2.773784	0.886955	0.041185	C	-2.839482	0.374880	-0.392897
C	-2.276176	1.724863	1.068820	C	-2.988203	0.993628	0.883649
H	-1.303451	2.216501	0.935873	H	-3.723031	-0.952145	-1.849809
H	-5.669918	-0.089798	1.595434	H	-5.803006	-1.397343	-0.528755
N	2.415376	-1.029654	0.809377	N	2.484348	-0.906122	0.739329
C	3.954553	-0.612666	-1.610994	C	3.634868	-0.683138	-1.917578
H	3.394772	-1.516707	-1.293031	H	3.068992	-1.525217	-1.469436
C	4.051280	0.325856	-0.409781	C	3.933007	0.322249	-0.807122
C	3.277722	0.121167	0.760053	C	3.370646	0.202037	0.489690
C	1.142733	-1.022425	0.279858	C	1.165843	-0.899878	0.334061
C	3.279604	1.016439	1.858154	C	3.617042	1.130641	1.531780
C	2.333503	0.818453	3.039907	C	2.918695	1.000568	2.883313
H	2.016171	-0.246262	3.040562	H	2.633520	-0.065652	3.010925
C	4.864512	1.476495	-0.451611	C	4.762203	1.436696	-1.047944
H	5.472678	1.676014	-1.347860	H	5.207670	1.572731	-2.045884
C	4.898689	2.375605	0.624861	C	5.022811	2.374472	-0.038369
H	5.540640	3.269426	0.571194	H	5.672737	3.238862	-0.248425
C	4.112756	2.149135	1.765846	C	4.458033	2.221922	1.237871
H	4.136456	2.873302	2.594734	H	4.667666	2.970987	2.016593
C	2.776292	-2.292927	1.281499	C	2.864523	-2.147520	1.249938
C	1.061426	1.667256	2.822444	C	1.610601	1.819988	2.866059
H	0.304667	1.462907	3.608368	H	1.028861	1.665777	3.798783
H	1.303082	2.751662	2.838203	H	1.827428	2.904426	2.762349
H	0.610915	1.427662	1.832339	H	0.976310	1.518042	2.004782
C	2.989193	1.107963	4.401708	C	3.814267	1.384422	4.074435
H	2.289407	0.856594	5.225721	H	3.296666	1.161700	5.030513
H	3.917828	0.516875	4.543616	H	4.774576	0.828162	4.062977
H	3.249569	2.181657	4.515195	H	4.049953	2.469672	4.081004
C	3.131827	0.048075	-2.736836	C	2.727720	-0.058943	-2.997386
H	3.639948	0.954465	-3.129150	H	3.229413	0.789129	-3.509815
H	2.979116	-0.658717	-3.579458	H	2.457415	-0.814745	-3.764084
H	2.127693	0.349315	-2.352257	H	1.784616	0.319103	-2.539353
C	5.335158	-1.082029	-2.107355	C	4.922328	-1.275958	-2.522855
H	5.922825	-1.552326	-1.291690	H	5.565609	-1.734000	-1.743054
H	5.218479	-1.826517	-2.922490	H	4.669058	-2.060018	-3.266774
H	5.935661	-0.241376	-2.515330	H	5.523979	-0.504781	-3.048676
C	1.702626	-3.111539	1.049505	C	1.759664	-2.952454	1.164918
H	1.546996	-4.176057	1.249536	H	1.607937	-4.002294	1.433471
H	3.757226	-2.487830	1.724846	H	3.879434	-2.340149	1.610085
N	0.719143	-2.324066	0.441993	N	0.738861	-2.181669	0.598908
C	-0.568981	-2.821911	0.024624	C	-0.572664	-2.689773	0.272951
C	-0.814555	-3.012478	-1.360658	C	-0.870522	-2.985290	-1.084715
C	-1.524407	-3.115397	1.032268	C	-1.492587	-2.885032	1.335607
C	-2.059982	-3.566939	-1.716910	C	-2.162816	-3.479356	-1.354186
C	-2.749019	-3.674659	0.617170	C	-2.769960	-3.374527	1.002017
C	-3.006775	-3.911626	-0.741532	C	-3.099167	-3.666723	-0.328424
H	-2.297948	-3.723093	-2.778444	H	-2.448534	-3.708672	-2.390015
H	-3.518581	-3.919191	1.363423	H	-3.522676	-3.519180	1.789749
H	-3.970448	-4.349899	-1.046253	H	-4.107611	-4.037071	-0.571441
C	0.221547	-2.612350	-2.410632	C	0.160055	-2.779193	-2.198463
H	0.629620	-1.632857	-2.066154	H	0.580289	-1.761981	-2.038916
C	-1.256073	-2.755042	2.494519	C	-1.109147	-2.550864	2.779618
H	-0.186166	-2.971750	2.705691	H	-0.045534	-2.844797	2.915458

C	1.390768	-3.617326	-2.478435
H	2.162615	-3.260629	-3.193058
H	1.884614	-3.754494	-1.495203
H	1.038834	-4.613154	-2.824392
C	-0.376779	-2.358296	-3.801350
H	0.402085	-1.932482	-4.467803
H	-0.741103	-3.292066	-4.282690
H	-1.210499	-1.631154	-3.740296
C	-2.086793	-3.569884	3.499382
H	-1.757041	-3.346146	4.534965
H	-3.165931	-3.312938	3.443387
H	-1.985836	-4.662942	3.334333
C	-1.467947	-1.239614	2.705191
H	-0.858426	-0.635731	2.003560
H	-2.529114	-0.969694	2.529477
H	-1.202959	-0.942871	3.742013
C	-1.361040	3.173387	-1.402982
C	-2.641110	3.681472	-1.689770
C	-0.330631	4.016944	-0.948504
C	-2.887031	5.052117	-1.507342
H	-3.428631	3.000218	-2.044166
C	-0.588669	5.386933	-0.782522
H	0.652853	3.573814	-0.722719
C	-1.866569	5.909802	-1.056648
H	-3.889755	5.453505	-1.724060
H	0.216358	6.050442	-0.428417
H	-2.067149	6.983532	-0.918631
H	-4.773997	1.396664	3.386176
C	-4.636906	-0.690356	-0.813315
H	-4.774978	-0.169230	-1.782340
H	-3.973382	-1.550496	-1.028296
H	-5.619346	-1.069143	-0.467033
Zero-point correction=			0.770525 (Hartree/Particle)
Thermal correction to Energy=			0.817293
Thermal correction to Enthalpy=			0.818237
Thermal correction to Gibbs Free Energy=			0.689953
Sum of electronic and zero-point Energies=			-1977.305237
Sum of electronic and thermal Energies=			-1977.258469
Sum of electronic and thermal Enthalpies=			-1977.257525
Sum of electronic and thermal Free Energies=			-1977.385809

C	1.317828	-3.800069	-2.115065
H	2.067518	-3.590592	-2.907287
H	1.849439	-3.772838	-1.144583
H	0.940918	-4.833909	-2.268894
C	-0.437951	-2.797606	-3.613291
H	0.341742	-2.506970	-4.347501
H	-0.792429	-3.811908	-3.899393
H	-1.271648	-2.077747	-3.706856
C	-1.924403	-3.325397	3.828820
H	-1.509914	-3.144222	4.842110
H	-2.984171	-2.994050	3.849936
H	-1.911368	-4.419205	3.641377
C	-1.195060	-1.031877	3.033030
H	-0.595046	-0.460521	2.297810
H	-2.246023	-0.692495	2.938452
H	-0.832322	-0.780068	4.051985
C	-1.606066	3.188816	-1.228050
C	-2.975497	3.411501	-1.488723
C	-0.816731	4.214645	-0.662280
C	-3.550856	4.646817	-1.149487
H	-3.574678	2.607024	-1.939015
C	-1.401341	5.448820	-0.342849
H	0.246746	4.005962	-0.465259
C	-2.773496	5.668954	-0.573574
H	-4.623141	4.812356	-1.341980
H	-0.781595	6.244228	0.101744
H	-3.232867	6.634523	-0.310763
H	-6.082565	-0.301983	1.735049
C	-1.983704	1.921472	1.517260
H	-0.954952	1.722027	1.135910
H	-2.223860	2.979821	1.291714
H	-1.972332	1.801233	2.618634
Zero-point correction=			0.770826 (Hartree/Particle)
Thermal correction to Energy=			0.817352
Thermal correction to Enthalpy=			0.818297
Thermal correction to Gibbs Free Energy=			0.691486
Sum of electronic and zero-point Energies=			-1977.302317
Sum of electronic and thermal Energies=			-1977.255791
Sum of electronic and thermal Enthalpies=			-1977.254847
Sum of electronic and thermal Free Energies=			-1977.381658

Ph(oMe)+B-Ph(pMe)-IPr-VI			
94			
IPrVI-MeOrto SCF Done: -1978.10322093 A.U.			
Pd	-0.222896	-0.837182	-0.409113
N	-2.598734	0.867956	0.141090
C	-2.932637	0.746139	-2.764909
H	-2.204412	1.340186	-2.175364
C	-3.652694	-0.201448	-1.811921
C	-3.450318	-0.155302	-0.412874
C	-1.247877	0.694340	0.306982
C	-4.012385	-1.097522	0.486227
C	-3.630672	-1.122822	1.965703
H	-3.103458	-0.175450	2.203826
C	-4.521023	-1.198845	-2.301459
H	-4.709706	-1.263324	-3.384380
C	-5.127094	-2.120558	-1.435677
H	-5.797166	-2.894994	-1.841501
C	-4.862047	-2.080411	-0.058001
H	-5.311584	-2.836123	0.604992
C	-3.040352	2.054710	0.724067
C	-2.635784	-2.274068	2.230436

Ph(oMeISOMER)+B-Ph(pMe)-IPR-VI			
94			
IPrVI-MeOrto180 SCF Done: -1978.09951008 A.U.			
Pd	0.053402	-0.758293	0.168731
N	-2.667933	0.246385	-0.381892
C	-2.516322	-1.446355	-2.757992
H	-2.041249	-0.461930	-2.572203
C	-3.121251	-1.929487	-1.445160
C	-3.149453	-1.110613	-0.292250
C	-1.368707	0.592914	-0.103796
C	-3.603376	-1.565601	0.972130
C	-3.473502	-0.708037	2.229326
H	-3.213666	0.324185	1.915826
C	-3.637654	-3.235103	-1.319506
H	-3.637649	-3.900758	-2.196795
C	-4.127749	-3.704718	-0.092290
H	-4.519336	-4.731403	-0.015163
C	-4.096239	-2.883184	1.044960
H	-4.447360	-3.277599	2.011347
C	-3.465973	1.369614	-0.592154
C	-2.309849	-1.225020	3.102597

H	-2.285142	-2.257904	3.283714	H	-2.155173	-0.565805	3.982239
H	-3.105119	-3.261533	2.037201	H	-2.511168	-2.252282	3.472464
H	-1.742986	-2.197989	1.572406	H	-1.357099	-1.263470	2.530722
C	-4.852198	-1.205708	2.899680	C	-4.785058	-0.618626	3.031331
H	-4.531454	-1.145585	3.960746	H	-4.664415	0.072709	3.891555
H	-5.565882	-0.378437	2.706685	H	-5.619427	-0.245360	2.402445
H	-5.401872	-2.162600	2.776862	H	-5.085735	-1.605419	3.442238
C	-2.106560	-0.040491	-3.802157	C	-1.388778	-2.388447	-3.226071
H	-2.754783	-0.620330	-4.493163	H	-1.779050	-3.383959	-3.526709
H	-1.494436	0.657264	-4.408580	H	-0.863628	-1.948597	-4.098449
H	-1.414370	-0.744304	-3.296146	H	-0.643299	-2.538826	-2.418580
C	-3.918574	1.726673	-3.431425	C	-3.598893	-1.259118	-3.839414
H	-4.475466	2.318873	-2.675167	H	-4.377279	-0.538476	-3.511646
H	-3.377016	2.434938	-4.092941	H	-3.149844	-0.876598	-4.779939
H	-4.666005	1.188741	-4.053248	H	-4.106795	-2.219539	-4.072800
C	-1.935617	2.646812	1.279290	C	-2.648839	2.458286	-0.435501
H	-1.819976	3.574034	1.847149	H	-2.850238	3.531592	-0.494863
H	-4.091854	2.355319	0.698358	H	-4.532377	1.286844	-0.821389
N	-0.850866	1.806171	1.014507	N	-1.373086	1.966990	-0.137294
C	0.484018	2.011541	1.523223	C	-0.265885	2.818773	0.222396
C	1.320835	2.959216	0.885126	C	0.377518	3.565058	-0.793653
C	0.904370	1.235472	2.638682	C	0.102430	2.905153	1.592950
C	2.607139	3.157631	1.429152	C	1.371254	4.484644	-0.393425
C	2.198129	1.477254	3.138726	C	1.110321	3.826960	1.932626
C	3.038052	2.433306	2.546593	C	1.724986	4.624717	0.954224
H	3.287266	3.880323	0.954327	H	1.885665	5.087427	-1.157726
H	2.564717	0.896263	3.997236	H	1.424024	3.922904	2.982244
H	4.049444	2.597849	2.950220	H	2.504965	5.345674	1.245833
C	0.866495	3.743802	-0.342858	C	0.044297	3.383062	-2.271516
H	0.021212	3.186763	-0.797434	H	-0.586031	2.475105	-2.364294
C	-0.000082	0.166634	3.251207	C	-0.571751	2.037287	2.653999
H	-0.563417	-0.286580	2.408517	H	-0.825421	1.075443	2.161197
C	0.363655	5.148462	0.055976	C	-0.754218	4.585078	-2.817339
H	-0.475206	5.101406	0.779427	H	-1.699745	4.740488	-2.257850
H	1.178985	5.737167	0.528171	H	-0.163989	5.523377	-2.741800
H	0.011550	5.706423	-0.836988	H	-1.012222	4.431432	-3.886115
C	1.968760	3.846445	-1.415313	C	1.315242	3.130445	-3.107876
H	1.540464	4.229406	-2.363816	H	1.039253	2.847877	-4.144274
H	2.776446	4.545397	-1.110978	H	1.957580	4.034800	-3.167166
H	2.426187	2.859119	-1.618668	H	1.917237	2.302210	-2.684609
C	-1.031155	0.782817	4.220582	C	-1.891791	2.674017	3.137125
H	-1.720001	0.000178	4.603318	H	-2.408310	2.004190	3.856684
H	-0.524842	1.251323	5.091309	H	-1.699890	3.643104	3.645203
H	-1.647711	1.559893	3.724984	H	-2.586428	2.862745	2.293026
C	0.777419	-0.980949	3.914933	C	0.351835	1.684042	3.830434
H	1.548336	-1.394876	3.232836	H	1.316170	1.268411	3.472258
H	1.276282	-0.663266	4.855224	H	0.570311	2.561030	4.476043
H	0.081832	-1.804224	4.178209	H	-0.130521	0.918562	4.472172
C	0.909268	0.396729	-1.473937	C	0.957253	-0.179116	-1.502842
O	0.428248	1.165598	-2.285949	O	0.358604	0.175823	-2.500116
O	0.590928	-2.592123	-1.034676	O	1.131133	-2.406934	0.632822
C	5.109504	-0.243610	-0.789082	C	5.148337	-1.157120	-1.539972
C	4.645082	0.049327	-2.083092	C	4.260555	-1.709336	-2.479468
H	4.547219	-0.594772	1.291696	H	5.374912	0.163237	0.166811
C	4.204334	-0.337047	0.279219	C	4.678322	-0.251468	-0.578514
C	3.279424	0.272808	-2.352507	C	2.907631	-1.348549	-2.444802
C	2.370487	0.178889	-1.255678	C	2.432956	-0.444001	-1.466452
C	2.841023	-0.145720	0.035562	C	3.321038	0.123191	-0.511846
H	2.111267	-0.238125	0.851906	H	2.192174	-1.776025	-3.163827
H	5.362707	0.101332	-2.918405	H	4.618731	-2.426924	-3.234211
C	1.746354	-2.991224	-0.503187	C	2.365595	-2.432530	1.128612
C	1.904152	-3.192671	0.901074	C	2.764529	-1.622821	2.232395
C	2.879798	-3.220188	-1.333934	C	3.339621	-3.301548	0.560224

C	3.139667	-3.571680	1.444758
H	1.022912	-3.032094	1.544115
C	4.111732	-3.593551	-0.780186
H	2.765966	-3.053252	-2.416047
C	4.257675	-3.768482	0.610519
H	3.232864	-3.714164	2.534783
H	4.980938	-3.735731	-1.443486
H	5.230353	-4.058214	1.038113
H	6.184167	-0.418558	-0.622092
C	2.822218	0.582299	-3.758039
H	3.656134	0.471695	-4.479132
H	1.994294	-0.086960	-4.070858
H	2.424219	1.615135	-3.831799

Zero-point correction= 0.771170 (Hartree/Particle)
Thermal correction to Energy= 0.818792
Thermal correction to Enthalpy= 0.819736
Thermal correction to Gibbs Free Energy= 0.690102
Sum of electronic and zero-point Energies= -1977.332051
Sum of electronic and thermal Energies= -1977.284429
Sum of electronic and thermal Enthalpies= -1977.283485
Sum of electronic and thermal Free Energies= -1977.413119

C	4.080605	-1.652758	2.713654
H	2.005631	-0.964307	2.686160
C	4.651539	-3.326638	1.049636
H	3.034575	-3.923671	-0.294815
C	5.039238	-2.498434	2.122032
H	4.363707	-1.007861	3.562611
H	5.392464	-3.992495	0.576708
H	6.074259	-2.518587	2.498012
H	6.210550	-1.447214	-1.543656
C	2.854466	1.142314	0.493543
H	1.882533	0.837627	0.939450
H	3.589666	1.273735	1.309724
H	2.679970	2.127596	0.012830

Zero-point correction= 0.771015 (Hartree/Particle)
Thermal correction to Energy= 0.818602
Thermal correction to Enthalpy= 0.819546
Thermal correction to Gibbs Free Energy= 0.690492
Sum of electronic and zero-point Energies= -1977.328495
Sum of electronic and thermal Energies= -1977.280908
Sum of electronic and thermal Enthalpies= -1977.279964
Sum of electronic and thermal Free Energies= -1977.409018

Ph(oMe)+B-Ph(pMe)-IPr-VII

100
IPrVII-MeOrto SCF Done: -3441.93401904 A.U.

Pd	-0.032504	0.209866	-0.321888
N	2.785492	-0.668774	-0.053019
C	2.705437	-0.317213	-2.959310
H	2.235354	-1.117394	-2.354069
C	3.277153	0.734498	-2.014472
C	3.275785	0.570860	-0.607442
C	1.465707	-0.945348	0.212105
C	3.723547	1.577224	0.291473
C	3.611350	1.408222	1.804200
H	2.744293	0.739629	1.976198
C	3.818164	1.935459	-2.527888
H	3.852385	2.087047	-3.618665
C	4.318734	2.927328	-1.668835
H	4.753242	3.849970	-2.087624
C	4.259156	2.752486	-0.275231
H	4.622511	3.551752	0.387633
C	3.610434	-1.726487	0.334451
C	3.298372	2.727025	2.533016
H	3.024191	2.512401	3.586471
H	4.175138	3.410421	2.557765
H	2.443658	3.248474	2.060674
C	4.875512	0.750496	2.399418
H	4.753145	0.608238	3.493661
H	5.081935	-0.243315	1.956012
H	5.769534	1.389791	2.234789
C	1.572954	0.267717	-3.826126
H	1.931639	1.076212	-4.499700
H	1.121754	-0.527917	-4.452223
H	0.759359	0.661981	-3.182131
C	3.814190	-0.959907	-3.816735
H	4.606773	-1.406691	-3.180740
H	3.392278	-1.764236	-4.454700
H	4.299117	-0.216360	-4.485758
C	2.794096	-2.676817	0.884582
H	3.013867	-3.644898	1.341735
H	4.691753	-1.702258	0.174740
N	1.489009	-2.180700	0.805345

Ph(oMeISOMER)+B-Ph(pMe)-IPR-VII

100
IPrVII-MeOrto180 SCF Done: -3441.93034439 A.U.

Pd	-0.096479	0.186547	-0.325297
N	2.839195	-0.174129	-0.084936
C	2.697658	0.052512	-2.988993
H	2.350653	-0.783625	-2.350495
C	3.048908	1.232883	-2.089832
C	3.092668	1.117285	-0.678771
C	1.592935	-0.681299	0.195435
C	3.359651	2.216772	0.181631
C	3.311351	2.077306	1.700868
H	2.576047	1.275656	1.913326
C	3.342654	2.497302	-2.649208
H	3.334577	2.617141	-3.744425
C	3.655032	3.593325	-1.828618
H	3.897829	4.568475	-2.282048
C	3.653798	3.453520	-0.429866
H	3.869941	4.327328	0.202552
C	3.844137	-1.062065	0.304236
C	2.792104	3.344472	2.402965
H	2.577389	3.117401	3.467414
H	3.540825	4.166436	2.389809
H	1.852961	3.701990	1.938246
C	4.684143	1.668089	2.277496
H	4.613546	1.538509	3.377890
H	5.052246	0.713356	1.853166
H	5.447891	2.449089	2.072704
C	1.519592	0.386386	-3.924205
H	1.778459	1.172491	-4.665554
H	1.203297	-0.520066	-4.478666
H	0.643743	0.726105	-3.332774
C	3.933637	-0.433195	-3.773111
H	4.756360	-0.722152	-3.086290
H	3.676801	-1.318060	-4.392175
H	4.323360	0.356426	-4.451417
C	3.216280	-2.133777	0.877011
H	3.609974	-3.039860	1.344288
H	4.902380	-0.847583	0.132237
N	1.842382	-1.881447	0.808404

C	0.346043	-2.856396	1.370546	C	0.854547	-2.747012	1.408187
C	-0.096086	-4.055249	0.755624	C	0.651628	-4.028953	0.837842
C	-0.264896	-2.305591	2.534908	C	0.167768	-2.297122	2.573728
C	-1.154326	-4.753004	1.376016	C	-0.240241	-4.901183	1.496893
C	-1.332155	-3.039866	3.091879	C	-0.726351	-3.209438	3.170057
C	-1.761684	-4.254802	2.533799	C	-0.919683	-4.498731	2.650895
H	-1.519249	-5.688317	0.925216	H	-0.414004	-5.906231	1.082447
H	-1.838377	-2.654461	3.987411	H	-1.281609	-2.906916	4.068354
H	-2.592295	-4.807869	3.000654	H	-1.618620	-5.190051	3.148227
C	0.507795	-4.583918	-0.544035	C	1.351529	-4.488536	-0.440103
H	1.112748	-3.766912	-0.987928	H	1.818536	-3.598941	-0.908486
C	0.195649	-0.985142	3.158263	C	0.374171	-0.899000	3.163181
H	0.275650	-0.232311	2.340990	H	0.296645	-0.160481	2.333113
C	1.428103	-5.795015	-0.281986	C	2.454635	-5.522019	-0.125880
H	2.250304	-5.553207	0.422282	H	3.208972	-5.126811	0.585423
H	0.854261	-6.639266	0.156883	H	2.021925	-6.438358	0.329912
H	1.884977	-6.151625	-1.229077	H	2.985916	-5.823357	-1.053240
C	-0.580539	-4.940355	-1.577226	C	0.351661	-5.053062	-1.469592
H	-0.111865	-5.163928	-2.557614	H	0.874041	-5.272482	-2.423668
H	-1.161086	-5.837579	-1.273567	H	-0.114421	-5.998938	-1.120114
H	-1.283035	-4.097888	-1.725172	H	-0.446264	-4.318844	-1.691085
C	1.586613	-1.114058	3.819835	C	1.775010	-0.738149	3.795964
H	1.899592	-0.130478	4.227201	H	1.898209	0.299199	4.169968
H	1.560613	-1.842396	4.659166	H	1.904269	-1.432581	4.654361
H	2.372661	-1.442397	3.111121	H	2.596708	-0.929813	3.077677
C	-0.808808	-0.391124	4.155381	C	-0.707628	-0.490700	4.172922
H	-1.813746	-0.285475	3.698605	H	-1.723415	-0.588272	3.737782
H	-0.894539	-0.999504	5.083033	H	-0.658785	-1.089647	5.109093
H	-0.480413	0.630735	4.423454	H	-0.574942	0.579078	4.420310
C	-0.718451	-1.223277	-1.495281	C	-0.486039	-1.293547	-1.590665
O	-0.051852	-1.908836	-2.268516	O	0.352024	-2.014191	-2.131210
O	-1.385056	1.644172	-1.132207	O	-1.728167	1.352895	-1.032504
C	-5.019219	-1.590705	-1.262592	C	-4.630969	-1.259984	-2.826173
C	-4.423244	-0.959901	-2.368729	C	-3.633019	-0.684166	-3.633994
H	-4.665095	-2.601767	0.639597	H	-5.058909	-2.343729	-0.994272
C	-4.213193	-2.110368	-0.236675	C	-4.275917	-1.897645	-1.629216
C	-3.023705	-0.846275	-2.488220	C	-2.293388	-0.744185	-3.226092
C	-2.223219	-1.363280	-1.435927	C	-1.940221	-1.363922	-2.008141
C	-2.818423	-1.976827	-0.317127	C	-2.933742	-1.961344	-1.194186
H	-2.179735	-2.335404	0.501388	H	-1.503534	-0.280931	-3.837212
H	-5.059859	-0.538139	-3.164087	H	-3.900300	-0.182039	-4.577669
K	0.664269	3.356593	-1.274894	K	-0.014770	3.353683	-1.320234
K	-2.562588	3.802658	2.056549	K	-3.123517	3.328076	2.138062
C	-0.057171	2.635817	1.479644	C	-0.475818	2.604407	1.487729
O	-0.180673	3.883197	1.105401	O	-0.829497	3.795359	1.078152
O	-0.732787	2.140186	2.441712	O	-1.007242	2.047063	2.504548
O	0.795577	1.880469	0.787075	O	0.458133	1.971619	0.777374
C	-2.613448	1.863012	-0.698844	C	-2.934531	1.279952	-0.504454
C	-3.177515	1.188126	0.429687	C	-3.216094	0.524976	0.678272
C	-3.438297	2.828795	-1.359098	C	-4.028607	1.976744	-1.108056
C	-4.492729	1.444489	0.844039	C	-4.513822	0.452369	1.205042
H	-2.550322	0.454694	0.958337	H	-2.373120	0.006961	1.161820
C	-4.743810	3.097531	-0.915665	C	-5.320800	1.908772	-0.562757
H	-3.023515	3.347337	-2.239240	H	-3.832427	2.543131	-2.032525
C	-5.291323	2.408513	0.188139	C	-5.583808	1.145020	0.595979
H	-4.904622	0.873779	1.693463	H	-4.693341	-0.162038	2.103748
H	-5.353115	3.844525	-1.452274	H	-6.145214	2.445370	-1.062244
H	-6.326235	2.598715	0.512832	H	-6.604575	1.076122	1.003411
H	-6.116558	-1.664237	-1.199675	H	-5.689382	-1.203438	-3.125891
C	-2.384198	-0.146392	-3.664192	C	-2.572085	-2.680094	0.082065
H	-3.141117	0.191518	-4.399233	H	-1.707641	-2.208263	0.590728
H	-1.819499	0.738812	-3.299492	H	-3.421492	-2.701007	0.793154
H	-1.658496	-0.808268	-4.179158	H	-2.275467	-3.731046	-0.120045

Zero-point correction= 0.789430 (Hartree/Particle)	Zero-point correction= 0.789503 (Hartree/Particle)
Thermal correction to Energy= 0.844782	Thermal correction to Energy= 0.844737
Thermal correction to Enthalpy= 0.845727	Thermal correction to Enthalpy= 0.845681
Thermal correction to Gibbs Free Energy= 0.699933	Thermal correction to Gibbs Free Energy= 0.700542
Sum of electronic and zero-point Energies= -3441.144589	Sum of electronic and zero-point Energies= -3441.140841
Sum of electronic and thermal Energies= -3441.089237	Sum of electronic and thermal Energies= -3441.085607
Sum of electronic and thermal Enthalpies= -3441.088292	Sum of electronic and thermal Enthalpies= -3441.084663
Sum of electronic and thermal Free Energies= -3441.234086	Sum of electronic and thermal Free Energies= -3441.229803

Ph(oMe)+B-Ph(pMe)-IPr-VII-VIII				**Ph(oMeISOMER)+B-Ph(pMe)-IPR-VII-VIII**			
100				100			
IPrVII-VIII-MeOrto SCF Done: -3441.90245240 A.U.				IPrVII-VIII-MeOrto180 SCF Done: -3441.90250427 A.U.			
Pd	-0.262614	-0.678218	0.138066	Pd	0.443234	-0.028678	0.006785
N	-2.462069	1.194226	0.605863	N	-1.510310	-2.003165	0.946683
C	-2.441803	2.239862	-2.101089	C	-2.740703	-2.243249	-1.668751
H	-1.468380	2.155007	-1.570581	H	-2.514336	-1.215389	-1.309254
C	-3.248774	0.997987	-1.713924	C	-1.565676	-3.123651	-1.238262
C	-3.256865	0.498551	-0.381504	C	-0.972496	-2.999948	0.049382
C	-1.107841	0.991061	0.742105	C	-1.245898	-0.658769	0.817071
C	-3.960377	-0.669673	0.010131	C	0.131396	-3.783660	0.474058
C	-3.926016	-1.179223	1.447654	C	0.753383	-3.621669	1.857820
H	-2.939684	-0.896005	1.872759	H	0.559024	-2.580295	2.190755
C	-4.004559	0.285225	-2.667451	C	-1.018923	-4.090399	-2.106247
H	-4.025674	0.630174	-3.711053	H	-1.439877	-4.215568	-3.113706
C	-4.724494	-0.866590	-2.309622	C	0.062907	-4.893201	-1.711020
H	-5.313907	-1.401331	-3.072640	H	0.465719	-5.648846	-2.405272
C	-4.699414	-1.339787	-0.988283	C	0.631308	-4.739869	-0.437016
H	-5.260053	-2.248322	-0.722847	H	1.480310	-5.373830	-0.139257
C	-2.908327	2.206360	1.457192	C	-2.426281	-2.239494	1.973677
C	-4.016562	-2.712295	1.547908	C	2.282974	-3.806229	1.852161
H	-3.773741	-3.033762	2.580333	H	2.706804	-3.464441	2.816464
H	-5.036197	-3.088829	1.312916	H	2.576096	-4.868793	1.705866
H	-3.284415	-3.197722	0.872869	H	2.756968	-3.189013	1.063371
C	-5.042303	-0.517648	2.286518	C	0.102631	-4.595704	2.865239
H	-4.994718	-0.871864	3.337468	H	0.539237	-4.453436	3.875784
H	-4.961250	0.587578	2.300334	H	-0.992515	-4.446519	2.946874
H	-6.044467	-0.777043	1.881751	H	0.275357	-5.650836	2.561202
C	-2.125310	2.329496	-3.602607	C	-2.917703	-2.152357	-3.191873
H	-3.032405	2.552211	-4.204884	H	-3.292827	-3.105187	-3.623547
H	-1.405736	3.155232	-3.781178	H	-3.660743	-1.365141	-3.433547
H	-1.666444	1.392732	-3.970837	H	-1.962853	-1.886626	-3.685570
C	-3.122273	3.547529	-1.636720	C	-4.064806	-2.692259	-1.009861
H	-3.271030	3.583155	-0.541158	H	-4.014652	-2.674242	0.095814
H	-2.494334	4.421257	-1.911397	H	-4.891632	-2.016921	-1.314841
H	-4.112372	3.669591	-2.125290	H	-4.329676	-3.723399	-1.326574
C	-1.805119	2.672117	2.122310	C	-2.763779	-1.014914	2.485827
H	-1.687804	3.461187	2.870236	H	-3.450575	-0.728209	3.287019
H	-3.959642	2.502412	1.505632	H	-2.760410	-3.247885	2.232145
N	-0.713197	1.933454	1.659657	N	-2.048278	-0.061825	1.757619
C	0.660926	2.291753	1.917927	C	-2.328587	1.354317	1.801624
C	1.215444	3.338589	1.136910	C	-3.398933	1.823519	0.995086
C	1.391879	1.581674	2.899299	C	-1.554128	2.196873	2.631611
C	2.546076	3.710242	1.410187	C	-3.673452	3.204295	1.026624
C	2.725702	1.984744	3.118902	C	-1.886998	3.568065	2.640741
C	3.291371	3.044376	2.394295	C	-2.927086	4.067946	1.843844
H	3.014727	4.513876	0.822127	H	-4.488285	3.607001	0.405644
H	3.329198	1.455495	3.871669	H	-1.307394	4.255486	3.276326
H	4.334995	3.342104	2.584226	H	-3.159394	5.144868	1.857422
C	0.413943	4.037683	0.039977	C	-4.279481	0.863451	0.196207
H	-0.462301	3.397674	-0.191747	H	-3.736841	-0.099049	0.111048
C	0.756307	0.452746	3.699745	C	-0.423267	1.657589	3.497532
H	-0.083100	0.038747	3.108805	H	-0.220388	0.611814	3.195952

C	-0.126353	5.397034	0.532073
H	-0.754122	5.283493	1.439024
H	0.708759	6.085311	0.783089
H	-0.745262	5.880477	-0.253144
C	1.204364	4.196807	-1.272576
H	0.533077	4.572861	-2.073406
H	2.034082	4.927613	-1.171515
H	1.634766	3.233055	-1.606900
C	0.181265	0.996728	5.024775
H	-0.319246	0.184069	5.591665
H	0.983867	1.422975	5.665226
H	-0.566544	1.797474	4.843651
C	1.713505	-0.727255	3.936515
H	2.201963	-1.029051	2.988463
H	2.507432	-0.491388	4.678243
H	1.140550	-1.601897	4.303079
C	0.319865	0.034688	-1.632777
O	-0.418034	-0.094538	-2.626105
O	1.348727	-2.481664	-1.393895
C	4.357080	1.561362	-1.823578
C	3.612814	1.423291	-3.008306
H	4.350922	1.292349	0.344238
C	3.782612	1.213767	-0.593005
C	2.289057	0.937538	-3.009778
C	1.698295	0.605050	-1.748398
C	2.463943	0.747777	-0.567377
H	1.991061	0.479401	0.389591
H	5.393790	1.931745	-1.869674
H	4.077525	1.689533	-3.972297
K	-1.188882	-2.542759	-2.226432
K	1.175106	-4.597221	0.389554
C	-0.771438	-2.953845	1.505239
O	-0.962710	-3.051351	0.193884
O	-0.552775	-3.975920	2.213823
O	-0.725355	-1.726547	1.977573
C	2.593701	-2.315292	-1.009475
C	2.936356	-2.168227	0.380686
C	3.683189	-2.259345	-1.938053
C	4.262716	-1.987775	0.804317
H	2.108736	-2.102995	1.111781
C	5.000384	-2.066810	-1.503690
H	3.443361	-2.333559	-3.010920
C	5.310550	-1.936009	-0.132277
H	4.470436	-1.853139	1.879495
H	5.809077	-2.002834	-2.251424
H	6.350297	-1.779487	0.194389
C	1.571512	0.785319	-4.329171
H	2.227940	1.092665	-5.168723
H	1.252909	-0.264935	-4.490823
H	0.643221	1.389243	-4.361817
Zero-point correction=			0.788250 (Hartree/Particle)
Thermal correction to Energy=			0.843293
Thermal correction to Enthalpy=			0.844237
Thermal correction to Gibbs Free Energy=			0.698799
Sum of electronic and zero-point Energies=			-3441.114202
Sum of electronic and thermal Energies=			-3441.059160
Sum of electronic and thermal Enthalpies=			-3441.058216
Sum of electronic and thermal Free Energies=			-3441.203653

C	-5.590111	0.584466	0.963497
H	-5.393747	0.199931	1.984998
H	-6.192780	1.512368	1.063259
H	-6.204585	-0.168652	0.426307
C	-4.565034	1.333537	-1.238011
H	-5.142268	0.557469	-1.783372
H	-5.165517	2.267023	-1.264232
H	-3.627571	1.515226	-1.793013
C	-0.836318	1.657640	4.984160
H	-0.029952	1.219435	5.608753
H	-1.032318	2.687981	5.352940
H	-1.759465	1.062276	5.148196
C	0.897119	2.416930	3.271943
H	1.171792	2.409870	2.198994
H	0.843141	3.471400	3.619140
H	1.717726	1.908592	3.816679
C	-0.242858	0.184516	-1.854577
O	-0.075291	-0.764302	-2.639257
O	2.381451	0.897019	-2.072674
C	-2.557699	3.482938	-3.472697
C	-2.451202	2.254100	-4.149720
H	-1.933994	4.639765	-1.746056
C	-1.863118	3.672572	-2.269874
C	-1.671926	1.234004	-3.593892
C	-0.983827	1.402393	-2.364249
C	-1.052859	2.661867	-1.702110
H	-1.577027	0.264477	-4.101674
H	-3.179210	4.294777	-3.883593
H	-2.980839	2.090805	-5.101769
K	2.264217	-1.690304	-2.049928
K	5.155233	0.232648	0.743268
C	2.558689	-0.649190	1.583955
O	2.746236	-0.775385	0.273505
O	3.515243	-0.753679	2.403083
O	1.330443	-0.373751	1.945712
C	3.390082	1.571506	-1.631625
C	3.338574	2.388554	-0.438063
C	4.680807	1.535573	-2.289849
C	4.440363	3.131735	0.008866
H	2.393848	2.404296	0.124130
C	5.781206	2.271398	-1.820730
H	4.765438	0.930446	-3.208940
C	5.684725	3.081445	-0.664705
H	4.332124	3.758609	0.911487
H	6.735283	2.225644	-2.374742
H	6.540856	3.681939	-0.320299
C	-0.237432	3.001101	-0.488018
H	-0.079183	2.103766	0.157529
H	0.768007	3.347671	-0.803206
H	-0.713202	3.793042	0.121070
Zero-point correction=			0.788525 (Hartree/Particle)
Thermal correction to Energy=			0.843275
Thermal correction to Enthalpy=			0.844220
Thermal correction to Gibbs Free Energy=			0.701029
Sum of electronic and zero-point Energies=			-3441.113980
Sum of electronic and thermal Energies=			-3441.059229
Sum of electronic and thermal Enthalpies=			-3441.058285
Sum of electronic and thermal Free Energies=			-3441.201476

Ph(oMe)+B-Ph(pMe)-IPr-VIIIpost	**Ph(oMeISOMER)+B-Ph(pMe)-IPR-VIIIpost**
100 IPrVIII-MeOrto SCF Done: -3441.92589630 A.U.	100 IPrVIII-MeOrto180 SCF Done: -3441.92486710 A.U.

Pd	-0.354808	-0.046842	-0.440488
N	0.826393	2.339954	0.898499
C	2.288692	2.749671	-1.569656
H	2.209515	1.698232	-1.223092
C	0.931146	3.408853	-1.308433
C	0.249053	3.239158	-0.068684
C	0.855311	0.967813	0.759226
C	-0.953358	3.921753	0.256487
C	-1.625698	3.787310	1.621475
H	-1.277669	2.830278	2.061178
C	0.326918	4.253502	-2.262391
H	0.807369	4.398642	-3.240224
C	-0.872770	4.929070	-1.979289
H	-1.317694	5.594293	-2.737289
C	-1.493698	4.778115	-0.729675
H	-2.421114	5.329642	-0.511151
C	1.500688	2.749152	2.050188
C	-3.161178	3.698942	1.541450
H	-3.573714	3.505153	2.553145
H	-3.618235	4.646891	1.182862
H	-3.487700	2.861742	0.893826
C	-1.210338	4.964003	2.535118
H	-1.635306	4.834903	3.552512
H	-0.110039	5.058027	2.636463
H	-1.585134	5.928547	2.129270
C	2.685453	2.705511	-3.052461
H	2.892321	3.719629	-3.457605
H	3.618815	2.116655	-3.167418
H	1.903494	2.217497	-3.664731
C	3.405027	3.432890	-0.744916
H	3.203645	3.407766	0.343576
H	4.373289	2.916026	-0.913745
H	3.525542	4.494739	-1.048358
C	1.977052	1.615956	2.646472
H	2.551954	1.462359	3.563487
H	1.581911	3.802431	2.329662
N	1.585628	0.543354	1.839852
C	2.048408	-0.798270	2.097031
C	3.398851	-1.077589	1.772291
C	1.172075	-1.747125	2.689394
C	3.910782	-2.336942	2.144153
C	1.741281	-2.990984	3.035076
C	3.094884	-3.274694	2.788614
H	4.956759	-2.588517	1.909954
H	1.111310	-3.758739	3.506007
H	3.508633	-4.253553	3.079730
C	4.277171	-0.069730	1.030064
H	3.620255	0.746538	0.663882
C	-0.316471	-1.458361	2.868480
H	-0.676657	-1.019283	1.906466
C	5.326517	0.561046	1.968083
H	4.851605	1.065966	2.833624
H	6.016741	-0.212723	2.366860
H	5.935867	1.314621	1.425763
C	4.943233	-0.693058	-0.211697
H	5.463519	0.091537	-0.800684
H	5.701624	-1.455554	0.063964
H	4.195617	-1.180272	-0.866310
C	-0.631613	-0.396548	3.942106
H	-1.717480	-0.178515	3.892377
H	-0.365549	-0.761667	4.958113
H	-0.097393	0.556512	3.763695
C	-1.163442	-2.714659	3.118179

Pd	-0.277369	-0.155880	-0.425269
N	0.862781	2.162977	1.107005
C	2.520289	2.726311	-1.200482
H	2.381498	1.653795	-0.943869
C	1.163308	3.404049	-0.989272
C	0.368763	3.131438	0.161359
C	0.866140	0.806797	0.880745
C	-0.876291	3.766031	0.418873
C	-1.693137	3.470715	1.675870
H	-1.431706	2.439384	1.997373
C	0.652097	4.339282	-1.912889
H	1.222791	4.572380	-2.823036
C	-0.575722	4.985888	-1.688207
H	-0.947157	5.721723	-2.420115
C	-1.326370	4.706427	-0.535316
H	-2.284518	5.222028	-0.370365
C	1.462840	2.476327	2.328847
C	-3.214521	3.492348	1.431890
H	-3.735835	3.092038	2.324322
H	-3.593135	4.523293	1.256715
H	-3.496636	2.841246	0.580883
C	-1.336249	4.468602	2.802015
H	-1.903986	4.225152	3.724135
H	-0.259077	4.461761	3.059214
H	-1.599469	5.505842	2.501542
C	3.021445	2.779995	-2.651042
H	3.295922	3.812194	-2.958043
H	3.934433	2.157747	-2.749092
H	2.261842	2.382197	-3.352031
C	3.597116	3.298417	-0.249569
H	3.324457	3.186564	0.817441
H	4.558841	2.764563	-0.400993
H	3.767798	4.377161	-0.452258
C	1.858790	1.290769	2.882689
H	2.369627	1.066507	3.822660
H	1.564054	3.506589	2.678369
N	1.498176	0.285416	1.984040
C	1.933452	-1.086106	2.112588
C	3.232234	-1.396874	1.633505
C	1.063967	-2.042927	2.695918
C	3.661535	-2.733651	1.753351
C	1.554579	-3.361085	2.803104
C	2.833208	-3.703066	2.337104
H	4.656953	-3.018227	1.381007
H	0.914370	-4.137712	3.246597
H	3.186009	-4.743431	2.422742
C	4.152491	-0.319324	1.060669
H	3.509687	0.515466	0.711720
C	-0.331161	-1.658239	3.172019
H	-0.739000	-0.893794	2.472224
C	5.089779	0.233797	2.157701
H	4.529211	0.629678	3.027245
H	5.765704	-0.565876	2.528960
H	5.718404	1.056188	1.755275
C	4.971555	-0.791321	-0.150688
H	5.503176	0.068849	-0.608580
H	5.743641	-1.536841	0.134699
H	4.326030	-1.245998	-0.922043
C	-0.286974	-1.016386	4.576163
H	-1.309466	-0.714275	4.884444
H	0.110284	-1.728772	5.332047
H	0.346631	-0.106768	4.597981
C	-1.334788	-2.824177	3.151411

H	-0.948647	-3.517637	2.382251
H	-1.003524	-3.132201	4.136565
H	-2.227814	-2.429544	3.010840
C	0.903143	-0.523572	-1.902147
O	0.832619	0.188610	-2.903524
O	-1.802446	-0.951230	-1.711002
C	3.327283	-4.091591	-1.611250
C	3.473765	-3.245566	-2.724392
H	2.268954	-4.421626	0.273034
C	2.396067	-3.776533	-0.608587
C	2.703987	-2.073030	-2.880433
C	1.766676	-1.752270	-1.847624
C	1.634749	-2.608875	-0.733573
H	0.914781	-2.322558	0.048225
H	4.210173	-3.501606	-3.504250
K	-2.632269	1.522532	-1.833916
K	-5.136502	-1.690889	0.635629
C	-3.121659	0.274757	0.896068
O	-4.110490	0.581426	0.092545
O	-3.255102	-0.581062	1.836596
O	-1.961000	0.889373	0.692354
C	-2.405348	-2.098758	-1.476847
C	-2.084651	-2.940645	-0.365917
C	-3.458925	-2.541278	-2.343459
C	-2.774310	-4.139940	-0.135787
H	-1.300366	-2.595709	0.322864
C	-4.145851	-3.742629	-2.100072
H	-3.708461	-1.914027	-3.214760
C	-3.819363	-4.556772	-0.991590
H	-2.495843	-4.757924	0.734587
H	-4.943736	-4.057123	-2.794513
H	-4.348145	-5.506574	-0.815465
H	3.947375	-4.999043	-1.530054
C	2.908479	-1.212923	-4.103871
H	3.728521	-1.613491	-4.733779
H	1.982780	-1.152541	-4.711103
H	3.144760	-0.165749	-3.827815
Zero-point correction=			0.789434 (Hartree/Particle)
Thermal correction to Energy=			0.844648
Thermal correction to Enthalpy=			0.845593
Thermal correction to Gibbs Free Energy=			0.699793
Sum of electronic and zero-point Energies=			-3441.136463
Sum of electronic and thermal Energies=			-3441.081248
Sum of electronic and thermal Enthalpies=			-3441.080304
Sum of electronic and thermal Free Energies=			-3441.226103

H	-1.266562	-3.403355	2.207805
H	-1.186321	-3.532659	3.996024
H	-2.362931	-2.413307	3.217600
C	0.932126	-0.233568	-2.009281
O	0.700070	0.627968	-2.873004
O	-1.583045	-1.069872	-1.850552
C	4.054231	-3.083557	-2.943892
C	3.064847	-3.441123	-2.015085
H	4.772421	-1.531796	-4.302686
C	4.005316	-1.823369	-3.567806
C	2.007417	-2.568845	-1.669283
C	1.977047	-1.282930	-2.286775
C	2.969557	-0.940820	-3.239961
H	2.900518	0.047666	-3.717115
H	3.100875	-4.434044	-1.537801
K	-2.017546	1.523779	-2.269321
K	-5.479632	-0.788844	0.027262
C	-3.052585	0.299703	0.848391
O	-3.457192	0.755316	-0.314220
O	-3.882285	-0.031211	1.761538
O	-1.758998	0.160534	1.086105
C	-2.483586	-1.987477	-1.565554
C	-2.567547	-2.649521	-0.299348
C	-3.454535	-2.356648	-2.555136
C	-3.557127	-3.610377	-0.043280
H	-1.863450	-2.344012	0.486953
C	-4.443568	-3.317101	-2.285199
H	-3.393603	-1.871125	-3.543147
C	-4.513999	-3.955877	-1.025307
H	-3.585558	-4.090790	0.949604
H	-5.166220	-3.583929	-3.075599
H	-5.276593	-4.725081	-0.825239
H	4.864976	-3.791037	-3.181306
C	0.932783	-3.055469	-0.735645
H	1.255101	-3.954659	-0.176902
H	0.648914	-2.264235	-0.006409
H	0.004790	-3.294550	-1.294874
Zero-point correction=			0.789691 (Hartree/Particle)
Thermal correction to Energy=			0.844874
Thermal correction to Enthalpy=			0.845818
Thermal correction to Gibbs Free Energy=			0.701308
Sum of electronic and zero-point Energies=			-3441.135176
Sum of electronic and thermal Energies=			-3441.079993
Sum of electronic and thermal Enthalpies=			-3441.079049
Sum of electronic and thermal Free Energies=			-3441.223559

Ph(oMe)+B-Ph(pMe)-IPr-VIII			
87			
IPrVIIImenysKOPh-MeOrto SCF Done: -2535.15646238 A.U.			
Pd	-0.009661	-0.782435	0.104447
N	2.331341	1.078643	0.175198
C	2.414100	0.176712	2.951013
H	1.657725	0.829889	2.471341
C	3.275746	-0.446598	1.857074
C	3.215796	-0.009557	0.512295
C	0.990208	0.907242	-0.041428
C	3.949232	-0.615080	-0.538022
C	3.811096	-0.161787	-1.990101
H	2.922806	0.501665	-2.053193
C	4.166686	-1.498791	2.149556
H	4.247473	-1.863691	3.185467

Ph(oMeISOMER)+B-Ph(pMe)-IPR-VIII			
87			
IPrVIIImenysKOPh-MeOrto180 SCF Done: -2535.14343565 A.U.			
Pd	0.606549	-0.658711	0.575461
N	0.792243	1.282967	-1.654615
C	-0.111267	3.528107	-0.059751
H	-0.609802	2.543757	0.080108
C	1.373718	3.225239	-0.269621
C	1.797994	2.075889	-0.988705
C	0.023237	0.335162	-1.025915
C	3.149679	1.672552	-1.074736
C	3.553615	0.332442	-1.680691
H	2.632512	-0.261836	-1.846630
C	2.381042	4.042321	0.278107
H	2.100977	4.943977	0.841415

C	4.939847	-2.093478	1.141333	C	3.739063	3.715820	0.133986
H	5.627983	-2.916576	1.392018	H	4.508528	4.378231	0.562206
C	4.824856	-1.661878	-0.188274	C	4.117194	2.532978	-0.514900
H	5.413228	-2.157450	-0.975909	H	5.182142	2.258846	-0.577666
C	2.727798	2.388328	-0.092489	C	0.414090	1.444238	-2.988361
C	3.549329	-1.339846	-2.948520	C	4.404363	-0.479516	-0.683105
H	3.377850	-0.956467	-3.977082	H	4.496100	-1.532137	-1.015375
H	4.418710	-2.029600	-2.998882	H	5.422586	-0.050735	-0.560613
H	2.651578	-1.906878	-2.627796	H	3.903023	-0.492407	0.306108
C	5.042643	0.664358	-2.418710	C	4.263745	0.509468	-3.036689
H	4.927629	1.031411	-3.460492	H	4.538390	-0.476681	-3.466407
H	5.198570	1.543511	-1.758960	H	3.612860	1.033179	-3.768134
H	5.965508	0.047163	-2.375905	H	5.195038	1.106563	-2.928406
C	1.617123	-0.892200	3.721803	C	-0.386664	4.340630	1.215605
H	2.275849	-1.552474	4.324936	H	-0.043978	5.393503	1.121812
H	0.895602	-0.404866	4.408613	H	-1.478511	4.367738	1.412123
H	1.039579	-1.522805	3.016304	H	0.112907	3.878548	2.090268
C	3.267177	1.050175	3.893241	C	-0.754580	4.211081	-1.286125
H	3.790582	1.854488	3.334813	H	-0.670213	3.593765	-2.201928
H	2.630456	1.526473	4.668339	H	-1.835716	4.389406	-1.104315
H	4.040747	0.444087	4.412399	H	-0.274035	5.192586	-1.485554
C	1.604750	3.060115	-0.498953	C	-0.648694	0.603319	-3.196707
H	1.456853	4.093190	-0.824378	H	-1.257873	0.411902	-4.084493
H	3.766068	2.711867	0.023569	H	0.933221	2.139876	-3.654037
N	0.550098	2.143251	-0.453114	N	-0.885277	-0.049094	-1.985956
C	-0.794939	2.434047	-0.882272	C	-2.044760	-0.855195	-1.691114
C	-1.607673	3.258715	-0.061401	C	-3.212380	-0.178225	-1.252429
C	-1.246674	1.895929	-2.117458	C	-1.955875	-2.263199	-1.795131
C	-2.888795	3.596236	-0.545652	C	-4.330825	-0.968456	-0.923143
C	-2.539112	2.261905	-2.546261	C	-3.111328	-3.004001	-1.471008
C	-3.347900	3.113347	-1.779101	C	-4.282663	-2.366336	-1.037739
H	-3.542140	4.238408	0.064205	H	-5.250922	-0.482225	-0.565611
H	-2.916649	1.869537	-3.503187	H	-3.082245	-4.101876	-1.540061
H	-4.351727	3.390425	-2.138653	H	-5.168171	-2.967046	-0.774875
C	-1.136862	3.772801	1.297167	C	-3.266960	1.346731	-1.182597
H	-0.265557	3.155863	1.600336	H	-2.223724	1.711291	-1.086310
C	-0.394562	0.967214	-2.979999	C	-0.670429	-2.949108	-2.242111
H	0.459508	0.612967	-2.370278	H	0.168965	-2.250500	-2.055467
C	-0.691753	5.248512	1.205333	C	-3.844059	1.928376	-2.491499
H	0.115874	5.397430	0.460172	H	-3.263397	1.604963	-3.378377
H	-1.542936	5.897947	0.907746	H	-4.894549	1.596872	-2.635787
H	-0.317861	5.606151	2.187656	H	-3.833082	3.038429	-2.463595
C	-2.210699	3.595670	2.388745	C	-4.035853	1.876619	0.037436
H	-1.783531	3.848181	3.381120	H	-3.906127	2.976032	0.119284
H	-3.082641	4.264294	2.225088	H	-5.126701	1.681890	-0.038539
H	-2.561355	2.546672	2.432555	H	-3.669532	1.418675	0.973944
C	0.182015	1.717030	-4.197375	C	-0.722668	-3.243584	-3.756296
H	0.829437	1.042164	-4.795573	H	0.226603	-3.708592	-4.095780
H	-0.627049	2.093210	-4.860020	H	-1.554140	-3.940090	-3.999667
H	0.792228	2.588478	-3.880176	H	-0.878882	-2.314969	-4.344844
C	-1.169822	-0.300282	-3.391120	C	-0.355278	-4.212585	-1.423730
H	-1.652639	-0.750124	-2.498990	H	-0.358113	-3.986285	-0.338833
H	-1.953180	-0.084990	-4.149394	H	-1.075436	-5.035602	-1.622543
H	-0.476081	-1.060128	-3.800993	H	0.660581	-4.576105	-1.674926
C	-1.157159	-0.016894	1.500497	C	-0.115609	0.579050	1.942229
O	-0.887662	0.750758	2.419109	O	0.635709	1.438243	2.403735
C	-5.125999	-1.681069	0.938483	C	-4.159638	0.528213	3.533039
C	-4.244476	-2.249582	1.882231	C	-3.329266	1.655668	3.664407
H	-5.394328	-0.103202	-0.550720	H	-4.320241	-1.510623	2.808769
C	-4.713263	-0.565941	0.181820	C	-3.670056	-0.625207	2.900909
C	-2.951169	-1.722971	2.094976	C	-2.029979	1.609067	3.145139
C	-2.556493	-0.589211	1.332919	C	-1.530802	0.457665	2.486152
C	-3.428439	-0.027700	0.378593	C	-2.358603	-0.699969	2.377424

H	-3.090833	0.833157	-0.216875	H	-1.358393	2.475045	3.233572
H	-4.570360	-3.118769	2.479308	H	-3.696038	2.567723	4.161804
K	-2.984597	-3.626279	-1.118248	K	3.646397	-2.381387	3.229971
C	-0.219913	-2.936661	-1.253941	C	2.241327	-2.626535	0.795567
O	-0.914926	-2.661266	-0.119184	O	1.632390	-2.008904	1.840567
O	-0.598076	-3.879261	-1.997284	O	3.167962	-3.454561	1.017876
O	0.751734	-2.105424	-1.490276	O	1.834121	-2.235095	-0.372780
H	-6.138885	-2.097415	0.810356	H	-5.190392	0.545713	3.922259
C	-1.976058	-2.361119	3.052487	C	-1.886721	-2.002386	1.784815
H	-1.107010	-2.749931	2.477572	H	-2.727098	-2.708013	1.637140
H	-1.579395	-1.621189	3.776513	H	-1.386416	-1.834376	0.804213
H	-2.434387	-3.198630	3.614751	H	-1.118386	-2.483911	2.425651
Zero-point correction= 0.696443 (Hartree/Particle)				Zero-point correction= 0.696981 (Hartree/Particle)			
Thermal correction to Energy= 0.743662				Thermal correction to Energy= 0.743848			
Thermal correction to Enthalpy= 0.744607				Thermal correction to Enthalpy= 0.744792			
Thermal correction to Gibbs Free Energy= 0.615180				Thermal correction to Gibbs Free Energy= 0.616584			
Sum of electronic and zero-point Energies= -2534.460020				Sum of electronic and zero-point Energies= -2534.446455			
Sum of electronic and thermal Energies= -2534.412800				Sum of electronic and thermal Energies= -2534.399587			
Sum of electronic and thermal Enthalpies= -2534.411856				Sum of electronic and thermal Enthalpies= -2534.398643			
Sum of electronic and thermal Free Energies= -2534.541282				Sum of electronic and thermal Free Energies= -2534.526851			

Ph(oMe)+B-Ph(pMe)-IPr-IX				**Ph(oMeISOMER)+B-Ph(pMe)-IPR-IX**			
103				103			
IPrIX-MeOrto SCF Done: -2943.17774131 A.U.				IPrIX-MeOrto180 SCF Done: -2943.17765554 A.U.			
Pd	0.135873	0.244631	-0.493705	Pd	-0.099869	-0.340686	-0.439895
K	-0.761579	5.289489	1.092248	K	2.920143	-4.351094	1.486837
O	0.413185	4.481921	-1.065773	O	1.705715	-4.214650	-0.807033
H	0.679309	4.679389	-1.979273	H	1.694613	-4.531198	-1.725676
B	-0.517196	3.327009	-1.068679	B	2.069588	-2.778293	-0.789671
O	-1.877432	3.843914	-1.278272	O	3.537517	-2.683119	-0.736114
H	-2.525958	3.118737	-1.199404	H	3.807276	-1.746040	-0.721116
C	-0.078828	2.149457	-2.159321	C	1.310956	-1.968294	-2.019094
C	-1.063536	1.721751	-3.109745	C	1.936571	-1.262960	-3.108536
C	1.259646	1.644473	-2.360671	C	-0.113152	-2.127976	-2.091882
C	-0.791309	0.837581	-4.155806	C	1.138928	-0.732331	-4.141624
H	-2.083207	2.124798	-3.012050	C	-0.897473	-1.580916	-3.138017
C	1.507286	0.702931	-3.402921	H	-0.604022	-2.792755	-1.362903
C	0.506408	0.303099	-4.289613	C	-0.262436	-0.872299	-4.161260
H	-1.591107	0.542245	-4.853137	H	1.632539	-0.191089	-4.966290
H	2.532331	0.310880	-3.512268	H	-1.989844	-1.719836	-3.128909
C	0.574036	2.606242	1.173262	C	0.456460	-2.649056	1.262321
O	0.821319	3.435917	2.080574	O	0.554954	-3.508307	2.169101
O	-0.548668	2.826078	0.398297	O	1.615415	-2.268189	0.606771
O	1.238688	1.537237	0.925334	O	-0.618415	-2.033487	0.921509
N	1.872038	-1.592180	1.064140	N	-2.587256	0.637240	0.850293
N	-0.177244	-1.833357	1.734662	N	-0.906528	1.736380	1.672977
C	0.585139	-1.206826	0.785798	C	-1.232750	0.810998	0.718442
C	1.910596	-2.432279	2.177712	C	-3.094186	1.432837	1.877334
C	0.618426	-2.582325	2.604727	C	-2.033821	2.123473	2.402012
C	3.022050	-1.245151	0.260677	C	-3.377456	-0.187872	-0.036482
C	3.963646	-0.323804	0.780640	C	-3.830125	-1.448627	0.421933
C	5.092268	-0.039774	-0.018219	C	-4.585060	-2.224966	-0.482752
C	5.250995	-0.624376	-1.280259	C	-4.863379	-1.764260	-1.776053
C	4.287175	-1.517729	-1.775421	C	-4.395493	-0.510095	-2.199674
C	3.151365	-1.860460	-1.016393	C	-3.638556	0.310693	-1.341746
C	3.796789	0.340547	2.144899	C	-3.558916	-1.945634	1.839432
H	6.132290	-0.376374	-1.893193	H	-5.448760	-2.391537	-2.467390
C	2.116131	-2.862693	-1.527706	C	-3.137059	1.684840	-1.782906
C	-1.615904	-1.756603	1.787212	C	0.419619	2.273292	1.854172
C	-2.357115	-2.756101	1.108414	C	0.745359	3.477078	1.180572
C	-3.762332	-2.655792	1.159380	C	2.045810	3.987048	1.372304
C	-4.384569	-1.612633	1.858551	C	2.964054	3.325214	2.198194

C	-3.619021	-0.631608	2.506511	C	2.614759	2.124085	2.833499
C	-2.211769	-0.667772	2.471907	C	1.337714	1.555996	2.662196
C	-1.661810	-3.903411	0.375528	C	-0.276433	4.208950	0.310156
H	-5.483764	-1.547808	1.876853	H	3.976766	3.737845	2.328697
C	-1.356924	0.417921	3.122833	C	0.955196	0.220387	3.297209
H	2.849688	-2.850276	2.549537	H	-4.157176	1.437179	2.132357
H	0.191887	-3.145041	3.439291	H	-1.972850	2.845411	3.220706
H	5.845719	0.672016	0.351365	H	-4.951355	-3.213009	-0.166087
H	4.425326	-1.960218	-2.772406	H	-4.616088	-0.165956	-3.220420
H	2.729746	0.243916	2.429819	H	-2.669432	-1.399420	2.214251
H	1.115423	-2.451876	-1.285672	H	-2.127423	1.819694	-1.344611
H	-4.378119	-3.397869	0.630628	H	2.346353	4.912056	0.858645
H	-4.126068	0.198176	3.020207	H	3.360633	1.600278	3.448966
H	-0.663613	-3.534247	0.057113	H	-1.006512	3.454110	-0.052404
H	-0.442177	0.527605	2.503222	H	0.253986	-0.283885	2.599204
C	-2.035585	1.798965	3.156836	C	2.148097	-0.734340	3.484153
H	-2.879147	1.833725	3.879503	H	2.838407	-0.392089	4.285234
H	-1.287220	2.559301	3.458486	H	1.766529	-1.738303	3.759014
H	-2.408805	2.087493	2.154293	H	2.718420	-0.849153	2.540676
C	-0.912642	-0.000682	4.541396	C	0.212726	0.433902	4.634340
H	-0.341364	-0.950471	4.530527	H	-0.699704	1.049827	4.504070
H	-0.260601	0.779360	4.986757	H	-0.096670	-0.541448	5.064395
H	-1.793666	-0.139408	5.204305	H	0.867917	0.947241	5.370530
C	-2.398912	-4.354536	-0.896288	C	0.342818	4.867921	-0.933905
H	-1.775893	-5.086342	-1.450492	H	-0.461060	5.262992	-1.588312
H	-3.362891	-4.854656	-0.662714	H	0.999767	5.722964	-0.667641
H	-2.591407	-3.499896	-1.570691	H	0.927463	4.138337	-1.523970
C	-1.447576	-5.104834	1.323673	C	-1.048700	5.255740	1.144220
H	-2.424179	-5.510843	1.663566	H	-0.356131	6.032941	1.532201
H	-0.898708	-5.917947	0.803594	H	-1.817623	5.759716	0.521682
H	-0.866730	-4.828889	2.225597	H	-1.563250	4.800203	2.013152
C	4.098149	1.850521	2.102647	C	-3.208499	-3.443451	1.892841
H	3.799945	2.320698	3.061591	H	-2.858599	-3.711028	2.910705
H	5.179408	2.055536	1.948464	H	-4.086008	-4.085613	1.662718
H	3.509296	2.338111	1.304053	H	-2.383595	-3.671890	1.192664
C	4.671724	-0.363423	3.204997	C	-4.763691	-1.633819	2.755373
H	5.749317	-0.279972	2.946513	H	-5.673100	-2.167352	2.404343
H	4.524799	0.100856	4.202964	H	-4.557667	-1.959789	3.796738
H	4.438213	-1.444421	3.295374	H	-5.005967	-0.551508	2.779869
C	2.124258	-3.047182	-3.051001	C	-2.947122	1.815183	-3.300000
H	3.041973	-3.560848	-3.411358	H	-3.912382	1.794342	-3.850760
H	1.253614	-3.663756	-3.351297	H	-2.449232	2.778114	-3.530575
H	2.030827	-2.074876	-3.571734	H	-2.292683	1.008870	-3.682671
C	2.251060	-4.229120	-0.818312	C	-4.048850	2.808697	-1.242601
H	1.460229	-4.922879	-1.174087	H	-3.640262	3.803311	-1.520550
H	3.237477	-4.693190	-1.033662	H	-5.072352	2.726225	-1.667245
H	2.145589	-4.145459	0.281753	H	-4.135814	2.780333	-0.137681
C	-2.579819	-0.394142	-1.370358	C	2.131207	1.391955	-1.188395
C	-2.938309	0.624821	-0.462580	C	2.805543	0.706717	-0.156134
C	-3.569130	-0.946659	-2.213061	C	2.860686	2.256312	-2.034460
C	-4.263804	1.079087	-0.392197	C	4.181865	0.896457	0.040878
C	-4.894172	-0.491732	-2.143816	C	4.237531	2.442592	-1.840206
C	-5.245719	0.523060	-1.232770	C	4.901781	1.766527	-0.798595
H	-2.157888	1.067991	0.178917	H	2.239358	0.007495	0.480345
H	-3.269764	-1.723116	-2.933950	H	2.326507	2.758737	-2.855515
H	-4.531528	1.865118	0.332180	H	4.690828	0.366712	0.862013
H	-5.659387	-0.924701	-2.808096	H	4.801017	3.113436	-2.508359
H	-6.286485	0.881077	-1.180013	H	5.983168	1.913431	-0.646899
C	-1.147144	-0.876547	-1.502654	C	0.647346	1.195644	-1.442264
O	-0.878898	-1.833145	-2.217940	O	0.055439	1.906268	-2.243221
H	0.730542	-0.422308	-5.087793	H	-0.844640	-0.432581	-4.986469
C	2.487036	2.196046	-1.655897	C	3.437813	-1.096981	-3.211848
H	2.237002	2.954691	-0.898218	H	3.722507	-0.649744	-4.185469

H 3.063043 1.386522 -1.166241	H 3.830522 -0.423137 -2.421368
H 3.153878 2.664612 -2.412536	H 3.962343 -2.065082 -3.090155
Zero-point correction= 0.820805 (Hartree/Particle)	Zero-point correction= 0.820987 (Hartree/Particle)
Thermal correction to Energy= 0.876224	Thermal correction to Energy= 0.876383
Thermal correction to Enthalpy= 0.877168	Thermal correction to Enthalpy= 0.877327
Thermal correction to Gibbs Free Energy= 0.734002	Thermal correction to Gibbs Free Energy= 0.733707
Sum of electronic and zero-point Energies= -2942.356936	Sum of electronic and zero-point Energies= -2942.356669
Sum of electronic and thermal Energies= -2942.301518	Sum of electronic and thermal Energies= -2942.301273
Sum of electronic and thermal Enthalpies= -2942.300574	Sum of electronic and thermal Enthalpies= -2942.300329
Sum of electronic and thermal Free Energies= -2942.443739	Sum of electronic and thermal Free Energies= -2942.443948

Ph(oMe)+B-Ph(pMe)-IPr-IX-X	**Ph(oMeISOMER)+B-Ph(pMe)-IPR-IX-X**
103	103
IPrIX-X-MeOrto SCF Done: -2943.15873355 A.U.	IPrIX-X-MeOrto180 SCF Done: -2943.15791670 A.U.
Pd 0.241813 0.289546 -0.354077	Pd -0.241166 -0.277038 -0.342298
K 2.173102 4.405665 2.703431	K -2.699684 -3.902265 2.937775
O 2.233467 3.782230 0.178813	O -2.661354 -3.544956 0.391017
H 2.446158 4.017575 -0.743180	H -2.952527 -3.761025 -0.513013
B 0.937774 3.156699 0.215150	B -1.331660 -2.964550 0.347773
O -0.111689 3.943700 -0.262749	O -0.334028 -3.869126 -0.052143
H -0.967793 3.472611 -0.209690	H 0.557320 -3.477099 0.042630
C 1.358757 1.786723 -1.501931	C -1.726813 -1.633890 -1.250556
C 0.711303 2.393960 -2.613851	C -1.615937 -2.306462 -2.517772
C 2.758177 1.479827 -1.671562	C -2.972697 -0.969894 -0.998430
C 1.348021 2.658069 -3.837025	C -2.725801 -2.348754 -3.396649
H -0.342110 2.696335 -2.510327	C -4.049582 -0.987752 -1.893339
C 3.392863 1.757979 -2.902997	H -3.102997 -0.424931 -0.050685
C 2.703823 2.328594 -3.987178	C -3.933437 -1.699590 -3.099693
H 0.785937 3.118679 -4.665983	H -2.623221 -2.887753 -4.354156
H 4.461933 1.508168 -3.015465	H -4.975355 -0.444205 -1.645998
C 1.547356 1.559248 2.073201	C -1.715737 -1.209515 2.149573
O 2.176444 1.916929 3.098702	O -2.354037 -1.403044 3.213809
O 0.699961 2.540505 1.499883	O -1.039593 -2.325676 1.627042
O 1.548978 0.424050 1.522413	O -1.582753 -0.116316 1.523565
N 0.497175 -2.641105 0.156892	N -0.272894 2.673583 -0.023994
N -1.523637 -2.083851 0.696365	N 1.721831 2.022052 0.515648
C -0.341148 -1.557573 0.240876	C 0.500887 1.547940 0.114144
C -0.151731 -3.817109 0.529172	C 0.458000 3.825916 0.257526
C -1.426871 -3.465957 0.882733	C 1.716372 3.416828 0.612114
C 1.897413 -2.564751 -0.191104	C -1.688461 2.631157 -0.320584
C 2.844833 -2.560113 0.865846	C -2.598975 2.729520 0.763446
C 4.206853 -2.548028 0.503761	C -3.971309 2.663961 0.451265
C 4.596828 -2.513372 -0.843262	C -4.405740 2.501415 -0.872400
C 3.633066 -2.476695 -1.860517	C -3.477331 2.389387 -1.916844
C 2.255980 -2.500866 -1.559817	C -2.092525 2.442540 -1.664896
C 2.419571 -2.586136 2.333431	C -2.126695 2.944873 2.200417
H 5.667538 -2.493204 -1.102172	H -5.484390 2.445164 -1.090720
C 1.212128 -2.501011 -2.671492	C -1.077854 2.322677 -2.797595
C -2.676073 -1.294781 1.050553	C 2.810120 1.173715 0.930352
C -3.818965 -1.343534 0.215902	C 3.949545 1.068771 0.096816
C -4.934893 -0.572335 0.602735	C 4.996983 0.234208 0.539586
C -4.905462 0.205325 1.766439	C 4.904747 -0.452851 1.756238
C -3.753215 0.241311 2.567642	C 3.757490 -0.333219 2.556803
C -2.604886 -0.498856 2.227020	C 2.673369 0.472409 2.160050
C -3.878538 -2.233894 -1.024718	C 4.076150 1.869546 -1.198130
H -5.786227 0.804434 2.046969	H 5.731978 -1.103881 2.080517
C -1.335781 -0.448625 3.077314	C 1.405462 0.588162 3.006538
H 0.354146 -4.785849 0.502558	H 0.016643 4.822911 0.179214
H -2.266461 -4.059774 1.253239	H 2.599674 3.978228 0.927541
H 4.973418 -2.543922 1.293173	H -4.710800 2.730047 1.263372
H 3.951401 -2.422793 -2.912710	H -3.830492 2.231892 -2.946462
H 1.374821 -2.213614 2.377551	H -1.088328 2.557245 2.266114

H	0.228681	-2.247633	-2.229050
H	-5.837511	-0.578137	-0.026658
H	-3.740414	0.871919	3.468630
H	-2.835471	-2.495878	-1.300037
H	-0.474017	-0.500286	2.381678
C	-1.163210	0.867510	3.852567
H	-1.901940	0.977240	4.676150
H	-0.149839	0.902509	4.301090
H	-1.249262	1.742249	3.175832
C	-1.242045	-1.670674	4.016061
H	-1.279069	-2.624279	3.450826
H	-0.284297	-1.650452	4.577159
H	-2.076007	-1.674263	4.750541
C	-4.500999	-1.532172	-2.244766
H	-4.432930	-2.191965	-3.134152
H	-5.575485	-1.298819	-2.087378
H	-3.964269	-0.595171	-2.479101
C	-4.642359	-3.539033	-0.706332
H	-5.699010	-3.318050	-0.443539
H	-4.642908	-4.217985	-1.584852
H	-4.198154	-4.087209	0.148974
C	3.260924	-1.651539	3.221222
H	2.836326	-1.629422	4.247018
H	4.311586	-2.001458	3.313337
H	3.244996	-0.617393	2.828720
C	2.445964	-4.028223	2.887689
H	3.479072	-4.436858	2.865916
H	2.093905	-4.047483	3.940827
H	1.802919	-4.717088	2.303953
C	1.483285	-1.424317	-3.736003
H	2.406401	-1.630649	-4.318808
H	0.633878	-1.379625	-4.446134
H	1.581956	-0.425884	-3.267490
C	1.096591	-3.910362	-3.290381
H	0.308041	-3.928128	-4.071991
H	2.053866	-4.221378	-3.761881
H	0.837475	-4.670658	-2.523148
C	-2.266916	1.374119	-1.391967
C	-2.452645	1.905438	-0.098360
C	-3.070074	1.845287	-2.453330
C	-3.444215	2.871223	0.139172
C	-4.043258	2.829846	-2.221384
C	-4.238662	3.339618	-0.923504
H	-1.814001	1.532143	0.718999
H	-2.906632	1.427588	-3.459160
H	-3.595770	3.253305	1.160853
H	-4.656060	3.203975	-3.057302
H	-5.010299	4.104732	-0.741677
C	-1.229970	0.292938	-1.668000
O	-1.388093	-0.463325	-2.619236
H	3.228448	2.520300	-4.937558
C	3.606852	0.902317	-0.561968
H	4.646544	0.722786	-0.900999
H	3.633142	1.595614	0.303100
H	3.202759	-0.051325	-0.176799
Zero-point correction=			0.819107 (Hartree/Particle)
Thermal correction to Energy=			0.874499
Thermal correction to Enthalpy=			0.875444
Thermal correction to Gibbs Free Energy=			0.730305
Sum of electronic and zero-point Energies=			-2942.339627
Sum of electronic and thermal Energies=			-2942.284234
Sum of electronic and thermal Enthalpies=			-2942.283290
Sum of electronic and thermal Free Energies=			-2942.428429

H	-0.117322	1.977958	-2.366050
H	5.895731	0.118654	-0.084902
H	3.694597	-0.896234	3.499713
H	3.057889	2.208280	-1.482969
H	0.550561	0.687253	2.307213
C	1.104048	-0.663497	3.846515
H	1.828421	-0.803700	4.678045
H	0.091587	-0.575814	4.290007
H	1.103100	-1.577360	3.217469
C	1.433835	1.859668	3.881519
H	1.565924	2.774893	3.268663
H	0.479062	1.963225	4.438452
H	2.264573	1.818112	4.618565
C	4.615494	1.040729	-2.376654
H	4.626712	1.658981	-3.298028
H	5.654683	0.690591	-2.200564
H	3.970903	0.163614	-2.566839
C	4.956932	3.117266	-0.962696
H	5.993089	2.817726	-0.696167
H	5.006584	3.743218	-1.878438
H	4.575008	3.750198	-0.135731
C	-2.955855	2.181246	3.248234
H	-2.494525	2.308829	4.250567
H	-3.992685	2.574714	3.321334
H	-2.986778	1.098350	3.023331
C	-2.106131	4.454172	2.534524
H	-3.135131	4.872110	2.501516
H	-1.700144	4.625132	3.554087
H	-1.490186	5.036714	1.820774
C	-1.467289	1.258664	-3.836008
H	-2.354828	1.553937	-4.435663
H	-0.624116	1.093554	-4.536337
H	-1.686911	0.293651	-3.339272
C	-0.836472	3.703762	-3.442358
H	-0.065934	3.634573	-4.239019
H	-1.770236	4.098076	-3.898346
H	-0.489067	4.445779	-2.692341
C	2.190173	-1.644471	-1.219469
C	2.269997	-2.102502	0.112396
C	3.016596	-2.236211	-2.199820
C	3.170984	-3.119366	0.466003
C	3.903017	-3.266138	-1.851749
C	3.986030	-3.708467	-0.517365
H	1.623316	-1.628896	0.869140
H	2.934073	-1.881810	-3.238949
H	3.236694	-3.446350	1.515565
H	4.534522	-3.731512	-2.625633
H	4.687105	-4.513809	-0.245648
C	1.225166	-0.541062	-1.629711
O	1.419986	0.080123	-2.670407
H	-4.773179	-1.740334	-3.812904
C	-0.332227	-2.937030	-2.999612
H	0.255883	-3.348788	-2.162917
H	-0.525435	-3.751520	-3.727798
H	0.289381	-2.173730	-3.514195
Zero-point correction=			0.819134 (Hartree/Particle)
Thermal correction to Energy=			0.874441
Thermal correction to Enthalpy=			0.875385
Thermal correction to Gibbs Free Energy=			0.731225
Sum of electronic and zero-point Energies=			-2942.338783
Sum of electronic and thermal Energies=			-2942.283476
Sum of electronic and thermal Enthalpies=			-2942.282532
Sum of electronic and thermal Free Energies=			-2942.426691

Ph(oMe)+B-Ph(pMe)-IPr-X				Ph(oMeISOMER)+B-Ph(pMe)-IPR-X			
103				103			
IPrX-MeOrto SCF Done: -2943.18504001 A.U.				IPrX-MeOrto180 SCF Done: -2943.18422570 A.U.			
Pd	0.241411	0.379543	-0.429521	Pd	-0.234588	0.482352	0.375492
K	3.974756	2.168031	1.074474	K	-4.088034	1.092401	-1.623908
O	1.776426	3.778950	1.370740	O	-2.185205	3.235619	-1.665201
H	1.623364	4.420006	0.642456	H	-2.244690	3.882698	-0.930915
B	0.551219	3.213950	1.724677	B	-0.845084	2.955318	-1.922498
O	-0.597863	3.924205	1.496858	O	0.109243	3.892352	-1.628012
H	-1.389971	3.354644	1.521791	H	1.012750	3.516685	-1.636598
C	1.119835	2.083762	-1.278897	C	-1.521917	1.983916	1.055806
C	0.477089	3.341155	-1.396874	C	-1.368047	3.346120	1.459591
C	2.503005	2.040020	-1.657922	C	-2.842779	1.459931	1.103633
C	1.155724	4.521364	-1.766958	C	-2.513883	4.133845	1.739422
H	-0.590358	3.426116	-1.145915	C	-3.973763	2.228223	1.448129
C	3.180086	3.224120	-2.044327	H	-2.996594	0.391244	0.876336
C	2.525428	4.469962	-2.078579	C	-3.813998	3.596533	1.728037
H	0.607393	5.477109	-1.817184	H	-2.374880	5.196156	2.005645
H	4.241607	3.164389	-2.350227	H	-4.970117	1.753878	1.519471
C	1.707740	1.205848	2.280052	C	-1.525505	0.773580	-2.550438
O	2.558551	1.400718	3.166651	O	-2.252143	0.698701	-3.557859
O	0.517679	1.971623	2.326373	O	-0.512690	1.760143	-2.538222
O	1.813679	0.423687	1.279020	O	-1.636967	0.083625	-1.482280
N	0.423561	-2.616559	-0.097892	N	-0.377586	-2.493627	0.523163
N	-1.565054	-2.072055	0.536599	N	1.653076	-2.082710	-0.087711
C	-0.372286	-1.518340	0.134626	C	0.456675	-1.458734	0.156312
C	-0.260209	-3.812611	0.114873	C	0.290801	-3.716844	0.536072
C	-1.517359	-3.469156	0.528982	C	1.575026	-3.460663	0.138745
C	1.799545	-2.556589	-0.525207	C	-1.781314	-2.317401	0.809705
C	2.814451	-2.543956	0.467404	C	-2.715150	-2.574309	-0.228583
C	4.148937	-2.546620	0.014279	C	-4.079929	-2.376086	0.070335
C	4.449439	-2.579193	-1.357699	C	-4.486810	-1.947299	1.345245
C	3.420944	-2.582366	-2.309708	C	-3.537005	-1.707395	2.349686
C	2.067391	-2.550178	-1.914873	C	-2.158450	-1.878287	2.104141
C	2.472429	-2.566641	1.956584	C	-2.273618	-3.141355	-1.576709
H	5.500931	-2.595484	-1.687070	H	-5.558509	-1.805865	1.561087
C	0.944555	-2.530981	-2.948962	C	-1.126126	-1.639055	3.202971
C	-2.707303	-1.336645	1.015972	C	2.820123	-1.425539	-0.619504
C	-3.865645	-1.284556	0.201537	C	3.940409	-1.247426	0.227354
C	-4.991852	-0.612915	0.720453	C	5.080973	-0.633714	-0.331416
C	-4.953679	-0.016964	1.986019	C	5.095693	-0.228058	-1.670707
C	-3.780968	-0.059450	2.757652	C	3.964324	-0.409869	-2.482277
C	-2.623001	-0.715327	2.294000	C	2.790958	-1.000816	-1.976996
C	-3.914052	-1.930557	-1.182812	C	3.955390	-1.751858	1.670419
H	-5.842915	0.505537	2.373092	H	5.995061	0.251995	-2.087657
C	-1.323303	-0.721968	3.105001	C	1.530700	-1.152853	-2.833340
H	0.209672	-4.786012	-0.050823	H	-0.204128	-4.647378	0.826116
H	-2.369340	-4.077772	0.841987	H	2.431765	-4.122294	-0.014172
H	4.968543	-2.535337	0.748310	H	-4.836552	-2.586970	-0.702276
H	3.669394	-2.591178	-3.382370	H	-3.866841	-1.361418	3.340200
H	1.516759	-2.014401	2.071705	H	-1.210490	-2.857389	-1.721529
H	0.000991	-2.271332	-2.427942	H	-0.145037	-1.457532	2.720187
H	-5.906502	-0.544177	0.112813	H	5.969512	-0.471943	0.297616
H	-3.767584	0.435029	3.739175	H	3.990286	-0.062680	-3.525046
H	-2.865241	-2.074924	-1.517839	H	2.905834	-1.962408	1.964974
H	-0.514552	-0.461059	2.387949	H	0.673721	-0.869507	-2.184588
C	-1.288401	0.336116	4.218294	C	1.492755	-0.213917	-4.049141
H	-1.989841	0.092545	5.045625	H	2.238495	-0.500946	-4.821662
H	-0.267752	0.391512	4.647339	H	0.489506	-0.253565	-4.519597
H	-1.525775	1.346489	3.831662	H	1.667811	0.840339	-3.756941
C	-0.998961	-2.115746	3.689162	C	1.307561	-2.616271	-3.275847

H	-0.899343	-2.894534	2.908127	H	1.242982	-3.311265	-2.414950
H	-0.037670	-2.079597	4.243163	H	0.359635	-2.701192	-3.847456
H	-1.790738	-2.439303	4.398301	H	2.136396	-2.960655	-3.930687
C	-4.602597	-1.040089	-2.234367	C	4.498239	-0.716667	2.671404
H	-4.465050	-1.476902	-3.244447	H	4.458969	-1.131607	3.699988
H	-5.695944	-0.959063	-2.054552	H	5.555361	-0.448383	2.462469
H	-4.174179	-0.021104	-2.245997	H	3.885140	0.202334	2.657340
C	-4.609453	-3.309068	-1.122682	C	4.759420	-3.068499	1.761499
H	-5.665468	-3.198026	-0.795424	H	5.825977	-2.893383	1.504379
H	-4.611277	-3.789068	-2.123819	H	4.720380	-3.483554	2.790579
H	-4.114693	-4.003751	-0.415188	H	4.377529	-3.842703	1.065051
C	3.512185	-1.856362	2.837225	C	-3.053613	-2.596831	-2.784925
H	3.138722	-1.785645	3.879097	H	-2.658691	-3.048893	-3.718600
H	4.476881	-2.407074	2.871411	H	-4.132751	-2.860620	-2.739382
H	3.685107	-0.820503	2.491004	H	-2.939005	-1.500230	-2.882784
C	2.261887	-4.014628	2.454693	C	-2.364048	-4.685260	-1.541527
H	3.195767	-4.606163	2.343539	H	-3.421429	-5.009511	-1.434675
H	1.979605	-4.016061	3.528469	H	-1.963706	-5.123203	-2.479880
H	1.459540	-4.537627	1.899314	H	-1.798136	-5.119357	-0.693896
C	1.143416	-1.438338	-4.013537	C	-1.418006	-0.386381	4.045190
H	2.069289	-1.590513	-4.608859	H	-2.334720	-0.495946	4.663689
H	0.283379	-1.434507	-4.712154	H	-0.567773	-0.194221	4.729103
H	1.172337	-0.438677	-3.536351	H	-1.528120	0.502847	3.393222
C	0.775134	-3.928279	-3.581330	C	-0.995524	-2.905340	4.077376
H	-0.069241	-3.930200	-4.302205	H	-0.216172	-2.761633	4.854861
H	1.692429	-4.236052	-4.128168	H	-1.954108	-3.136940	4.590006
H	0.569325	-4.700121	-2.810139	H	-0.715257	-3.791764	3.469907
C	-2.276285	1.559132	-1.365820	C	2.320760	1.800014	0.844455
C	-2.602553	1.840405	-0.023486	C	2.374924	1.887511	-0.562689
C	-2.954907	2.242213	-2.397927	C	3.250472	2.531941	1.612433
C	-3.612335	2.764646	0.285817	C	3.349419	2.676802	-1.192841
C	-3.932335	3.202413	-2.088231	C	4.210067	3.342986	0.985026
C	-4.270297	3.459774	-0.746527	C	4.264807	3.416389	-0.418828
H	-2.064840	1.299309	0.771125	H	1.636611	1.317668	-1.151584
H	-2.698155	2.005008	-3.442051	H	3.189265	2.468041	2.710119
H	-3.896401	2.933382	1.337431	H	3.403598	2.703070	-2.293310
H	-4.441754	3.748730	-2.898373	H	4.920616	3.924286	1.594580
H	-5.050683	4.198987	-0.505048	H	5.023274	4.045898	-0.911015
C	-1.233526	0.514732	-1.730535	C	1.263225	0.960336	1.555267
O	-1.382343	-0.151761	-2.750937	O	1.431623	0.631960	2.725833
H	3.072219	5.378920	-2.377912	H	-4.680533	4.229873	1.977834
C	3.265499	0.728346	-1.688873	C	-0.002091	3.966416	1.629840
H	4.361964	0.871571	-1.814817	H	0.540182	3.468546	2.460731
H	3.076753	0.097573	-0.794636	H	0.611985	3.837969	0.720887
H	2.932894	0.110015	-2.545332	H	-0.061465	5.049282	1.860714
Zero-point correction=			0.820423 (Hartree/Particle)	Zero-point correction=			0.820620 (Hartree/Particle)
Thermal correction to Energy=			0.876380	Thermal correction to Energy=			0.876495
Thermal correction to Enthalpy=			0.877324	Thermal correction to Enthalpy=			0.877439
Thermal correction to Gibbs Free Energy=			0.731385	Thermal correction to Gibbs Free Energy=			0.732282
Sum of electronic and zero-point Energies=			-2942.364617	Sum of electronic and zero-point Energies=			-2942.363606
Sum of electronic and thermal Energies=			-2942.308660	Sum of electronic and thermal Energies=			-2942.307731
Sum of electronic and thermal Enthalpies=			-2942.307716	Sum of electronic and thermal Enthalpies=			-2942.306787
Sum of electronic and thermal Free Energies=			-2942.453655	Sum of electronic and thermal Free Energies=			-2942.451943

Ph(oMe)+B-Ph(pMe)-IPr-XI				**Ph(oMeISOMER)+B-Ph(pMe)-IPR-XI**			
93				93			
IPrXI-MeOrto SCF Done: -1902.90040782 A.U.				IPrXI-MeOrto180 SCF Done: -1902.89979882 A.U.			
Pd	0.435654	0.877505	-0.149808	Pd	0.593407	0.715791	-0.128405
C	0.837409	2.898754	-0.323337	C	1.675301	2.447163	-0.156040
C	-0.020616	3.950276	-0.728658	C	1.612005	3.680618	-0.862197
C	2.187742	3.243838	-0.015306	C	2.827594	2.179870	0.623973
C	0.414261	5.285889	-0.809999	C	2.686248	4.592910	-0.748762

H	-1.068129	3.734913	-0.993948	C	3.898579	3.089520	0.722052
C	2.620030	4.585675	-0.096110	H	2.918110	1.221197	1.170860
C	1.742703	5.610108	-0.487622	C	3.820454	4.310579	0.033683
H	-0.287348	6.073734	-1.131736	H	2.635042	5.549123	-1.298080
H	3.670170	4.827347	0.146735	H	4.781578	2.842456	1.334752
N	1.438614	-2.007002	-0.062729	N	1.060168	-2.218269	-0.100683
N	-0.715463	-2.083884	0.052310	N	-1.090807	-2.013564	-0.049855
C	0.332309	-1.192292	-0.005849	C	0.064496	-1.273734	-0.058445
C	1.099495	-3.359071	-0.049907	C	0.550493	-3.514430	-0.125119
C	-0.266465	-3.407415	0.023565	C	-0.814650	-3.385007	-0.094213
C	2.788723	-1.507972	-0.015521	C	2.443709	-1.821410	0.001054
C	3.373595	-1.305420	1.260336	C	2.994794	-1.676775	1.300588
C	4.692509	-0.811445	1.293113	C	4.321804	-1.211229	1.390523
C	5.385650	-0.530814	0.105920	C	5.052269	-0.889148	0.237117
C	4.770775	-0.724157	-1.140010	C	4.472825	-1.027635	-1.032185
C	3.453524	-1.217329	-1.231682	C	3.153585	-1.499773	-1.183105
C	2.581679	-1.529140	2.547494	C	2.170104	-1.926673	2.561844
H	6.413584	-0.137895	0.152872	H	6.081110	-0.507441	0.329559
C	2.745629	-1.338402	-2.577315	C	2.505897	-1.585808	-2.561900
C	-2.103288	-1.725598	0.227781	C	-2.413823	-1.459415	0.118541
C	-2.996412	-1.918781	-0.855760	C	-3.301009	-1.470353	-0.984548
C	-4.352425	-1.600189	-0.639797	C	-4.608066	-0.985836	-0.768367
C	-4.787577	-1.091237	0.589419	C	-4.994398	-0.485990	0.480764
C	-3.878471	-0.897694	1.639339	C	-4.080851	-0.450937	1.544931
C	-2.515340	-1.217020	1.491421	C	-2.770429	-0.941650	1.395758
C	-2.543010	-2.483613	-2.201697	C	-2.886333	-2.000091	-2.356115
H	-5.846261	-0.822744	0.728422	H	-6.013549	-0.094265	0.624109
C	-1.519759	-1.030763	2.638707	C	-1.775814	-0.936687	2.557152
H	1.856807	-4.147729	-0.085018	H	1.197169	-4.396364	-0.155483
H	-0.958685	-4.252176	0.072203	H	-1.610981	-4.134424	-0.084913
H	5.178494	-0.628203	2.263777	H	4.780778	-1.074486	2.382112
H	5.317421	-0.470618	-2.061277	H	5.048738	-0.743939	-1.926468
H	1.681169	-2.125393	2.293689	H	1.206217	-2.383164	2.256397
H	1.826085	-1.940779	-2.418857	H	1.516638	-2.074821	-2.437758
H	-5.074560	-1.733049	-1.459489	H	-5.326996	-0.984437	-1.601831
H	-4.238338	-0.476317	2.587917	H	-4.394054	-0.023780	2.507676
H	-1.438230	-2.381480	-2.253384	H	-1.776982	-2.053383	-2.369508
H	-0.620472	-0.553083	2.192695	H	-0.800202	-0.622915	2.127744
C	-2.014946	-0.098387	3.754686	C	-2.116622	0.070081	3.666002
H	-2.844891	-0.552558	4.337432	H	-3.013861	-0.235835	4.246057
H	-1.188644	0.104436	4.466930	H	-1.272175	0.135742	4.382608
H	-2.365553	0.872400	3.355188	H	-2.297127	1.082361	3.255014
C	-1.089335	-2.386002	3.244825	C	-1.600491	-2.349195	3.159175
H	-0.642441	-3.066437	2.494120	H	-1.280144	-3.094951	2.405237
H	-0.333508	-2.228247	4.042958	H	-0.832731	-2.333727	3.961371
H	-1.960681	-2.904748	3.698335	H	-2.553677	-2.704301	3.605839
C	-3.123549	-1.712081	-3.402707	C	-3.307671	-1.061267	-3.503476
H	-2.692822	-2.104008	-4.347655	H	-2.898844	-1.432623	-4.466303
H	-4.225771	-1.828430	-3.475120	H	-4.411976	-1.015040	-3.614797
H	-2.875565	-0.636069	-3.333589	H	-2.917245	-0.039132	-3.335966
C	-2.902445	-3.983282	-2.303394	C	-3.444805	-3.422428	-2.582072
H	-4.004283	-4.121070	-2.270862	H	-4.555667	-3.410379	-2.579044
H	-2.533028	-4.413215	-3.258115	H	-3.111322	-3.825634	-3.561389
H	-2.472627	-4.577910	-1.471974	H	-3.120506	-4.131334	-1.793067
C	2.083917	-0.182180	3.113701	C	1.835181	-0.592129	3.260431
H	1.450427	-0.345783	4.010578	H	1.192570	-0.765833	4.148948
H	2.935761	0.466872	3.406692	H	2.755570	-0.071441	3.599046
H	1.476037	0.372659	2.365169	H	1.293529	0.093418	2.573371
C	3.370332	-2.325584	3.603700	C	2.855594	-2.915584	3.524319
H	4.246384	-1.757129	3.981070	H	3.804493	-2.505092	3.929762
H	2.724221	-2.547923	4.478505	H	2.194510	-3.133607	4.389123
H	3.741221	-3.287881	3.194388	H	3.091677	-3.875104	3.019532
C	2.298224	0.058867	-3.060070	C	2.244131	-0.173163	-3.126755

H	3.174417	0.722427	-3.219402
H	1.734458	-0.015659	-4.012309
H	1.633329	0.545371	-2.308090
C	3.598697	-2.064801	-3.634236
H	3.010390	-2.214975	-4.563125
H	4.499188	-1.477454	-3.912856
H	3.939626	-3.058393	-3.275322
C	-2.448812	1.629841	-0.378604
C	-2.335887	2.146170	0.927864
C	-3.700165	1.662101	-1.032789
C	-3.455340	2.691998	1.571351
C	-4.821443	2.201191	-0.384975
C	-4.701534	2.718563	0.917866
H	-1.344466	2.124084	1.410698
H	-3.773163	1.253762	-2.051630
H	-3.355755	3.106726	2.587001
H	-5.795864	2.218110	-0.898748
C	-1.265687	1.059289	-1.122867
O	-1.342029	0.693188	-2.282998
H	2.097453	6.651860	-0.550025
C	3.171020	2.176906	0.424471
H	3.214229	2.079862	1.530321
H	2.897656	1.175186	0.021963
H	4.203360	2.381919	0.073060
H	-5.581013	3.148394	1.423847
Zero-point correction=			0.766624 (Hartree/Particle)
Thermal correction to Energy=			0.813105
Thermal correction to Enthalpy=			0.814049
Thermal correction to Gibbs Free Energy=			0.688359
Sum of electronic and zero-point Energies=			-1902.133784
Sum of electronic and thermal Energies=			-1902.087303
Sum of electronic and thermal Enthalpies=			-1902.086358
Sum of electronic and thermal Free Energies=			-1902.212049

H	3.193397	0.382864	-3.277639
H	1.716420	-0.234749	-4.100828
H	1.613076	0.416464	-2.423124
C	3.332966	-2.451202	-3.533207
H	2.802183	-2.556173	-4.502388
H	4.321550	-1.993387	-3.748927
H	3.513401	-3.467701	-3.125070
C	-2.056443	2.061911	-0.191131
C	-1.732851	2.636311	1.055195
C	-3.369095	2.185568	-0.696779
C	-2.712374	3.320214	1.790915
C	-4.350786	2.854034	0.048267
C	-4.025877	3.421931	1.293854
H	-0.694838	2.545978	1.417724
H	-3.602851	1.735988	-1.673004
H	-2.450255	3.778897	2.757541
H	-5.377759	2.931302	-0.343042
C	-1.036810	1.332481	-1.029072
O	-1.241503	1.056649	-2.200936
H	4.641406	5.043132	0.099591
C	0.434454	4.017429	-1.749684
H	0.289963	3.239939	-2.527787
H	-0.510876	4.055825	-1.168850
H	0.561797	4.996602	-2.254536
H	-4.796210	3.952992	1.875945
Zero-point correction=			0.766828 (Hartree/Particle)
Thermal correction to Energy=			0.813376
Thermal correction to Enthalpy=			0.814320
Thermal correction to Gibbs Free Energy=			0.687672
Sum of electronic and zero-point Energies=			-1902.132971
Sum of electronic and thermal Energies=			-1902.086423
Sum of electronic and thermal Enthalpies=			-1902.085479
Sum of electronic and thermal Free Energies=			-1902.212127

Ph(oMe)+B-Ph(pMe)-IPr-XI-XII			
93			
IPrXI-XII-MeOrto SCF Done: -1902.88990799 A.U.			
Pd	0.368952	0.708141	0.094487
C	0.361944	2.838277	-0.051185
C	0.116663	3.573059	1.150070
C	1.359338	3.290439	-0.949016
C	0.901307	4.724489	1.394443
C	2.148056	4.414627	-0.670365
H	1.476489	2.749172	-1.902034
C	1.907886	5.141918	0.508831
H	0.723244	5.300827	2.318240
H	2.931747	4.733167	-1.376481
H	2.501261	6.041690	0.739196
N	1.691464	-1.977955	0.157565
N	-0.443312	-2.307728	0.136376
C	0.493089	-1.302748	0.126242
C	1.512373	-3.360105	0.194033
C	0.157215	-3.570171	0.180646
C	2.948253	-1.285705	0.026319
C	3.578625	-0.787539	1.192222
C	4.781175	-0.073642	1.019517
C	5.319873	0.132051	-0.259633
C	4.659287	-0.357491	-1.396826
C	3.450980	-1.072712	-1.281713
C	2.930919	-0.926701	2.567798
H	6.259472	0.695855	-0.373032
C	2.668665	-1.502124	-2.521098

Ph(oMeISOMER)+B-Ph(pMe)-IPR-XI-XII			
93			
IPrXI-XII-MeOrto180 SCF Done: -1902.89551951 A.U.			
Pd	0.308528	0.700672	0.254037
C	0.383629	2.822773	0.194463
C	-0.336782	3.543414	1.178861
C	1.639691	3.337301	-0.265442
C	0.168894	4.727112	1.741320
H	-1.320257	3.174956	1.505656
C	2.121490	4.534162	0.304399
C	1.404218	5.225088	1.297591
H	-0.406133	5.260860	2.515044
H	3.090735	4.932919	-0.040253
H	1.811062	6.159173	1.718021
N	1.559453	-2.029994	0.217806
N	-0.587004	-2.283731	0.258654
C	0.384286	-1.312805	0.220501
C	1.330749	-3.405016	0.266001
C	-0.030993	-3.566639	0.291682
C	2.833932	-1.389056	0.012436
C	3.523072	-0.857425	1.129220
C	4.735745	-0.183855	0.879488
C	5.234208	-0.055616	-0.425591
C	4.523354	-0.586941	-1.512131
C	3.300704	-1.260968	-1.319957
C	2.936608	-0.931113	2.536404
H	6.181562	0.478743	-0.599641
C	2.475051	-1.738154	-2.512788

C	-1.866688	-2.089095	0.065691	C	-2.001914	-2.010822	0.190237
C	-2.440816	-1.731797	-1.182815	C	-2.564560	-1.654261	-1.064318
C	-3.841234	-1.576490	-1.216235	C	-3.957890	-1.449428	-1.101978
C	-4.621683	-1.773414	-0.068747	C	-4.744136	-1.594772	0.049689
C	-4.020450	-2.096880	1.156168	C	-4.153043	-1.912041	1.281006
C	-2.622890	-2.246845	1.254468	C	-2.761761	-2.114678	1.381419
C	-1.576011	-1.515205	-2.426184	C	-1.690612	-1.487773	-2.308440
H	-5.713771	-1.643013	-0.123838	H	-5.831094	-1.427311	-0.008017
C	-1.928359	-2.472230	2.599003	C	-2.074608	-2.336497	2.729221
H	2.356133	-4.056246	0.214682	H	2.148836	-4.131489	0.264959
H	-0.434463	-4.490750	0.189858	H	-0.654180	-4.465681	0.322724
H	5.296885	0.339888	1.899988	H	5.293719	0.256523	1.720383
H	5.078929	-0.163098	-2.396274	H	4.911576	-0.454419	-2.533848
H	2.134277	-1.696862	2.486168	H	2.108449	-1.671183	2.513087
H	1.853020	-2.179803	-2.193437	H	1.653664	-2.378123	-2.129350
H	-4.330545	-1.279403	-2.154115	H	-4.436252	-1.152860	-2.045798
H	-4.646426	-2.214750	2.053022	H	-4.781177	-1.987511	2.180956
H	-0.684646	-0.942241	-2.092199	H	-0.773642	-0.957875	-1.973613
H	-1.030162	-3.100419	2.413710	H	-1.185632	-2.980151	2.552937
C	-1.425701	-1.124039	3.166190	C	-1.555690	-0.986883	3.277490
H	-2.281580	-0.447225	3.374290	H	-2.403044	-0.292708	3.461866
H	-0.869732	-1.277508	4.115088	H	-1.012588	-1.131268	4.235203
H	-0.751550	-0.607635	2.450022	H	-0.866691	-0.493525	2.558314
C	-2.796002	-3.214960	3.628610	C	-2.956432	-3.054230	3.764688
H	-3.204027	-4.161875	3.218088	H	-3.378166	-3.999094	3.363204
H	-2.195943	-3.459386	4.529431	H	-2.362504	-3.298198	4.669700
H	-3.651970	-2.595463	3.971164	H	-3.803518	-2.418017	4.098523
C	-2.258659	-0.666715	-3.508879	C	-2.326339	-0.612941	-3.398508
H	-1.523854	-0.418823	-4.301070	H	-1.573794	-0.394043	-4.182575
H	-3.102612	-1.205803	-3.991620	H	-3.185773	-1.117360	-3.891231
H	-2.628233	0.292475	-3.096941	H	-2.669856	0.357176	-2.990399
C	-1.082119	-2.853783	-3.018378	C	-1.263421	-2.852599	-2.892761
H	-1.937380	-3.469206	-3.370986	H	-2.148993	-3.426053	-3.240906
H	-0.416187	-2.663895	-3.886484	H	-0.589655	-2.701808	-3.762256
H	-0.508639	-3.454837	-2.284776	H	-0.720537	-3.477093	-2.155574
C	2.243515	0.398491	2.961013	C	2.321923	0.428797	2.926343
H	1.708410	0.298322	3.928402	H	1.842429	0.379712	3.925968
H	2.980246	1.224139	3.047945	H	3.089058	1.230741	2.939288
H	1.495093	0.703761	2.186152	H	1.537637	0.742218	2.189345
C	3.920358	-1.396065	3.650780	C	3.959544	-1.411849	3.582942
H	4.706147	-0.636521	3.847582	H	4.782046	-0.678834	3.721986
H	3.389334	-1.570280	4.609827	H	3.469319	-1.541778	4.570295
H	4.426896	-2.339204	3.358616	H	4.415380	-2.380912	3.292116
C	1.996662	-0.272645	-3.170491	C	1.814511	-0.531402	-3.211856
H	2.757881	0.440061	-3.553683	H	2.580832	0.155043	-3.630243
H	1.354504	-0.580304	-4.022259	H	1.165960	-0.869906	-4.047037
H	1.357420	0.269636	-2.441792	H	1.189387	0.054068	-2.508173
C	3.533124	-2.282187	-3.528970	C	3.296066	-2.593009	-3.496414
H	2.908081	-2.643354	-4.372254	H	2.639719	-2.991612	-4.298046
H	4.332646	-1.646129	-3.964175	H	4.093262	-1.999792	-3.992339
H	4.019240	-3.161569	-3.057417	H	3.780570	-3.451859	-2.986876
C	-2.354093	1.901310	-0.636192	C	-2.210374	2.009676	-0.740637
C	-2.832249	1.259617	0.521562	C	-2.765125	1.451296	0.428133
C	-3.263353	2.602984	-1.460072	C	-3.056332	2.666195	-1.660496
C	-4.190265	1.329102	0.865815	C	-4.138767	1.561221	0.687603
C	-4.619620	2.684607	-1.109698	C	-4.431942	2.774653	-1.403043
C	-5.086915	2.048961	0.056854	C	-4.976263	2.226164	-0.226017
H	-2.122241	0.684578	1.134658	H	-2.092573	0.901838	1.109618
H	-2.880659	3.078061	-2.376620	H	-2.610281	3.081012	-2.577748
H	-4.550054	0.805547	1.765021	H	-4.558039	1.106735	1.598332
H	-5.319195	3.245695	-1.750179	H	-5.085983	3.291914	-2.123599
H	-6.152570	2.110666	0.330616	H	-6.056382	2.311947	-0.025042
C	-0.914046	1.810049	-1.093087	C	-0.736168	1.877906	-1.082269

O	-0.666534	1.848483	-2.302828
C	-0.905960	3.163593	2.187046
H	-1.940456	3.297057	1.808732
H	-0.800860	2.093141	2.455774
H	-0.799347	3.765538	3.111602

Zero-point correction=	0.765891 (Hartree/Particle)
Thermal correction to Energy=	0.811819
Thermal correction to Enthalpy=	0.812763
Thermal correction to Gibbs Free Energy=	0.687337
Sum of electronic and zero-point Energies=	-1902.124017
Sum of electronic and thermal Energies=	-1902.078089
Sum of electronic and thermal Enthalpies=	-1902.077145
Sum of electronic and thermal Free Energies=	-1902.202571

O	-0.373801	1.951846	-2.260023
C	2.462764	2.619635	-1.309009
H	3.348656	3.214617	-1.608960
H	2.819641	1.637409	-0.932494
H	1.840516	2.405536	-2.201142

Zero-point correction=	0.766492 (Hartree/Particle)
Thermal correction to Energy=	0.812077
Thermal correction to Enthalpy=	0.813021
Thermal correction to Gibbs Free Energy=	0.690038
Sum of electronic and zero-point Energies=	-1902.129028
Sum of electronic and thermal Energies=	-1902.083442
Sum of electronic and thermal Enthalpies=	-1902.082498
Sum of electronic and thermal Free Energies=	-1902.205482

Ph(oMe)+B-Ph(pMe)-IPr-XII			
93			
IPrXII-MeOrto SCF Done: -1902.92116053 A.U.			
Pd	0.212459	-0.676832	-0.269252
C	-0.015161	-2.832531	-0.598080
C	-0.290711	-3.162189	-1.983305
C	1.357294	-2.587593	-0.201535
C	0.785315	-3.197217	-2.882288
C	2.408493	-2.630965	-1.156734
H	1.606136	-2.602456	0.870647
C	2.117981	-2.923743	-2.487412
H	0.584386	-3.476397	-3.929967
H	3.438853	-2.435212	-0.823499
H	2.924430	-2.964633	-3.237026
N	1.765701	1.722210	0.699531
N	-0.239963	2.354707	0.213169
C	0.568750	1.242280	0.216105
C	1.704896	3.084309	0.991955
C	0.431871	3.488662	0.679367
C	2.900287	0.855570	0.886565
C	3.847622	0.749301	-0.161454
C	4.905422	-0.163636	0.016218
C	4.999766	-0.940623	1.182126
C	4.040878	-0.815610	2.198349
C	2.968590	0.091573	2.076602
C	3.666070	1.517363	-1.469169
H	5.828682	-1.657203	1.296604
C	1.929800	0.225985	3.188498
C	-1.615974	2.343541	-0.208652
C	-2.623592	2.268262	0.787933
C	-3.962009	2.350744	0.358379
C	-4.276853	2.473809	-1.004243
C	-3.260416	2.477922	-1.969788
C	-1.901796	2.415585	-1.593661
C	-2.266442	1.997132	2.248095
H	-5.330991	2.539156	-1.318046
C	-0.800768	2.373890	-2.651355
H	2.563452	3.633658	1.389917
H	-0.056598	4.465726	0.743483
H	5.657167	-0.282722	-0.778791
H	4.122583	-1.436748	3.104202
H	3.018448	2.394104	-1.252633
H	1.184082	0.980917	2.863367
H	-4.773800	2.296987	1.098393
H	-3.523332	2.537007	-3.037518
H	-1.260014	2.430548	2.435549
H	0.171880	2.508780	-2.133036
C	-0.763171	0.983335	-3.320632

Ph(oMeISOMER)+B-Ph(pMe)-IPR-XII			
93			
IPrXII-MeOrto180 SCF Done: -1902.92174621 A.U.			
Pd	0.301872	-0.312570	-0.779839
C	-0.357180	-1.784621	-2.289179
C	-1.110163	-1.168397	-3.351043
C	1.097872	-1.694298	-2.316947
C	-0.493377	-0.450206	-4.369733
H	-2.200175	-1.312120	-3.371664
C	1.673078	-0.877288	-3.350137
C	0.912184	-0.274827	-4.348704
H	-1.097717	-0.011160	-5.178659
H	2.769697	-0.772573	-3.360723
H	1.407133	0.325836	-5.128278
N	1.698705	0.929141	1.602108
N	-0.242047	1.849007	1.381753
C	0.561997	0.879120	0.826963
C	1.609795	1.898834	2.601190
C	0.378042	2.485264	2.459871
C	2.823347	0.060559	1.364233
C	3.864736	0.525587	0.522734
C	4.919848	-0.366993	0.249687
C	4.929588	-1.660418	0.796514
C	3.886855	-2.086225	1.631785
C	2.807983	-1.232731	1.939530
C	3.802344	1.909293	-0.122621
H	5.759279	-2.346588	0.563508
C	1.652612	-1.715007	2.814134
C	-1.572989	2.136787	0.914887
C	-2.668847	1.638976	1.669763
C	-3.961583	1.960942	1.215556
C	-4.150704	2.712603	0.044504
C	-3.048850	3.157367	-0.697815
C	-1.729474	2.891510	-0.272866
C	-2.442682	0.725455	2.875328
H	-5.172076	2.944804	-0.297558
C	-0.542157	3.396885	-1.090469
H	2.423980	2.080441	3.309225
H	-0.111333	3.289916	3.017281
H	5.742033	-0.048519	-0.409237
H	3.902119	-3.106682	2.045354
H	3.100292	2.526190	0.478075
H	1.003247	-0.839954	3.028589
H	-4.837683	1.596937	1.771431
H	-3.211429	3.734054	-1.621810
H	-1.511620	1.063886	3.379726
H	0.384067	3.168605	-0.522956
C	-0.441651	2.638820	-2.429491

H	-1.730736	0.747191	-3.812502
H	0.038050	0.936638	-4.087044
H	-0.549118	0.194209	-2.561437
C	-0.934051	3.504621	-3.689329
H	-0.973079	4.501602	-3.203336
H	-0.068366	3.492077	-4.384047
H	-1.850110	3.393212	-4.307289
C	-2.158298	0.471220	2.475731
H	-1.863015	0.251341	3.522706
H	-3.127902	-0.029289	2.270680
H	-1.402276	0.012516	1.802099
C	-3.238421	2.643756	3.249865
H	-4.240821	2.166668	3.216920
H	-2.858358	2.518215	4.284660
H	-3.369549	3.729308	3.058325
C	2.915331	0.642324	-2.497083
H	2.685036	1.223884	-3.414704
H	3.527474	-0.237312	-2.786270
H	1.964299	0.252787	-2.071344
C	4.987436	2.057327	-2.044847
H	5.656426	1.237632	-2.383062
H	4.787679	2.695671	-2.930594
H	5.543575	2.663087	-1.299413
C	1.161266	-1.089360	3.414624
H	1.838165	-1.919094	3.707891
H	0.410156	-0.967595	4.222471
H	0.621014	-1.397559	2.497242
C	2.578969	0.745794	4.488096
H	1.808105	0.908681	5.270480
H	3.315958	0.019856	4.892593
H	3.110556	1.706040	4.321341
C	-2.416889	-2.480095	0.433111
C	-2.804904	-1.449076	-0.452348
C	-3.372522	-3.001937	1.332968
C	-4.121105	-0.965907	-0.452658
C	-4.691151	-2.522741	1.331419
C	-5.069560	-1.504310	0.435542
H	-2.047849	-0.983196	-1.112189
H	-3.046902	-3.779496	2.040905
H	-4.396801	-0.152073	-1.138009
H	-5.428443	-2.940947	2.035358
H	-6.103453	-1.122828	0.435884
C	-0.993854	-2.974229	0.552354
O	-0.616071	-3.471786	1.621913
C	-1.667289	-3.550969	-2.474609
H	-2.230527	-4.137030	-1.721219
H	-2.292698	-2.662157	-2.703168
H	-1.593162	-4.152850	-3.402511

Zero-point correction= 0.767295 (Hartree/Particle)	
Thermal correction to Energy= 0.813611	
Thermal correction to Enthalpy= 0.814555	
Thermal correction to Gibbs Free Energy= 0.688034	
Sum of electronic and zero-point Energies= -1902.153866	
Sum of electronic and thermal Energies= -1902.107549	
Sum of electronic and thermal Enthalpies= -1902.106605	
Sum of electronic and thermal Free Energies= -1902.233127	

H	-1.352245	2.780191	-3.048873
H	0.434883	2.985825	-3.014782
H	-0.312930	1.546090	-2.239013
C	-0.593484	4.924126	-1.295156
H	-0.665269	5.463635	-0.327736
H	0.321639	5.272664	-1.818409
H	-1.462523	5.228158	-1.916332
C	-2.204169	-0.729664	2.410286
H	-1.914499	-1.367821	3.271010
H	-3.123116	-1.153741	1.956716
H	-1.403353	-0.792057	1.646041
C	-3.570784	0.788622	3.918656
H	-4.510460	0.338589	3.533904
H	-3.285729	0.209745	4.821299
H	-3.791482	1.830535	4.231528
C	3.210219	1.808202	-1.544158
H	3.071214	2.816168	-1.988854
H	3.883455	1.225792	-2.208430
H	2.225641	1.288531	-1.529301
C	5.160249	2.634904	-0.123406
H	5.896464	2.132630	-0.786096
H	5.041444	3.671990	-0.500790
H	5.599566	2.684395	0.894598
C	0.788813	-2.739810	2.054071
H	1.375013	-3.640802	1.777103
H	-0.072679	-3.068438	2.670669
H	0.390012	-2.292041	1.120161
C	2.142213	-2.266047	4.167747
H	1.277016	-2.526183	4.812835
H	2.745129	-3.190012	4.041268
H	2.767904	-1.525841	4.708849
C	-2.468224	-2.353857	-0.846129
C	-3.074418	-1.077690	-0.938185
C	-3.209845	-3.414368	-0.274657
C	-4.402464	-0.890824	-0.523156
C	-4.527442	-3.220236	0.163298
C	-5.134837	-1.957873	0.026436
H	-2.493383	-0.212396	-1.294373
H	-2.717022	-4.394801	-0.187448
H	-4.855329	0.106862	-0.610493
H	-5.088563	-4.059211	0.605355
H	-6.174381	-1.803026	0.357705
C	-1.058253	-2.688650	-1.301724
O	-0.529946	-3.736835	-0.906869
C	2.053454	-2.603923	-1.562301
H	2.999706	-2.064386	-1.351634
H	1.642099	-2.984670	-0.615121
H	2.288896	-3.493001	-2.188913

Zero-point correction= 0.767744 (Hartree/Particle)	
Thermal correction to Energy= 0.813932	
Thermal correction to Enthalpy= 0.814877	
Thermal correction to Gibbs Free Energy= 0.689411	
Sum of electronic and zero-point Energies= -1902.154003	
Sum of electronic and thermal Energies= -1902.107814	
Sum of electronic and thermal Enthalpies= -1902.106870	
Sum of electronic and thermal Free Energies= -1902.232336	