

Electronic Effects in Iridium C–H Borylations: Insights from Unencumbered Substrates and Variation of

Boryl Ligand Substituents

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General Methods:

All commercially available chemicals were used as received unless otherwise indicated. Pinacolborane (HBpin containing 1% NEt₃) was generously supplied by BASF. (η^5 -Indenyl)(cyclooctadiene)iridium(I) {(Ind)Ir(COD)}, bis-(di-*iso*-propylphosphino)-ethane (dippe), (dippe)Ir(Bpin)₃ (**2**), (η^6 -MesH)Ir(Bcat)₃ and (dtbpy)Ir(Bpin)₃(coe) (**5**) were prepared per the literature procedures.¹⁻⁵ Solvents were refluxed over sodium benzophenone, distilled, and degassed. All the experiments were carried out in a glove box under a nitrogen atmosphere or by using standard Schlenk techniques.

¹H and ¹³C NMR spectra were recorded on a Varian Inova-300 (300.11 and 75.47 MHz respectively), Varian VXR-500 or Varian Unity-500-Plus spectrometer (499.74 and 125.67 MHz respectively) and referenced to residual solvent signals. ¹¹B spectra were recorded on Varian VXR-500 or Varian Inova-300 operating at 160.41 and 96.29 MHz respectively, and were referenced to neat BF₃·Et₂O as the external standard. ³¹P spectra were recorded on Varian Unity-500-Plus or Varian Inova-300 operating at 202.29 and 121.36 MHz respectively, and were referenced to neat 85% H₃PO₄ as the external standard. All coupling constants are apparent *J* values measured at the indicated field strengths. Elemental analyses were performed at Michigan State University using a Perkin Elmer Series II 2400 CHNS/O Analyzer. Melting points were measured on a MEL-TEMP[®] capillary melting apparatus and are uncorrected.

Synthesis of (dippe)Ir(Bcat[†])₃ (**7**)

A THF solution of 1,2'-bis(diisopropylphosphino)ethane (dippe) (39 mg, 0.15 mmol, 1 equiv) was added to (η^6 MesH)Ir(Bcat[†])₃ (150 mg, 0.15 mmol, 1 equiv) in a 20 mL vial equipped with a magnetic stirring bar. The reaction was stirred at room temperature for 2 h, when the crude reaction mixture was pumped down under high vacuum to give the desired complex as a yellow solid (yield 172 mg, 97%, mp 136-138 °C (dec)). ¹H NMR (C₆D₆, 500 MHz): δ 7.25 (d, *J* = 1.8 Hz, 6 H), 7.08 (d, *J* = 1.8 Hz, 6 H), 2.42 (h, *J* = 7.4 Hz, 4H), 1.49 (s, 27 H), 1.29 (s, 27 H), 1.00-0.87 (m, 24 H); ¹³C NMR {¹H} (C₇D₈, 125 MHz): δ 151.1 (s), 146.7 (s), 143.1 (s), 133.1 (s), 114.3 (s), 106.8 (s), 34.9 (s), 34.4 (s), 32.1 (s), 30.1 (s), 27.0-26.7 (m), 24.1 (t, *J* = 18 H), 19.0 (s),

18.6 (s); ^{11}B NMR (C_6D_6 , 160 MHz): δ 40.8; ^{31}P NMR (C_6D_6 , 202 MHz): δ 84.3.

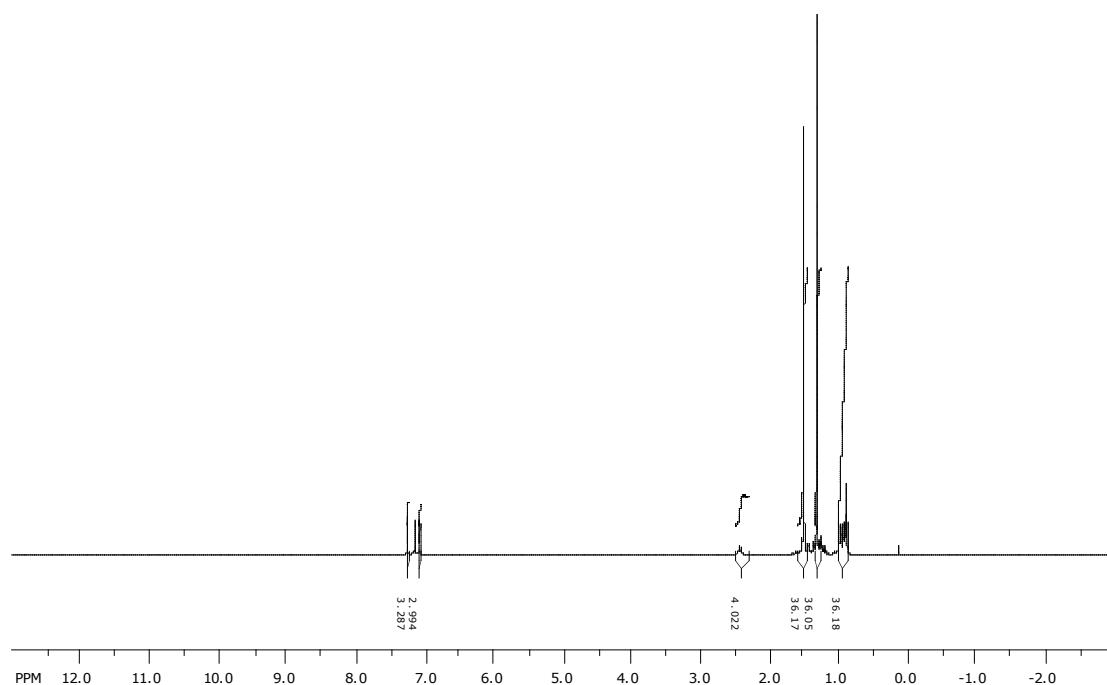


Figure S1. ^1H NMR spectrum of **7**.

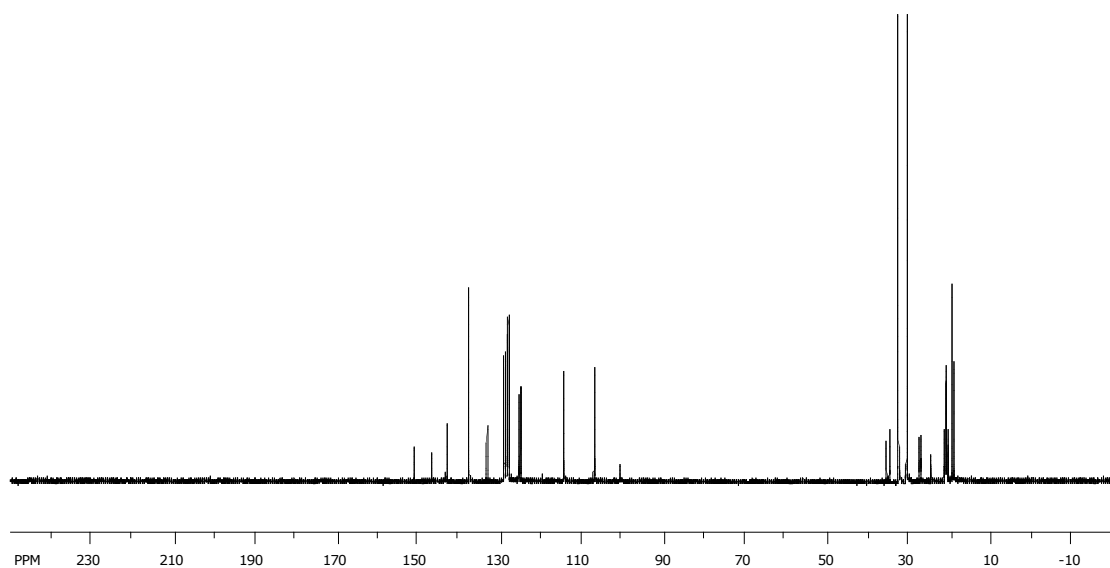


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **7**.

*Synthesis of (dippe)Ir(Bcat)₃ (**8**).*

A THF solution of 1,2'-bis(diisopropylphosphino)ethane (dippe) (50 mg, 0.19 mmol, 1 equiv) was added to (η^6 MesH)Ir(Bcat)₃ (125 mg, 0.19 mmol, 1 equiv) in a 20 mL vial equipped with a magnetic stirring bar. The reaction was stirred at room temperature for 3 h, when the crude reaction mixture was pumped down under high vacuum to give the desired complex as a yellow solid (yield 33 mg, 22%, mp 136-138 °C (dec)). ^1H NMR (C_6D_6 , 500 MHz): δ 7.05 (dd, $J = 5.7$ Hz, 3.2 Hz, 6H), 6.72 (dd, $J = 5.7$ Hz, 3.2 Hz, 6H), 2.30-2.20 (m, 4 H), 0.94-0.80 (m, 24 H); ^{13}C NMR $\{^1\text{H}\}$ (C_6D_6 , 125 MHz): δ 151.11 (s), 121.03 (s), 111.45 (s), 26.86-26.30 (m), 18.90 (s) 18.60 (s); ^{11}B NMR (C_6D_6 , 160 MHz): δ 42.4; ^{31}P NMR (C_6D_6 , 202 MHz): δ 83.0;

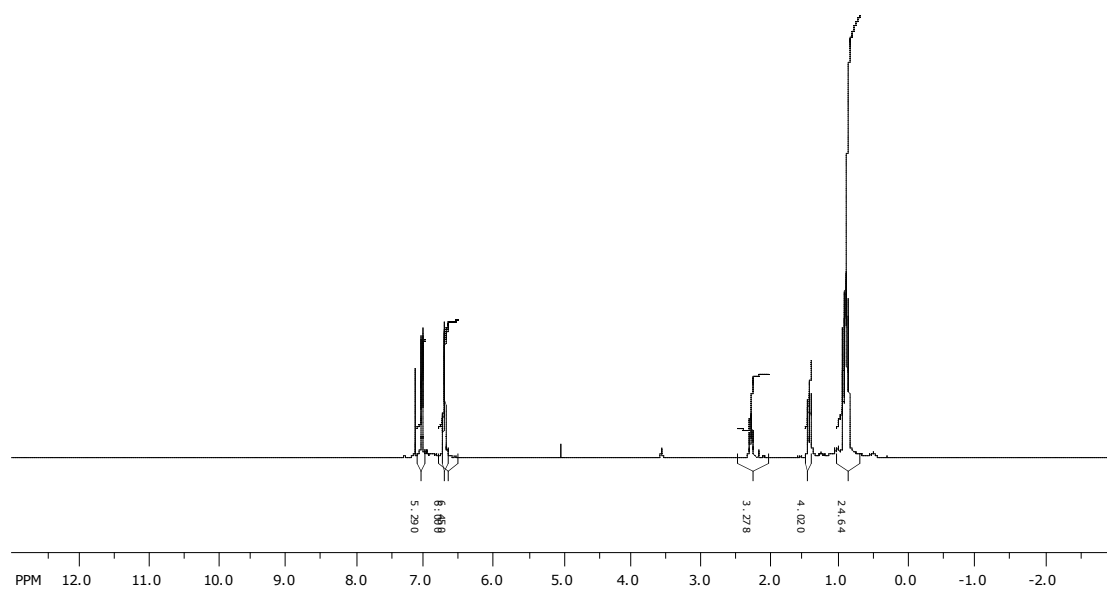


Figure S3. ^1H NMR Spectrum of **8**.

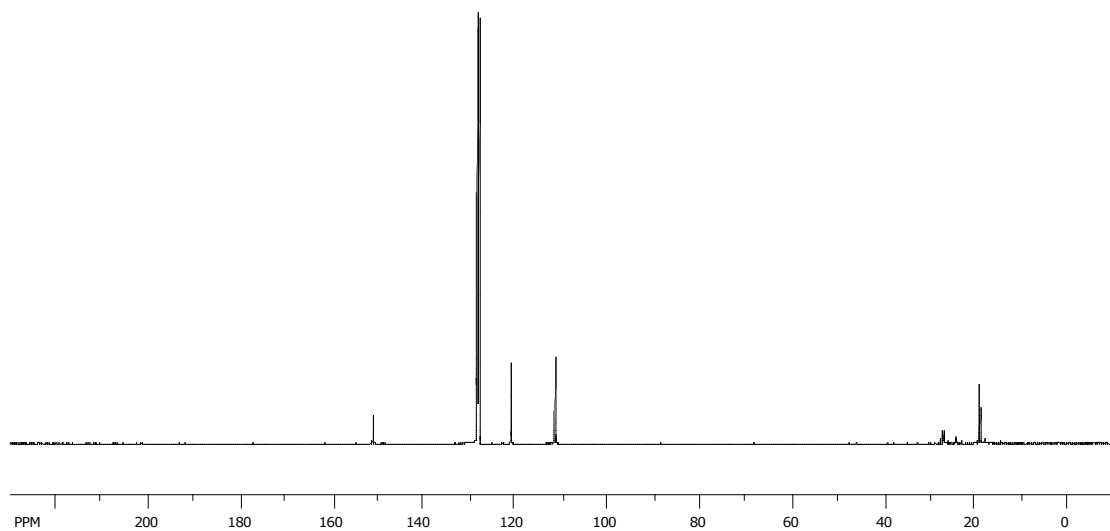
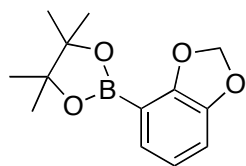


Figure S4: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **8**.

Borylation of anisole with catalysts generated in situ from (Ind)Ir(COD) and dmpe.

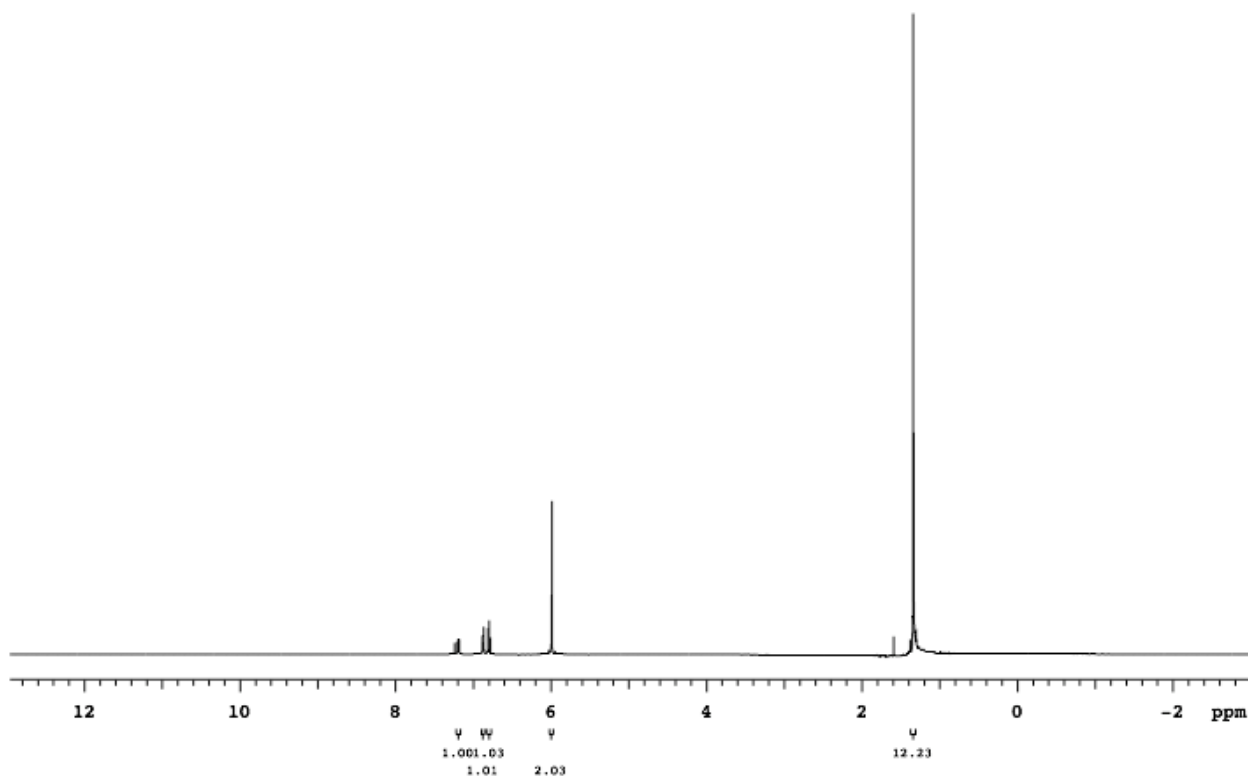
In a glove box, two separate test tubes were charged with (Ind)Ir(COD) (2.8 mg, 0.0066 mmol, 2 mol % Ir) and dmpe (1 mg, 0.0066 mmol, 2 mol %). HBpin (48 μ L, 43mg, 0.336mmol, 1.0 equiv) was added to the dmpe test tube. The dmpe and HBpin mixture was added to the (Ind)Ir(COD) test tube. After mixing for one minute, the resulting solution was transferred to a J-Young NMR tube. The two test tubes were washed three times with 166 μ L each of anisole, a total of 500 μ L of the substrate, and the washings were transferred to a J-Young NMR tube. The NMR tube was sealed, brought out of the glove box, and heated at 150 °C in a constant temperature oil bath. The reaction was monitored by ^{11}B -NMR and judged to be complete after 3 h. At this time, GC-FID samples of the reaction mixture were run in triplicate yielding the distribution of meta (76%), para (19%), and ortho (5%) isomers. After removing the excess anisole in vacuo, the isomer distribution in the crude reaction was confirmed by NMR (^1H , gCOSY).

Synthesis of 2-(benzo[d][1,3]dioxol-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane.

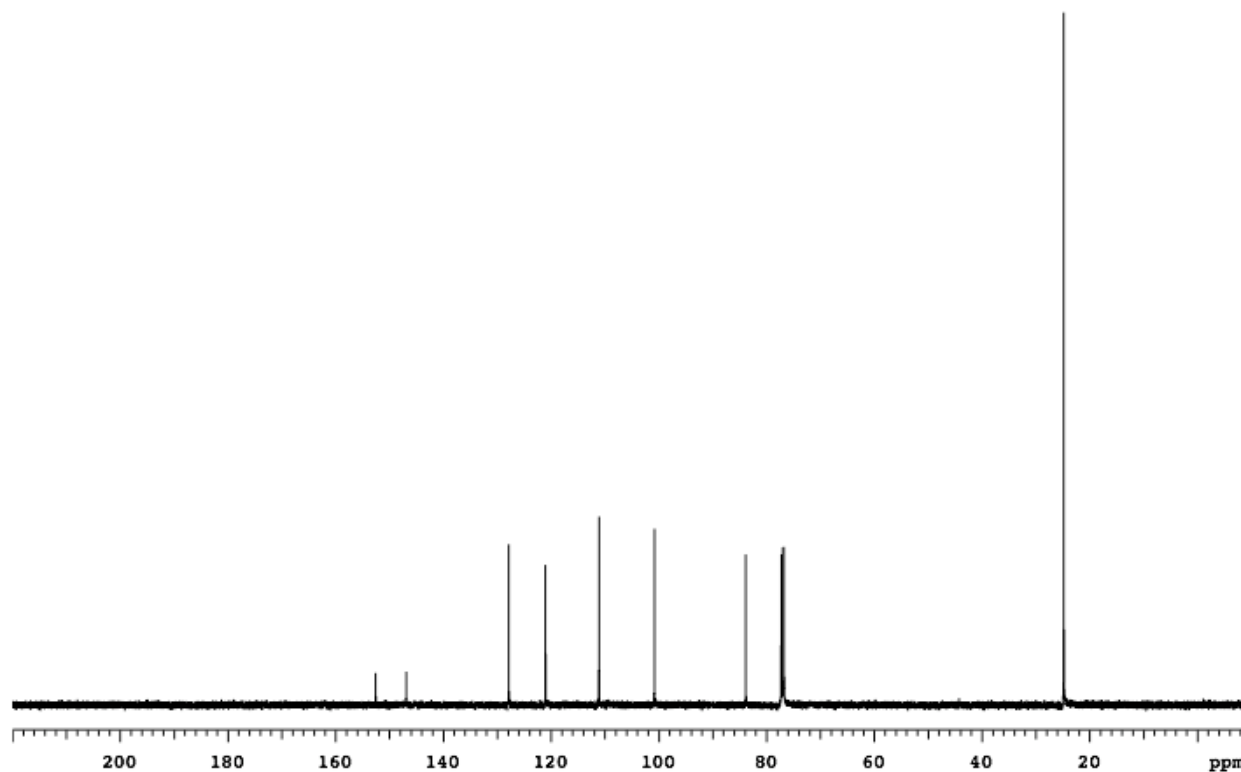


In a glovebox, an air free flask fitted with a stir bar, 127 mg (0.5 mmol) B_2Pin_2 and 573 μL (5.0 mmol) 1,3-benzodioxole. A solution of 6.6 mg (0.01 mmol) $[\text{Ir}(\text{OMe})\text{COD}]_2$, 3.3mg (0.02 mmol) 2,2'-bisoxazoline in 2.0 mL cyclohexane was then added to the air free flask and stirred at 70 °C under N_2 . After 24 hours the solution was transferred to a 20 mL scintillation vial, the air free flask rinsed with methanol and all volatiles removed in vacuo. The obtained liquid was passed through a short pad of silica-gel with dichloromethane as the eluent. Vacuum transfer (0.01 mmHg, 40 °C) into a -78 °C cold bath yielded 315 mg 1,3-benzodioxole (52% recovery). The contaminating *meta*-borylated isomer was removed via sublimation (0.01 mmHg, 50 °C) providing 63 mg of the product (25% yield, mp = 88 °C) as a white solid. ^1H NMR (500 MHz, CDCl_3 = 7.24 ppm): δ 7.189 (dd, 3J = 7.8 Hz, 4J = 1.5 Hz, 1H), 6.872 (dd, 3J = 7.6 Hz, 4J = 1.2 Hz, 1H), 6.796 (t, 3J = 7.8 Hz, 1H), 5.988 (s, 2H), 1.340 (s, 12H); ^{13}C NMR (126 MHz, CDCl_3 = 77 ppm): δ 152.537, 146.89, 127.83, 121.03, 111.11, 100.79, 83.84, 24.80; ^{11}B NMR

(96 MHz, $\text{BF}_3 \cdot \text{OEt}_2$ = 0 ppm) δ 30.3; FT-IR(thin film): 3076, 2998, 2975, 2926, 1638, 1492, 1441, 1407, 1390, 1370, 1351, 1320, 1268, 1248, 1199, 1164, 1142, 1128, 1058, 1028, 1002, 973, 944, 921, 852, 839, 778, 739, 690, 672, 484, 452 cm^{-1} ; HRMS calcd. for $\text{C}_{13}\text{H}_{17}\text{BO}_4$ $[\text{M}]^+$ 248.1220, found 248.1223.



^1H NMR of 2-(benzo[*d*][1,3]dioxol-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (CDCl_3).



^{13}C NMR of 2-(benzo[*d*][1,3]dioxol-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (CDCl_3).

Stoichiometric borylation of veratrole (3) with 2 (Table 1, entry 1)

2 (20 mg, 0.024 mmol, 1 equiv) was weighed into a small vial. Veratrole (24.5 μL , 0.19 mmol, 8 equiv) was added to the vial *via* microliter syringe. Cyclohexane (2.4 mL) was added to the vial and the solution was divided four J. Young NMR tubes (600 μL per tube). The tubes were heated in an oil bath at 100 $^\circ\text{C}$ and monitored by GC. After 15 min, 0.20 equiv of veratrole were converted to the 4- and 3-substituted boronic esters in a ratio greater than 99:1.

Borylation of veratrole (3) with catalysts generated in situ from (Ind)Ir(COD) and dippe (Table 1, entry 2).

(Ind)Ir(COD) (2.0 mg, 0.005 mmol, 0.02 equiv) was weighed in a test tube and was transferred to a J. Young NMR tube using C_6H_{12} (100 $\mu\text{L} \times 4$). A standard solution of dippe (13.2 mg, 0.05 mmol, 0.2 equiv) in C_6H_{12} (500 μL) was prepared in a small vial. A 50 μL portion of this solution was then transferred to the J. Young NMR tube (0.02 equiv dippe). Veratrole (255 μL , 2.0 mmol, 8 equiv) and HBpin (36 μL , 0.25 mmol, 1

equiv) were syringed into the J. Young NMR tube, which was then capped and heated in an oil bath at 130 °C. After 4 h, GC analysis showed that 0.26 equiv. of veratrole were converted to the 4- and 3-substituted boronic esters in a 98:2 ratio.

Stoichiometric borylation of veratrole (3) with (dtbpy)Ir(Bpin)₃COE (5) (Table 1, entry 3).

Compound **5** (dtbpy)Ir(Bpin)₃COE (30 mg, 0.0315 mmol, 1 equiv) was weighed in a test tube and was dissolved in C₆D₁₂ (300 µL). Veratrole (34.8 mg, 0.252 mmol, 8 equiv) was weighed in a test tube and mixed with the solution containing **5**. The mixture was then transferred via pipette into a J. Young NMR tube. The J. Young NMR tube was capped and the reaction was monitored by ¹H NMR. The reaction was quenched at 1h (19 % conversion by NMR) with wet EtOAc and the product ratios were determined by GC/FID (99:1 4-isomer to 3-isomer.)

Catalytic borylation of veratrole (3) with (dtbpy)Ir(Bpin)₃COE (5) (Table 1, entry 4).

Compound **5** (dtbpy)Ir(Bpin)₃COE (19 mg, 0.02 mmol) was weighed in a test tube and was dissolved in C₆H₁₂ (2 mL) in a 20 mL scintillation vial containing a magnetic stir bar. 145 µL HBpin (1 mmol, 1 equiv) was added to the solution via syringe. Veratrole (127 µL, 1 mmol, 1 equiv) was added via syringe to the mixture and the vial was loosely sealed. Reaction was quenched at 12h with wet EtOAc and product ratios determined by GC/FID (98:2 4-isomer to 3-isomer at 26% conversion.)

Stoichiometric borylation of 1,3-benzodioxole (4) with 2 (Table 1, entry 5).

2 (20 mg, 0.024 mmol, 1 equiv) was weighed into a small vial. 1,3-benzodioxole (22.1 µL, 0.19 mmol, 8 equiv) was added to the vial *via* microliter syringe. Cyclohexane (2.4 mL) was added to the vial and the solution was divided four J. Young NMR tubes (600 µL per tube). The tubes were heated in an oil bath at 100 °C and monitored by GC. After 15 min, 1.3 equiv of 1,3-benzodioxole were converted to the 5- and 4-substituted boronic esters in a 2:98 ratio.

Catalytic Borylation of 1,3-benzodioxole (4) with 2 (Table 1, entry 6).

Compound **2** (4.2 mg, 0.005 mmol, 0.02 equiv) was weighed in a test tube and was transferred to a J.

Young NMR tube using C₆H₁₂ (100 μ L $\times$ 4). 1,3-benzodioxole (230 μ L, 2.0 mmol, 8 equiv) and HBpin (36 μ L, 0.25 mmol, 1 equiv) were syringed into the J. Young NMR tube, which was then capped and heated in an oil bath at 130 °C. After 4 h, GC analysis showed that 0.34 equiv. of 1,3-benzodioxole were converted to the 5- and 4-substituted boronic esters in a 4:96 ratio.

Stoichiometric borylation of 1,3-benzodioxole (4) with (dtbpy)Ir(Bpin)₃COE (5) (Table 1, entry 7).

Compound **5** (dtbpy)Ir(Bpin)₃COE (30 mg, 0.0315 mmol, 1 equiv) was weighed in a test tube and was dissolved in C₆D₁₂ (300 μ L). 1,3-benzodioxole (30.8 mg, 0.252 mmol, 8 equiv) was weighed in a test tube and mixed with the solution containing **5**. The mixture was then transferred via pipette into a J. Young NMR tube. The J. Young NMR tube was capped and the reaction was monitored by ¹H NMR. The reaction was quenched at 15 min at room temperature (51 % conversion by NMR) with wet EtOAc and the product ratios were determined by GC/FID (95:5 4-isomer to 5-isomer.)

Catalytic borylation of 1,3-benzodioxole (4) with (dtbpy)Ir(Bpin)₃COE (5) (Table 1, entry 8).

Compound **5** (dtbpy)Ir(Bpin)₃COE (19 mg, 0.02 mmol) was weighed in a test tube and was dissolved in C₆H₁₂ (2 mL) in a 20 mL scintillation vial containing a magnetic stir bar. 145 μ L HBpin (1 mmol, 1 equiv) was added to the solution via syringe. 1,3-benzodioxole (122 mg, 1 mmol, 1 equiv) was added to the mixture and the vial was loosely sealed. Reaction was quenched at 1h with wet EtOAc and product ratios determined by GC/FID (91:3 4-isomer to 5-isomer with 6% diborylation at 30% conversion.)

t_{1/2} determination for the stoichiometric borylation of 2-methylthiophene with 2.

Compound **2** (10.0 mg, 0.012 mmol, 1 equiv) was weighed in a test tube and was transferred to an NMR tube using C₆D₆ (125 μ L $\times$ 4) which was then closed with a rubber septum. 2-methylthiophene (11.6 μ L, 0.120 mmol, 10 equiv) was syringed in to the NMR tube. The tube was inserted into the spectrometer at 30 °C and the reaction was monitored by ¹H NMR. The ratio of starting materials to product after 5 minutes was 7:1, corresponding to the production of 3 equiv. of 4,4,5,5-tetramethyl-2-(5-methylthiophen-2-yl)-1,3,2-

dioxaborolane.

$t_{1/2}$ determination for the stoichiometric borylation of 2-methylthiophene with 7.

7 (13.7 mg, 0.012 mmol, 1 equiv) was weighed in a test tube and was transferred to an NMR tube using C_6D_6 ($125\ \mu L \times 4$) which was then closed with a rubber septum. 2-methylthiophene ($11.6\ \mu L$, 0.120 mmol, 10 equiv) was syringed in to the NMR tube. The tube was inserted into the spectrometer at 30 °C and the reaction was monitored by 1H NMR every 15 minutes. The ratio of starting materials to product after 3.5 h was 19:1, corresponding to the production of 0.5 equiv. of 2-methyl-5-Bcat^{''}-thiophene.

$t_{1/2}$ determination for the stoichiometric borylation of 2-methylthiophene with 8.

8 (9.7 mg, 0.012 mmol, 1 equiv) was weighed in a test tube and was transferred to an NMR tube using C_6D_6 ($125\ \mu L \times 4$) which was then closed with a rubber septum. 2-methylthiophene ($11.6\ \mu L$, 0.120 mmol, 10 equiv) was syringed in to the NMR tube. The tube was inserted into the spectrometer at 30 °C and the reaction was monitored by 1H NMR every 15 minutes. The ratio of starting materials to product after 3.5 h was 19:1, corresponding to the production of 0.5 equiv. of 2-methyl-5-Bcat-thiophene.

Crystallographic Details:

Data were collected using a Bruker CCD (charge coupled device) based diffractometer equipped with an Oxford Cryostream low-temperature apparatus operating at 173 K. Data were measured using omega and phi scans of 0.5° per frame for 30 s. Cell parameters were retrieved using ASTRO software⁶ and refined using SAINT on all observed reflections. Data reduction was performed using the SAINT software⁷ which corrects for Lp. Scaling and absorption corrections were applied using SADABS⁸ multi-scan technique, supplied by George Sheldrick. The structures are solved by the direct method using the SHELXS-97⁹ program and refined by least squares method on F^2 , SHELXL- 97,¹⁰ incorporated in SHELXTL-PC V 6.10.¹¹

All non-hydrogen atoms are refined anisotropically. Hydrogens were calculated by geometrical methods and refined as a riding model. Two disordered octane solvent molecules in **7** were refined at half occupancy. Translational disorder of the B3 boryl group in **8** was modeled using standard commands in the SHELXTL suite. The conformer population was optimized by least squares analysis and the major conformer consists of 58% of the total population. The crystals used for the diffraction study showed no decomposition during data collection. All drawings are done at 50% probabilities for the thermal ellipsoids.

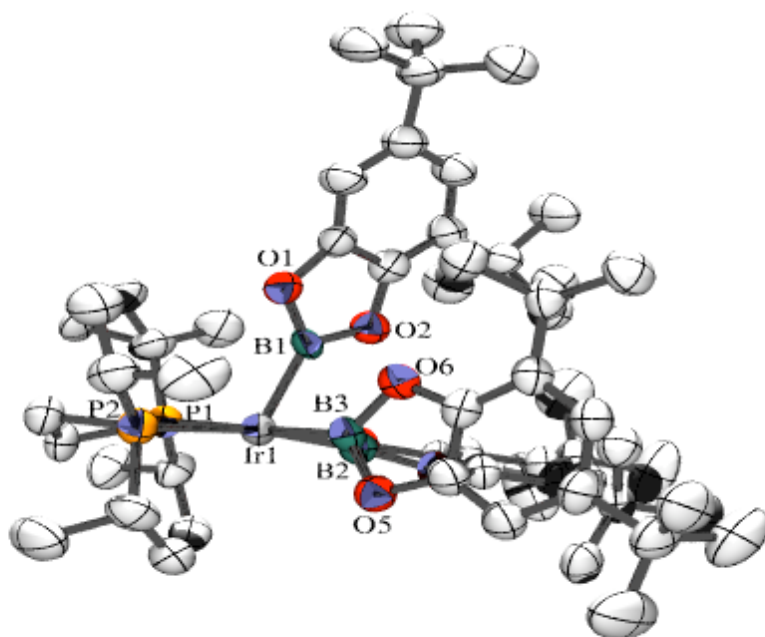


Figure 5. ORTEP plot for 7. Hydrogen atoms are removed for clarity. Thermal ellipsoids are shown at 50% probability.

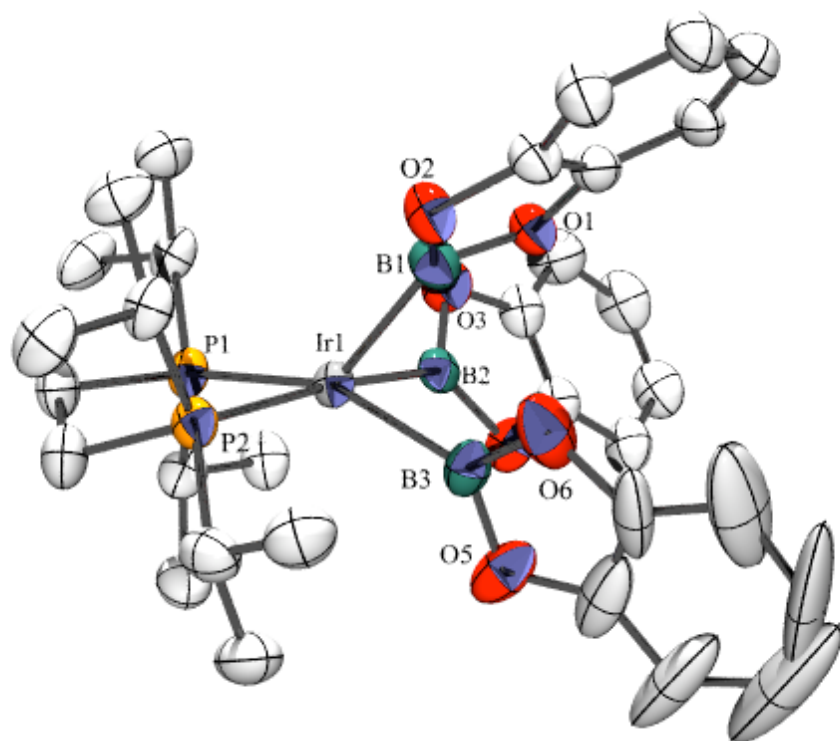


Figure 6. ORTEP plot for 8. Hydrogen atoms and a minor disorder component in the B3 boryl ligand (~ 42 %) have been removed for clarity. Thermal ellipsoids are shown at 50% probability.

Theoretical Methods

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anisole.....	30
benzodioxole5D.....	30
bisCF3benzene5D.....	31
metaxylene5D.....	31
methylthiophene5D.....	32
veratroleoutout5D.....	32
benzene5D.....	33
pyrrole.....	33
metadibromobenzene.....	34
bpyBpin32PyrroleCHactTS.....	34
bpyBpin32PyrroleCHOpttoprod.....	35
bpyBpin33PyrroleCHactTS.....	37
bpyBpin33PyrroleCHOpttoprod.....	38
dmpeBpin3MetaAnisCHactTSParParBackA.....	39
dmpeBpin3MetaAnisCHactTSParSptBackA.....	40
dmpeBpin3MetaAnisCHactTSSptSptBackA.....	42
dmpeBpin3MetaAnisCHactTSSptSptBackAoOpttoprod.....	43
dmpeBpin3MetaAnisCHactTSSptSptBackS.....	44
dmpeBpin3MetaAnisCHactTSSptSptFrntA.....	45
dmpeBpin3MetaAnisprodbetter.....	47
dmpeBpin3MetaBr2PhHCHactTSSptSptBack.....	48
dmpeBpin3MetaXyleneHCHactopttoprod.....	49
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dmpeBpin3MetaXyleneprodbetter.....	52
dmpeBpin3OrthoAnisCHactTSParSptBackA.....	53
dmpeBpin3OrthoAnisCHactTSParSptBackAoOpttoprod.....	55
dmpeBpin3OrthoAnisCHactTSSptSptBackS.....	56
dmpeBpin3OrthoAnisprodbetter.....	57
dmpeBpin3ParaAnisCHactTSParSptBackA.....	59
dmpeBpin3ParaAnisCHactTSParSptBackAoOpttoprod.....	60
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dmpeBpin3ParaAnisCHactTSSptSptFrntS.....	64
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methiophenedmpeIrBcat3TS.....	78
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veratroleIrBeg3TSPSBA.....	81
veratroleIrBeg3TSSSB1.....	82
veratroleIrBeg3TSSSBout.....	83
bpyIrBcat3HPhts.....	85
dmpeBcat3benzeneTS.....	86
dmpeBcat3Ir.....	88
dmpeBcat3IrconfB.....	89
dmpeBcat3TSBisCF3.....	90
hartwigbpyIrBcat3.....	92
hartwigbpyIrBcat3HPh.....	93

hartwigdmpeIrBcat3.....	94
dmpeBpin3PhHCHactTSParSptBack.....	95
dmpeBpin3PhHCHactTSParWrdBack.....	97
dmpeBpin3PhHCHactTSSptParBack.....	98
dmpeBpin3PhHCHactTSSptSptBack11.....	99
dmpeBpin3PhHCHactTSSptSptFrnt.....	100
IrDMPE_Bpin2_n2BpinH_Ph_goodgs.....	102
IrDMPE_Bpin2_n2BpinH_Ph_goodgsB.....	103
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dmpeBpin3BisMetaCF3CHacttoprod.....	108
methiophenebpyIrBeg3toprod.....	109
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General

The structures and energies for all stationary points were obtained using Gaussian 03.¹² Vibrational frequency analyses were carried out on all stationary points. Default methods were employed unless otherwise stated. Free energies in the main text were calculated using a 1 M standard state.

Choice of Methods and Method Details

To gauge theoretical methods for the study of iridium-mediated C-H activations, diverse combinations of functionals (B3LYP,¹³ mPW1K,¹⁴ TPSS,¹⁵ VXSC,¹⁶ B1B95,¹⁷ mPWLYP1M¹⁸) and basis sets were applied to the highly simplified model reaction of benzene with (dhpe)Ir(H)₂Beg [eg (ethyleneglycolato) = OCH₂CH₂O]. With the exception of the VXSC functional, the various methods afforded very similar C-H activation transition structure geometries, and the familiar B3LYP functional provided a middle-range geometry. Barriers varied modestly (< 3 kcal/mol) with basis set, generally increasing with diffuse functions on the light atoms and decreasing with an increased basis set for iridium. The B3LYP barrier was similar to that obtained with the mPWLYP1M functional, but was approximately 8 kcal/mol higher than that obtained with the mPW1k, B1B95, and TPSS functionals. In single-point energy tests of the latter functionals on catalytic cycle structures, they appeared to systematically favor higher-coordination complexes (which includes the C-H activation transition structure) but otherwise did not qualitatively differ from the B3LYP results. For the

practical study of large numbers of structures, geometry optimizations were carried out in B3LYP calculations employing an SDD basis set and core potential on iridium¹⁹ and a 6-31G** basis set on the remaining atoms (this basis set is designated here as BS1). Single-point energies were then calculated using for iridium an extension of the SDD basis set augmented with three f-functions and a separated d-function (a 3111 contraction instead of the normal 411), along with a 6-31+G** basis set on the remaining atoms (designated here as BS2). These single point energies using BS2 were determined for the complete set of structures using both B3LYP and mPW1K functionals. Selected small structures were fully optimized using B3LYP/BS2 and mPW1K/BS2 calculations as a check against qualitative errors.

For BS2, the listing below specifies the basis set and core potential in Gaussian format:

C H O B P 0

6-31+G**

IR 0

S	3	1.00	
		15.2937090	-1.6750339
		13.5736820	2.3934648
		5.8162740	-1.6504979
S	1	1.00	
		1.1955210	1.0000000
S	1	1.00	
		0.5657760	1.0000000
S	1	1.00	
		0.1405270	1.0000000
S	1	1.00	
		0.0508200	1.0000000
S	1	1.00	
		0.0150000	1.0000000
P	2	1.00	
		8.6697960	0.8677142
		6.2456140	-1.8144826
P	2	1.00	
		1.9663840	0.2709454
		1.0202060	0.7540443
P	1	1.00	
		0.4065800	1.0000000
P	1	1.00	
		0.0901160	1.0000000
P	1	1.00	
		0.0273640	1.0000000
D	3	1.00	
		3.6994850	-0.5973104
		3.3617430	0.6112252
		1.1745250	0.4732939
D	1	1.00	
		0.4701760	0.5755302
D	1	1.00	
		0.1576780	1.0000000
D	1	1.00	

		0.0500000	1.0000000
F	1	1.00	
		2.03336960E+00	1.00000000
F	1	1.00	
		7.82065200E-01	1.00000000
F	1	1.00	
		3.12826100E-01	1.00000000

IR 0			
IR-ECP 5 60			
H POTENTIAL			
	1		
2		1.000000000	0.000000000
S-H POTENTIAL			
	2		
2		13.652203000	732.269200000
2		6.826101000	26.484721000
P-H POTENTIAL			
	2		
2		10.279868000	299.489474000
2		5.139934000	26.466234000
D-H POTENTIAL			
	2		
2		7.349859000	124.457595000
2		3.674929000	14.035995000
F-H POTENTIAL			
	1		
2		3.034072000	21.531031000
G-H POTENTIAL			
	1		
2		4.808857000	-21.607597000

Tables of Energies for Calculated Structures

Table S1.

B3LYP/BS1 Potential Energies, E + zpe, harmonic entropy, Enthalpy at 25 °C, harmonic free energy at 25 °C and 1 atm. Energies are in Hartrees, entropies are in e.u.

Structure Title (see Key to Structure Titles section)	potential energy	E + zpe	S 1atm 25°C	Enthalpy 25 °C	G 1atm 25 °C
<u>organic starting materials</u>					
bisCF3benzene5D	-906.317889	-906.207527	111.2	-906.195104	-906.247938
benzodioxole5D	-420.778372	-420.662073	81.449	-420.654603	-420.693302
methylthiophene5D	-592.323829	-592.229219	76.781	-592.222461	-592.258942
veratroleoutout5D	-461.294083	-461.128027	94.339	-461.117684	-461.162508
benzene5D	-232.253118	-232.152485	69.024	-232.147152	-232.179948
pyrrole	-210.171917	-210.089233	65.941	-210.084305	-210.115635
metaxylene5D	-310.892755	-310.737334	91.3	-310.728292	-310.771672
anisole	-346.776574	-346.643204	81.743	-346.635410	-346.674248
metadibromobenzene	-5373.855750	-5373.775025	88.8	-5373.766979	-5373.809171
<u>metal complex starting materials</u>					
IrDMPE_Bpin3	-1787.534069	-1787.111805	199.742	-1787.080451	-1787.175355
hartwigdmpelrBeg3	-1787.532253	-1787.110479	205.274	-1787.078831	-1787.176363
hartwigbpyIrBeg3	-1361.886313	-1361.515002	189.734	-1361.487330	-1361.577479
Irbpy_Bpin3	-1361.886040	-1361.514774	189.409	-1361.487070	-1361.577065
dmpeBcat3Ir	-2244.848326	-2244.356031	229.537	-2244.319041	-2244.428101
dmpeBcat3IrconfB	-2244.848105	-2244.356039	231.544	-2244.319041	-2244.428948
hartwigdmpelrBcat3	-2244.848456	-2244.355988	229.421	-2244.319055	-2244.428060
hartwigbpyIrBcat3	-1819.202284	-1818.760879	217.405	-1818.727677	-1818.830973
	-2102.027925	-2101.376084	244.627	-2101.334234	-2101.450464
<u>dmpe Beg system</u>					
dmpeBpin3PhHCHactTSSptSptBack	-2019.753626	-2019.232820	217.942	-2019.196557	-2019.300108
IrDMPE_Bpin2_n2BpinH_Ph_goodgsD	-2019.766459	-2019.242978	218.721	-2019.206629	-2019.310550
hartwigdmpelrBeg3HPh	-2019.765862	-2019.242061	216.22	-2019.205928	-2019.308662
dmpeBpin3BisMetaCF3CHactTSA	-2693.826526	-2693.296336	260.158	-2693.252560	-2693.376170
dmpeBpin3BisMetaCF3CHacttoprod	-2693.841705	-2693.307967	257.015	-2693.264436	-2693.386553
dioxmetaParSptBackA	-2208.278721	-2207.742341	229.864	-2207.703766	-2207.812982
dioxmetaSptSptBackS best	-2208.279081	-2207.742998	232.774	-2207.704274	-2207.814872
dioxmetaSptSptFrntA	-2208.277423	-2207.741003	230.933	-2207.702354	-2207.812078
dioxorthoParSptBackA best	-2208.284353	-2207.747673	226.898	-2207.709412	-2207.817218
dioxorthoSptSptBackS	-2208.278953	-2207.742886	227.804	-2207.704416	-2207.812653
methiophenedmpeBeg3TS	-2379.833227	-2379.318571	226.08	-2379.280717	-2379.388135
methiophenedmpeBeg3toprod	-2379.848310	-2379.330120	224.133	-2379.292516	-2379.399009
veratroleIrBeg3orthoTSPSBA	-2248.792641	-2248.207051	242.572	-2248.165490	-2248.280744
veratroleIrBeg3TSPSBA	-2248.793024	-2248.207230	245.274	-2248.165485	-2248.282022
veratroleIrBeg3TSSSB1	-2248.794040	-2248.207915	243.377	-2248.166324	-2248.281961
veratroleIrBeg3TSSSBout	-2248.793459	-2248.207163	242.944	-2248.165715	-2248.281145
dmpeBpin3MetaXyleneHCHactTSSptSptBack	-2098.392596	-2097.817161	241.404	-2097.776969	-2097.891668
dmpeBpin3MetaXyleneHCHactopttoprod	-2098.404554	-2097.825921	237.605	-2097.785962	-2097.898856
dmpeBpin3MetaXyleneprod better	-2098.405085	-2097.827146	238.943	-2097.786927	-2097.900457
dmpeBpin3MetaBr2PhHCHactTSSptSptBack	-7161.362083	-7160.861758	231.759	-7160.823110	-7160.933226

dmpeBpin3MetaBr2PhHCHactopttoprod	-7161.377235	-7160.873177	236.143	-7160.833907	-7160.946106
dmpeBpin3OrthoAnisCHactTSParSptBackA	-2134.274894	-2133.721799	230.383	-2133.682882	-2133.792344
dmpeBpin3OrthoAnisCHactTSParSptBackAopttoprod	-2134.286324	-2133.729384	226.187	-2133.690918	-2133.798387
dmpeBpin3OrthoAnisprodbetter	-2134.287130	-2133.731118	230.471	-2133.692252	-2133.801756
dmpeBpin3MetaAnisCHactTSSptSptBackA	-2134.277704	-2133.724461	232.055	-2133.685444	-2133.795700
dmpeBpin3MetaAnisCHactTSSptSptBackAopttoprod	-2134.290282	-2133.733380	229.02	-2133.694680	-2133.803495
dmpeBpin3MetaAnisprodbetter	-2134.289877	-2133.733863	230.526	-2133.694892	-2133.804423
dmpeBpin3ParaAnisCHactTSParSptBackA	-2134.275854	-2133.722766	233.314	-2133.683676	-2133.794531
dmpeBpin3ParaAnisCHactTSParSptBackAopttoprod	-2134.286489	-2133.729876	224.867	-2133.692031	-2133.798872
dmpeBpin3ParaAnisprodbetter	-2134.289254	-2133.732732	228.78	-2133.693973	-2133.802674
<u>dmpe Bcat system</u>					
dmpeBcat3benzeneTS	-2477.064471	-2476.474013	247.767	-2476.431927	-2476.549649
dmpeIrBcat3HPhprodfromts	-2477.077431	-2476.483818	245.005	-2476.441956	-2476.558365
hartwigdmpeIrBcat3HPh	-2477.076964	-2476.483253	244.357	-2476.441460	-2476.557562
dmpeBcat3TSBisCF3	-3151.134929	-3150.534812	288.743	-3150.485367	-3150.622558
dmpeBcat3BisCF3toprod	-3151.150449	-3150.547287	286.128	-3150.497979	-3150.633928
methiophenedmpeIrBcat3TS	-2837.143505	-2836.559000	255.308	-2836.515425	-2836.636731
methiophenedmpeIrBcat3toprod	-2837.159363	-2836.571944	253.459	-2836.528455	-2836.648882
<u>bpy Beg system</u>					
Ir_bpy_Bpin3_PhH_CHact_ts_lit	-1594.107185	-1593.638306	211.847	-1593.605289	-1593.705944
Irbpy_Bpin3_H_Ph	-1594.120807	-1593.649580	209.011	-1593.616690	-1593.715998
hartwigbpyIrBeg3HPh	-1594.120592	-1593.649626	205.802	-1593.617386	-1593.715169
bypbpin3methylenedioxyMetaTS	-1782.632753	-1782.148300	223.415	-1782.112998	-1782.219149
bypbpin3methylenedioxyMetatoprod	-1782.647121	-1782.160354	220.338	-1782.125187	-1782.229877
bypbpin3methylenedioxyOrthoTS	-1782.636641	-1782.151770	218.655	-1782.116816	-1782.220706
bypbpin3methylenedioxyOrthotoprod	-1782.651077	-1782.163668	216.313	-1782.128837	-1782.231615
methiophenebpyIrBeg3TS	-1954.185934	-1953.722795	219.333	-1953.688276	-1953.792488
methiophenebpyIrBeg3toprod	-1954.202069	-1953.736317	215.963	-1953.701931	-1953.804542
bypbeg3veratroleMetaTSC	-1823.146546	-1822.612848	238.633	-1822.574374	-1822.687756
bypbeg3veratroleMetaCtoprod	-1823.160635	-1822.624632	234.836	-1822.586294	-1822.697872
bypbeg3veratroleMetaTSB	-1823.147433	-1822.613180	236.226	-1822.574937	-1822.687176
bypbeg3veratroleMetaBtoprod	-1823.161114	-1822.624659	234.063	-1822.586500	-1822.697712
bypbeg3veratroleMetaTSA	-1823.146462	-1822.612699	238.153	-1822.574267	-1822.687421
bypbeg3veratroleMetaAtoprod	-1823.160746	-1822.624733	235.824	-1822.586353	-1822.698400
bypbeg3veratroleOrthoTSB	-1823.145650	-1822.611487	232.862	-1822.573373	-1822.684013
bypbeg3veratroleOrthoTSBtoprod	-1823.159541	-1822.623075	231.741	-1822.585005	-1822.695113
bpyBpin32PyrroleCHactTS	-1572.035328	-1571.583917	201.391	-1571.552489	-1571.648177
bpyBpin32PyrroleCHopttoprod	-1572.048745	-1571.595047	204.549	-1571.562806	-1571.659994
bpyBpin33PyrroleCHactTS	-1572.027688	-1571.576696	207.84	-1571.544204	-1571.642956
bpyBpin33PyrroleCHopttoprod	-1572.040237	-1571.587121	206.984	-1571.554611	-1571.652956
<u>bpy Bcat system</u>					
bpyIrBcat3HPhts	-2051.418708	-2050.879626	238.243	-2050.841081	-2050.954278
hartwigbpyIrBcat3HPh	-2051.432031	-2050.891254	237.309	-2050.852622	-2050.965376
bpyBcat3methiopheneTS	-2411.496947	-2410.963842	246.714	-2410.923716	-2411.040938
bpyBcat3methiophenetoprod	-2411.511992	-2410.976975	247.149	-2410.936705	-2411.054134

Table S2.

MPW1K/BS2//B3LYP/BS1 potential energies (in Hartrees), MPW1K/BS2//B3LYP/BS1 E + zpe (in Hartrees), entropy adjusted to a 1 M standard state at 25 °C, harmonic free energy at 25 °C and 1 M standard state (in Hartrees), free energy of transition structures and intermediates relative to separate starting materials (in kcal/mol).

Structure Title (see Key to Structure Titles section)	potential energy	E + zpe	S at 1 M, 25 °C	G at 1 M, 25 °C	$\Delta G^\ddagger$ or ΔG 25 °C
<u>organic starting materials</u>					
bisCF3benzene5D	-906.090993	-905.980631	104.846	-906.018024	
benzodioxole5D	-420.665239	-420.548940	75.095	-420.577150	
methylthiophene5D	-592.285927	-592.191316	70.427	-592.218021	
veratroleoutout5D	-461.170490	-461.004434	87.985	-461.035896	
benzene5D	-232.197776	-232.097143	62.67	-232.121587	
pyrrole	-210.123101	-210.040417	59.587	-210.063800	
metaxylene5D	-310.822531	-310.667110	84.946	-310.698429	
anisole	-346.686968	-346.553597	75.389	-346.581623	
metadibromobenzene	-5374.069679	-5373.988954	82.446	-5374.020081	
<u>metal complex starting materials</u>					
IrDMPE_Bpin3	-1787.258059	-1786.835795	193.388	-1786.896326	
hartwigdmpeIrBeg3	-1787.256125	-1786.834351	198.92	-1786.897217	
hartwigbpyIrBeg3	-1361.503251	-1361.131940	183.38	-1361.191398	
Irbpy_Bpin3	-1361.502223	-1361.130957	183.055	-1361.190228	
dmpeBcat3Ir	-2244.454403	-2243.962108	223.183	-2244.031160	
dmpeBcat3IrconfB	-2244.454254	-2243.962188	225.19	-2244.032185	
hartwigdmpeIrBcat3	-2244.454389	-2243.961920	223.067	-2244.030974	
hartwigbpyIrBcat3	-1818.699811	-1818.258406	211.051	-1818.325481	
	-2101.696460	-2101.044619	238.273	-2101.115980	
<u>dmpe Beg system</u>					
dmpeBpin3PhHCHactTSSptSptBack	-2019.434258	-2018.913452	211.588	-2018.977722	25.8
IrDMPE_Bpin2_n2BpinH_Ph_goodgsD	-2019.450579	-2018.927099	212.367	-2018.991652	17.0
hartwigdmpeIrBeg3HPh	-2019.449455	-2018.925654	209.866	-2018.989235	18.6
dmpeBpin3BisMetaCF3CHactTSA	-2693.335306	-2692.805116	253.804	-2692.881931	20.9
dmpeBpin3BisMetaCF3CHacttoprod	-2693.353690	-2692.819952	250.661	-2692.895518	12.4
dioxmetaParSptBackA	-2207.902120	-2207.365741	223.51	-2207.433362	25.7
dioxmetaSptSptBackS best	-2207.902226	-2207.366143	226.42	-2207.434999	24.7
dioxmetaSptSptFrntA	-2207.899824	-2207.363404	224.579	-2207.431460	26.9
dioxorthoParSptBackA best	-2207.907107	-2207.370427	220.544	-2207.436954	23.5
dioxorthoSptSptBackS	-2207.902508	-2207.366441	221.45	-2207.433189	25.8
methiophenedmpeBeg3TS	-2379.532082	-2379.017426	219.726	-2379.083971	19.6
methiophenedmpeBeg3toprod	-2379.549892	-2379.031703	217.779	-2379.097573	11.1
veratroleIrBeg3orthoTSPSBA	-2248.404058	-2247.818467	236.218	-2247.889141	27.6
veratroleIrBeg3TSPSBA	-2248.405662	-2247.819869	238.92	-2247.891642	26.0
veratroleIrBeg3TSSSB1	-2248.406542	-2247.820417	237.023	-2247.891443	26.1
veratroleIrBeg3TSSSBout	-2248.405976	-2247.819681	236.59	-2247.890644	26.6
dmpeBpin3MetaXyleneHCHactTSSptSptBack	-2098.058299	-2097.482863	235.05	-2097.554351	25.9
dmpeBpin3MetaXyleneHCHactopttoprod	-2098.073258	-2097.494624	231.251	-2097.564540	19.0
dmpeBpin3MetaXyleneprodbetter	-2098.074342	-2097.496403	232.589	-2097.566695	17.6
dmpeBpin3MetaBr2PhHCHactTSSptSptBack	-7161.313882	-7160.813558	225.405	-7160.882007	21.6
dmpeBpin3MetaBr2PhHCHactopttoprod	-7161.331564	-7160.827506	229.789	-7160.897416	11.9
dmpeBpin3OrthoAnisCHactTSParSptBackA	-2133.920965	-2133.367871	224.029	-2133.435397	26.7

dmpeBpin3OrthoAnisCHactTSParSptBackAoptytoprod	-2133.934648	-2133.377709	219.833	-2133.443692	21.5
dmpeBpin3OrthoAnisprodbetter	-2133.936583	-2133.380572	224.117	-2133.448191	18.7
dmpeBpin3MetaAnisCHactTSSptSptBackA	-2133.924484	-2133.371241	225.701	-2133.439462	24.2
dmpeBpin3MetaAnisCHactTSSptSptBackAoptytoprod	-2133.939725	-2133.382822	222.666	-2133.449918	17.6
dmpeBpin3MetaAnisprodbetter	-2133.939713	-2133.383699	224.172	-2133.451239	16.8
dmpeBpin3ParaAnisCHactTSParSptBackA	-2133.922536	-2133.369448	226.96	-2133.438195	24.9
dmpeBpin3ParaAnisCHactTSParSptBackAoptytoprod	-2133.935566	-2133.378953	218.513	-2133.444930	20.7
dmpeBpin3ParaAnisprodbetter	-2133.939002	-2133.382480	222.426	-2133.449402	17.9
<u>dmpe Bcat system</u>					
dmpeBcat3benzeneTS	-2476.626391	-2476.035933	241.413	-2476.108550	28.4
dmpeIrBcat3HPhprodfromts	-2476.642144	-2476.048531	238.651	-2476.120060	21.2
hartwigdmpeIrBcat3HPh	-2476.641456	-2476.047745	238.003	-2476.119035	21.8
dmpeBcat3TSBisCF3	-3150.524954	-3149.924837	282.389	-3150.009564	25.5
dmpeBcat3BisCF3toprod	-3150.543460	-3149.940298	279.774	-3150.023920	16.5
methiophenedmpeIrBcat3TS	-2836.723841	-2836.139336	248.954	-2836.214047	22.7
methiophenedmpeIrBcat3toprod	-2836.742420	-2836.155002	247.105	-2836.228920	13.4
<u>bpy Beg system</u>					
Ir_bpy_Bpin3_PhH_CHact_ts_lit	-1593.678078	-1593.209199	205.493	-1593.273818	24.6
Irbpy_Bpin3_H_Ph	-1593.696916	-1593.225689	202.657	-1593.289088	15.0
hartwigbpyIrBeg3HPh	-1593.696415	-1593.225449	199.448	-1593.287973	15.7
bypbpin3methylenedioxyMetaTS	-1782.146362	-1781.661909	217.061	-1781.729740	24.4
bypbpin3methylenedioxyMetatoprod	-1782.166023	-1781.679256	213.984	-1781.745760	14.3
bypbpin3methylenedioxyOrthoTS	-1782.150981	-1781.666110	212.301	-1781.732027	22.9
bypbpin3methylenedioxyOrthotoprod	-1782.170306	-1781.682898	209.959	-1781.747825	13.0
methiophenebpyIrBeg3TS	-1953.775279	-1953.312141	212.979	-1953.378815	19.2
methiophenebpyIrBeg3toprod	-1953.796228	-1953.330476	209.609	-1953.395682	8.6
bypbeg3veratroleMetaTSC	-1822.649546	-1822.115848	232.279	-1822.187738	24.8
bypbeg3veratroleMetaCtoprod	-1822.668696	-1822.132692	228.482	-1822.202914	15.3
bypbeg3veratroleMetaTSB	-1822.650385	-1822.116131	229.872	-1822.187108	25.2
bypbeg3veratroleMetaBtoprod	-1822.669275	-1822.132820	227.709	-1822.202853	15.3
bypbeg3veratroleMetaTSA	-1822.649360	-1822.115597	231.799	-1822.187300	25.1
bypbeg3veratroleMetaAtoprod	-1822.668917	-1822.132903	229.47	-1822.203552	14.9
bypbeg3veratroleOrthoTSB	-1822.647989	-1822.113826	226.508	-1822.183333	27.6
bypbeg3veratroleOrthoTSBtoprod	-1822.667063	-1822.130597	225.387	-1822.199616	17.4
bpyBpin32PyrroleCHactTS	-1571.612647	-1571.161236	195.037	-1571.222476	20.5
bpyBpin32PyrroleCHopttoprod	-1571.631481	-1571.177782	198.195	-1571.239710	9.7
bpyBpin33PyrroleCHactTS	-1571.605482	-1571.154491	201.486	-1571.217731	23.5
bpyBpin33PyrroleCHopttoprod	-1571.622692	-1571.169576	200.63	-1571.232392	14.3
<u>bpy Bcat system</u>					
bpyIrBcat3HPhts	-2050.870953	-2050.331872	231.889	-2050.403505	27.3
hartwigbpyIrBcat3HPh	-2050.888128	-2050.347351	230.955	-2050.418453	18.0
bpyBcat3methiopheneTS	-2410.967714	-2410.434609	240.36	-2410.508686	21.8
bpyBcat3methiophenetoprod	-2410.986413	-2410.451396	240.795	-2410.525536	11.3

Data for Figures 5a and 5b

List of Reactions

Metal Complex Starting Materials

(dmpe)Ir(Beg)₃ (**1a**), (bpy)Ir(Beg)₃ (**6a**), (dmpe)Ir(Bcat)₃ (**1b**), and (bpy)Ir(Bcat)₃ (**6b**)

Arene Starting Materials

benzene, veratrole, benzodioxole, *meta*-bis(trifluoromethyl)benzene, *meta*-dibromobenzene, *meta*-xylene, 2-methylthiophene, pyrrole

Reactions

- A. **6a** + benzodioxole, ortho position
- B. **6a** + benzodioxole, meta position
- C. **6b** + methylthiophene, reaction at 5 position
- D. **6a** + benzene
- E. **6a** + veratrole, meta position, transition structure conformer B
- F. **6a** + veratrole, meta position, transition structure conformer C
- G. **6a** + veratrole, meta position, transition structure conformer A
- H. **6b** + benzene
- I. **6a** + veratrole, ortho position
- J. **6a** + methylthiophene, reaction at 5 position
- K. **6a** + pyrrole, reaction at 2 position
- L. **6a** + pyrrole, reaction at 3 position
- M. **1a** + methylthiophene, reaction at 5 position
- N. **1b** + methylthiophene, reaction at 5 position
- O. **1a** + benzene
- P. **1b** + benzene
- Q. **1b** + *meta*-bis(trifluoromethyl)benzene, reaction at 5 position
- R. **1a** + *meta*-bis(trifluoromethyl)benzene, reaction at 5 position
- S. **1a** + *meta*-dibromobenzene, reaction at 5 position
- T. **1a** + anisole, ortho position
- U. **1a** + anisole, meta position
- V. **1a** + anisole, para position
- W. **1a** + *meta*-xylene, reaction at 5 position

Table S3

$\Delta E^\ddagger$ for reactions (B3LYP/BS1, E + zpe); ΔE for reactions (B3LYP/BS1, E + zpe), total charge on arene in intermediate structure from an NPA calculation.

Reaction	$\Delta E^\ddagger$	ΔE	Arene charge
A	15.9	8.4	-0.3161
B	18.1	10.5	-0.2961
C	16.5	8.2	-0.2838
D	18.3	11.2	-0.2875
E	18.7	11.5	-0.2860
F	18.9	11.5	-0.2886
G	19.0	11.5	-0.2894

H	21.2	13.9	-0.2526
I	19.8	12.5	-0.3041
J	13.4	5.0	-0.3279
K	12.7	5.8	-0.2786
L	17.3	10.7	-0.2568
M	14.1	6.8	-0.3058
N	16.5	8.4	-0.2779
O	19.7	13.4	-0.2769
P	21.7	15.5	-0.2503
Q	18.0	10.2	-0.3038
R	14.4	7.1	-0.3314
S	15.7	8.6	-0.3285
T	20.8	15.0	-0.2656
U	19.2	13.3	-0.2771
V	20.2	14.0	-0.2667
W	20.1	13.8	-0.2718

Calculated Structures

Key to structure titles

The structure titles in the following section have retained the original file names for the computational output files. This lets us use a single code name for structures, single-point energies in tables, charge calculations, and our records, but a problem is that the titles are sometime clear and sometimes relatively cryptic. We will give here some general explanation of the titles along with structural drawings.

The titles anisole, benzodioxole5D, bisCF₃benzene5D, metaxylene5D, methylthiophene5D, veratroleoutout5D, pyrrole, metadibromobenzene, and benzene5D are largely self-explanatory. "5D" in a title means five d functions were used in the calculation (as opposed to 6), though this is true of every calculation here. bisCF₃benzene is the *meta* isomer of bis(trifluoromethyl)benzene. methylthiophene is 2-methylthiophene. veratroleoutout is the lowest-energy conformer of veratrole as depicted in the main text.

Structures with TS in the title are transition structures and in every case had one imaginary frequency. Every TS here is a transition structure for C-H activation of an arene from reaction of the arene with (dmpe)Ir(Beg)₃, (dmpe)Ir(Bcat)₃, (bpy)Ir(Beg)₃, or (bpy)Ir(Bcat)₃. The use of "dmpe", "DMPE", "bpy", and "Bcat" in titles is self-explanatory, but the use of "Bpin" in title actually refers to Beg ligands, not Bpin ligands.

Structures with "toprod", "opttoprod", or "goodgs" in the title are the intermediates following C-H activation. In general these intermediates were located by a geometry optimization process after stepping forward from the transition structures; in four test cases these structures were verified by an IRC analysis.

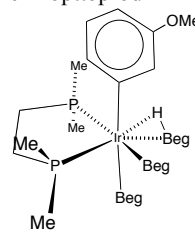
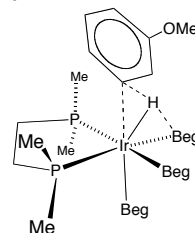
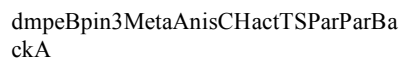
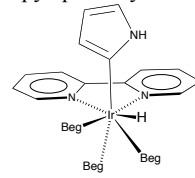
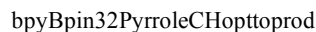
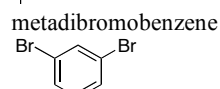
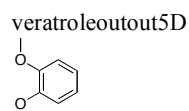
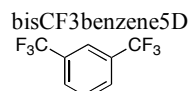
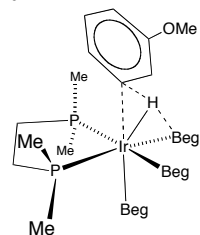
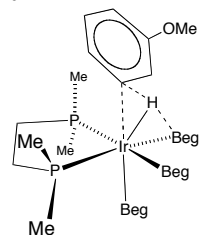
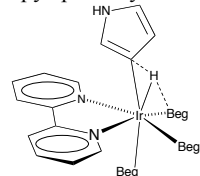
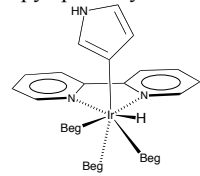
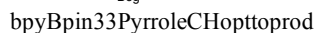
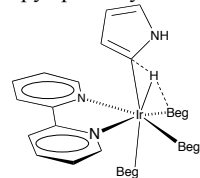
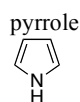
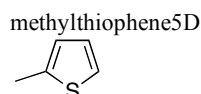
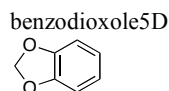
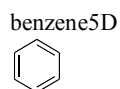
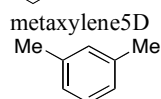
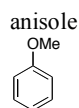
In most of the title names, the arene involved is identified; otherwise benzene is the arene. Pyrrole, MetaBr2Ph, MetaXylene, veratrole, and PhH are self-explanatory. "Anis" refers to reactions of anisole. "diox" or "methylenedioxy" refer to benzodioxole. "BisMetaCF₃" refers to meta-bis(trifluoromethyl)benzene. The position of reaction of the arene is designated by either a number (2Pyrrole and 3Pyrrole refer to reactions at the 2 or 3 position of pyrrole) or by "Ortho", "Meta", or "Para". For meta-xylene, meta-dibromobenzene, and meta-bis(trifluoromethyl)benzene, only substitution at the least-hindered 5 position was considered. "methiophene" refers to 2-methylthiophene and only substitution at the 5 position was considered.

Designations "ParParBackA", "ParSptBackA", "SptSptBackA", "SptSptBackS", "SptSptFrntA", etc., refer to different transition structure conformers located for the dmpe-containing structures. In general, the Beg group anti to the incoming arene could adopt two conformations that we designated as Par or Spt, the incoming arene could approach in the Ir in two ways that we designated as Par or Spt, and the C-H activation could occur in two ways relative to the cant of the (dmpe)Ir 5-membered ring, which we designated as Back or Frnt. After

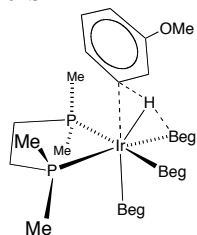
exploring the various possibilities in detail with benzene, only the lower-energy possibilities were explored with other arenes. For arenes desymmetrized by substituents, two more possibilities arose in general, which we designated as A or S. In some cases the conformer designation is abbreviated further as "PSBA" for ParSptBackA or "SSB" for SptSptBack. "Out", "ConfB", "A", "B", "C", "D", and "better" were also used to designate particular conformers that could not otherwise be described in a systematic way.

The use of "lit" in a title means that the general structure reported here was previously reported in Tamura, H.; Yamazaki, H.; Sato, H.; Sakaki, S. *J. Am. Chem. Soc.* **2003**, *125*, 16114-16126. The use of "hartwig" in a title means that the general structure reported here was previously reported in Liskey, C. W., Wei C. S., Pahls, D. R., Hartwig J. F. "Pronounced Effects of Substituents on the Iridium-Catalyzed Borylation of Aryl C–H Bonds" *Chem. Commun.* **2009**, 5603-5605. In the supporting information for the latter paper, the bpyIr(Beg)3(H)(Ph) structure is missing 6 atoms, and structure 6 was not an optimized structure. Of course, due to the larger basis set here, none of the structures are identical, and in some cases we have located lower-energy conformations.

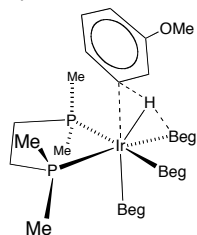
The structures below are meant as a guide but they are not drawn to be geometrically meaningful – differing conformers are drawn identically.



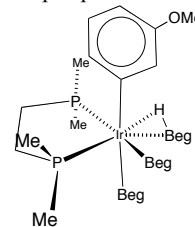
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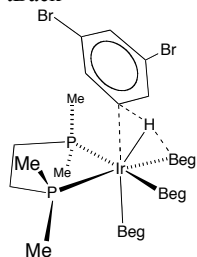
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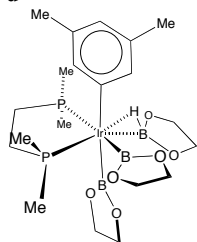
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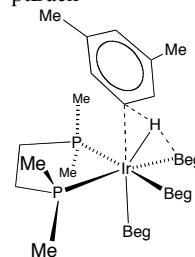
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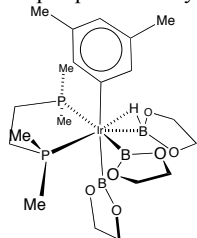
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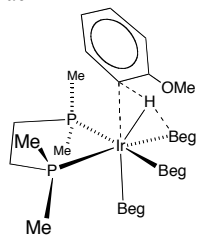
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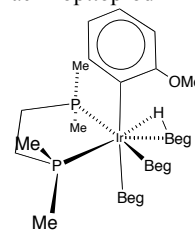
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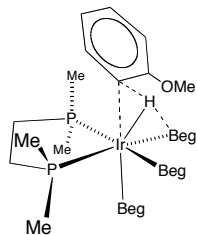
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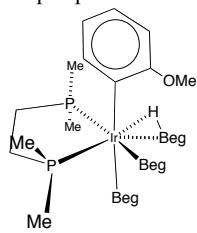
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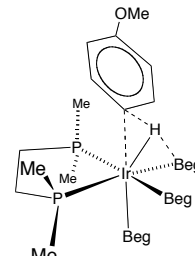
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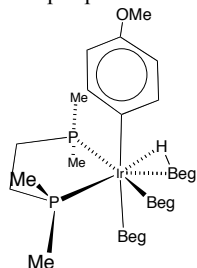
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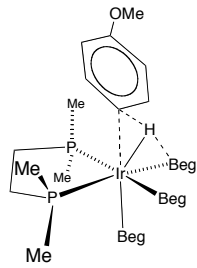
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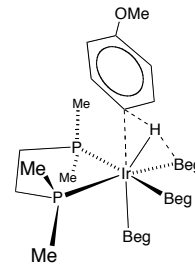
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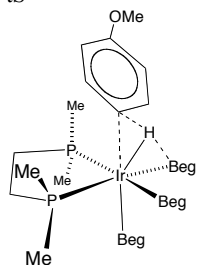
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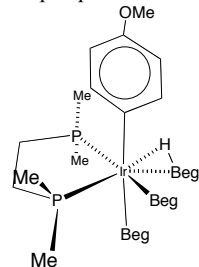
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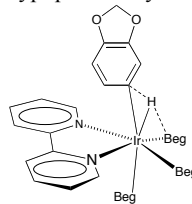
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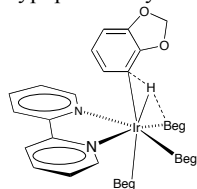
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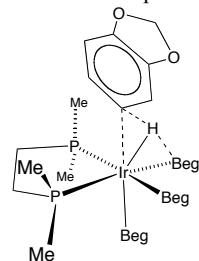
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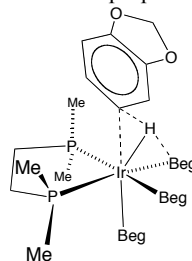
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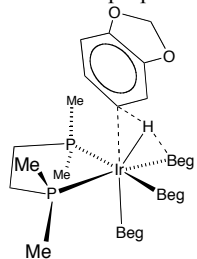
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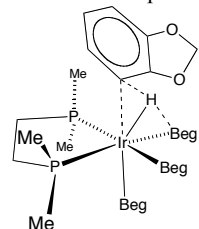
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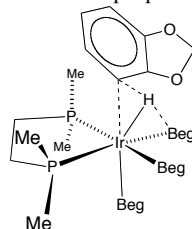
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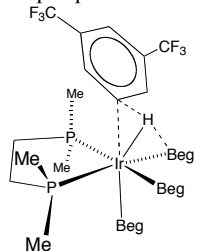
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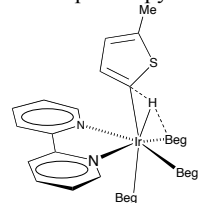
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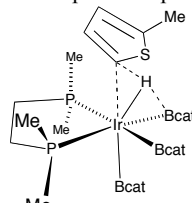
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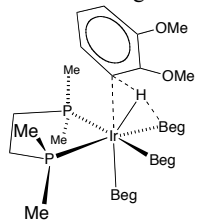
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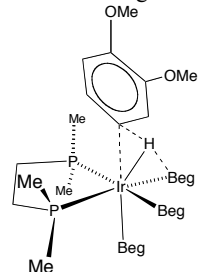
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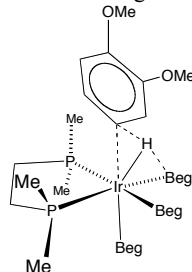
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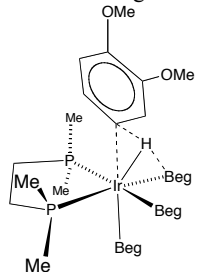
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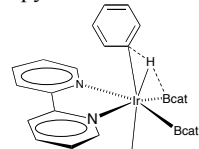
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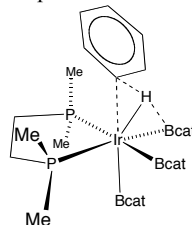
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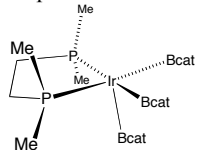
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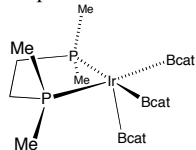
dmpeBcat3benzeneTS



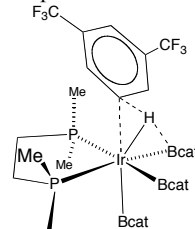
dmpeBcat3Ir



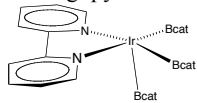
dmpeBcat3IrconfB



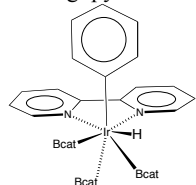
dmpeBcat3TSBisCF3



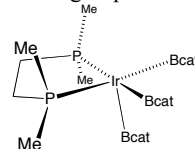
hartwigbpyIrBcat3



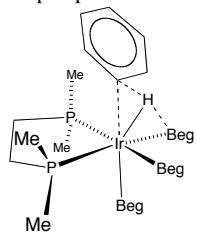
hartwigbpyIrBcat3HPh



hartwigdmpeIrBcat3

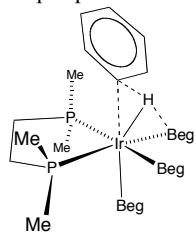


dmpeBpin3PhHCHactTSParSptBack



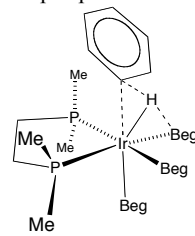
conformer

dmpeBpin3PhHCHactTSParWrdBack



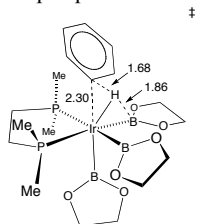
conformer

dmpeBpin3PhHCHactTSSptParBack



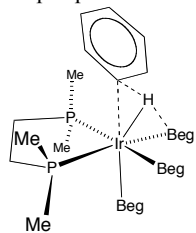
conformer

dmpeBpin3PhHCHactTSSptSptBack11

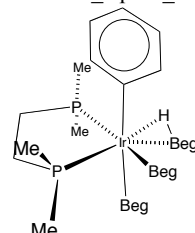


†

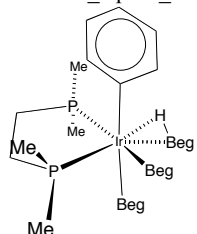
dmpeBpin3PhHCHactTSSptSptFmt



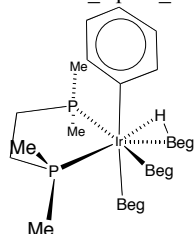
IrDMPE_Bpin2_n2BpinH_Ph_goodgs



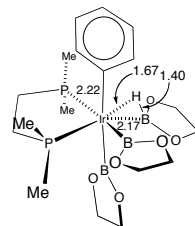
IrDMPE_Bpin2_n2BpinH_Ph_goodgsB



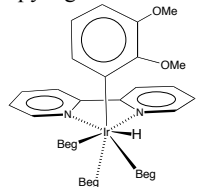
IrDMPE_Bpin2_n2BpinH_Ph_goodgsC



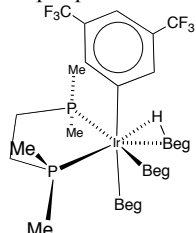
IrDMPE_Bpin2_n2BpinH_Ph_goodgsD
12



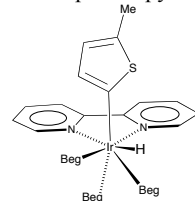
bpybeg3veratroleOrthoTSBtoprod



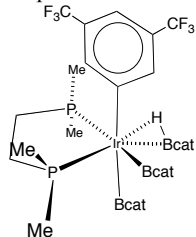
dmpeBpin3BisMetaCF3CHacttoprod



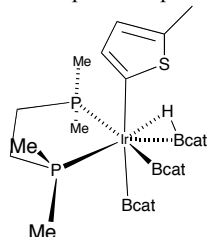
methiophenebpyIrBpin3toprod



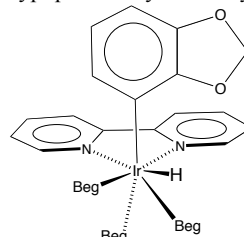
dmpeBcat3BisCF3toprod



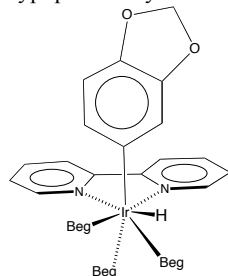
methiophenedmpeIrBcat3toprod



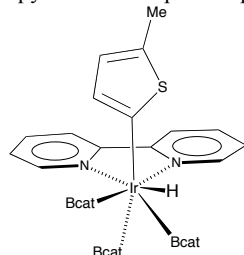
bybpin3methylenedioxyOrthotoprod



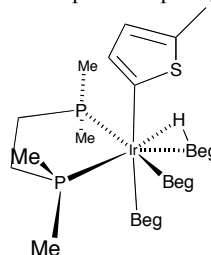
bybpin3methylenedioxyMetatoprod



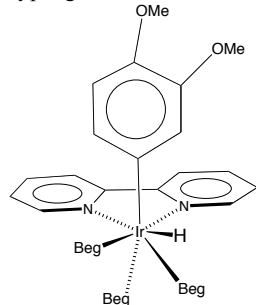
bpyBcat3methiophenetoprod



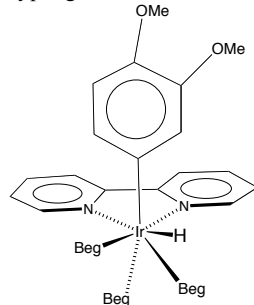
methiophenedmpeBeg3toprod



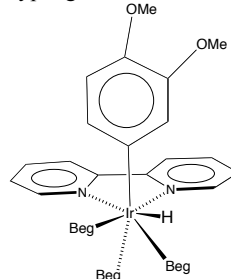
bypbeg3veratroleMetaCtoprod



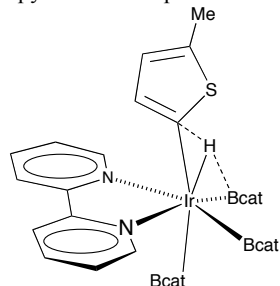
bypbeg3veratroleMetaBtoprod



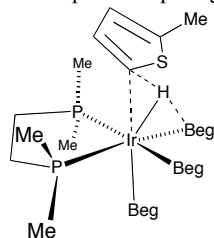
bypbeg3veratroleMetaAtoprod



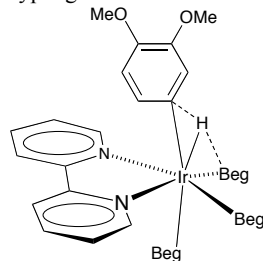
bpyBcat3methiopheneTS



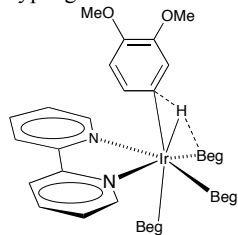
methiophenedmpeBeg3TS



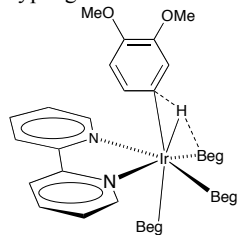
bypbeg3veratroleMetaTSC



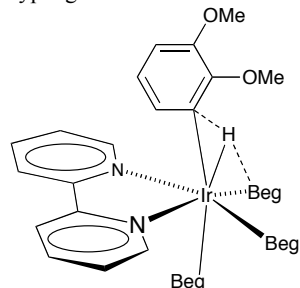
bypbeg3veratroleMetaTSB



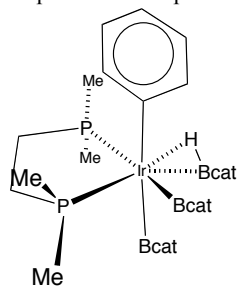
bypbeg3veratroleMetaTSA



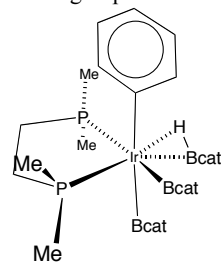
bypbeg3veratroleOrthoTSB



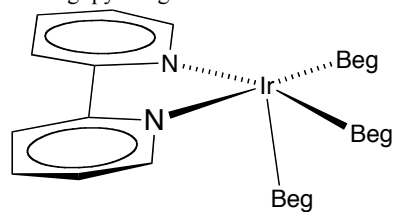
dmpIrBcat3HPhprodfromts



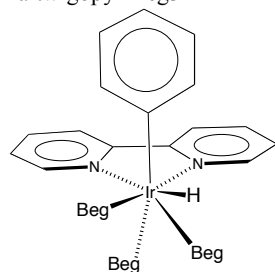
hartwigdmpIrBcat3HPh



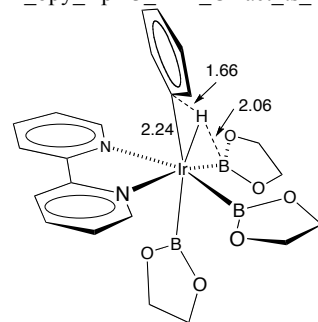
hartwigbpyIrBeg3



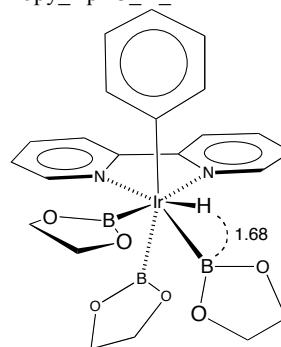
hartwigbpyIrBeg3HPh



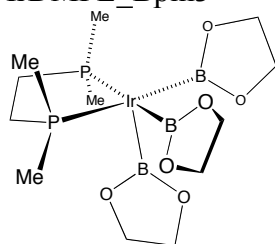
Ir_bpy_Bpin3_PhH_CHact_ts_lit



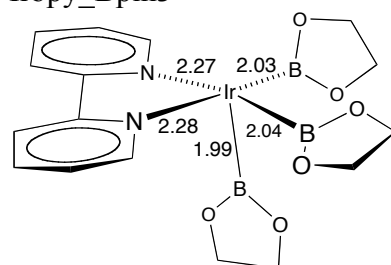
Irbpy_Bpin3_H_Ph



IrDMPE_Bpin3



Irbpy_Bpin3



anisole

anisole 5D
E(RB+HF-LYP) = -346.776574246

Zero-point correction= 0.133370 (Hartree/Particle)
Thermal correction to Energy= 0.140220
Thermal correction to Enthalpy= 0.141165
Thermal correction to Gibbs Free Energy= 0.102326
Sum of electronic and ZPE= -346.643204
Sum of electronic and thermal Energies= -346.636354
Sum of electronic and thermal Enthalpies= -346.635410
Sum of electronic and thermal Free Energies= -346.674248

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 87.990	26.285	81.743

C,0,0.7348489203,0.,-0.7692469004
C,0,-0.5126775006,0.,-0.1337280919
C,0,-0.5822563177,0.,1.2678257943
C,0,0.5855453267,0.,2.0220622781
C,0,1.8371862945,0.,1.3957747273
C,0,1.9004054447,0.,0.0043578993
O,0,-1.7143688012,0.,-0.7842773606
H,0,-1.561192389,0.,1.7362341139
H,0,0.5191456944,0.,3.1065126734
H,0,2.747567797,0.,1.9871120222
H,0,2.8648470934,0.,-0.4962024607
H,0,0.8106672336,0.,-1.8502084889
C,0,-1.7092665629,0.,-2.2017258303
H,0,-2.7567218978,0.,-2.5077899096
H,0,-1.2160383757,0.8934893974,-2.6066791619
H,0,-1.2160383757,-0.8934893974,-2.6066791619

benzodioxole5D

benzodioxolane
B3LYP/6-31G**
E(RB+HF-LYP) = -420.778371565

Zero-point correction= 0.116298 (Hartree/Particle)
Thermal correction to Energy= 0.122824
Thermal correction to Enthalpy= 0.123769
Thermal correction to Gibbs Free Energy= 0.085070
Sum of electronic and ZPE= -420.662073
Sum of electronic and thermal Energies= -420.655547
Sum of electronic and thermal Enthalpies= -420.654603
Sum of electronic and thermal Free Energies= -420.693302

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 77.073	25.411	81.449

C,0,0.3725482922,-0.599322845,-0.0998285698
C,0,-0.0103365634,0.7401981849,-0.0694953232
C,0,-1.3359386097,1.1209314486,0.0010795211
C,0,-2.2903423908,0.0864238319,0.0384090128
C,0,-1.9072451673,-1.2538225242,0.0080688646
C,0,-0.5509180787,-1.6254141904,-0.0610971369
O,0,1.1079406297,1.5413009663,-0.0954695126
H,0,-1.6206886333,2.1667374899,0.0271082156
H,0,-3.3438126929,0.3430275327,0.0899802202
H,0,-2.6654793609,-2.0300892638,0.0362659274
H,0,-0.2398993524,-2.6638216079,-0.0822316643

O,0,1.7448476732,-0.6868949071,-0.1459024392
C,0,2.2132440382,0.656344747,-0.307433391
H,0,2.9926036669,0.8623565274,0.4330774253
H,0,2.6008055492,0.7902286097,-1.3280671501

bisCF3benzene5D

Ir dmpw bcat3 bistrifluoromethylbenzene
B3LYP/6-31G**
E(RB+HF-LYP) = -906.317888632

Zero-point correction= 0.110362 (Hartree/Particle)
Thermal correction to Energy= 0.121841
Thermal correction to Enthalpy= 0.122785
Thermal correction to Gibbs Free Energy= 0.069950
Sum of electronic and ZPE= -906.207527
Sum of electronic and thermal Energies= -906.196048
Sum of electronic and thermal Enthalpies= -906.195104
Sum of electronic and thermal Free Energies= -906.247938

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 76.456	42.381	111.200

C,0,-0.0214906361,-0.0397157022,0.0274248792
F,0,0.2100384881,0.0059850529,1.357188097
F,0,1.1621944826,-0.2465370689,-0.5882210369
F,0,-0.7834316157,-1.1333796892,-0.2031432914
C,0,-0.695898102,1.215252944,-0.4623503245
C,0,-0.4849309638,1.6500142016,-1.7712929165
C,0,-1.1571660701,2.7811979661,-2.2353816899
C,0,-2.0360582342,3.4744174289,-1.3988920812
C,0,-2.240589026,3.0343854779,-0.0918651038
C,0,-1.5717132149,1.9056550524,0.3796783684
H,0,0.1953867931,1.1135701341,-2.4220714355
C,0,-0.8890779609,3.2929900766,-3.6267296242
H,0,-2.5583664974,4.3477866089,-1.7738261981
H,0,-2.9219842046,3.5716791257,0.5599440513
H,0,-1.7213692534,1.5621430737,1.3974002478
F,0,-1.9693364459,3.9165283529,-4.1446155395
F,0,0.125929836,4.1871061032,-3.6382405454
F,0,-0.546685719,2.2964698479,-4.470898205

metaxylene5D

meta-xylene 5D
B3LYP/6-31G**
E(RB+HF-LYP) = -310.892754831

Zero-point correction= 0.155421 (Hartree/Particle)
Thermal correction to Energy= 0.163519
Thermal correction to Enthalpy= 0.164463
Thermal correction to Gibbs Free Energy= 0.121083
Sum of electronic and ZPE= -310.737334
Sum of electronic and thermal Energies= -310.729236
Sum of electronic and thermal Enthalpies= -310.728292
Sum of electronic and thermal Free Energies= -310.771672

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 102.609	29.288	91.300

C,0,0.0136013377,-0.0572116649,0.0247833156
H,0,-0.0633113986,-0.1692420225,1.1108048076
H,0,1.0750423353,-0.056556827,-0.2409586306
H,0,-0.433829717,-0.9524917135,-0.4254529843

C,0,-0.6781798741,1.1990730633,-0.4523522288
C,0,-0.1922654867,1.9093350286,-1.5571721849
C,0,-0.8284767274,3.0603257853,-2.0383988013
C,0,-1.9806577002,3.5085669164,-1.3798352197
C,0,-2.4781352901,2.816838725,-0.2755399549
C,0,-1.8321812577,1.6702675601,0.1866448422
H,0,0.7096373227,1.5577550098,-2.0552261753
C,0,-0.2969936457,3.7880788134,-3.2518122192
H,0,-2.4854399426,4.4055970945,-1.7304460673
H,0,-3.3685135843,3.177744265,0.2323899407
H,0,-2.2216811041,1.1399452534,1.0523497705
H,0,0.7772938664,3.6243449162,-3.3794692302
H,0,-0.7900118307,3.4429174485,-4.1695449873
H,0,-0.468648303,4.8666233484,-3.1792899928

methythiophene5D

methythiophene
B3LYP/6-31G**
E(RB+HF-LYP) = -592.323829226

Zero-point correction= 0.094610 (Hartree/Particle)
Thermal correction to Energy= 0.100424
Thermal correction to Enthalpy= 0.101368
Thermal correction to Gibbs Free Energy= 0.064887
Sum of electronic and ZPE= -592.229219
Sum of electronic and thermal Energies= -592.223405
Sum of electronic and thermal Enthalpies= -592.222461
Sum of electronic and thermal Free Energies= -592.258942

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	63.017	21.162	76.781

S,0,-1.0854407548,-0.5600888785,-0.0606834796
C,0,0.2413514315,-1.6818703987,-0.0283177226
C,0,1.440383645,-1.0306201767,0.0208672481
C,0,1.2965104436,0.3924643442,0.0329308794
C,0,-0.0054898709,0.8157055356,-0.0069381036
H,0,0.0515962446,-2.7459953368,-0.0476153488
H,0,2.3965178221,-1.5412902752,0.0477524685
H,0,2.1330748237,1.0825115218,0.0700490844
C,0,-0.5309893921,2.2206061493,-0.008279049
H,0,-1.1758452711,2.418617578,0.8555491213
H,0,0.3033805434,2.9265923454,0.0291931533
H,0,-1.114551665,2.4398715918,-0.9097372516

veratroleoutout5D

veratrole
B3LYP/6-31G**
E(RB+HF-LYP) = -461.294082741

Zero-point correction= 0.166056 (Hartree/Particle)
Thermal correction to Energy= 0.175454
Thermal correction to Enthalpy= 0.176398
Thermal correction to Gibbs Free Energy= 0.131575
Sum of electronic and ZPE= -461.128027
Sum of electronic and thermal Energies= -461.118629
Sum of electronic and thermal Enthalpies= -461.117684
Sum of electronic and thermal Free Energies= -461.162508

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	110.099	35.418	94.339

C,0,-0.162839369,0.,-0.7028035036
C,0,-0.0979168113,0.,0.7149536471
C,0,1.1450832707,0.,1.3445203077
C,0,2.3259869842,0.,0.5879697905
C,0,2.2624767167,0.,-0.7979059334
C,0,1.0173892274,0.,-1.443306513
O,0,-1.3020259722,0.,1.3560034143
H,0,1.2047747432,0.,2.4264172016
H,0,3.2850763359,0.,1.0967942795
H,0,3.1710058217,0.,-1.3923189337
H,0,0.9779860902,0.,-2.5261605199
O,0,-1.4203284219,0.,-1.2314612733
C,0,-1.5445870433,0.,-2.6422522721
H,0,-2.6158739477,0.,-2.8500102417
H,0,-1.0903189518,0.893421945,-3.0911949303
H,0,-1.0903189518,-0.893421945,-3.0911949303
C,0,-1.2977346957,0.,2.7722383433
H,0,-2.345762658,0.,3.0763143227
H,0,-0.8047011542,-0.8934456079,3.178171504
H,0,-0.8047011542,0.8934456079,3.178171504

benzene5D

benzene
E(RB+HF-LYP) = -232.253117949

Zero-point correction= 0.100633 (Hartree/Particle)
Thermal correction to Energy= 0.105022
Thermal correction to Enthalpy= 0.105966
Thermal correction to Gibbs Free Energy= 0.073170
Sum of electronic and ZPE= -232.152485
Sum of electronic and thermal Energies= -232.148096
Sum of electronic and thermal Enthalpies= -232.147152
Sum of electronic and thermal Free Energies= -232.179948

	E	CV	S
KCAL/MOL	CAL/MOL-K	CAL/MOL-K	
TOTAL	65.902	17.142	69.024

6	-1.209447	0.698521	0.000000
6	0.000000	1.396658	0.000000
6	1.209672	0.698143	0.000000
6	1.209571	-0.698301	0.000000
6	-0.000204	-1.396658	0.000000
6	-1.209548	-0.698364	0.000000
1	2.150448	1.241684	0.000000
1	-2.150576	1.241422	0.000000
1	2.150389	-1.241748	0.000000
1	-0.000188	-2.483153	0.000000
1	-2.150640	-1.241348	0.000000
1	0.000297	2.483154	0.000000

pyrrole

pyrrole
B3LYP/6-31G**
E(RB+HF-LYP) = -210.171917378

Zero-point correction= 0.082684 (Hartree/Particle)
Thermal correction to Energy= 0.086667
Thermal correction to Enthalpy= 0.087612
Thermal correction to Gibbs Free Energy= 0.056933
Sum of electronic and ZPE= -210.089233
Sum of electronic and thermal Energies= -210.085250
Sum of electronic and thermal Enthalpies= -210.084306
Sum of electronic and thermal Free Energies= -210.114984

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	54.385	14.815	64.568

C,0,-0.9677821422,0.,-0.6630813911
C,0,-0.9817442121,0.,0.7151165375
C,0,0.3739127973,0.,1.1555962012
C,0,1.1727016626,0.,0.0324039566
N,0,0.3469046553,0.,-1.0676627467
H,0,-1.7735737226,0.,-1.3820662026
H,0,-1.865590945,0.,1.3376114172
H,0,0.7230665147,0.,2.1787172126
H,0,2.247209414,0.,-0.0756345672
H,0,0.6580275178,0.,-2.0252004587

metadibromobenzene

meta-dibromobenzene 5D
B3LYP/6-31G**
E(RB+HF-LYP) = -5373.85575037

Zero-point correction= 0.080726 (Hartree/Particle)
Thermal correction to Energy= 0.087827
Thermal correction to Enthalpy= 0.088771
Thermal correction to Gibbs Free Energy= 0.046580
Sum of electronic and ZPE= -5373.775025
Sum of electronic and thermal Energies= -5373.767923
Sum of electronic and thermal Enthalpies= -5373.766979
Sum of electronic and thermal Free Energies= -5373.809171

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	55.112	25.479	88.800

Br,0,-0.0035613296,0.0061684936,-0.0088392117
C,0,-0.9048971954,1.5673283347,-0.6381260911
C,0,-1.0219697523,1.7701036989,-2.0125142089
C,0,-1.6826129184,2.9143714716,-2.4574505379
C,0,-2.2180000749,3.8416897114,-1.5647673207
C,0,-2.0847341326,3.6108665714,-0.1952926935
C,0,-1.4290349486,2.4751620366,0.2808730547
H,0,-0.6107568326,1.0578616543,-2.7156474467
Br,0,-1.8533267107,3.2100560939,-4.3360286972
H,0,-2.7272726753,4.7237759119,-1.9338017642
H,0,-2.4973167868,4.3254810671,0.5101826205
H,0,-1.3259227835,2.2965667167,1.3444014554

bpyBpin32PyrroleCHactTS

Ir Bpin3 bpy pyrrole at C2
B3LYP/gen
E(RB+HF-LYP) = -1572.03532752

Zero-point correction= 0.451410 (Hartree/Particle)
Thermal correction to Energy= 0.481894
Thermal correction to Enthalpy= 0.482838
Thermal correction to Gibbs Free Energy= 0.387151
Sum of electronic and ZPE= -1571.583917
Sum of electronic and thermal Energies= -1571.553433
Sum of electronic and thermal Enthalpies= -1571.552489
Sum of electronic and thermal Free Energies= -1571.648177

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	302.393	113.804	201.391

C,0,-2.4040211185,1.50070161,-3.5863334747
C,0,-1.8596726823,2.6667746142,-3.0891314073
N,0,-0.9546810249,2.3209446222,-2.1138160341
C,0,-0.918191193,0.9510913236,-1.9366414536
C,0,-1.805193865,0.4221133499,-2.872054319
Ir,0,0.2133932144,0.0614033533,-0.2750709866
N,0,-1.4071373638,-1.5710288919,-0.2230811591
C,0,-2.5231459427,-1.2723782517,0.4808771087
C,0,-3.6267031938,-2.1365588519,0.4909990466
C,0,-3.5763728209,-3.3243662403,-0.2292051597
C,0,-2.4186860138,-3.6263396822,-0.941387582
C,0,-1.3589816782,-2.7231318715,-0.9110507294
C,0,-2.5077500252,0.0022272177,1.2371526037
N,0,-1.4111781348,0.7856355549,1.0944246405
C,0,-1.3423523838,1.9486448777,1.7646192935
C,0,-2.3551614379,2.3896089535,2.6096300432
C,0,-3.4847851881,1.5914783477,2.7722698166
C,0,-3.5587898711,0.3887419276,2.08028725
B,0,1.1259226554,-0.643778313,1.5193234963
O,0,1.3345563046,-1.9784496361,1.8650116037
C,0,1.830685395,-2.0549678996,3.2072817548
C,0,2.1103734335,-0.5896923293,3.6065070973
O,0,1.4935778871,0.1908548521,2.5743549885
B,0,1.78317918,-1.1480161213,-0.9160172821
O,0,3.1412880243,-1.035385642,-0.6709345546
C,0,3.8411626501,-2.0575097287,-1.3826314153
C,0,2.7426118558,-3.0447224606,-1.8183057318
O,0,1.5325593733,-2.2866585969,-1.7015032397
B,0,1.4795539577,1.6712983036,-0.1334179914
O,0,0.9585037063,2.9911897227,-0.0098580713
C,0,2.041368166,3.9335117257,-0.0400001157
C,0,3.2990447855,3.0628741668,0.1381511599
O,0,2.8626508897,1.7351154389,-0.1457493942
H,0,0.5371041796,0.1311234991,-1.8552630445
H,0,-0.43138134,-2.9047541878,-1.4419854392
H,0,-4.5220302619,-1.8837664037,1.0448135893
H,0,-2.3287549889,-4.5414942673,-1.5167735657
H,0,-4.4276018348,-3.9983156576,-0.2326491639
H,0,-4.427371636,-0.2459007094,2.2008934467
H,0,-4.2957901925,1.8967688836,3.4263019843
H,0,-2.2497743065,3.3383495577,3.1244521284
H,0,-0.4496994125,2.5347186193,1.5885924074
H,0,2.6873647147,-3.9183853563,-1.1559556384
H,0,2.8594913881,-3.3942066476,-2.8490647633
H,0,4.5910437528,-2.5150679267,-0.7293532301
H,0,4.3584031323,-1.6104871436,-2.2417296111
H,0,-0.4307562655,2.9487559898,-1.5174861831
H,0,-2.0451964363,3.7011522336,-3.3431612576
H,0,-3.1388376924,1.4306122686,-4.3777605807
H,0,-1.9875173757,-0.6320737429,-3.0344809219
H,0,1.0703605859,-2.5228955239,3.8457560416
H,0,2.7294911234,-2.6801135243,3.2323360229
H,0,1.678941223,-0.3235517454,4.5774932303
H,0,3.183580196,-0.3650338536,3.6327809597
H,0,2.0332660066,4.458810387,-1.003903911
H,0,1.9114217593,4.6728992476,0.7570554412
H,0,4.1085001286,3.3413468248,-0.5445770874
H,0,3.6844400299,3.1051387301,1.1652284921

bpyBpin32PyrroleCHopttoprod

bpyBpin32PyrroleCHopttoprod

B3LYP/gen

E(RB+HF-LYP) = -1572.04874526

Zero-point correction= 0.453698 (Hartree/Particle)

Thermal correction to Energy= 0.484995
 Thermal correction to Enthalpy= 0.485939
 Thermal correction to Gibbs Free Energy= 0.388752
 Sum of electronic and ZPE= -1571.595047
 Sum of electronic and thermal Energies= -1571.563750
 Sum of electronic and thermal Enthalpies= -1571.562806
 Sum of electronic and thermal Free Energies= -1571.659994

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	304.339	116.549	204.549

C,0,2.3223325809,-1.9093409361,-3.4462574468
 C,0,1.7937717037,-3.0009562693,-2.7933028669
 N,0,0.9519020778,-2.5230140932,-1.8121116222
 C,0,0.9158247833,-1.1380008639,-1.8009893586
 C,0,1.7740025196,-0.7453968105,-2.8262542006
 Ir,0,-0.2265741133,-0.0044432058,-0.3849924559
 N,0,1.5385823256,1.4531396266,-0.3902558845
 C,0,2.6209163051,1.0272739935,0.2982616629
 C,0,3.8425290974,1.709543475,0.2245123139
 C,0,3.9435488945,2.8469255721,-0.5686138176
 C,0,2.8177529728,3.2845914009,-1.2621787854
 C,0,1.6355433085,2.5580184696,-1.1440067029
 C,0,2.4291720899,-0.1791535285,1.1349180683
 N,0,1.2223530792,-0.7963236599,1.0568980987
 C,0,0.9830787253,-1.8802976109,1.8174864274
 C,0,1.9325590503,-2.4084404452,2.6851661413
 C,0,3.1769349374,-1.7889474976,2.7746660324
 C,0,3.4219084331,-0.6647446896,1.995695259
 B,0,-1.1046538028,0.7426778286,1.4427798934
 O,0,-0.8022768688,1.9419465016,2.0826213679
 C,0,-1.3078088286,1.8979312401,3.4249111002
 C,0,-2.1974083523,0.6375051215,3.4623558363
 O,0,-1.8414279092,-0.0880028086,2.2786485092
 B,0,-1.7078853611,1.4765749431,-0.5584410808
 O,0,-3.0769902762,1.3917613644,-0.3270833744
 C,0,-3.6999946458,2.5816054768,-0.8184916192
 C,0,-2.5392787963,3.5809700773,-0.9687645272
 O,0,-1.3776529862,2.7493039062,-1.0479140648
 B,0,-1.6063092292,-1.5205299129,-0.4372679605
 O,0,-1.3550692663,-2.8058480714,0.0944637103
 C,0,-2.4415679435,-3.6782468656,-0.2528171366
 C,0,-3.530665324,-2.7315578772,-0.7959207579
 O,0,-2.8464690055,-1.5059531765,-1.0545993725
 H,0,-1.0431862819,0.4105762665,-1.696231162
 H,0,0.7227930721,2.8604859581,-1.6417252952
 H,0,4.7103547812,1.3532721937,0.7653376998
 H,0,2.8458685079,4.1695239398,-1.8887510687
 H,0,4.8863605551,3.3802884764,-0.6414894972
 H,0,4.3788963509,-0.1632652534,2.0620534974
 H,0,3.9445481231,-2.1701563257,3.4410200405
 H,0,1.6905752667,-3.2875686856,3.2722150513
 H,0,0.0048509386,-2.3266147873,1.6942154883
 H,0,-2.4514908968,4.2428877875,-0.0972115035
 H,0,-2.6148364764,4.1971424455,-1.8703462606
 H,0,-4.4668784851,2.9153036494,-0.1124073112
 H,0,-4.1835361561,2.3643377838,-1.7798579272
 H,0,0.398126332,-3.0828512377,-1.1802576236
 H,0,1.9456880748,-4.0614634432,-2.9394262918
 H,0,3.0197925278,-1.9417243867,-4.2737038911
 H,0,1.9743587368,0.2788955405,-3.1143060754
 H,0,-0.4638846747,1.8337345964,4.1234658272
 H,0,-1.860417549,2.8182452315,3.6394662449
 H,0,-2.0193343665,0.0146262601,4.3449816998
 H,0,-3.2656038424,0.8833466815,3.4217352055
 H,0,-2.0984364556,-4.3928307101,-1.0122629906
 H,0,-2.7610753407,-4.2392757377,0.6312199587

H,0,-3.9904888828,-3.1005512215,-1.7183586302
H,0,-4.3251920341,-2.5543536966,-0.0597545706

bpyBpin33PyrroleCHactTS

Ir Bpin3 bpy pyrrole 3-position

B3LYP/gen

E(RB+HF-LYP) = -1572.02768754

Zero-point correction= 0.450991 (Hartree/Particle)

Thermal correction to Energy= 0.482539

Thermal correction to Enthalpy= 0.483483

Thermal correction to Gibbs Free Energy= 0.384732

Sum of electronic and ZPE= -1571.576696

Sum of electronic and thermal Energies= -1571.545148

Sum of electronic and thermal Enthalpies= -1571.544204

Sum of electronic and thermal Free Energies= -1571.642956

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 302.798	116.303	207.840

C,0,2.3317884728,-1.7710620075,-3.4712886288
N,0,1.2063975343,-2.5459665342,-3.6242450192
C,0,0.2325177547,-2.1180623737,-2.7491548499
C,0,0.7296274915,-1.0627990941,-1.9973255016
C,0,2.0650250023,-0.8421470895,-2.4881900031
Ir,0,-0.1889807531,-0.0562544916,-0.2579936462
N,0,1.5565827737,1.4124570288,-0.1726544688
C,0,2.6335133678,1.0229492277,0.5468983049
C,0,3.7589046294,1.8509295879,0.6661499283
C,0,3.7694024563,3.0883991721,0.0322584393
C,0,2.6520334751,3.4776241826,-0.7041277962
C,0,1.5656365422,2.6102364444,-0.7781269012
C,0,2.5412826767,-0.3059445449,1.1996241043
N,0,1.3765168844,-0.983193596,1.0435113071
C,0,1.2222114837,-2.179375101,1.6376697422
C,0,2.2252830139,-2.7669565552,2.4025244189
C,0,3.4321943199,-2.0897446034,2.5617293329
C,0,3.5880299883,-0.8475498034,1.9578057053
B,0,-0.9427209049,0.7712289624,1.5688435804
O,0,-0.7917886423,2.1133199947,1.9362960061
C,0,-1.2653915815,2.2959496989,3.2763854193
C,0,-1.9546374318,0.9608879082,3.6293049671
O,0,-1.5485880984,0.0581326484,2.5951276316
B,0,-1.705987222,1.2647740181,-0.7672652573
O,0,-3.0470599416,1.2100844558,-0.3980764671
C,0,-3.7592236933,2.2574388689,-1.0613505057
C,0,-2.6579116573,3.2131026045,-1.5549541363
O,0,-1.472857506,2.4087822531,-1.5482207313
B,0,-1.6214923365,-1.514608234,-0.2140049249
O,0,-1.7112308372,-2.5075753315,0.7733124814
C,0,-2.8652107593,-3.3166478061,0.5373876923
C,0,-3.308286271,-2.9455162618,-0.8939105587
O,0,-2.5862092202,-1.7522762266,-1.1990915305
H,0,-0.4766560069,0.0737461067,-1.8345458825
H,0,0.6605406455,2.8610293395,-1.3211008447
H,0,4.6178694828,1.5382381605,1.2469181068
H,0,2.6136667508,4.4349044737,-1.2128316631
H,0,4.6359243226,3.7373071092,0.1160407023
H,0,4.5188052045,-0.3066311147,2.0743950199
H,0,4.2396876225,-2.5171561917,3.1484156582
H,0,2.0529561603,-3.7354274917,2.8594649535
H,0,0.2558572571,-2.6489657861,1.490314719
H,0,-2.5210000312,4.0668823496,-0.8780987395
H,0,-2.8392232144,3.5943731311,-2.5650038792
H,0,-4.4563676989,2.7319728326,-0.3631288486

H,0,-4.3366758961,1.8315151932,-1.8923424241
H,0,-0.7495438541,-2.566168291,-2.743012442
H,0,1.1041114147,-3.2973363424,-4.2870374324
H,0,3.2169134407,-1.9454395763,-4.0668745508
H,0,2.7601874816,-0.0860063762,-2.1501019612
H,0,-0.4132319579,2.5116837522,3.9342521297
H,0,-1.9488042211,3.1511463898,3.3133313629
H,0,-1.6481693928,0.5674216658,4.6045181957
H,0,-3.0485678127,1.0458215068,3.6216753579
H,0,-2.6058200502,-4.3761571855,0.6423508863
H,0,-3.6328502361,-3.0745815853,1.2833904061
H,0,-3.0476520351,-3.727004547,-1.6215799884
H,0,-4.3847791352,-2.7576407718,-0.968681973

bpyBpin33PyrroleCHopttoprod

bpyBpin33PyrroleCHopttoprod

B3LYP/gen

E(RB+HF-LYP) = -1572.04023714

Zero-point correction= 0.453116 (Hartree/Particle)

Thermal correction to Energy= 0.484682

Thermal correction to Enthalpy= 0.485626

Thermal correction to Gibbs Free Energy= 0.387281

Sum of electronic and ZPE= -1571.587121

Sum of electronic and thermal Energies= -1571.555555

Sum of electronic and thermal Enthalpies= -1571.554611

Sum of electronic and thermal Free Energies= -1571.652956

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 304.143	117.033	206.984

C,0,-1.823790789,3.4309049727,-2.354881211
N,0,-0.5588021933,3.5725294431,-2.8703433116
C,0,0.2671565106,2.6120721774,-2.3188187683
C,0,-0.4585104725,1.8262880834,-1.4347220038
C,0,-1.7917063206,2.3699327362,-1.4725917546
Ir,0,0.2785753318,0.1392141656,-0.3250549404
N,0,-1.5599512191,-1.0435251693,-1.0177628664
C,0,-2.6629337449,-0.8976849139,-0.252472272
C,0,-3.8742520109,-1.5113671833,-0.60149045
C,0,-3.9425586415,-2.2761112893,-1.7603041839
C,0,-2.7996765497,-2.4117502377,-2.5460913211
C,0,-1.6293059587,-1.7794415874,-2.1359617568
C,0,-2.5134464866,-0.0396727535,0.9455902894
N,0,-1.3078346974,0.5612990396,1.1237075176
C,0,-1.1261603253,1.3791894356,2.1783959614
C,0,-2.1294457095,1.6300165153,3.1079164154
C,0,-3.3664405338,1.0096377979,2.9480431355
C,0,-3.5566462715,0.1703427353,1.8573987976
B,0,0.7820970032,-1.2750430392,1.2328596485
O,0,0.1634867839,-2.5135917143,1.4077498395
C,0,0.4482236469,-2.9943900124,2.729290445
C,0,1.5575575944,-2.0561291314,3.2478051924
O,0,1.5303800298,-0.9401511764,2.3517046177
B,0,1.6501066607,-1.3673868311,-0.8114021589
O,0,2.9790498832,-1.5064937675,-0.4131342026
C,0,3.5934219006,-2.5179712723,-1.214857606
C,0,2.4077394939,-3.2910172138,-1.8201240506
O,0,1.3158285999,-2.3717445191,-1.7345842744
B,0,1.7422111164,1.4298369403,0.2926669212
O,0,1.6947985295,2.2002976971,1.4615914015
C,0,2.9208333002,2.9246800875,1.5993582547
C,0,3.5908401377,2.802247676,0.2156153158
O,0,2.8963035737,1.7330742224,-0.4279101373
H,0,1.2679615274,0.0578193463,-1.5784969645

H,0,-0.704725808,-1.870280452,-2.6915806005
H,0,-4.7570905035,-1.3885866384,0.0136046881
H,0,-2.8063709544,-2.9952012762,-3.4604725729
H,0,-4.8749337464,-2.7540750985,-2.0450805574
H,0,-4.5114202494,-0.3200735263,1.7161810939
H,0,-4.171653518,1.1761034045,3.6571105459
H,0,-1.931557922,2.2987899103,3.9383922483
H,0,-0.1423257303,1.8284434168,2.2535380133
H,0,2.168752633,-4.1944002912,-1.2429060691
H,0,2.5694184817,-3.5784456303,-2.8642261628
H,0,4.2415956285,-3.1418968608,-0.5912345582
H,0,4.2104978285,-2.0416011979,-1.9883832261
H,0,1.3121111664,2.5654987231,-2.5904241139
H,0,-0.2802084615,4.2657240383,-3.5455014126
H,0,-2.6284089678,4.0885714645,-2.6535201864
H,0,-2.6500755362,2.0264555895,-0.9085695642
H,0,-0.4639619379,-2.9355487419,3.3371665656
H,0,0.7598040442,-4.0428133445,2.6804722811
H,0,1.3827291818,-1.712189796,4.2724008647
H,0,2.548743668,-2.525301724,3.2054601944
H,0,2.70940287,3.9616182875,1.8817551737
H,0,3.5238774261,2.463884593,2.3922887697
H,0,3.475278937,3.7191174861,-0.3780452414
H,0,4.6582967706,2.5662584045,0.280732308

dmpeBpin3MetaAnisCHactTSParParBackA

Ir Bpin3 bpy meta anisole
B3LYP/gen
E(RB+HF-LYP) = -2134.27447502

Zero-point correction= 0.553169 (Hartree/Particle)
Thermal correction to Energy= 0.591298
Thermal correction to Enthalpy= 0.592242
Thermal correction to Gibbs Free Energy= 0.479907
Sum of electronic and ZPE= -2133.721306
Sum of electronic and thermal Energies= -2133.683177
Sum of electronic and thermal Enthalpies= -2133.682233
Sum of electronic and thermal Free Energies= -2133.794568

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 371.045	138.796	236.430

C,0,2.713461871,1.1913254302,0.3891227466
C,0,1.9790035187,0.0507420332,0.7777685978
C,0,2.6360485012,-0.9018355885,1.5732458151
C,0,3.9897812146,-0.7612675026,1.9064967693
C,0,4.7161780127,0.3417303918,1.4781555427
C,0,4.0660849485,1.3292983224,0.7247304023
Ir,0,-0.1857907159,-0.1755833113,0.0373545434
P,0,0.3250900006,-0.0018739105,-2.3178925168
C,0,0.1026971435,-1.6954245075,-3.0754416376
C,0,0.6824537834,-2.7819683109,-2.1615064244
P,0,0.0361409515,-2.6141425313,-0.4117530617
B,0,-2.2389928438,-0.0285794663,-0.5168581548
O,0,-2.8532003787,1.156605111,-0.9346295781
C,0,-4.2712962722,0.9704711741,-0.9953311412
C,0,-4.45773027,-0.5581486291,-0.9468323007
O,0,-3.1880436,-1.0593619668,-0.5088472145
B,0,-1.2531669776,-0.6604879024,1.8028123164
O,0,-1.0639119162,-1.8821206871,2.4646528837
C,0,-2.0337825898,-1.9941262574,3.5166478449
C,0,-2.6195219205,-0.5737918012,3.647429106
O,0,-2.219923559,0.0927534349,2.4457328374
B,0,-0.4041330805,1.8997824529,0.2297657249
O,0,-0.7758231836,2.5813849218,1.3792177253

C,0,-0.6484341058,3.9891842909,1.1706368362
C,0,-0.4156367589,4.13799683,-0.3463636751
O,0,-0.0686350291,2.8167603041,-0.7825417965
H,0,-4.7348756207,1.4698886746,-0.1360008938
H,0,-4.6655252754,1.421601284,-1.9121303668
H,0,-5.2381181095,-0.870718185,-0.2455468525
H,0,-4.6936694567,-0.9807366768,-1.9325268824
H,0,-2.7948184409,-2.7304715289,3.2278497846
H,0,-1.5443754359,-2.3426275182,4.4315050401
H,0,-3.711340558,-0.5688059215,3.7260235005
H,0,-2.2079671731,-0.033845067,4.5092580832
H,0,-1.3213407917,4.4646490847,-0.8728870199
H,0,0.3953254538,4.8329909426,-0.5902158299
H,0,-1.5562045213,4.4974965208,1.5119284198
H,0,0.1985234624,4.3665312045,1.7586627036
H,0,0.5084253533,0.0793180165,1.4847032767
H,0,2.2186645954,1.9685883362,-0.1785015135
O,0,4.8465352882,2.3980581315,0.3637556566
H,0,2.0828205447,-1.7440171556,1.9710606002
H,0,4.474541168,-1.515554211,2.5221055945
H,0,5.7633299893,0.4759759699,1.729368578
C,0,-0.6811118941,1.0706684399,-3.4282294906
C,0,2.0398544171,0.4465880214,-2.8456300341
C,0,-1.4897173851,-3.6573598369,-0.4415857598
C,0,1.1790565707,-3.7649746441,0.4825786624
H,0,0.4712257084,-3.7840170725,-2.5532400132
H,0,1.7731049248,-2.6821736677,-2.1023316116
H,0,-0.9758842635,-1.8444783888,-3.2063176641
H,0,0.5588360096,-1.7247417526,-4.0723403001
H,0,2.1632576405,0.300708903,-3.9237305052
H,0,2.220833877,1.4960222783,-2.6040782204
H,0,2.7718182205,-0.1533331153,-2.3019802576
H,0,-0.3916574242,0.9343291475,-4.4752952216
H,0,-1.7408312722,0.8453567995,-3.2976441434
H,0,-0.5231686159,2.1061199266,-3.1226297713
H,0,1.144569555,-4.7632028175,0.0334973808
H,0,2.2027972485,-3.38846858,0.4485615439
H,0,0.8642227443,-3.8320097457,1.5267677956
H,0,-1.2754156871,-4.6560162265,-0.8365892137
H,0,-1.859462591,-3.7413080465,0.5829656168
H,0,-2.2650906487,-3.165347932,-1.0284133248
C,0,4.2380573192,3.4690400496,-0.3335535641
H,0,5.0202460814,4.2158368764,-0.4843410399
H,0,3.8504906691,3.1545395085,-1.3119925196
H,0,3.4169403937,3.9169848837,0.2415057696

dmpeBpin3MetaAnisCHactTSParSptBackA

Ir Bpin3 C-H act of meta-anisole Par Spt Back A
B3LYP/gen
E(RB+HF-LYP) = -2134.27655396

Zero-point correction= 0.553193 (Hartree/Particle)
Thermal correction to Energy= 0.591257
Thermal correction to Enthalpy= 0.592201
Thermal correction to Gibbs Free Energy= 0.481746
Sum of electronic and ZPE= -2133.723361
Sum of electronic and thermal Energies= -2133.685297
Sum of electronic and thermal Enthalpies= -2133.684353
Sum of electronic and thermal Free Energies= -2133.794808

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 371.019	138.951	232.473

C,0,4.0455379452,1.4527487208,0.4006472369
C,0,2.6744200814,1.2759936771,0.1620896593

C,0,1.9649701409,0.1854851784,0.6801074033
C,0,2.6789236489,-0.691820484,1.5242124895
C,0,4.0393071877,-0.514015622,1.7739427326
C,0,4.7457965686,0.5500244612,1.2071148581
Ir,0,-0.2087794231,-0.1427969742,0.0715655326
B,0,-0.5126765357,1.9154079732,-0.1860282409
O,0,-1.1044356869,2.5122005468,-1.3115870012
C,0,-1.2753413267,3.9138736835,-1.0586815276
C,0,-0.4027486043,4.1895448589,0.1826656683
O,0,-0.1219730218,2.8940848484,0.7169859642
H,0,5.8027372128,0.6721531538,1.4125108919
P,0,0.4000313886,-0.4760549391,-2.2520593586
C,0,2.1706486341,-0.2325665335,-2.7257074272
P,0,-0.125462743,-2.61908936,0.1212814542
C,0,0.8048751895,-3.6890682286,1.3150799766
B,0,-2.2513716338,-0.1907419566,-0.5406503021
O,0,-2.7308507591,-0.8563004087,-1.6870381929
C,0,-4.1161006306,-0.5375098598,-1.8848511863
C,0,-4.5503069576,0.1119377334,-0.5577515149
O,0,-3.3236435308,0.4193732922,0.1104441834
B,0,-1.2544650632,-0.1091475401,1.9217546086
O,0,-1.6658972368,1.0003694045,2.6353631103
C,0,-2.5165733747,0.5761688611,3.7021557249
C,0,-2.2332326372,-0.9317919977,3.8390879287
O,0,-1.6177384118,-1.2867924918,2.5911441316
C,0,0.120446941,-2.2761729458,-2.6613562706
C,0,0.5885834746,-3.1828585985,-1.5147055368
C,0,-0.4702329149,0.3935213891,-3.6232605229
C,0,-1.7681892024,-3.4678939838,0.1542404246
H,0,-5.1406751352,-0.5728958035,0.0647662504
H,0,-5.1298027856,1.0291775224,-0.7032188762
H,0,-4.6743312244,-1.4496610613,-2.120213063
H,0,-4.2087965262,0.1532908466,-2.7324066124
H,0,-3.1392554683,-1.5282672563,3.9867943489
H,0,-1.5360010285,-1.1500308741,4.6583142997
H,0,-3.5608161123,0.7736476433,3.4283638592
H,0,-2.2804159954,1.141095939,4.6093280563
H,0,-2.3369876346,4.1165045294,-0.8692106017
H,0,-0.9655862463,4.4888872165,-1.9379258669
H,0,-0.9157571579,4.7951830882,0.9366453187
H,0,0.541295834,4.6876720808,-0.0750859734
H,0,0.4761073623,0.3634741608,1.4492778243
H,0,2.1819842818,2.0296048492,-0.4409030777
O,0,4.6094187785,2.5471751708,-0.2062400322
H,0,2.1604492634,-1.5020506183,2.0219863664
H,0,4.5618249804,-1.2057508218,2.4310836145
H,0,0.3193913094,-4.2285632076,-1.7061563204
H,0,1.6802870835,-3.1430403094,-1.4168294115
H,0,-0.9581923681,-2.3808509278,-2.8138142008
H,0,0.6232425357,-2.5306850126,-3.601980729
H,0,2.3390124863,-0.5804804321,-3.7502275394
H,0,2.4295939554,0.8262054374,-2.6602495553
H,0,2.8247554003,-0.7716156325,-2.0380937251
H,0,-0.0491321437,0.111980155,-4.5937393039
H,0,-1.527392476,0.1294100093,-3.5821668804
H,0,-0.3825864131,1.4700091482,-3.4679947338
H,0,0.6426251355,-4.7485743464,1.0906105206
H,0,1.8743028428,-3.4761495825,1.2700923826
H,0,0.4444862618,-3.4812908799,2.3258808319
H,0,-1.6608146195,-4.5529124816,0.0534687035
H,0,-2.2430587839,-3.2270358939,1.1077680335
H,0,-2.3905440893,-3.0769637508,-0.6524472243
C,0,5.9779966899,2.8118565914,0.0389964164
H,0,6.2155294879,3.7243989029,-0.5113355665
H,0,6.1770932134,2.9744950761,1.1068181078
H,0,6.6237534441,1.9989439451,-0.3207044204

dmpeBpin3MetaAnisCHactTSSptSptBackA

dmpe Bpin3 meta-anisole spt spt back A
B3LYP/gen
E(RB+HF-LYP) = -2134.27770407

Zero-point correction= 0.553243 (Hartree/Particle)
Thermal correction to Energy= 0.591316
Thermal correction to Enthalpy= 0.592261
Thermal correction to Gibbs Free Energy= 0.482004
Sum of electronic and ZPE= -2133.724461
Sum of electronic and thermal Energies= -2133.686388
Sum of electronic and thermal Enthalpies= -2133.685444
Sum of electronic and thermal Free Energies= -2133.795700

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 371.057	138.917	232.055

C,0,3.1755398497,-0.6961767473,0.7900930997
C,0,2.275751457,0.3678075002,0.6339856849
C,0,2.8169117111,1.6692400848,0.7183239772
C,0,4.1844488093,1.8708165132,0.8981361379
C,0,5.0750597373,0.7996817456,1.0180080474
C,0,4.5539801028,-0.4948869928,0.9668911289
Ir,0,0.0797699321,0.0072154989,0.0788919832
P,0,0.7227799292,-0.7240342544,-2.1309869502
C,0,0.5233824276,-2.5854572396,-2.1998828493
C,0,0.9022847177,-3.2618900216,-0.8719675947
P,0,0.061404722,-2.4056343714,0.5651595365
B,0,-1.9492065338,-0.0453748459,-0.5634837943
O,0,-2.458187879,-0.9192066899,-1.542301675
C,0,-3.8223526728,-0.5783299716,-1.8296904643
C,0,-4.2247815053,0.3736784813,-0.6882414727
O,0,-2.9839742899,0.765144429,-0.0936581927
B,0,-1.008432933,0.3971370273,1.867546524
O,0,-1.5504785294,-0.6423278029,2.6394615988
C,0,-2.1420809166,-0.0779973445,3.8191030342
C,0,-2.1984671488,1.4333910618,3.5251409557
O,0,-1.2789975473,1.6207585729,2.447036225
B,0,-0.1541149946,2.0052442794,-0.5342951119
O,0,0.0638440487,3.1425671863,0.2367661208
C,0,-0.1139623519,4.3168312176,-0.5579695751
C,0,-0.7613456383,3.8064256881,-1.8596724296
O,0,-0.5542536428,2.3889373423,-1.8276907238
H,0,-3.8726270579,-0.0912430009,-2.8118700537
H,0,-4.4300917809,-1.4884466229,-1.8644572944
H,0,-4.760340596,1.2604936714,-1.041637855
H,0,-4.8455407919,-0.1261649657,0.0665200388
H,0,-3.1295224213,-0.5207278825,3.9852494469
H,0,-1.5087673389,-0.308896078,4.6856597499
H,0,-3.1982223469,1.7519267011,3.2038227956
H,0,-1.8950481567,2.0476151597,4.3787363698
H,0,-1.8389037486,4.0124881629,-1.8923884867
H,0,-0.3025794194,4.2278903587,-2.7606197759
H,0,-0.7440107887,5.0323545566,-0.0199656608
H,0,0.8630438971,4.7856418604,-0.7377567722
H,0,0.8203615355,0.4441725095,1.4622006789
H,0,2.852854155,-1.7290777498,0.7606808593
O,0,5.3028025195,-1.6417959249,1.0739421465
H,0,2.1560655609,2.5252599462,0.6632224435
H,0,4.5712574054,2.8857890231,0.9563369058
H,0,6.1338298877,0.9827920072,1.1588980327
C,0,-0.1592359111,-0.1786281346,-3.6543840333
C,0,2.4818258828,-0.4512099056,-2.6252135046
C,0,-1.5920382338,-3.2312188236,0.6003756168
C,0,0.8279234639,-3.1826941959,2.0614356538
H,0,0.6398673286,-4.3265600085,-0.8879470307

H,0,1.9839275649,-3.1971037419,-0.7073947247
H,0,-0.5350203451,-2.7587016073,-2.423192837
H,0,1.1086868872,-2.9937154771,-3.0322675957
H,0,2.6894690361,-0.9165394834,-3.5942505888
H,0,2.6615910226,0.624802789,-2.6956229183
H,0,3.1577566142,-0.8496862695,-1.867371805
H,0,0.2793544686,-0.642209074,-4.5439175774
H,0,-1.2102108195,-0.454676128,-3.5668513625
H,0,-0.0923342695,0.9083860208,-3.7192905833
H,0,0.8025645023,-4.2757891649,2.0003237905
H,0,1.8580752577,-2.8517442884,2.2004539657
H,0,0.2447075984,-2.8582915474,2.9272019673
H,0,-1.494407502,-4.3164040357,0.7118608255
H,0,-2.1449311377,-2.8191206703,1.4473555516
H,0,-2.1344396291,-2.9939308824,-0.3161480769
C,0,6.6973406444,-1.5065275371,1.2771801724
H,0,7.0960453734,-2.5208162817,1.3424884789
H,0,7.1833353969,-0.9834740466,0.4424024486
H,0,6.9236094309,-0.9711565851,2.2090523771

dmpeBpin3MetaAnisCHactTSSptSptBackAopttoprod

dmpeBpin3MetaAnisCHactTSSptSptBackAopttoprod

B3LYP/gen

E(RB+HF-LYP) = -2134.29028228

Zero-point correction= 0.556902 (Hartree/Particle)

Thermal correction to Energy= 0.594658

Thermal correction to Enthalpy= 0.595602

Thermal correction to Gibbs Free Energy= 0.486787

Sum of electronic and ZPE= -2133.733380

Sum of electronic and thermal Energies= -2133.695624

Sum of electronic and thermal Enthalpies= -2133.694680

Sum of electronic and thermal Free Energies= -2133.803495

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 373.154	138.691	229.020

C,0,3.0403919806,-0.1275576018,-0.0658235889
C,0,1.9387401392,0.6287527576,0.3649986417
C,0,2.2649880118,1.7970844779,1.0992948263
C,0,3.5850076634,2.1599805421,1.3618112968
C,0,4.6635584214,1.3903422682,0.9119725782
C,0,4.3745552652,0.2334797218,0.1888644061
Ir,0,-0.1923145611,0.0495291823,0.1114208525
P,0,0.1026675264,-0.454212716,-2.171717554
C,0,0.2613700499,-2.3118756987,-2.3405756944
C,0,0.9953836933,-2.9690034557,-1.1619326237
P,0,0.3399489455,-2.3365662261,0.478318557
B,0,-2.2797795808,-0.3535124287,-0.2926680049
O,0,-2.7276562557,-1.5333731265,-0.9152239723
C,0,-4.1330910506,-1.4444767124,-1.1889355534
C,0,-4.5828879601,-0.1446951505,-0.4901397678
O,0,-3.3671064419,0.4910312338,-0.0829652585
B,0,-1.3899868166,0.1893585931,1.942788974
O,0,-1.7416821064,-0.9611526985,2.6614369239
C,0,-2.5902283508,-0.558894842,3.7476592227
C,0,-3.018839035,0.8723421167,3.3745575954
O,0,-2.0175106788,1.3080755053,2.4556621581
B,0,-0.5869273709,2.0504727367,-0.3756675516
O,0,-0.5986933046,3.1096148124,0.520295055
C,0,-0.7328114024,4.3442776232,-0.1867740763
C,0,-1.1093203124,3.9298809467,-1.6235201674
O,0,-0.814363231,2.5275661403,-1.678120669
H,0,-4.2882626241,-1.4079224615,-2.2749996215
H,0,-4.6382743728,-2.3355470619,-0.802331866

H,0,-5.1402366394,0.523981646,-1.1539876462
H,0,-5.2010429014,-0.3412215809,0.3945374738
H,0,-3.4314320311,-1.2537280171,3.8349919132
H,0,-2.0155788921,-0.5880176427,4.682536258
H,0,-3.9957561599,0.8899173984,2.8739742707
H,0,-3.0519935667,1.5504450638,4.2325612331
H,0,-2.1760284445,4.0816772427,-1.8319213096
H,0,-0.5292035705,4.4588859718,-2.3871110031
H,0,-1.4996613591,4.9616427883,0.2921365402
H,0,0.2208895795,4.8867760545,-0.1503374233
H,0,-0.0450224211,0.4577586073,1.7261265518
H,0,2.9156023051,-1.0487754278,-0.6254383814
O,0,5.3208903644,-0.6291135186,-0.3165878684
H,0,1.4719026717,2.4381325336,1.468386489
H,0,3.7868275188,3.0641728014,1.9327587203
H,0,5.6816719213,1.6932286673,1.1272629413
C,0,-1.2266633489,-0.0769451838,-3.3923957123
C,0,1.5538378121,0.2699311544,-3.0473704034
C,0,-0.9855309577,-3.5645796678,0.8661050091
C,0,1.645658439,-2.8341786378,1.6874218134
H,0,0.8946147529,-4.0598221675,-1.2076564512
H,0,2.0662406104,-2.7469910377,-1.2027788158
H,0,-0.7713622082,-2.6732816336,-2.3806344836
H,0,0.7390810325,-2.5586200502,-3.2960707395
H,0,1.6226047924,-0.1320270181,-4.0633103604
H,0,1.3981114634,1.3506616251,-3.0939591137
H,0,2.4787572474,0.0817814719,-2.5048039861
H,0,-0.908970077,-0.3713880482,-4.3975671705
H,0,-2.1345375069,-0.6170189744,-3.1249863541
H,0,-1.414570136,0.9967751936,-3.3560186403
H,0,1.9153077807,-3.8902725113,1.5824506649
H,0,2.5300579083,-2.2089779795,1.5518280313
H,0,1.2563546695,-2.6665150712,2.6958278882
H,0,-0.5864766324,-4.5843707986,0.8781573534
H,0,-1.4048098114,-3.3164522188,1.8429880027
H,0,-1.7790794395,-3.4759975334,0.1229503324
C,0,6.68202557,-0.3320721171,-0.0713480037
H,0,7.2597346781,-1.1318633225,-0.5396468218
H,0,6.977718453,0.6292083547,-0.5135252591
H,0,6.9080642925,-0.3085768942,1.0035113427

dmpeBpin3MetaAnisCHactTSSptSptBackS

Ir Bpin3 dmpe C-H activation with meta-anisole spt spt back S
B3LYP/gen
E(RB+HF-LYP) = -2134.27720315

Zero-point correction= 0.553671 (Hartree/Particle)
Thermal correction to Energy= 0.591468
Thermal correction to Enthalpy= 0.592412
Thermal correction to Gibbs Free Energy= 0.483421
Sum of electronic and ZPE= -2133.723532
Sum of electronic and thermal Energies= -2133.685735
Sum of electronic and thermal Enthalpies= -2133.684791
Sum of electronic and thermal Free Energies= -2133.793782

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 371.152	138.713	229.391

C,0,3.0123338812,-0.1592511065,0.3898857142
C,0,1.9111629199,0.7250208937,0.4427887832
C,0,2.2042749421,2.0827631608,0.6222651422
C,0,3.5255508578,2.5545444348,0.694706907
C,0,4.602725813,1.6682314378,0.6108393023
C,0,4.3240693354,0.3066953094,0.4621031217
Ir,0,-0.2360546163,0.0066376542,0.0524105509

P,0,0.2871430789,-0.3744830302,-2.2733758766
C,0,0.4331649742,-2.222393181,-2.5361517718
C,0,1.0627479017,-2.9400226413,-1.3309027279
P,0,0.2311712028,-2.3994563835,0.2592656904
B,0,-2.2825208557,-0.3660517447,-0.4003274948
O,0,-2.7385263232,-1.228299207,-1.4151839494
C,0,-4.1649844381,-1.1203609754,-1.5332076129
C,0,-4.5955768494,-0.3661220418,-0.2619270635
O,0,-3.383235006,0.1940091253,0.2505444857
B,0,-1.1721798087,0.0222065859,1.9659075747
O,0,-1.4275993185,-1.1662952749,2.667298193
C,0,-1.9889003181,-0.8329308692,3.9457566131
C,0,-2.3500694659,0.6599586352,3.8203585798
O,0,-1.5982197304,1.114810836,2.6936018415
B,0,-0.8746637759,1.9769936823,-0.3094651452
O,0,-0.788418077,3.0527535507,0.5666248304
C,0,-1.2187807723,4.2508568895,-0.083574168
C,0,-1.8843216576,3.7636492571,-1.3848672556
O,0,-1.4431436544,2.4067164871,-1.5227307407
H,0,-4.4095733144,-0.5641936846,-2.4471423831
H,0,-4.6052364797,-2.1199520781,-1.6095771759
H,0,-5.3147421955,0.4339713734,-0.4638766505
H,0,-5.0295507389,-1.038370364,0.4895093812
H,0,-2.8570784564,-1.4694634971,4.1451736942
H,0,-1.239386418,-1.0147717776,4.7270603263
H,0,-3.4190402351,0.8080926647,3.6215450269
H,0,-2.076443491,1.2431210064,4.705243181
H,0,-2.9798730686,3.7810654033,-1.3197663224
H,0,-1.5820056841,4.3425982019,-2.2641729711
H,0,-1.9072563669,4.7960395511,0.5698138918
H,0,-0.3475571487,4.8904770947,-0.2778594623
H,0,0.5601999104,0.4369783752,1.4069600956
H,0,2.8593763026,-1.2241361013,0.2675091014
H,0,1.4080363851,2.8097457654,0.7282056033
O,0,3.6531866977,3.910381008,0.8533170042
H,0,5.6294462252,2.0097957105,0.6683790756
C,0,-0.8507351357,0.1194119653,-3.6359239555
C,0,1.8947674671,0.2921460873,-2.8912294249
C,0,-1.224198277,-3.5365051048,0.3426716166
C,0,1.2771056751,-3.1443231648,1.5944991542
H,0,0.995859853,-4.0284169426,-1.4472275954
H,0,2.1261273833,-2.6877066707,-1.2517000824
H,0,-0.5922053373,-2.5757208809,-2.6886166756
H,0,0.9935713778,-2.4265935204,-3.4560855452
H,0,2.0808046277,-0.0327432279,-3.9200815592
H,0,1.8527320533,1.3839891153,-2.8597858832
H,0,2.7139291743,-0.024901861,-2.2444176375
H,0,-0.4371349367,-0.1595632727,-4.6105241093
H,0,-1.8112471321,-0.3729639577,-3.4808512097
H,0,-1.0023154875,1.1983607622,-3.5800694918
H,0,1.4514171247,-4.2113211772,1.4204629798
H,0,2.2340267421,-2.6280933479,1.6837477682
H,0,0.7327366608,-3.0176834332,2.5339942582
H,0,-0.9105891288,-4.5854059321,0.3126073721
H,0,-1.7469066738,-3.3350503662,1.2802893586
H,0,-1.9022295183,-3.3216151995,-0.4845549798
C,0,4.9572786092,4.4478151306,0.966040683
H,0,4.8329170314,5.5243803187,1.0978934151
H,0,5.4937874069,4.0398174305,1.8334016471
H,0,5.5553557892,4.2644547973,0.0627509717
H,0,5.1497894879,-0.3992566838,0.402626985

dmpeBpin3MetaAnisCHactTSSptSptFrntA

Ir Bpin3 dmpe C-H activation for meta anisole, ring splitting Ps, OMe n
B3LYP/gen
E(RB+HF-LYP) = -2134.27607120

Zero-point correction= 0.553291 (Hartree/Particle)
Thermal correction to Energy= 0.591369
Thermal correction to Enthalpy= 0.592313
Thermal correction to Gibbs Free Energy= 0.481633
Sum of electronic and ZPE= -2133.722780
Sum of electronic and thermal Energies= -2133.684702
Sum of electronic and thermal Enthalpies= -2133.683758
Sum of electronic and thermal Free Energies= -2133.794438

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	371.090	138.867	232.945

C,0,0.0054220221,-3.4478032636,-0.6156472746
C,0,-1.0841638483,-2.8921187372,-1.5448429875
P,0,-0.7932291614,-1.0838271194,-1.9270450291
Ir,0,-0.0378847631,-0.0277043638,0.0982585519
B,0,-0.1207780571,1.8355839646,-0.8764128365
O,0,-0.2863401085,3.0946381084,-0.3173237298
C,0,-0.1660880727,4.098555621,-1.3265048123
C,0,-0.2448832914,3.3223984205,-2.6557826294
O,0,-0.0440857248,1.9541740954,-2.2803111492
P,0,0.318330974,-2.336396942,0.8659306003
B,0,1.0449474518,0.8353419387,1.725965396
O,0,1.8449392664,0.0709900527,2.5861888673
C,0,2.3447000699,0.9199148452,3.6295445735
C,0,2.0386478004,2.3457471097,3.133331245
O,0,1.0560505698,2.1624773982,2.1114178353
B,0,1.9629427425,0.0390151645,-0.6246173145
O,0,2.6284690098,-1.0172709381,-1.2721572107
C,0,3.9136055669,-0.5708118358,-1.7293706202
C,0,4.1228818529,0.7797526784,-1.0193216681
O,0,2.825195438,1.1330641694,-0.5311093212
C,0,2.0077146294,-2.8860902655,1.3735119859
C,0,-0.6756284814,-3.1102193041,2.2301451946
H,0,-0.2387585122,-4.4644136558,-0.2854949504
H,0,0.9605370482,-3.4995535133,-1.1503110737
C,0,0.2918876861,-1.1257771788,-3.4169207368
C,0,-2.3947141685,-0.5371682749,-2.6573263685
H,0,-1.1391236136,-3.4675055843,-2.4769381182
H,0,-2.0679224429,-2.961175287,-1.0668024932
H,0,0.5241379267,3.6259120847,-3.3740619298
H,0,-1.2262304443,3.4259887147,-3.1379186615
H,0,0.79427374,4.6157031646,-1.2062187649
H,0,-0.9695441374,4.8344460624,-1.2144711994
H,0,2.923092138,2.8281933191,2.6983280618
H,0,1.6380540068,2.9964337395,3.916970017
H,0,3.4138645835,0.7351754091,3.7755852074
H,0,1.8218651307,0.6851778342,4.5659524194
H,0,4.4901188092,1.5622617197,-1.6909475673
H,0,4.8171070389,0.698201795,-0.1731189511
H,0,3.8903145404,-0.4660702181,-2.8217184486
H,0,4.6750645358,-1.3138366307,-1.4709249563
H,0,2.0319629772,-3.9636651194,1.5677302999
H,0,2.7086815267,-2.6344556092,0.576344606
H,0,2.2914776971,-2.3343645002,2.2711795601
H,0,-0.423393486,-4.1692120344,2.3505506071
H,0,-0.4431150525,-2.5834777689,3.1603857503
H,0,-1.7471840511,-3.0138053065,2.051983479
H,0,-2.7035124014,-1.1990285593,-3.4729887272
H,0,-3.1643417282,-0.5165123516,-1.8840584473
H,0,-2.2568587706,0.4755419822,-3.042780158
H,0,-0.1800687432,-1.6871915419,-4.2297917223
H,0,0.4609449903,-0.0920521562,-3.7262135512
H,0,1.2507407334,-1.5723826829,-3.1526809997
H,0,-0.7354408775,0.413797616,1.5012937625
C,0,-2.2153961011,0.2649159044,0.7569753505

C,0,-3.105458404,-0.8140215385,0.8501629746
C,0,-4.4773452424,-0.633394895,1.0918107681
C,0,-4.99602784,0.6501564438,1.2775682526
C,0,-4.1125837278,1.7325362245,1.2184853487
C,0,-2.7529637385,1.5535325584,0.9695397518
H,0,-2.7790431102,-1.8383226431,0.7175277487
O,0,-5.221994368,-1.7869749116,1.1226607764
H,0,-6.0490153534,0.8154984613,1.4729394476
H,0,-4.4987223328,2.7368212221,1.3775554043
H,0,-2.0981360588,2.4161928827,0.9384453243
C,0,-6.6103746184,-1.6738138559,1.3766153735
H,0,-7.0070854466,-2.6908349087,1.3620591861
H,0,-6.810027823,-1.2247808314,2.3588075013
H,0,-7.1196183995,-1.0792003777,0.6061541794

dmpeBpin3MetaAnisprodbetter

dmpeBpin3MetaAnisbetterprod
B3LYP/gen
E(RMPW+HF-PW91) = -2133.93971296

Zero-point correction= 0.556015 (Hartree/Particle)
Thermal correction to Energy= 0.594041
Thermal correction to Enthalpy= 0.594985
Thermal correction to Gibbs Free Energy= 0.485455
Sum of electronic and ZPE= -2133.733863
Sum of electronic and thermal Energies= -2133.695837
Sum of electronic and thermal Enthalpies= -2133.694892
Sum of electronic and thermal Free Energies= -2133.804423

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	372.766	139.033	230.526

C,0,-2.6961605636,0.8722799494,-1.6086859986
C,0,-2.2536524684,-0.0349760951,-0.6289361649
C,0,-3.2548290085,-0.8966098908,-0.1189136913
C,0,-4.581462872,-0.8457094672,-0.5485844058
C,0,-4.9928352114,0.069295632,-1.5200644702
C,0,-4.0287931876,0.9318043127,-2.0487022401
Ir,0,-0.094728056,-0.0685014018,-0.0795303109
P,0,-0.5619154781,-0.0313110281,2.2185754504
C,0,-0.3711246448,-1.7672620215,2.8938030369
C,0,-0.8193814656,-2.8489125925,1.8988316684
P,0,-0.1106650941,-2.5283560411,0.1902055007
B,0,1.9493204067,0.2608758223,0.5322306217
O,0,2.47525976,1.5217381009,0.7991668971
C,0,3.8772254924,1.4149882367,1.0600642143
C,0,4.1076725116,-0.0899533691,1.3014892866
O,0,2.9150916687,-0.7174051849,0.806203554
B,0,1.2886086236,-0.3142141734,-1.7431348161
O,0,1.4949572567,-1.5556405136,-2.3571835227
C,0,2.6883882357,-1.4736426446,-3.1456858184
C,0,2.9396309423,0.0393231416,-3.2904042126
O,0,2.1862246171,0.6291328863,-2.2266742811
B,0,-0.1945601964,2.0226015112,-0.1497428108
O,0,-0.0075774894,2.7810836874,-1.2967129518
C,0,-0.086692758,4.1711808894,-0.9694743322
C,0,-0.6467755467,4.2030940237,0.4685237893
O,0,-0.532881303,2.8496192076,0.9290274443
H,0,4.432482819,1.7832749884,0.1886148444
H,0,4.1421270972,2.0323328332,1.9248541807
H,0,4.9786240648,-0.4821944841,0.7666083785
H,0,4.2256183702,-0.3288942346,2.366664142
H,0,3.5077437004,-1.9778230846,-2.616521156
H,0,2.5293967537,-1.9777601154,-4.1038077015
H,0,3.9953047792,0.309993316,-3.1897085283

H,0,2.571529387,0.4289539709,-4.24801911
H,0,-0.0800185117,4.8663726922,1.1306650312
H,0,-1.7015636517,4.503890999,0.496317862
H,0,0.9158090438,4.6121409412,-1.0326035956
H,0,-0.7362575723,4.6814342899,-1.6881470472
H,0,-0.066375533,0.0383201954,-1.7481906008
H,0,-2.0105397331,1.5782586663,-2.0661397182
O,0,-4.2874838742,1.8812675609,-3.00689784
H,0,-3.0136514895,-1.6359388693,0.6383871994
H,0,-5.3127636828,-1.5299189189,-0.1221427714
H,0,-6.026977649,0.0965735745,-1.8428291126
C,0,0.5182475918,0.9419611609,3.35168123
C,0,-2.2224051501,0.5520566074,2.7600192335
C,0,1.4628843676,-3.4976123041,0.2475439168
C,0,-1.1359690497,-3.595712589,-0.9149593695
H,0,-0.517748027,-3.8427611524,2.2492653072
H,0,-1.9103771512,-2.8596106961,1.8137016624
H,0,0.6989960103,-1.8790436664,3.1047344061
H,0,-0.9009925454,-1.8576333363,3.8494156291
H,0,0.1536514546,0.8656343301,4.3810292208
H,0,1.5463246334,0.5793796121,3.3035118035
H,0,0.4967886565,1.9810705063,3.0202004441
H,0,-2.3355835241,0.4407237498,3.8431044493
H,0,-2.2872947226,1.6077678978,2.486221582
H,0,-3.0144247478,0.016724068,2.2375575898
H,0,1.2728093274,-4.5388428092,0.5289234108
H,0,1.9162510691,-3.4607666664,-0.7442672157
H,0,2.1568698324,-3.0319745228,0.9481824865
H,0,-1.1863462876,-4.628130025,-0.5530581081
H,0,-2.1416177378,-3.1803761102,-1.0007041114
H,0,-0.6738188483,-3.5843272838,-1.9057364842
C,0,-5.6125088457,1.997118968,-3.4863147604
H,0,-5.6008374339,2.7995640093,-4.2268771124
H,0,-5.9573430102,1.0713588193,-3.9673700044
H,0,-6.3168673504,2.2597901345,-2.6847480987

dmpeBpin3MetaBr2PhHCHactTSSptSptBack

Ir Bpin3 CH activation for meta-dibromobenzene
B3LYP/gen
E(RB+HF-LYP) = -7161.36208279

Zero-point correction= 0.500325 (Hartree/Particle)
Thermal correction to Energy= 0.538029
Thermal correction to Enthalpy= 0.538973
Thermal correction to Gibbs Free Energy= 0.428857
Sum of electronic and ZPE= -7160.861758
Sum of electronic and thermal Energies= -7160.824054
Sum of electronic and thermal Enthalpies= -7160.823110
Sum of electronic and thermal Free Energies= -7160.933226

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	337.618	136.306	231.759

C,0,2.2032267017,-0.8744206449,0.6384472503
C,0,1.3125867207,0.2036088104,0.4797174369
C,0,1.8576053729,1.5007154226,0.5498675699
C,0,3.2287946486,1.6842713466,0.7147348033
C,0,4.1189470972,0.6201443332,0.8397525125
C,0,3.5702914907,-0.6576398731,0.8024695732
Ir,0,-0.8812055694,-0.1564735809,-0.1081788641
P,0,-0.2299463476,-0.8852386728,-2.3204371774
C,0,-0.4313679376,-2.7451389419,-2.3974852531
C,0,-0.0736248387,-3.4285752007,-1.0671174088
P,0,-0.9255188964,-2.5736822473,0.3656759495
B,0,-2.9038678794,-0.1834653018,-0.7586406278

O,0,-3.4130592304,-1.0453076844,-1.7455694191
C,0,-4.7770943001,-0.6975503426,-2.0298649233
C,0,-5.1740676798,0.2540458437,-0.8854961599
O,0,-3.9313056445,0.6300624845,-0.283410289
B,0,-1.9693066812,0.238136717,1.6835749824
O,0,-2.5142685942,-0.7972127255,2.4562170521
C,0,-3.1062422369,-0.2251926645,3.6339536058
C,0,-3.1561500088,1.2851119172,3.3340843676
O,0,-2.2318560248,1.4646868561,2.2572980873
B,0,-1.0941807938,1.8464837852,-0.7196787147
O,0,-0.8345528481,2.9782011836,0.044655219
C,0,-0.9950111066,4.1560232944,-0.753366491
C,0,-1.6745708532,3.6560551845,-2.0425713986
O,0,-1.5016397714,2.2324714574,-2.0075318356
H,0,-4.8266774543,-0.2092521551,-3.0111520555
H,0,-5.3880558277,-1.6052950458,-2.0643801567
H,0,-5.6980379713,1.1482448653,-1.2371108077
H,0,-5.8026922172,-0.2417809529,-0.1349679923
H,0,-4.0954066897,-0.6636578557,3.7993682873
H,0,-2.4747885434,-0.4557653928,4.5015948973
H,0,-4.1528172323,1.6059745498,3.0064700861
H,0,-2.8529440409,1.9021115476,4.1853892747
H,0,-2.7471134031,3.887013426,-2.0603013914
H,0,-1.2189625091,4.0612330102,-2.9521585226
H,0,-1.5993027531,4.8871351025,-0.2077238902
H,0,-0.0090626825,4.5978166023,-0.9473936436
H,0,-0.1193383166,0.2703754906,1.2712865086
H,0,1.8483295054,-1.8939936687,0.6155337018
Br,0,4.739565977,-2.1722048832,0.9739654652
H,0,1.2049723353,2.3616749944,0.488546082
Br,0,3.9313198459,3.4693952805,0.7775564186
H,0,5.1811401877,0.7790598366,0.9690427763
C,0,-1.100010277,-0.3316922155,-3.8465120034
C,0,1.5351078744,-0.6192523187,-2.7970705231
C,0,-2.5877094842,-3.3782605374,0.3808752078
C,0,-0.1813912391,-3.3642782198,1.8664395581
H,0,-0.3409056762,-4.4917241157,-1.0922811876
H,0,1.0068644979,-3.3742365462,-0.8899853431
H,0,-1.4852046626,-2.9192659371,-2.6397742593
H,0,0.1673005892,-3.1507869661,-3.2214511649
H,0,1.7433838523,-1.0633366922,-3.7756497654
H,0,1.7302271969,0.4554005213,-2.8413204285
H,0,2.2049306184,-1.0479671023,-2.0501328564
H,0,-0.6660396846,-0.8063206812,-4.7323461513
H,0,-2.1548040781,-0.5928648372,-3.7590599574
H,0,-1.0173675767,0.7538529467,-3.9180041263
H,0,-0.2364461643,-4.456283454,1.8089288872
H,0,0.8584578068,-3.0659681532,2.009412106
H,0,-0.7569380626,-3.0208064497,2.7299757856
H,0,-2.5038072143,-4.4638078974,0.4962775909
H,0,-3.1464683156,-2.9574669968,1.21949598
H,0,-3.1143078017,-3.1355361043,-0.5428983055

dmpeBpin3MetaXyleneHCHactopttoprod

dmpeBpin3MetaXyleneHCHact
B3LYP/gen
E(RB+HF-LYP) = -2098.40455449

Zero-point correction= 0.578634 (Hartree/Particle)
Thermal correction to Energy= 0.617648
Thermal correction to Enthalpy= 0.618592
Thermal correction to Gibbs Free Energy= 0.505698
Sum of electronic and ZPE= -2097.825921
Sum of electronic and thermal Energies= -2097.786907
Sum of electronic and thermal Enthalpies= -2097.785962
Sum of electronic and thermal Free Energies= -2097.898856

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	387.580	141.793	237.605

C,0,2.9832811673,-0.9229183839,-0.1609627829
 C,0,2.077343636,0.0979915902,0.1906576211
 C,0,2.6700034083,1.2405695394,0.7736700642
 C,0,4.0491176666,1.363955244,0.9956341096
 C,0,4.896834216,0.3184325176,0.6144673321
 C,0,4.3726708822,-0.8349654459,0.0282005675
 Ir,0,-0.1411741792,-0.009986253,0.0571682294
 P,0,-0.1000907985,-1.0184928661,-2.067062229
 C,0,-0.3279488564,-2.8646809822,-1.8446090083
 C,0,0.3038602083,-3.4096791155,-0.5535135206
 P,0,-0.0927358427,-2.3235273189,0.9248450191
 B,0,-2.2828446569,-0.0064221604,-0.2564437444
 O,0,-3.0275393535,-1.1746066495,-0.505230126
 C,0,-4.4185793404,-0.8399482873,-0.6246882181
 C,0,-4.4243190081,0.6902427662,-0.7898404509
 O,0,-3.1228623121,1.0999066203,-0.3565299121
 B,0,-1.2317154461,0.7931116031,1.7706077071
 O,0,-1.822699026,-0.0472227232,2.7251986694
 C,0,-2.507813289,0.7795930025,3.6772639465
 C,0,-2.6045419472,2.1482314634,2.978741333
 O,0,-1.5635058789,2.1159307993,2.0031662013
 B,0,-0.0442316459,1.8822690514,-0.8412851815
 O,0,0.2516592564,3.0715154872,-0.1915871636
 C,0,0.4207001455,4.1162953248,-1.1520311367
 C,0,-0.1514025704,3.5332013536,-2.457638957
 O,0,-0.2042165723,2.119513679,-2.2184155475
 H,0,-4.854227027,-1.3668930151,-1.4800616842
 H,0,-4.9435767717,-1.162381842,0.2832190757
 H,0,-4.5677992661,0.9938223924,-1.8346698454
 H,0,-5.1889375913,1.1844353835,-0.1821175686
 H,0,-3.4836887566,0.342152488,3.9104862572
 H,0,-1.9175093849,0.8286442411,4.6015901971
 H,0,-3.5687348029,2.280701557,2.4704221596
 H,0,-2.4476949451,2.9915658975,3.657980982
 H,0,-1.1648699561,3.9007589998,-2.6636081358
 H,0,0.4765047319,3.7382831583,-3.3309959883
 H,0,-0.1081904711,5.0146019068,-0.8178801618
 H,0,1.488797828,4.3550126842,-1.2411404383
 H,0,0.1422107271,0.6654340572,1.5606756879
 H,0,2.6191411652,-1.8476813599,-0.6024183201
 C,0,5.2860487092,-1.9567784942,-0.4157946927
 H,0,2.0396042807,2.0768374402,1.0604266206
 C,0,4.612810234,2.6008213177,1.6603252526
 H,0,5.9705773826,0.4036056262,0.7766971091
 C,0,-1.4106754932,-0.6216513403,-3.3022921664
 C,0,1.3934228645,-0.7926682583,-3.1243202956
 C,0,-1.608296961,-3.1252465271,1.6139344537
 C,0,1.175996288,-2.8226683042,2.1716817114
 H,0,-0.0390152105,-4.4335618465,-0.3634769346
 H,0,1.3930856114,-3.4522771355,-0.6463989886
 H,0,-1.4130949439,-3.0099450549,-1.8137031426
 H,0,0.0507403357,-3.3939786043,-2.7269784047
 H,0,1.3154197251,-1.4049180155,-4.0284079087
 H,0,1.4264992603,0.2642534116,-3.3994278421
 H,0,2.3066536818,-1.0323531752,-2.5829665338
 H,0,-1.2355117313,-1.1749204508,-4.2305297597
 H,0,-2.3885958203,-0.8861991732,-2.9004380731
 H,0,-1.3692252769,0.4517655696,-3.4927867565
 H,0,1.229807422,-3.9107720686,2.2826307025
 H,0,2.1510215627,-2.4281309963,1.8799308727
 H,0,0.9005180802,-2.3825929885,3.1345886468
 H,0,-1.4272507872,-4.1769587852,1.8602927883
 H,0,-1.9073079827,-2.5769765043,2.5095716875

H,0,-2.4131942198,-3.0384306015,0.8828001166
H,0,5.7803697581,-1.721126994,-1.3673601265
H,0,6.0789204555,-2.1454285689,0.3163379365
H,0,4.7345138509,-2.8919421557,-0.5597231783
H,0,5.509393893,2.9625873356,1.1441384521
H,0,3.8798106073,3.4126552875,1.6759334598
H,0,4.9021700814,2.3997916493,2.6999779549

dmpeBpin3MetaXyleneHCHactTSSptSptBack

Ir Bpin3 dmpe C-H activation for meta-xylene split on top, split on bo
B3LYP/gen
E(RB+HF-LYP) = -2098.39259645

Zero-point correction= 0.575435 (Hartree/Particle)
Thermal correction to Energy= 0.614683
Thermal correction to Enthalpy= 0.615627
Thermal correction to Gibbs Free Energy= 0.500928
Sum of electronic and ZPE= -2097.817161
Sum of electronic and thermal Energies= -2097.777914
Sum of electronic and thermal Enthalpies= -2097.776969
Sum of electronic and thermal Free Energies= -2097.891668

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 385.719	141.806	241.404

C,0,3.1788883104,-0.7302499198,0.7077118435
C,0,2.2581994406,0.3368661673,0.6626214089
C,0,2.7775570083,1.6203441131,0.8964085955
C,0,4.1458281049,1.8467514797,1.1242012539
C,0,5.0228403766,0.7613078,1.1267197629
C,0,4.549496458,-0.5406487122,0.9213960168
Ir,0,0.0632495366,-0.0118654285,0.0728948957
P,0,0.6960028948,-0.7524135921,-2.1407398804
C,0,0.4660578934,-2.6092103602,-2.1994502428
C,0,0.8496969709,-3.2917064109,-0.8768483677
P,0,0.0374583281,-2.4204680196,0.5696647048
B,0,-1.9617043966,-0.0574920311,-0.5831956434
O,0,-2.482704254,-0.9777127623,-1.5136460174
C,0,-3.8389779812,-0.6276798292,-1.8279435419
C,0,-4.2268977388,0.3995568209,-0.7483946254
O,0,-2.9805913654,0.8034495496,-0.1735847975
B,0,-1.0417910145,0.4111587223,1.8426893009
O,0,-1.6328745455,-0.6083784186,2.604420496
C,0,-2.2235261361,-0.0244274996,3.7750137456
C,0,-2.222560516,1.4881801249,3.4817762422
O,0,-1.2792236533,1.6434359253,2.419392902
B,0,-0.1125492178,1.9888122849,-0.5479214179
O,0,0.0900563631,3.1247767496,0.2296872488
C,0,-0.0101887822,4.297589982,-0.5802107526
C,0,-0.6202452062,3.7983035022,-1.902859235
O,0,-0.4407611547,2.3774273286,-1.8605465604
H,0,-3.875805891,-0.1999493004,-2.8381159015
H,0,-4.4649147662,-1.5257760418,-1.8108340184
H,0,-4.7447436345,1.2730210868,-1.1570629994
H,0,-4.8589516529,-0.0419035871,0.0329173117
H,0,-3.2283261476,-0.4325531336,3.9247576111
H,0,-1.6128638934,-0.2775500735,4.6515721292
H,0,-3.2047501629,1.8418474399,3.1443393595
H,0,-1.911709994,2.0912389917,4.3407866015
H,0,-1.6921354827,4.0240176317,-1.9727770839
H,0,-0.1223632876,4.2094834101,-2.787607528
H,0,-0.6343218507,5.0416723988,-0.0750785813
H,0,0.9908132146,4.7273306131,-0.7233839896
H,0,0.7895089308,0.3843115723,1.4739773777
H,0,2.8403912491,-1.7471472361,0.542958405

C,0,5.5059783404,-1.7127859284,0.9227856321
H,0,2.1005971535,2.4679153288,0.91335578
C,0,4.647357311,3.2475396203,1.396445941
H,0,6.0851303959,0.9265009453,1.2999667205
C,0,-0.2001324514,-0.2070079617,-3.6561513623
C,0,2.4502117564,-0.4990692049,-2.6621617171
C,0,-1.6050632824,-3.2648037094,0.6608887829
C,0,0.8534657845,-3.1593051017,2.0587454536
H,0,0.5691024315,-4.3517474216,-0.8896724922
H,0,1.9341825979,-3.2484205947,-0.7264789427
H,0,-0.5996485383,-2.757827559,-2.4035104962
H,0,1.0280617012,-3.0312745085,-3.0410731134
H,0,2.644326437,-0.9858238288,-3.6235582719
H,0,2.6316345367,0.5746653098,-2.7603010377
H,0,3.1356129185,-0.881873162,-1.9050251067
H,0,0.2174528545,-0.6858074123,-4.5477917287
H,0,-1.2535194691,-0.4677876694,-3.5506860829
H,0,-0.1179786167,0.8780468496,-3.7308760079
H,0,0.8587765353,-4.2535216008,2.0154440106
H,0,1.8749764025,-2.7919974731,2.1687276758
H,0,0.2801511218,-2.8395705342,2.9330562798
H,0,-1.4891308356,-4.34687213,0.7842963485
H,0,-2.1419941908,-2.8493169672,1.5164437829
H,0,-2.1758171783,-3.0487898424,-0.2436586203
H,0,6.226531683,-1.646365692,0.0982723326
H,0,6.0880528869,-1.7544822087,1.8508076212
H,0,4.9745926621,-2.6643284851,0.8214406226
H,0,5.732142521,3.3179978867,1.2695163419
H,0,4.1791512005,3.9775780956,0.7280307757
H,0,4.415271512,3.5592126216,2.4226958492

dmpeBpin3MetaXyleneprodbetter

dmpeBpin3MetaXylenebetterprod
B3LYP/gen
E(RmPW+HF-PW91) = -2098.07434212

Zero-point correction= 0.577939 (Hartree/Particle)
Thermal correction to Energy= 0.617213
Thermal correction to Enthalpy= 0.618158
Thermal correction to Gibbs Free Energy= 0.504628
Sum of electronic and ZPE= -2097.827146
Sum of electronic and thermal Energies= -2097.787871
Sum of electronic and thermal Enthalpies= -2097.786927
Sum of electronic and thermal Free Energies= -2097.900457

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 387.307	142.172	238.943

C,0,-2.6604508698,0.9126168349,-1.6649085556
C,0,-2.2408806141,0.0309334949,-0.6429117554
C,0,-3.257335021,-0.7933228552,-0.1205518651
C,0,-4.5933963662,-0.7560757798,-0.5536567037
C,0,-4.943901447,0.1344358565,-1.5698815027
C,0,-3.9791054212,0.9736441486,-2.1372873886
Ir,0,-0.0854525104,-0.0286287975,-0.0880961234
P,0,-0.5372898767,-0.034261577,2.2186434522
C,0,-0.3809438352,-1.7866041582,2.8579756174
C,0,-0.855593291,-2.833726998,1.8400195668
P,0,-0.1343859723,-2.4889578717,0.1433687037
B,0,1.9608176409,0.2892520951,0.5289001015
O,0,2.515826548,1.5501460661,0.7259900087
C,0,3.907001509,1.422317005,1.0308250716
C,0,4.082493329,-0.0651950507,1.3919605493
O,0,2.890904191,-0.6939169087,0.8952258518
B,0,1.2974348604,-0.2920792043,-1.7444328645

O,0,1.4702565206,-1.5404870438,-2.3580470895
C,0,2.6693853716,-1.4935177032,-3.1407611526
C,0,2.960745562,0.0114094795,-3.2908653841
O,0,2.2229658134,0.6244172608,-2.2296400703
B,0,-0.17154634,2.0634568091,-0.1090006708
O,0,0.0036772545,2.8564360855,-1.2353297974
C,0,-0.034164907,4.2354390604,-0.8567588608
C,0,-0.5864693795,4.2288687697,0.5837197125
O,0,-0.4789976645,2.8613445955,1.0016805384
H,0,4.4944316458,1.7050215939,0.1483509042
H,0,4.1709714677,2.0962762313,1.8523849611
H,0,4.9616533767,-0.5210619104,0.9256098371
H,0,4.1491780417,-0.2255907815,2.4763579317
H,0,3.4727267655,-2.0154187808,-2.6039964971
H,0,2.503011079,-1.9985373226,-4.097107801
H,0,4.0231544921,0.2544063644,-3.1902766215
H,0,2.6038722095,0.4068535247,-4.250429978
H,0,-0.0122939487,4.8685222828,1.2623560814
H,0,-1.6392289831,4.5358209412,0.6256594739
H,0,0.9804814155,4.6494053235,-0.9079784817
H,0,-0.6711177763,4.7916144052,-1.5524795502
H,0,-0.0405865986,0.1175916804,-1.7541544429
H,0,-1.9374270884,1.5867409157,-2.1161135798
C,0,-4.3491283238,1.9137165595,-3.2634377895
H,0,-3.0278695698,-1.5126112712,0.6620013897
C,0,-5.6385524186,-1.6435828335,0.0866208891
H,0,-5.973314033,0.1741983308,-1.923529833
C,0,0.5781627678,0.8876436622,3.3604577292
C,0,-2.1780152581,0.5743656137,2.793450187
C,0,1.4264236117,-3.4809633739,0.1987775094
C,0,-1.1719515575,-3.5182011963,-0.9850331442
H,0,-0.5785604659,-3.8430268288,2.1658785594
H,0,-1.946279414,-2.8149654625,1.752610157
H,0,0.6864518659,-1.9274160718,3.0644502193
H,0,-0.911630627,-1.8837882691,3.8123685181
H,0,0.2331702878,0.7835854322,4.3941743193
H,0,1.5977036201,0.5067945757,3.2798312173
H,0,0.5673175389,1.9374819652,3.0641346962
H,0,-2.2693953979,0.4637745694,3.8787430304
H,0,-2.2328592821,1.6307461696,2.5210942236
H,0,-2.9894576337,0.0499125884,2.2907023799
H,0,1.2207914625,-4.5218398179,0.4708833765
H,0,1.887891331,-3.444468592,-0.7892354115
H,0,2.1215214223,-3.0318730783,0.9096915716
H,0,-1.2555671721,-4.5521885308,-0.6340620207
H,0,-2.164419365,-3.0729002443,-1.0763108285
H,0,-0.6985763604,-3.5091941288,-1.9703064227
H,0,-6.3697697372,-1.9978723931,-0.6477633566
H,0,-5.1862648768,-2.5219817223,0.5592468969
H,0,-6.1999080339,-1.1093549956,0.8646010066
H,0,-5.3158767274,2.3975648182,-3.0842456323
H,0,-3.5964178839,2.6974129111,-3.3913022866
H,0,-4.4305639525,1.3802175329,-4.2194257776

dmpeBpin3OrthoAnisCHactTSParSptBackA

Ir Bpin3 bpy ortho anisole
B3LYP/gen
E(RB+HF-LYP) = -2134.27489358

Zero-point correction= 0.553095 (Hartree/Particle)
Thermal correction to Energy= 0.591067
Thermal correction to Enthalpy= 0.592011
Thermal correction to Gibbs Free Energy= 0.482549
Sum of electronic and ZPE= -2133.721799
Sum of electronic and thermal Energies= -2133.683826
Sum of electronic and thermal Enthalpies= -2133.682882

Sum of electronic and thermal Free Energies= -2133.792344

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	370.900	138.953	230.383

6	3.140816	-0.031857	0.383722
6	1.986067	-0.812137	0.627899
6	2.207463	-2.055464	1.242405
6	3.482166	-2.549351	1.543477
6	4.596293	-1.771428	1.251144
6	4.425357	-0.509685	0.676837
77	-0.112794	-0.109061	0.048085
15	0.441252	0.133469	-2.311068
6	-0.522837	-1.158634	-3.249122
6	-0.439662	-2.512177	-2.529792
15	-0.902799	-2.340102	-0.724014
5	-1.999822	0.762176	-0.395817
8	-2.835922	1.427516	0.502329
6	-4.053518	1.807867	-0.144153
6	-3.780894	1.583943	-1.642372
8	-2.609813	0.755386	-1.667405
5	-1.149639	-0.388338	1.880765
8	-1.848649	-1.573129	2.163582
6	-2.361618	-1.495470	3.502697
6	-2.190614	-0.012920	3.884924
8	-1.240476	0.488312	2.944167
5	0.319987	1.892204	0.502855
8	0.826263	2.341398	1.716810
6	1.059995	3.746330	1.650694
6	0.352503	4.196942	0.356537
8	0.111490	2.980952	-0.361135
1	-4.872787	1.176980	0.225067
1	-4.288635	2.849880	0.095096
1	-4.602991	1.077680	-2.158941
1	-3.568347	2.523690	-2.167899
1	-3.405098	-1.826472	3.518699
1	-1.776388	-2.161131	4.150187
1	-3.128335	0.548294	3.782626
1	-1.811272	0.126157	4.902231
1	-0.605932	4.691064	0.561772
1	0.962599	4.873680	-0.252578
1	0.657519	4.231800	2.546028
1	2.141661	3.936431	1.615973
1	0.664301	-0.271005	1.458545
8	2.950058	1.208264	-0.184156
1	5.300219	0.093743	0.462672
1	1.345050	-2.649518	1.524712
1	3.592978	-3.521103	2.017182
1	5.598304	-2.126171	1.476675
6	0.086773	1.680041	-3.244116
6	2.167964	-0.247833	-2.854905
6	-2.737294	-2.571172	-0.775204
6	-0.377348	-3.987760	-0.059807
1	-1.079116	-3.259212	-3.015090
1	0.586487	-2.898208	-2.560390
1	-1.556552	-0.803092	-3.285085
1	-0.150260	-1.232532	-4.277928
1	2.219572	-0.318277	-3.946427
1	2.832205	0.541604	-2.503702
1	2.502591	-1.187773	-2.411106
1	0.378518	1.580245	-4.294567
1	-0.980900	1.887422	-3.169538
1	0.626113	2.503081	-2.773347
1	-0.839114	-4.801402	-0.629004
1	0.708903	-4.087293	-0.108028
1	-0.690463	-4.061478	0.984733
1	-3.007348	-3.530415	-1.229348

1 -3.109453 -2.525422 0.249914
1 -3.183070 -1.754361 -1.346054
6 4.044298 2.106407 -0.236742
1 3.639277 3.051447 -0.603781
1 4.488724 2.261138 0.754470
1 4.827672 1.764079 -0.927357

dmpeBpin3OrthoAnisCHactTSParSptBackAopttoprod

dmpeBpin3OrthoAnisCHactTSParSptBackAopttoprod
B3LYP/gen
E(RB+HF-LYP) = -2134.28632375

Zero-point correction= 0.556940 (Hartree/Particle)
Thermal correction to Energy= 0.594462
Thermal correction to Enthalpy= 0.595406
Thermal correction to Gibbs Free Energy= 0.487937
Sum of electronic and ZPE= -2133.729384
Sum of electronic and thermal Energies= -2133.691862
Sum of electronic and thermal Enthalpies= -2133.690918
Sum of electronic and thermal Free Energies= -2133.798387

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 373.030	138.604	226.187

C,0,3.2017286763,0.0137205261,0.2313517825
C,0,2.0676836196,-0.8069266149,0.4388155615
C,0,2.347602328,-2.0308149386,1.0749366632
C,0,3.6337624791,-2.4498160205,1.4418987716
C,0,4.7192997684,-1.6240141646,1.1797045011
C,0,4.5001938871,-0.3842863108,0.5754041399
Ir,0,-0.0369701786,-0.2002290642,0.075470107
P,0,0.3732362568,0.1111805125,-2.2362243402
C,0,-0.579681348,-1.1809325651,-3.1826029777
C,0,-0.4159797029,-2.5551455454,-2.5211875156
P,0,-0.8257384747,-2.4549192072,-0.6994970564
B,0,-1.9704168103,0.6880949668,-0.3086191046
O,0,-2.6766868987,1.5793456627,0.5000464859
C,0,-3.9281700788,1.921552666,-0.1019826761
C,0,-3.8370582802,1.3602967811,-1.5320034979
O,0,-2.7049305019,0.4796231455,-1.4942153402
B,0,-1.23567893,-0.3341565227,1.9207007993
O,0,-2.0921914142,-1.4207851917,2.1269094255
C,0,-2.8236976421,-1.1786925399,3.3396720041
C,0,-2.5792136302,0.3140446002,3.6316962497
O,0,-1.3931427482,0.62379857,2.9003094724
B,0,0.5050084717,1.7592629505,0.5810256545
O,0,1.0096930569,2.1201493355,1.8220497118
C,0,1.2552816616,3.5245305121,1.8523844672
C,0,0.6166985811,4.0640706973,0.5533564072
O,0,0.3318594416,2.8954910113,-0.2239184447
H,0,-4.7434661455,1.4612497297,0.4710938462
H,0,-4.0626625955,3.0075154276,-0.0776229821
H,0,-4.7285952943,0.8007945447,-1.833037632
H,0,-3.6568749826,2.1475240363,-2.2754259453
H,0,-3.8801465068,-1.4210356374,3.1870805524
H,0,-2.4275380658,-1.8270560413,4.1316611151
H,0,-3.3995242659,0.9425466695,3.2625236574
H,0,-2.4225870626,0.5250405456,4.6937599288
H,0,-0.3188371746,4.6041272751,0.7464222788
H,0,1.2854770315,4.7287971059,-0.0060035042
H,0,0.8081730102,3.9575512785,2.7535805226
H,0,2.3377902867,3.7055733422,1.8873420531
H,0,0.1028015371,-0.5572538457,1.6981655305
O,0,2.9736368154,1.253957201,-0.3450252741
H,0,5.3474609311,0.2649647338,0.3844590001

H,0,1.5213743816,-2.6865714598,1.3297819927
H,0,3.7731866818,-3.4079420582,1.936729001
H,0,5.7292220737,-1.9225548975,1.4479398702
C,0,-0.0865421018,1.6819134082,-3.0751701002
C,0,2.0796019584,-0.176049774,-2.8795882769
C,0,-2.6501146879,-2.7652470644,-0.7123356507
C,0,-0.2174957381,-4.1023617099,-0.1039893129
H,0,-1.0483699906,-3.3066521993,-3.0083965874
H,0,0.6208207396,-2.9022384445,-2.6037716309
H,0,-1.6266471191,-0.8682413846,-3.1676347094
H,0,-0.2379444968,-1.1950428359,-4.2243075022
H,0,2.0558288102,-0.2261320733,-3.9729095433
H,0,2.7254486036,0.6384709425,-2.5556021883
H,0,2.4828789264,-1.1050527864,-2.4732535379
H,0,0.2093675422,1.6543173967,-4.1285308923
H,0,-1.1658416159,1.8182751448,-2.9979916148
H,0,0.4033620665,2.5064282348,-2.5556764487
H,0,-0.6691537711,-4.9144628017,-0.6835301165
H,0,0.8692829354,-4.158730359,-0.1908445597
H,0,-0.4882025317,-4.2290377633,0.9479682204
H,0,-2.8857979188,-3.7081376363,-1.2171456482
H,0,-3.0008038384,-2.7954647543,0.3204512413
H,0,-3.1452643428,-1.9356908936,-1.2203831132
C,0,4.0218246675,2.2035346401,-0.3585053826
H,0,3.5839846573,3.1304505874,-0.7356132903
H,0,4.4269348825,2.3746043045,0.6471827378
H,0,4.8451671185,1.9054066198,-1.0232443549

dmpeBpin3OrthoAnisCHactTSSptSptBackS

Ir Bpin3 dmpe C-H activation for ortho-anisole spt spt back
B3LYP/gen
E(RB+HF-LYP) = -2134.27130714

Zero-point correction= 0.552663 (Hartree/Particle)
Thermal correction to Energy= 0.590695
Thermal correction to Enthalpy= 0.591639
Thermal correction to Gibbs Free Energy= 0.482176
Sum of electronic and ZPE= -2133.718644
Sum of electronic and thermal Energies= -2133.680612
Sum of electronic and thermal Enthalpies= -2133.679668
Sum of electronic and thermal Free Energies= -2133.789131

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 370.667	139.012	230.384

C,0,3.19753338,-0.6942817488,0.5976640227
C,0,2.2573495147,0.3473053818,0.625005926
C,0,2.7747454179,1.6316444524,0.9251472697
C,0,4.1473756042,1.8521496567,1.1056340072
C,0,5.0470368912,0.7878185833,1.0261746208
C,0,4.5722596455,-0.4953065056,0.7792642027
Ir,0,0.0551053458,-0.0157943072,0.0439980564
P,0,0.6358161972,-0.7379938864,-2.177111761
C,0,0.3627418302,-2.5875565119,-2.264144731
C,0,0.7491981915,-3.290190668,-0.9517590806
P,0,0.0026390179,-2.4109102437,0.5271621326
B,0,-1.9995041859,-0.066678251,-0.4930286194
O,0,-2.5363525255,-0.84290664,-1.5432764069
C,0,-3.9353325254,-0.5558170971,-1.684358971
C,0,-4.2983377105,0.1955109225,-0.3910930742
O,0,-3.0400616277,0.6037915127,0.1473027064
B,0,-0.9149830384,0.4654892881,1.8879536511
O,0,-1.4752468944,-0.5357252785,2.6962697694
C,0,-2.0076302807,0.0754216788,3.8800591568
C,0,-1.9860203866,1.5840780753,3.5670529965

O,0,-1.0762042561,1.7061069019,2.4719987126
B,0,-0.0675567276,1.9653526346,-0.6734062701
O,0,-0.939742972,2.9801779071,-0.3036264572
C,0,-0.6369306988,4.168523578,-1.0301475681
C,0,0.3242349244,3.713802647,-2.1491711112
O,0,0.7115183631,2.3899730251,-1.7710795586
H,0,-4.0891221432,0.0626002283,-2.5783125675
H,0,-4.4934042664,-1.489278504,-1.8120033395
H,0,-4.926698921,1.0739322027,-0.5695020554
H,0,-4.8100384007,-0.4539387058,0.3316583985
H,0,-3.0150844912,-0.3072790004,4.0733563823
H,0,-1.3698015797,-0.1803100116,4.736666729
H,0,-2.9715375476,1.9515553028,3.2552818398
H,0,-1.6359894488,2.1916850679,4.4078317151
H,0,-0.1687862915,3.6840479834,-3.1310062941
H,0,1.2112860244,4.3513209052,-2.2353194753
H,0,-1.5610721884,4.6121009975,-1.4172551136
H,0,-0.1670369595,4.8995212467,-0.3584803174
H,0,0.8275185298,0.3486210337,1.4361929509
H,0,2.8613346852,-1.7073272312,0.4057887401
H,0,5.2554658968,-1.3390268083,0.7286001019
O,0,1.8578170252,2.6402594692,1.0482342658
H,0,4.5201948416,2.8482142656,1.3155850223
H,0,6.1086178643,0.9699140088,1.1696798664
C,0,-0.2703152659,-0.1259384071,-3.6606738832
C,0,2.3844691437,-0.4971652713,-2.7141359724
C,0,-1.6570625391,-3.2093920734,0.6742826105
C,0,0.8654341051,-3.1836039907,1.9721551218
H,0,0.4407289912,-4.3426046876,-0.9659109212
H,0,1.8377915555,-3.2774541495,-0.821348241
H,0,-0.7072477988,-2.7164839265,-2.4586042904
H,0,0.9085662728,-3.0131304302,-3.1146387291
H,0,2.5442910322,-0.9097849251,-3.7156292628
H,0,2.5751664409,0.5785566546,-2.7204032572
H,0,3.0772349455,-0.956920026,-2.0084717779
H,0,0.0756456537,-0.6316440062,-4.5680320273
H,0,-1.3365017211,-0.3006318901,-3.5172720355
H,0,-0.084562073,0.9465677776,-3.7448672164
H,0,0.8334525274,-4.2774843796,1.9287098811
H,0,1.9040003764,-2.8519116391,2.0261950486
H,0,0.3532188565,-2.8463603943,2.8771700394
H,0,-1.5731299648,-4.2936405692,0.802856607
H,0,-2.1562561511,-2.7694589257,1.5406720406
H,0,-2.2446500729,-2.9834506954,-0.2174259637
C,0,2.2771062619,3.9068308815,1.5179381231
H,0,1.3653638311,4.494459397,1.6343216776
H,0,2.7840768738,3.8312938759,2.4889198087
H,0,2.9464495958,4.4091232431,0.8058431488

dmpeBpin3OrthoAnisprodbetter

dmpeBpin3OrthoAnisbetterprod
B3LYP/gen
E(RmPW+HF-PW91) = -2133.93658349

Zero-point correction= 0.556012 (Hartree/Particle)
Thermal correction to Energy= 0.593934
Thermal correction to Enthalpy= 0.594878
Thermal correction to Gibbs Free Energy= 0.485374
Sum of electronic and ZPE= -2133.731118
Sum of electronic and thermal Energies= -2133.693196
Sum of electronic and thermal Enthalpies= -2133.692252
Sum of electronic and thermal Free Energies= -2133.801756

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 372.699	138.952	230.471

C,0,-2.7302058517,0.6752220349,-1.8255309347
C,0,-2.2744748497,0.0078021561,-0.6568825435
C,0,-3.2819638506,-0.701792978,0.0188259856
C,0,-4.6283566314,-0.7448521014,-0.3733494323
C,0,-5.0248934205,-0.0524549287,-1.5091467861
C,0,-4.0688655908,0.6564656556,-2.2402667764
Ir,0,-0.1201207459,0.0448013559,-0.0771769198
P,0,-0.5489647866,-0.0006793138,2.2376922889
C,0,-0.4151495049,-1.7703750907,2.8419421021
C,0,-0.8816819874,-2.7992272103,1.8014014974
P,0,-0.1760881117,-2.4217738699,0.1042132603
B,0,1.920285194,0.3450154016,0.5359698256
O,0,2.4895000423,1.5918323188,0.7802256981
C,0,3.8848766412,1.4405937298,1.0520720534
C,0,4.0575650947,-0.064223346,1.3379166025
O,0,2.8480630679,-0.6611772645,0.8466775094
B,0,1.2185754453,-0.2067159206,-1.7768928292
O,0,1.3040299552,-1.4308745641,-2.4516591125
C,0,2.4978863277,-1.429459377,-3.2434824044
C,0,2.9138313526,0.0536243979,-3.2972455335
O,0,2.2107833663,0.6631294881,-2.2114211626
B,0,-0.187176512,2.1451027871,-0.0434168807
O,0,0.2147278456,3.0033223962,-1.0561080456
C,0,0.2080295594,4.3448323341,-0.567208788
C,0,-0.6269058861,4.2800210867,0.7254723835
O,0,-0.6434549571,2.8861232692,1.0613837513
H,0,4.4580956416,1.7623094746,0.173761302
H,0,4.169025547,2.0718219642,1.9006435341
H,0,4.9201641187,-0.5025977514,0.825775538
H,0,4.154367556,-0.2757955233,2.4112652466
H,0,3.258307393,-2.0524129556,-2.7542685599
H,0,2.2836605023,-1.8526579517,-4.2296755015
H,0,3.9909060502,0.2004167943,-3.169133045
H,0,2.608205797,0.5339903447,-4.2354069497
H,0,-0.1884704555,4.8549192926,1.5481549571
H,0,-1.6573699562,4.6264050123,0.5716595529
H,0,1.2403587676,4.6635151382,-0.3723287431
H,0,-0.2246336907,5.0131099003,-1.3195292317
H,0,-0.0640611056,0.319989635,-1.7269243396
O,0,-1.7727692897,1.3409286572,-2.5580652409
H,0,-4.3754858692,1.1855831178,-3.1356309305
H,0,-3.020265284,-1.2675290382,0.9072541947
H,0,-5.3475555081,-1.3156796435,0.2092226824
H,0,-6.0606673203,-0.0601848992,-1.8380364595
C,0,0.6172859676,0.8690283902,3.3725738289
C,0,-2.1476621456,0.6507721645,2.8882586693
C,0,1.3800846998,-3.4220725179,0.1138014551
C,0,-1.2417281791,-3.4231584415,-1.0221784794
H,0,-0.5956170602,-3.8121564268,2.107671181
H,0,-1.9725544081,-2.790312158,1.7141688402
H,0,0.6483635881,-1.9223271416,3.059932996
H,0,-0.9572012654,-1.8832491904,3.7882399081
H,0,0.2899954407,0.756497172,4.4111051034
H,0,1.6250126287,0.4647699253,3.2653319226
H,0,0.6291407694,1.9243703857,3.0970347749
H,0,-2.2091940015,0.4935396356,3.9698470852
H,0,-2.1558121817,1.7195015566,2.6642231137
H,0,-3.0027462705,0.1924170821,2.3949991645
H,0,1.1779934723,-4.4635122385,0.3863854794
H,0,1.8155919074,-3.3864147228,-0.8864308763
H,0,2.0945934099,-2.9766418697,0.8075566765
H,0,-1.2885019655,-4.4718849414,-0.710198589
H,0,-2.2465956882,-2.9972874785,-1.0478082223
H,0,-0.813887258,-3.3625172134,-2.0260779092
C,0,-2.1599551656,2.1303384516,-3.6631702105
H,0,-1.2478946279,2.6133322726,-4.0180726226
H,0,-2.5894032543,1.5246432574,-4.4736912971

dmpeBpin3ParaAnisCHactTSParSptBackA

dmpe Bpin3 Ir para-anisaldehyde C-H act Par Spt Back A
 B3LYP/gen
 E(RB+HF-LYP) = -2134.27585367

Zero-point correction= 0.553088 (Hartree/Particle)
 Thermal correction to Energy= 0.591233
 Thermal correction to Enthalpy= 0.592177
 Thermal correction to Gibbs Free Energy= 0.481323
 Sum of electronic and ZPE= -2133.722766
 Sum of electronic and thermal Energies= -2133.684620
 Sum of electronic and thermal Enthalpies= -2133.683676
 Sum of electronic and thermal Free Energies= -2133.794531

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 371.004	138.981	233.314

C,0,3.9590141604,1.6562994104,0.3834842086
 C,0,2.5857277235,1.4599786227,0.1899621019
 C,0,1.9218434143,0.285677192,0.5822092227
 C,0,2.7144634009,-0.6591501417,1.264515773
 C,0,4.0818804484,-0.4871660692,1.4735519659
 C,0,4.7206321687,0.6720674671,1.0203387361
 Ir,0,-0.2578238803,-0.0782294948,0.0185234413
 B,0,-0.5966062085,1.9714020641,-0.2585890779
 O,0,-1.207262474,2.5441019155,-1.3875655895
 C,0,-1.4147045226,3.9424112713,-1.1484742214
 C,0,-0.5443377821,4.2535129137,0.0856888524
 O,0,-0.2253654138,2.9719232487,0.6313073402
 O,0,6.067605846,0.7536735308,1.2624477088
 P,0,0.3516207404,-0.4393030075,-2.2908544874
 C,0,2.1311872508,-0.2015137547,-2.7276407202
 P,0,-0.1991376057,-2.5548583269,0.0983514497
 C,0,0.7021164315,-3.6337685481,1.3094364569
 B,0,-2.3034914644,-0.1448236132,-0.5853128663
 O,0,-2.774227359,-0.7630484521,-1.7606568672
 C,0,-4.1686820408,-0.4704885717,-1.9329051001
 C,0,-4.6102408861,0.0840723658,-0.5664955507
 O,0,-3.3871980217,0.4016359232,0.1038194695
 B,0,-1.2703802,-0.0183839302,1.8902011038
 O,0,-1.7237935044,1.0949687433,2.5703773979
 C,0,-2.5560871394,0.6679588477,3.6504341138
 C,0,-2.20671245,-0.8208355972,3.8357279144
 O,0,-1.5772128542,-1.1886343679,2.5981304019
 C,0,0.0632831656,-2.2403497524,-2.6902466852
 C,0,0.5077449982,-3.1463914237,-1.5324745849
 C,0,-0.4917110952,0.4269439822,-3.6795433778
 C,0,-1.8547853427,-3.3811985681,0.1342672825
 H,0,-5.1627001809,-0.6602650415,0.021791918
 H,0,-5.2285856808,0.9833349949,-0.6510647645
 H,0,-4.7039099391,-1.3813974783,-2.2206146125
 H,0,-4.2852975282,0.2680070643,-2.7361260229
 H,0,-3.0858733725,-1.4510189185,4.0041848095
 H,0,-1.5002880682,-0.9820495602,4.6602058715
 H,0,-3.6073915123,0.8097965853,3.3694178995
 H,0,-2.3466068909,1.2717723604,4.53888853
 H,0,-2.4803765936,4.1195910012,-0.9560218395
 H,0,-1.1244884002,4.5166679085,-2.034947205
 H,0,-1.0689585067,4.853125616,0.8363408264
 H,0,0.3842745322,4.7753857734,-0.1829242383
 H,0,0.4299883159,0.3894792169,1.4134664709
 H,0,2.0264663717,2.2656308594,-0.2721121752
 H,0,4.4119534606,2.5825116892,0.0462198675

H,0,2.2527256784,-1.5503110899,1.6715409341
H,0,4.6692347401,-1.2330832797,2.0015025274
H,0,0.2187275774,-4.188110756,-1.7165184847
H,0,1.5997596023,-3.1282378232,-1.4316346533
H,0,-1.014140904,-2.3362016686,-2.8579994559
H,0,0.5758565239,-2.5082030436,-3.621952657
H,0,2.3244369349,-0.5350739108,-3.7523535076
H,0,2.3873380396,0.856380391,-2.6382757165
H,0,2.7676001452,-0.748816424,-2.029888333
H,0,-0.0817130284,0.1105151151,-4.6440460175
H,0,-1.5563814072,0.1988035462,-3.6288979981
H,0,-0.368496389,1.5032297366,-3.5497048167
H,0,0.4759668709,-4.6895932421,1.1278249274
H,0,1.7814363879,-3.4896699434,1.2338616701
H,0,0.3791299943,-3.3683995494,2.3191898802
H,0,-1.7588630809,-4.4683980981,0.0455442009
H,0,-2.332312256,-3.129275817,1.0836615381
H,0,-2.4698732599,-2.9956911326,-0.6805278965
C,0,6.743774658,1.9290284146,0.856369104
H,0,7.7878251963,1.7953157153,1.1462810554
H,0,6.6898800342,2.0770299819,-0.2308981033
H,0,6.3444285967,2.8228450409,1.3542185188

dmpeBpin3ParaAnisCHactTSParSptBackAopttprod

dmpeBpin3ParaAnisCHactTSParSptBackAopttprod
B3LYP/gen
E(RB+HF-LYP) = -2134.28648927

Zero-point correction= 0.556613 (Hartree/Particle)
Thermal correction to Energy= 0.593514
Thermal correction to Enthalpy= 0.594458
Thermal correction to Gibbs Free Energy= 0.487617
Sum of electronic and ZPE= -2133.729876
Sum of electronic and thermal Energies= -2133.692975
Sum of electronic and thermal Enthalpies= -2133.692031
Sum of electronic and thermal Free Energies= -2133.798872

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	372.436	136.563	224.867

6	4.270289	0.525989	-0.270280
6	2.883363	0.577081	-0.481836
6	1.959636	-0.230912	0.203802
6	2.539776	-1.084423	1.171614
6	3.911517	-1.156928	1.407871
6	4.794331	-0.353450	0.678149
77	-0.237481	-0.053352	0.053782
5	0.147860	1.997510	0.025786
8	0.225469	2.782050	-1.136751
6	0.440865	4.150101	-0.760293
6	0.810813	4.083196	0.736616
8	0.449315	2.761413	1.139893
8	6.128792	-0.493793	0.974840
15	-0.249771	-0.192487	-2.308072
6	1.332342	-0.087703	-3.254924
15	-0.570387	-2.538755	-0.094728
6	0.513164	-3.795039	0.727960
5	-2.322586	0.450812	-0.243764
8	-3.272126	-0.406914	-0.828393
6	-4.545836	0.254251	-0.885526
6	-4.218570	1.730542	-0.589710
8	-2.896768	1.700854	-0.043926
5	-1.309744	0.048013	1.944505
8	-1.676800	1.178391	2.653930
6	-2.648594	0.805768	3.629549

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6 -2.496823 -0.722483 3.754520
8 -1.835104 -1.107063 2.541441
6 -0.898202 -1.871052 -2.794390
6 -0.305303 -2.963032 -1.896079
6 -1.313035 0.957343 -3.279606
6 -2.237691 -3.268898 0.231335
1 -4.905517 2.185438 0.130967
1 -4.220507 2.345437 -1.498982
1 -5.211909 -0.184333 -0.132018
1 -4.997161 0.102338 -1.871629
1 -3.454572 -1.246591 3.834576
1 -1.871493 -1.006692 4.610641
1 -3.648086 1.090286 3.272879
1 -2.452492 1.335754 4.566501
1 -0.481757 4.718380 -0.933005
1 1.234752 4.582338 -1.378704
1 0.264056 4.815292 1.339917
1 1.885290 4.230243 0.904206
1 0.075535 0.048115 1.687209
1 2.527636 1.308877 -1.200916
1 4.916687 1.185369 -0.840303
1 1.898223 -1.703439 1.791486
1 4.317831 -1.820138 2.166746
1 -0.743349 -3.942088 -2.123195
1 0.776601 -3.045140 -2.055142
1 -1.985170 -1.825188 -2.672683
1 -0.683864 -2.057210 -3.853270
1 1.156330 -0.390458 -4.292177
1 1.694796 0.941840 -3.242117
1 2.094713 -0.722926 -2.802210
1 -1.175468 0.794944 -4.353126
1 -2.359852 0.790222 -3.020946
1 -1.033209 1.977319 -3.011305
1 0.264545 -4.803516 0.380942
1 1.563064 -3.585588 0.516160
1 0.363222 -3.749321 1.810176
1 -2.266905 -4.327538 -0.048198
1 -2.457771 -3.155085 1.294340
1 -2.984403 -2.704651 -0.328719
6 7.044349 0.349455 0.304600
1 8.033978 0.093923 0.689254
1 7.031238 0.189153 -0.782585
1 6.845180 1.411338 0.504881

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dmpeBpin3ParaAnisCHactTSParWrdBackA

Ir Bpin3 bpy para anisole
B3LYP/gen
E(RB+HF-LYP) = -2134.27375331

Zero-point correction= 0.552920 (Hartree/Particle)
Thermal correction to Energy= 0.591250
Thermal correction to Enthalpy= 0.592194
Thermal correction to Gibbs Free Energy= 0.479774
Sum of electronic and ZPE= -2133.720834
Sum of electronic and thermal Energies= -2133.682504
Sum of electronic and thermal Enthalpies= -2133.681560
Sum of electronic and thermal Free Energies= -2133.793979

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	371.015	138.967	236.607

```

C,0,2.6256561976,1.276860249,0.2528065961
C,0,1.8894497623,0.149697513,0.6564995344
C,0,2.5859813595,-0.7871822271,1.4470554358
C,0,3.9388643503,-0.6512317718,1.7525243771

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C,0,4.656187174,0.4575584976,1.2893806748
C,0,3.9874561249,1.431850552,0.5417287372
Ir,0,-0.281135342,-0.080335101,-0.0278391415
P,0,0.186945152,0.0729347164,-2.3878153658
C,0,-0.2380173617,-1.5847375271,-3.131660041
C,0,0.335379229,-2.7256324061,-2.2817305654
P,0,-0.0940463111,-2.5200567832,-0.4658721214
B,0,-2.3268431638,0.0758119623,-0.6174632136
O,0,-2.9812703863,1.2870001294,-0.8549999154
C,0,-4.3827983964,1.052231568,-1.0206189618
C,0,-4.483966858,-0.4607965154,-1.2870569372
O,0,-3.2181738183,-0.9810616221,-0.8575745417
B,0,-1.3532033011,-0.5419081436,1.7407984116
O,0,-1.0583527052,-1.6736785991,2.5149388382
C,0,-2.0512464054,-1.8062019173,3.5426859511
C,0,-2.7986020254,-0.458211003,3.5261556685
O,0,-2.437560214,0.1361383656,2.2747141124
B,0,-0.4873546217,1.9941406278,0.1992984332
O,0,-0.7730472347,2.6460391587,1.3916827938
C,0,-0.6674928288,4.0593953142,1.2080952557
C,0,-0.5344378443,4.2450167857,-0.317503612
O,0,-0.2272130556,2.9342231043,-0.8098242801
H,0,-4.9064142545,1.3439372667,-0.1020025753
H,0,-4.7662060313,1.6601466632,-1.8467737634
H,0,-5.2904349035,-0.9419550691,-0.7245350405
H,0,-4.6256122714,-0.6876045225,-2.3523526704
H,0,-2.7121725288,-2.6485321858,3.299270715
H,0,-1.5632584863,-2.0153742679,4.4996158807
H,0,-3.885945565,-0.5720988455,3.5799941535
H,0,-2.478580294,0.2028215232,4.341101984
H,0,-1.4703304453,4.5906806507,-0.7744272185
H,0,0.2646279976,4.9404579205,-0.5962733269
H,0,-1.5547812142,4.5527817925,1.6183965074
H,0,0.2134865776,4.4291912598,1.7486275982
H,0,0.4236998704,0.1615692262,1.4130905747
H,0,2.1346379953,2.0661276428,-0.3077817486
H,0,4.5045875322,2.3169403152,0.1868631858
H,0,2.0517404534,-1.6336870173,1.8643593173
H,0,4.4538649084,-1.3848111814,2.3661386387
O,0,5.9822988467,0.5048718219,1.6332342011
C,0,-0.7376000541,1.2490295579,-3.462492766
C,0,1.9284081971,0.3419667451,-2.9474365162
C,0,-1.5913509182,-3.5863084907,-0.2684308016
C,0,1.1781297324,-3.628742048,0.3003764416
H,0,-0.0091016298,-3.7012484803,-2.6438173029
H,0,1.4301327824,-2.7283693205,-2.3480317945
H,0,-1.3326603514,-1.6390318429,-3.1483081575
H,0,0.1154705152,-1.6413658824,-4.1682994541
H,0,1.1383530388,-4.6257347391,-0.151249947
H,0,2.1776922706,-3.2109533904,0.1676367411
H,0,0.976742811,-3.7165675667,1.3710262179
H,0,-1.4099628781,-4.5984258744,-0.6454721634
H,0,-1.8310977244,-3.6345951908,0.796735059
H,0,-2.4343380953,-3.1256083838,-0.7831276488
H,0,2.0168120728,0.2096821379,-4.0307928755
H,0,2.2363289687,1.3560833691,-2.6843484216
H,0,2.5969253254,-0.3506912765,-2.4321532652
H,0,-0.4895395411,1.0997522388,-4.5183263852
H,0,-1.8101623426,1.1179907038,-3.3069779997
H,0,-0.4816961526,2.261825159,-3.1480961656
C,0,6.7360965884,1.6285469836,1.2175395187
H,0,7.7482063131,1.473143942,1.5961750531
H,0,6.7722191465,1.7146208079,0.1229294458
H,0,6.337682687,2.5643959353,1.6320672937

dmpeBpin3ParaAnisCHactTSSptSptBackA

dmpe Bpin3 para-anisole C-H act away spt spt back
B3LYP/gen
E(RB+HF-LYP) = -2134.27646546

Zero-point correction= 0.553391 (Hartree/Particle)
Thermal correction to Energy= 0.591415
Thermal correction to Enthalpy= 0.592359
Thermal correction to Gibbs Free Energy= 0.482422
Sum of electronic and ZPE= -2133.723074
Sum of electronic and thermal Energies= -2133.685050
Sum of electronic and thermal Enthalpies= -2133.684106
Sum of electronic and thermal Free Energies= -2133.794044

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 371.119	138.825	231.383

C,0,2.839403597,-0.7616116838,0.6240291087
C,0,1.9144704741,0.2948222778,0.5966940935
C,0,2.4501061561,1.5767706288,0.850892328
C,0,3.8096586963,1.7869217067,1.0673993046
C,0,4.7076642881,0.7130873113,1.0553136791
C,0,4.2134730034,-0.5745762153,0.8338889773
Ir,0,-0.2797538294,-0.0362679709,0.0115606724
P,0,0.336929885,-0.7648412316,-2.2085379109
C,0,0.1083847895,-2.622223059,-2.2780683217
C,0,0.4952025874,-3.3126410429,-0.9604814491
P,0,-0.3103005595,-2.4490380914,0.494981702
B,0,-2.3080546513,-0.069020007,-0.6347944013
O,0,-2.8411442785,-0.9939827271,-1.5539539198
C,0,-4.1966742745,-0.6373093972,-1.8639630381
C,0,-4.5693790924,0.4086053633,-0.7967207865
O,0,-3.3170759023,0.8054514767,-0.2302097593
B,0,-1.3752323296,0.3850758082,1.7868782146
O,0,-1.9663696991,-0.6351793339,2.547737052
C,0,-2.5482775713,-0.053740002,3.7237913574
C,0,-2.542361438,1.4601733084,3.4370071948
O,0,-1.6060888243,1.616142989,2.3686445507
B,0,-0.4340910453,1.9701378109,-0.5968421832
O,0,-0.2176131809,3.0978150808,0.1887288003
C,0,-0.2996753581,4.2775224919,-0.6138773369
C,0,-0.9093844605,3.7946365493,-1.9429270073
O,0,-0.7511687213,2.3707270609,-1.9082555272
H,0,-4.2372825206,-0.2242506371,-2.8800881589
H,0,-4.8296816124,-1.529967894,-1.8295320399
H,0,-5.0779105303,1.2827137143,-1.2156201848
H,0,-5.204839413,-0.0147424484,-0.0082120596
H,0,-3.5539480483,-0.4583689834,3.8772509738
H,0,-1.9340848575,-0.3131711224,4.5960428352
H,0,-3.5256591387,1.8196793332,3.1082584786
H,0,-2.2230321423,2.0579914113,4.2964268115
H,0,-1.9773752428,4.0365183383,-2.0179846567
H,0,-0.4000481413,4.2034416604,-2.8221895801
H,0,-0.91759612,5.0252419613,-0.1065217952
H,0,0.7070557711,4.6958337354,-0.7487588226
H,0,0.4483092987,0.3439531773,1.4158114211
H,0,2.5100342051,-1.779532486,0.4486084187
H,0,4.8726439633,-1.436061036,0.8234051456
H,0,1.7819009437,2.429602024,0.8882295365
H,0,4.1967541826,2.7835780189,1.2594890321
O,0,6.024717546,1.0213942171,1.2758047958
C,0,-0.5693331287,-0.2116103255,-3.7151239523
C,0,2.0870586832,-0.5030694861,-2.7389545443
C,0,-1.9523780739,-3.2923754828,0.5916813916
C,0,0.5169112232,-3.1939174786,1.9747749443
H,0,0.2134733163,-4.3723147458,-0.9786546786

H,0,1.5804679486,-3.2719012005,-0.8139220612
H,0,-0.9575520399,-2.7708297892,-2.4807517204
H,0,0.6687362415,-3.0389006104,-3.1234498743
H,0,2.2781314633,-0.9850698826,-3.703337978
H,0,2.2613175324,0.5720747445,-2.8341980614
H,0,2.7801191916,-0.8839845635,-1.9879695468
H,0,-0.1600965488,-0.687950531,-4.611936636
H,0,-1.6226103145,-0.4701143219,-3.6025794769
H,0,-0.4842754131,0.8735344024,-3.7858952669
H,0,0.5216538023,-4.2879685219,1.9280573375
H,0,1.5396387781,-2.8277792099,2.0780141801
H,0,-0.0488870916,-2.8766369712,2.8548608745
H,0,-1.8377934833,-4.375548457,0.7060899989
H,0,-2.4819774013,-2.8814271078,1.4538731871
H,0,-2.5291007084,-3.0675316829,-0.30688715
C,0,6.9611922757,-0.0394914062,1.2847473567
H,0,7.9349385062,0.4147567649,1.4778417214
H,0,6.7434715146,-0.7706760385,2.0751507292
H,0,6.9951694443,-0.5631299533,0.3194545317

dmpeBpin3ParaAnisCHactTSSptSptFrntS

Ir Bpin3 dmpe C-H activation for anisole, ring splitting Ps, OMe near P
B3LYP/gen
E(RB+HF-LYP) = -2134.27536754

Zero-point correction= 0.553494 (Hartree/Particle)
Thermal correction to Energy= 0.591500
Thermal correction to Enthalpy= 0.592445
Thermal correction to Gibbs Free Energy= 0.482400
Sum of electronic and ZPE= -2133.721874
Sum of electronic and thermal Energies= -2133.683867
Sum of electronic and thermal Enthalpies= -2133.682923
Sum of electronic and thermal Free Energies= -2133.792967

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 371.172	138.766	231.608

C,0,0.0418590209,-3.4592430759,-0.6226109997
C,0,-1.0301249323,-2.9092395683,-1.5756373618
P,0,-0.7483650742,-1.0971003797,-1.951267415
Ir,0,-0.0211741474,-0.0398809512,0.0823286188
B,0,-0.1131624935,1.8195285958,-0.895528921
O,0,-0.3183272168,3.0764411711,-0.3441988019
C,0,-0.1933199115,4.0801910026,-1.3533712505
C,0,-0.2241710491,3.2993778287,-2.6820097877
O,0,-0.0054149603,1.9362978545,-2.2979857444
P,0,0.334535089,-2.3427755274,0.8590847368
B,0,1.0563912662,0.8264438668,1.7109968902
O,0,1.8437623649,0.0615020572,2.5825474739
C,0,2.3558380947,0.9178195291,3.6138976945
C,0,2.0702818139,2.3410060774,3.0980440667
O,0,1.083371244,2.1580836026,2.0802852411
B,0,1.9882948243,0.032144191,-0.6214353643
O,0,2.6578017893,-1.0193644394,-1.2740607382
C,0,3.9442187318,-0.5676226949,-1.7218126332
C,0,4.1553001354,0.7678816446,-0.9851508312
O,0,2.8541826504,1.1217102116,-0.5061746855
C,0,2.0200170775,-2.8918797708,1.3812428953
C,0,-0.6666432709,-3.1120600067,2.2209942461
H,0,-0.2068385221,-4.4748445435,-0.2927151676
H,0,1.0058455483,-3.5120952729,-1.1407128004
C,0,0.3450966857,-1.1273279642,-3.4351340817
C,0,-2.3504554271,-0.5608094996,-2.6882182375
H,0,-1.0596699504,-3.4850778091,-2.5085608798
H,0,-2.0243126904,-2.985281323,-1.1221766701

H,0,0.5558007609,3.6167735987,-3.3821749277
H,0,-1.1952506329,3.382725681,-3.1884038701
H,0,0.753502664,4.6162878384,-1.2112137126
H,0,-1.0136103326,4.8003224751,-1.2630529336
H,0,2.961050077,2.8039510782,2.6548022694
H,0,1.6808329149,3.0086495335,3.8730130496
H,0,3.4224076337,0.7200528192,3.7618765572
H,0,1.8302099626,0.703498365,4.5536057983
H,0,4.5365403148,1.559708713,-1.6376725755
H,0,4.8381305576,0.6646816239,-0.1320133525
H,0,3.9212584429,-0.4403555258,-2.8118716246
H,0,4.7037966922,-1.3175397521,-1.4783730685
H,0,2.0488767331,-3.9736766505,1.5503279556
H,0,2.7307883646,-2.6178636822,0.6003783595
H,0,2.2878438631,-2.3611805348,2.2961564698
H,0,-0.4277867869,-4.1744092132,2.3382258822
H,0,-0.4245022551,-2.590904735,3.1520119194
H,0,-1.7372478792,-2.9992957896,2.0470216635
H,0,-2.6458708045,-1.2178514306,-3.5125818679
H,0,-3.126849252,-0.5530733143,-1.9215729091
H,0,-2.2191454524,0.4565598506,-3.0635976921
H,0,-0.1249926541,-1.6784619435,-4.2560171458
H,0,0.5187322074,-0.0908935312,-3.7322488655
H,0,1.3014843745,-1.5799267802,-3.1713077944
H,0,-0.7103163764,0.4126199791,1.483861029
C,0,-2.2041978354,0.238057043,0.7331565472
C,0,-3.1105786733,-0.8390387305,0.8257018386
C,0,-4.4695220089,-0.6579363789,1.0776459629
C,0,-4.9824325337,0.6287403962,1.2814895553
C,0,-4.1102356756,1.7186255711,1.2254552788
C,0,-2.7499645371,1.5135396466,0.9599991587
H,0,-2.7673116167,-1.8566893019,0.6749235967
H,0,-5.1501740405,-1.503297465,1.1261666349
O,0,-6.3275514351,0.7083704952,1.53125905
H,0,-4.4665865085,2.729455486,1.3918252962
H,0,-2.0996545905,2.3808474221,0.925460183
C,0,-6.8831964745,1.990783616,1.7600867353
H,0,-7.9488688994,1.8334725566,1.9373336643
H,0,-6.4403391309,2.476213215,2.6400308736
H,0,-6.7568928676,2.6511699494,0.8916545191

dmpeBpin3ParaAnisprodbetter

dmpeBpin3ParaAnisbetterprod
B3LYP/gen
E(RmPW+HF-PW91) = -2133.93900151

Zero-point correction= 0.556522 (Hartree/Particle)
Thermal correction to Energy= 0.594337
Thermal correction to Enthalpy= 0.595281
Thermal correction to Gibbs Free Energy= 0.486580
Sum of electronic and ZPE= -2133.732732
Sum of electronic and thermal Energies= -2133.694917
Sum of electronic and thermal Enthalpies= -2133.693973
Sum of electronic and thermal Free Energies= -2133.802674

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 372.952	138.811	228.780

C,0,-2.6553023578,0.9656893671,-1.6249457886
C,0,-2.2246484499,0.0413043585,-0.6500540065
C,0,-3.2526438715,-0.7949490159,-0.1614536871
C,0,-4.582411756,-0.7183870583,-0.5803502615
C,0,-4.9602927462,0.2219130914,-1.5426943798
C,0,-3.9809572627,1.0661164055,-2.0704648089
Ir,0,-0.0721800993,-0.049218153,-0.0930424552

P,0,-0.5430989885,-0.1198847184,2.2113328337
C,0,-0.4011598972,-1.8908873676,2.7992805484
C,0,-0.8742570099,-2.9071469969,1.7497395535
P,0,-0.1447378092,-2.5194979179,0.0656466446
B,0,1.9696526149,0.2229241215,0.5500087937
O,0,2.5355085459,1.4639687661,0.8253288907
C,0,3.9263350756,1.3052733321,1.1175225498
C,0,4.0906757143,-0.2037682696,1.3825108069
O,0,2.8920418817,-0.7897600215,0.8521109148
B,0,1.318675103,-0.2581170911,-1.7474984179
O,0,1.4874689155,-1.477753411,-2.4164733918
C,0,2.6860659804,-1.4000789431,-3.1971852894
C,0,2.9827252412,0.1089455356,-3.2789363114
O,0,2.2496991661,0.675198312,-2.1888202616
B,0,-0.1473367359,2.0422433447,-0.0589805621
O,0,0.0226484963,2.8562507536,-1.172295208
C,0,0.0037514542,4.2277642467,-0.7662183019
C,0,-0.5342615069,4.1977500912,0.6792829329
O,0,-0.4357830243,2.8215324587,1.0690787863
H,0,4.5141887585,1.6386668828,0.2532381203
H,0,4.1979197229,1.9233310861,1.9795646905
H,0,4.9641083092,-0.6358769684,0.8837324326
H,0,4.161254014,-0.4336761394,2.4540528744
H,0,3.4879664643,-1.9496649767,-2.6865785504
H,0,2.516677514,-1.8599820026,-4.1755885334
H,0,4.0462930938,0.3436323005,-3.1711532787
H,0,2.624020131,0.5487939117,-4.2183187328
H,0,0.0526551666,4.8185166018,1.3644932929
H,0,-1.5835541527,4.5138229396,0.7377158488
H,0,1.0223333536,4.6317595083,-0.8192747272
H,0,-0.6335359574,4.8050626544,-1.4442525095
H,0,-0.0247192948,0.148257753,-1.750505107
H,0,-1.9375201792,1.652570973,-2.063469194
H,0,-4.2274348782,1.8058703863,-2.8251053405
H,0,-3.0303918067,-1.552044198,0.5856011244
H,0,-5.3410548153,-1.3805478576,-0.1715935884
O,0,-6.2885717396,0.2340963958,-1.8935984257
C,0,0.5657223383,0.7612117127,3.3919149079
C,0,-2.1857017836,0.481096567,2.7900475438
C,0,1.4101544164,-3.5197513006,0.0934400675
C,0,-1.1839000167,-3.5111192507,-1.0949924494
H,0,-0.6030597389,-3.9260816838,2.0499958538
H,0,-1.9646589158,-2.8831725309,1.6582618084
H,0,0.6645673661,-2.0418509766,3.0070583119
H,0,-0.9371865051,-2.0135428085,3.7476872751
H,0,0.2054865616,0.6326334694,4.4177044905
H,0,1.5837778727,0.3753406794,3.3153920445
H,0,0.5683608802,1.8187458712,3.1238309114
H,0,-2.3043388887,0.2987914776,3.862988354
H,0,-2.2163542846,1.5547436979,2.5908249891
H,0,-2.9951298866,0.0096723508,2.2343304075
H,0,1.2010708784,-4.5669489502,0.3368332638
H,0,1.8718606977,-3.4566654341,-0.8934601
H,0,2.1052374824,-3.0896299986,0.8156830919
H,0,-1.2562761547,-4.5587080137,-0.7840312828
H,0,-2.1814562992,-3.0738965875,-1.1650035211
H,0,-0.7167972385,-3.459877253,-2.0820552922
C,0,-6.7076956904,1.1900498887,-2.8481150315
H,0,-7.7827126828,1.0452656542,-2.9742289344
H,0,-6.5218594596,2.2177978827,-2.5068387217
H,0,-6.2111633263,1.0474450656,-3.8177815078

bybpin3methylenedioxyMetaTS

Ir bpy Bpin3 methylenedioxybenzene meta ts
B3LYP/gen
E(RB+HF-LYP) = -1782.63275272

Zero-point correction= 0.484453 (Hartree/Particle)
Thermal correction to Energy= 0.518811
Thermal correction to Enthalpy= 0.519755
Thermal correction to Gibbs Free Energy= 0.413604
Sum of electronic and ZPE= -1782.148300
Sum of electronic and thermal Energies= -1782.113942
Sum of electronic and thermal Enthalpies= -1782.112998
Sum of electronic and thermal Free Energies= -1782.219149

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	325.559	126.878	223.415

C,0,-3.0915421631,2.9953664257,-2.6038395237
C,0,-2.3146584584,3.511040107,-1.5710307688
C,0,-1.3253855741,2.7741921682,-0.9493010481
C,0,-1.1210949096,1.4377620623,-1.376916462
C,0,-1.9027326338,0.9452108787,-2.4349927208
C,0,-2.9074341102,1.7080747951,-3.0645522849
Ir,0,0.2202912255,0.1212022159,-0.1553232987
N,0,-1.2635192321,-1.5979005813,-0.4839956701
C,0,-2.3074712455,-1.6621374837,0.3722622351
C,0,-3.2829448107,-2.6613786553,0.2492902865
C,0,-3.177901076,-3.6015418309,-0.7695010637
C,0,-2.0950378729,-3.527377359,-1.6426997156
C,0,-1.1605781779,-2.5111030193,-1.4621315028
C,0,-2.3435996855,-0.637393179,1.4432900776
N,0,-1.3113959793,0.2415487348,1.4807577371
C,0,-1.2742392687,1.1741359305,2.4492623156
C,0,-2.2677497131,1.2857667562,3.4175580508
C,0,-3.3407785012,0.3988917332,3.3835731838
C,0,-3.3752954724,-0.5717978065,2.3889730323
B,0,1.3420238637,-1.0813435862,1.2054202637
O,0,1.3363083665,-2.4792684575,1.1890784117
C,0,2.0757922834,-2.9682654111,2.3156886132
C,0,2.7650148846,-1.7171034727,2.8988995093
O,0,2.1016104581,-0.6143244331,2.270826175
B,0,1.7854797628,-0.6676672499,-1.2681457908
O,0,3.1436969579,-0.6580341524,-0.9775479295
C,0,3.8654609955,-1.2365637311,-2.0677692791
C,0,2.7899267839,-1.965067843,-2.8948994936
O,0,1.5576704747,-1.3734541895,-2.4620339321
B,0,1.4429274456,1.6939631334,0.330602194
O,0,1.303933311,2.4668536717,1.4957155094
C,0,2.1871690794,3.5927514952,1.4329589504
C,0,3.1054025365,3.2887919619,0.2317202664
O,0,2.4357920002,2.2453259296,-0.4765374973
H,0,0.3900969163,0.796782548,-1.6076860914
H,0,-0.2931984815,-2.4021836332,-2.1046560436
H,0,-4.1157665653,-2.7099813589,0.9396320536
H,0,-1.9676078783,-4.2401301245,-2.4504323144
H,0,-3.9286118502,-4.3787821529,-0.8751452559
H,0,-4.2021412168,-1.2696001819,2.3488958086
H,0,-4.1382224805,0.4574271892,4.1180303147
H,0,-2.1919688649,2.0575155175,4.1758430586
H,0,-0.4141322901,1.8342840169,2.4253598956
H,0,2.7678680181,-3.0426816351,-2.6850652813
H,0,2.9063734344,-1.8230701888,-3.9738468238
H,0,4.6381686743,-1.9103989865,-1.68394141
H,0,4.3544104189,-0.4377736242,-2.6399338533
O,0,-2.7233551754,4.8021268231,-1.2917538751
O,0,-4.0108863011,3.941014275,-3.0127702924
H,0,-0.7412150667,3.2099609412,-0.1462557771
H,0,-1.7249152074,-0.0608933199,-2.8023110868
H,0,-3.5030816167,1.3074559972,-3.8783653912
H,0,1.381657797,-3.4314898149,3.0291996044
H,0,2.7875726815,-3.7326037359,1.9863564994

H,0,2.6612869083,-1.6399479669,3.9863878781
H,0,3.8330388871,-1.6806191455,2.6505560677
H,0,1.5976094197,4.507119561,1.2832174573
H,0,2.7340800027,3.6852741389,2.3769136056
H,0,3.2451671288,4.1532132197,-0.4259049828
H,0,4.0939649699,2.9338619281,0.5508103304
C,0,-3.6256151713,5.1457592591,-2.3451258494
H,0,-3.1208558637,5.8161257598,-3.0589970927
H,0,-4.512798772,5.6284081366,-1.9237819828

bypbpin3methylenedioxyOrthoTS

Ir bpy Bpin3 methylenedioxybenzene ortho ts
B3LYP/gen
E(RB+HF-LYP) = -1782.63664076

Zero-point correction= 0.484871 (Hartree/Particle)
Thermal correction to Energy= 0.518880
Thermal correction to Enthalpy= 0.519825
Thermal correction to Gibbs Free Energy= 0.415935
Sum of electronic and ZPE= -1782.151770
Sum of electronic and thermal Energies= -1782.117760
Sum of electronic and thermal Enthalpies= -1782.116816
Sum of electronic and thermal Free Energies= -1782.220706

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 325.602	126.578	218.655

C,0,-3.0883321383,2.9388658665,-2.7648479778
C,0,-2.370891044,3.4262831205,-1.6899029931
C,0,-1.3873871056,2.6726087567,-1.0491049324
C,0,-1.0547116504,1.3752360349,-1.4104154496
C,0,-1.7795404271,0.8904424184,-2.5290478192
C,0,-2.7640436384,1.6359266357,-3.1804725143
Ir,0,0.2628193501,0.1019400919,-0.1235951654
N,0,-1.2825727162,-1.5823476083,-0.4215319211
C,0,-2.3584868363,-1.5442174801,0.3968547759
C,0,-3.4151853359,-2.4516647564,0.241216652
C,0,-3.3504651074,-3.4141611364,-0.7606217907
C,0,-2.2267523728,-3.4558947803,-1.5829410296
C,0,-1.2153925059,-2.51992771,-1.379506382
C,0,-2.3295096437,-0.5219365292,1.4725622376
N,0,-1.239909206,0.2823496346,1.515217994
C,0,-1.1124618368,1.1772059124,2.5091516392
C,0,-2.0840767406,1.3366720334,3.4931473164
C,0,-3.2234810198,0.5373444609,3.4477608022
C,0,-3.3427454141,-0.4056894571,2.4325744257
B,0,1.3379211811,-1.1313079472,1.238475766
O,0,1.869331054,-2.3897663199,0.9378341775
C,0,2.5690463455,-2.889964151,2.0835833587
C,0,2.105113549,-1.9820167175,3.2395487145
O,0,1.5045798524,-0.8546512025,2.591518749
B,0,1.8092256065,-0.6514275117,-1.287418693
O,0,3.1695459902,-0.4088480212,-1.1601008411
C,0,3.8658857738,-1.060823212,-2.2246571765
C,0,2.8317216448,-2.0344302252,-2.8211243496
O,0,1.5721068631,-1.5359666777,-2.3509489041
B,0,1.4992663005,1.6686405355,0.3488209179
O,0,1.7263771736,2.1543957398,1.6442244723
C,0,2.4405193968,3.3907791064,1.555784765
C,0,2.9766198467,3.4163294369,0.1118570354
O,0,2.1695322259,2.464665308,-0.5808228311
H,0,0.4243873144,0.7797690067,-1.582798937
H,0,-0.3148227698,-2.4969267529,-1.9848691383
H,0,-4.2804011876,-2.4108716414,0.8912633923
H,0,-2.1280961858,-4.1940888007,-2.3716398972

H,0,-4.1641890355,-4.1209642929,-0.8916742112
H,0,-4.2140417984,-1.0473809963,2.3939923296
H,0,-4.0048210622,0.6360103399,4.1952322408
H,0,-1.9392660637,2.0740629151,4.2751698862
H,0,-0.1963458147,1.7568887716,2.4962829619
H,0,2.9732891129,-3.0594383005,-2.4553014905
H,0,2.8357302228,-2.0495445678,-3.915717075
H,0,4.7514648348,-1.5701924851,-1.8310630304
H,0,4.1937531438,-0.3098306081,-2.9552483202
O,0,-0.902983213,3.4117188047,0.0253442801
O,0,-2.5162455494,4.6463078495,-1.0605031775
H,0,-3.849707845,3.5344765158,-3.2559814408
H,0,-1.5464216503,-0.1009835394,-2.9066410036
H,0,-3.2794991194,1.2086444952,-4.0362662117
H,0,2.3190658381,-3.9448057526,2.2384457735
H,0,3.649670979,-2.8130476851,1.9073506869
H,0,1.3584873615,-2.4732300949,3.8777971151
H,0,2.9301164629,-1.6444854136,3.8752142489
H,0,1.7505267065,4.2234996272,1.7507955657
H,0,3.2332861998,3.4149617621,2.3107249757
H,0,2.8835699568,4.4002563977,-0.3606734423
H,0,4.0292066072,3.1073055993,0.0598885798
C,0,-1.3810397606,4.7343946253,-0.1964714589
H,0,-0.5961953898,5.3357968529,-0.6845619687
H,0,-1.6811597098,5.1809797198,0.7548827379

dioxmetaParSptBackA

Ir bpin3 tempdioxmetaParSptBackA
B3LYP/gen
E(RB+HF-LYP) = -2208.27872086

Zero-point correction= 0.536380 (Hartree/Particle)
Thermal correction to Energy= 0.574010
Thermal correction to Enthalpy= 0.574954
Thermal correction to Gibbs Free Energy= 0.465739
Sum of electronic and ZPE= -2207.742341
Sum of electronic and thermal Energies= -2207.704711
Sum of electronic and thermal Enthalpies= -2207.703766
Sum of electronic and thermal Free Energies= -2207.812982

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 360.197	137.975	229.864

C,0,4.277297906,0.0826569134,0.4162012273
C,0,2.9579842254,0.4171529047,0.1851388577
C,0,1.9468382004,-0.4861292466,0.6041118651
C,0,2.3516709819,-1.6403198668,1.2964324819
C,0,3.7026332769,-1.9720005159,1.5363470789
C,0,4.6510535907,-1.087091937,1.0699139469
Ir,0,-0.2300416914,-0.0728624388,0.0452149855
B,0,0.1205778395,1.988919171,-0.1020880868
O,0,-0.3149690267,2.8053495501,-1.1586029555
C,0,-0.0337560817,4.1743082319,-0.8363566147
C,0,0.9450589878,4.095852854,0.3526724102
O,0,0.8446855809,2.744992099,0.81051001
O,0,6.0274356686,-1.1680034918,1.1335395228
P,0,0.2254374334,-0.4600105268,-2.295022888
C,0,1.9780412995,-0.8157156906,-2.7643745144
P,0,-0.9756757226,-2.4349915893,-0.0254043803
C,0,-0.4350022651,-3.8267666727,1.0754280017
B,0,-2.186052139,0.5584885385,-0.5162147268
O,0,-2.8316190421,0.1983422669,-1.716012406
C,0,-4.0622744968,0.927038856,-1.8369618134
C,0,-4.301200877,1.5029018631,-0.4293801302
O,0,-3.0395162956,1.3706162942,0.2313016166

B,0,-1.1618958571,0.2059483109,1.9391090243
O,0,-1.2245284484,1.3688557382,2.681691872
C,0,-2.1390501251,1.1768543597,3.7630524559
C,0,-2.2924284063,-0.3527391153,3.866162227
O,0,-1.8248387261,-0.8381240985,2.5975791905
C,0,-0.6538291139,-2.0277052313,-2.7989190397
C,0,-0.5263340336,-3.1079318843,-1.7150190082
C,0,-0.2763425502,0.73109699,-3.6062539727
C,0,-2.8076417529,-2.688331609,0.031970368
H,0,-5.0611168905,0.936717978,0.1249440403
H,0,-4.6005853781,2.5556534446,-0.4450115464
H,0,-4.8592534116,0.2523038081,-2.1664659319
H,0,-3.9419250338,1.7148738795,-2.5911466302
H,0,-3.3278118247,-0.671072912,4.0242351776
H,0,-1.6718339309,-0.7794570977,4.6645564455
H,0,-3.0893887394,1.6683932808,3.5193028049
H,0,-1.7339990317,1.6297815349,4.6733174923
H,0,-0.970002937,4.6787395226,-0.5663416127
H,0,0.3911362675,4.6801820458,-1.7099681768
H,0,0.6825213853,4.7799666515,1.1658429164
H,0,1.9812478872,4.3010118693,0.0520467389
H,0,0.5738305647,0.0644708921,1.4504808292
H,0,2.7183180213,1.3583395702,-0.2921412775
O,0,5.4121441223,0.7794542253,0.0427053691
H,0,1.5966493816,-2.3022139585,1.701479258
H,0,3.9819634826,-2.8727418936,2.0732985304
H,0,-1.147530876,-3.9793010979,-1.9542717495
H,0,0.510323366,-3.4596709658,-1.6493199642
H,0,-1.7021431138,-1.7475250659,-2.939480253
H,0,-0.265832917,-2.3841482596,-3.7606685695
H,0,2.0351198916,-1.1543577251,-3.8041359029
H,0,2.580412706,0.0879936436,-2.6488584651
H,0,2.3987084161,-1.5746528412,-2.1019200134
H,0,-0.026434019,0.3441853169,-4.5993605709
H,0,-1.3506191778,0.896367523,-3.5254489387
H,0,0.2288431132,1.6828808072,-3.4348357518
H,0,-0.9748648116,-4.7466593788,0.8279208387
H,0,0.6361272244,-4.0084219507,0.9695439957
H,0,-0.6468394097,-3.5576647399,2.1133789183
H,0,-3.0703318659,-3.7407259393,-0.1179319203
H,0,-3.1581477475,-2.3553568104,1.0110475775
H,0,-3.2817209311,-2.0753303136,-0.736626227
C,0,6.4930714339,0.1126861431,0.6974671583
H,0,6.8158090535,0.702438746,1.5700829565
H,0,7.3202623907,-0.0209729593,-0.0062351514

dioxmetaSptSptBackS

Ir bpin3 tempdioxmetaSptSptBackS
B3LYP/gen
E(RB+HF-LYP) = -2208.27908090

Zero-point correction= 0.536083 (Hartree/Particle)
Thermal correction to Energy= 0.573863
Thermal correction to Enthalpy= 0.574807
Thermal correction to Gibbs Free Energy= 0.464209
Sum of electronic and ZPE= -2207.742998
Sum of electronic and thermal Energies= -2207.705218
Sum of electronic and thermal Enthalpies= -2207.704274
Sum of electronic and thermal Free Energies= -2207.814872

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 360.105	138.094	232.774

C,0,2.4254110836,-1.8471454541,0.6679865958
C,0,1.9709007327,-0.5299423767,0.4717149357

C,0,2.9453322042,0.5010604651,0.4320249605
C,0,4.2780772127,0.1519160058,0.5365895492
C,0,4.7008406075,-1.1620201322,0.7017757777
C,0,3.7888504883,-2.1937067288,0.7768931637
Ir,0,-0.2477315065,-0.0784933227,0.0460392581
P,0,-0.1399658284,-1.2053533466,-2.0854330004
C,0,-1.0208628415,-2.849286374,-1.906317754
C,0,-0.7994295257,-3.4896134421,-0.526761057
P,0,-1.1193006307,-2.2404044517,0.8323503982
B,0,-2.1980811247,0.5922205841,-0.4731997399
O,0,-3.1035760454,-0.1192325631,-1.2824597864
C,0,-4.2605338349,0.6908903438,-1.5389530135
C,0,-4.1374879708,1.8595589498,-0.5427892172
O,0,-2.7877338094,1.7921245765,-0.0736564945
B,0,-0.91393955,0.8744632532,1.8330223543
O,0,-1.7196961471,0.2049430686,2.7660815723
C,0,-1.9334477326,1.0699081256,3.891747532
C,0,-1.4557211046,2.4500096313,3.4009245596
O,0,-0.6475783137,2.1605118152,2.2578471539
B,0,0.2511180023,1.7775467433,-0.8076807171
O,0,0.9524117664,2.811386321,-0.1946594076
C,0,1.1952439288,3.8634768064,-1.13187692
C,0,0.2927360289,3.5218155992,-2.3321156565
O,0,-0.06413102,2.148698118,-2.1278108167
H,0,-4.2375310224,1.0315075814,-2.5819097691
H,0,-5.1671463444,0.0950418587,-1.3910780924
H,0,-4.317594144,2.8346238712,-1.0065975456
H,0,-4.8223660236,1.7516220758,0.3080534271
H,0,-2.991515985,1.0561771849,4.1724302239
H,0,-1.3442306123,0.7050067682,4.7431201033
H,0,-2.2934929534,3.0890736096,3.0947142504
H,0,-0.8607935742,2.9880177985,4.1454556832
H,0,-0.6195685019,4.131792632,-2.3479445572
H,0,0.7999522441,3.6335905446,-3.2963545037
H,0,0.9509427669,4.8270943492,-0.6739323406
H,0,2.2596945376,3.8700757098,-1.4025381895
H,0,0.7080053091,0.1663659591,1.3420424369
H,0,1.7130908342,-2.6606437737,0.7158481454
H,0,2.652582531,1.5395606836,0.3400781384
O,0,5.3785286595,0.9886965074,0.5461048104
O,0,6.0740523708,-1.2044789086,0.8171383244
C,0,-0.9145902467,-0.5198856816,-3.6102183822
C,0,1.5378501966,-1.6567857755,-2.7123626736
C,0,-2.947072983,-2.3810004389,1.0708627023
C,0,-0.5359267381,-3.0852812933,2.373342402
H,0,-1.4439446596,-4.3674452949,-0.3971111658
H,0,0.236536556,-3.8328333848,-0.4279462287
H,0,-2.0833624597,-2.6226057603,-2.0455996265
H,0,-0.7181542627,-3.5284254747,-2.7120708543
H,0,1.4633150226,-2.2793574048,-3.6098047082
H,0,2.073387481,-0.7355463683,-2.9573213813
H,0,2.1091913006,-2.1768461758,-1.9421437396
H,0,-0.7584570925,-1.1900259185,-4.4616920888
H,0,-1.9815928572,-0.3876243615,-3.4290867749
H,0,-0.473383199,0.4582375188,-3.8071930317
H,0,-0.9617443019,-4.0895721319,2.4691768907
H,0,0.552955758,-3.1468371268,2.4033006572
H,0,-0.8652714023,-2.4732060076,3.2169783545
H,0,-3.2385192542,-3.4076585821,1.3165458506
H,0,-3.2253861863,-1.7116083023,1.8879754652
H,0,-3.4577377334,-2.0513751959,0.1648891824
C,0,6.5141946306,0.1237496083,0.5128566181
H,0,7.2428544263,0.4460157292,1.2632565529
H,0,6.9615907968,0.1389368016,-0.4937232803
H,0,4.1054830467,-3.2219536452,0.9196904849

dioxmetaSptSptFrntA

Ir bpin3 tempdioxmetaSptSptFrntA
B3LYP/gen
E(RB+HF-LYP) = -2208.27742316

Zero-point correction= 0.536420 (Hartree/Particle)
Thermal correction to Energy= 0.574125
Thermal correction to Enthalpy= 0.575069
Thermal correction to Gibbs Free Energy= 0.465345
Sum of electronic and ZPE= -2207.741003
Sum of electronic and thermal Energies= -2207.703298
Sum of electronic and thermal Enthalpies= -2207.702354
Sum of electronic and thermal Free Energies= -2207.812078

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 360.269	137.897	230.933

C,0,-0.2706376537,-3.2954019133,-0.9886212317
C,0,-1.1062770587,-2.4636515504,-1.9732061125
P,0,-0.4392546611,-0.7205672927,-2.1261473306
Ir,0,0.243868006,-0.0074457058,0.068055488
B,0,0.6552996336,1.8976273959,-0.7117333
O,0,0.6063000877,3.1225685176,-0.0612566691
C,0,1.06706014,4.158671082,-0.9305707543
C,0,1.1090500743,3.5041235397,-2.3261587334
O,0,0.9969854167,2.0994539322,-2.0647803664
P,0,0.0336962417,-2.4010487997,0.633403284
B,0,1.2708783227,0.4682368592,1.8801644486
O,0,1.7417368329,-0.5201911059,2.7550771366
C,0,2.3003210349,0.117522246,3.9135035603
C,0,2.4173453098,1.5994719526,3.5084877405
O,0,1.5573134298,1.7264793857,2.3738213856
B,0,2.2895862463,-0.3234526093,-0.4284261699
O,0,2.7852467181,-1.4397873872,-1.1288923318
C,0,4.1843310596,-1.2581179219,-1.3949237289
C,0,4.5910858062,-0.0697965751,-0.5034271433
O,0,3.3506773338,0.523930529,-0.1082283104
C,0,1.5068797014,-3.3169956638,1.2698956541
C,0,-1.2565813375,-3.0823772897,1.7839528169
H,0,-0.7298290017,-4.274476991,-0.8083809236
H,0,0.7258605986,-3.4708660858,-1.4084790206
C,0,0.780295041,-0.8511429931,-3.5030007269
C,0,-1.8149525958,0.1945471519,-2.9439218601
H,0,-1.1365785398,-2.9390488272,-2.9611091241
H,0,-2.14274731,-2.381426574,-1.6276058202
H,0,2.0410470605,3.7068706906,-2.864328211
H,0,0.2704342182,3.823548327,-2.9592503341
H,0,2.0591319384,4.4900555559,-0.5993775007
H,0,0.3840907681,5.0134907523,-0.8816265738
H,0,3.4404908049,1.8660228228,3.214731122
H,0,2.0917916428,2.2866453899,4.2957314952
H,0,3.2650165897,-0.339108214,4.1571847364
H,0,1.6235001479,-0.0278134988,4.7654582454
H,0,5.2023040707,0.6693438152,-1.0309335222
H,0,5.1374841795,-0.3934788201,0.3916868323
H,0,4.3223521178,-1.0423500068,-2.4622027232
H,0,4.7272001181,-2.1785673767,-1.1566978582
H,0,1.3065615063,-4.3916278729,1.3374249578
H,0,2.3453610854,-3.1367766256,0.5958580829
H,0,1.7595432585,-2.917317877,2.2530543893
H,0,-1.2019592297,-4.1750364873,1.8316090453
H,0,-1.0690206525,-2.6753059602,2.7818968059
H,0,-2.2645928478,-2.7883615998,1.4897499364
H,0,-2.1426465751,-0.3149668737,-3.8557983292
H,0,-2.6524253562,0.2952619306,-2.25185867
H,0,-1.4496347502,1.192411645,-3.1978073631

H,0,0.3044395652,-1.2418495819,-4.4082937493
H,0,1.1743278053,0.1499233547,-3.6902910798
H,0,1.6027394533,-1.4979224309,-3.1962522914
H,0,-0.5022872149,0.4874212855,1.4278334698
C,0,-1.9048854681,0.6635130088,0.5355602736
C,0,-2.9827442091,-0.2524405692,0.426025816
C,0,-4.274724939,0.220180235,0.5640951696
C,0,-4.55229609,1.5548246907,0.8337915282
C,0,-3.5352683356,2.4755886509,0.9769968176
C,0,-2.2144861871,2.0053666587,0.8267486753
H,0,-2.8243523661,-1.3011030792,0.215008607
O,0,-5.456483902,-0.4938411989,0.5019368804
O,0,-5.9160161498,1.7310303769,0.9581958117
H,0,-3.742031377,3.5161122343,1.2050910174
H,0,-1.4040264519,2.7164597408,0.9354619567
C,0,-6.4933752741,0.4919524102,0.5410632443
H,0,-7.2601445801,0.1860073887,1.2594747991
H,0,-6.9278312507,0.607651803,-0.4646233667

dioxorthoParSptBackA

Ir bpin3 tempdioxorthoParSptBackA
B3LYP/gen
E(RB+HF-LYP) = -2208.28435264

Zero-point correction= 0.536679 (Hartree/Particle)
Thermal correction to Energy= 0.573997
Thermal correction to Enthalpy= 0.574941
Thermal correction to Gibbs Free Energy= 0.467135
Sum of electronic and ZPE= -2207.747673
Sum of electronic and thermal Energies= -2207.710356
Sum of electronic and thermal Enthalpies= -2207.709412
Sum of electronic and thermal Free Energies= -2207.817218

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 360.188	137.692	226.898

C,0,3.0995053423,-0.0502117239,0.3584635394
C,0,1.9758826161,-0.8342903333,0.5875728571
C,0,2.2863131623,-2.0961698792,1.1607500278
C,0,3.5895708888,-2.5337790415,1.4061645022
C,0,4.6978704749,-1.7207561049,1.1185140727
C,0,4.4078568484,-0.4744151114,0.5993095557
Ir,0,-0.1183486933,-0.1402580644,0.0336990916
P,0,0.43542117,0.1011395097,-2.3211747401
C,0,-0.5187020553,-1.2036602646,-3.2535071244
C,0,-0.4508665911,-2.5521862484,-2.5225994422
P,0,-0.9262759706,-2.3623156074,-0.7219343544
B,0,-2.0053918726,0.7369707861,-0.4062639309
O,0,-2.8318063699,1.4220358328,0.4836339336
C,0,-4.0538716076,1.7923523541,-0.1605146898
C,0,-3.8017922737,1.5203801002,-1.6552715316
O,0,-2.6246994079,0.6994427639,-1.6720380143
B,0,-1.1679583593,-0.3609685324,1.8676750356
O,0,-1.9462396723,-1.491801701,2.1549288206
C,0,-2.453729865,-1.3729533535,3.4931288426
C,0,-2.1806573875,0.0956611051,3.869029788
O,0,-1.1949896982,0.5246651066,2.9281970996
B,0,0.3465122772,1.8550247503,0.4926514208
O,0,0.9788913027,2.2700868142,1.6584434803
C,0,1.230779085,3.6729171995,1.5890776508
C,0,0.3818091568,4.1585560076,0.3983434183
O,0,0.0640105421,2.9611428932,-0.3219432886
H,0,-4.8733679514,1.1806150699,0.2385848095
H,0,-4.2764456733,2.8434595571,0.0487348175
H,0,-4.627759319,0.9906845527,-2.1412617421

H,0,-3.6055835883,2.4431168426,-2.2158182372
H,0,-3.5176384674,-1.6305456038,3.5084415634
H,0,-1.917105884,-2.0749783633,4.1442843809
H,0,-3.0763823037,0.7203380222,3.7602651931
H,0,-1.7950786058,0.2131195069,4.8866242105
H,0,-0.5493211398,4.638754153,0.7257508231
H,0,0.9174701961,4.8549802507,-0.2559727835
H,0,0.9499272441,4.1472606127,2.5350618319
H,0,2.3038119726,3.8431925212,1.4237270338
H,0,0.6812058833,-0.3545904352,1.4293460608
O,0,3.160139911,1.2189121873,-0.2138515944
O,0,5.3026312774,0.5029975515,0.2141622191
H,0,1.4667881118,-2.7431469889,1.4530177623
H,0,3.7493372672,-3.5124034177,1.8505315296
H,0,5.7185598316,-2.0363537093,1.3028803818
C,0,0.0615629497,1.6423088182,-3.2559663082
C,0,2.1701119565,-0.2523077095,-2.8533035631
C,0,-2.762709491,-2.5734550263,-0.7787317113
C,0,-0.4215307119,-4.0055892438,-0.0321854514
H,0,-1.0953965117,-3.2955327171,-3.0067063706
H,0,0.5711936127,-2.9494731269,-2.5454971867
H,0,-1.5504541206,-0.844001766,-3.2989734064
H,0,-0.1383105692,-1.2879756286,-4.2786225783
H,0,2.2336899257,-0.2902041797,-3.9457255633
H,0,2.8244531545,0.5317392216,-2.4705489825
H,0,2.5063018217,-1.2031029991,-2.4339709574
H,0,0.3477523405,1.539951171,-4.3077572193
H,0,-1.0076382323,1.8409209503,-3.1760776809
H,0,0.598560805,2.4734069562,-2.7961561423
H,0,-0.9013722043,-4.8227096507,-0.5809611394
H,0,0.6622991444,-4.1238199136,-0.0899641623
H,0,-0.7246568317,-4.0552002994,1.0170034128
H,0,-3.0422302274,-3.5357518308,-1.2204844964
H,0,-3.1367808866,-2.50894771,0.244826443
H,0,-3.197225434,-1.758399269,-1.3607803995
C,0,4.4900632417,1.6637835876,0.0328569497
H,0,4.5113171597,2.272997702,0.9512012788
H,0,4.8527123041,2.2331870969,-0.826140045

dioxorthoSptSptBackS

Ir bpin3 tempdioxorthoSptSptBackS
B3LYP/gen
E(RB+HF-LYP) = -2208.27895340

Zero-point correction= 0.536067 (Hartree/Particle)
Thermal correction to Energy= 0.573593
Thermal correction to Enthalpy= 0.574537
Thermal correction to Gibbs Free Energy= 0.466300
Sum of electronic and ZPE= -2207.742886
Sum of electronic and thermal Energies= -2207.705361
Sum of electronic and thermal Enthalpies= -2207.704416
Sum of electronic and thermal Free Energies= -2207.812653

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	359.935	137.927	227.804

C,0,-2.377322766,-2.0017544136,-1.0168428361
C,0,-1.9920854279,-0.6845512363,-0.6467634293
C,0,-3.0700277426,0.1860109914,-0.5463871847
C,0,-4.4014986406,-0.1891381023,-0.7440879065
C,0,-4.7622447749,-1.4785154225,-1.0779607829
C,0,-3.7031724855,-2.3925683289,-1.2124928367
Ir,0,0.1509662632,-0.1229699337,-0.0721201706
P,0,0.1204784417,-1.5842742963,1.8438146308
C,0,1.2170297366,-3.0505354057,1.4582134367

C,0,1.1053404008,-3.4819458673,-0.0141730731
P,0,1.2685108169,-2.006759222,-1.1596706838
B,0,2.0262921452,0.6457367786,0.5603660342
O,0,2.9376872498,-0.0509123777,1.3820805318
C,0,4.0492608928,0.8015888023,1.6948142233
C,0,3.9155680302,1.9757253739,0.7071974485
O,0,2.5786974949,1.8754205722,0.2134612815
B,0,0.6629344288,1.200548218,-1.6711005438
O,0,1.5916964556,0.8312330403,-2.6550575624
C,0,1.6767668505,1.8863382013,-3.6245424423
C,0,0.9158409782,3.0601366221,-2.9761523289
O,0,0.1516880727,2.455264695,-1.9305217234
B,0,-0.5999259523,1.4381466593,1.1341354998
O,0,-0.3506000167,2.7991371566,1.055686294
C,0,-1.1730962949,3.4889760021,1.9940506198
C,0,-1.6639690212,2.3915704027,2.9581606437
O,0,-1.4109323057,1.1688091889,2.2571915883
H,0,3.9706606089,1.1289612344,2.7396500403
H,0,4.9853434192,0.2454130033,1.5787071758
H,0,4.06110328,2.9512381015,1.1819920742
H,0,4.6200012131,1.8912734355,-0.1306912009
H,0,2.7275375048,2.1178396411,-3.8269211839
H,0,1.2091174825,1.5537924694,-4.5605880064
H,0,1.5972128873,3.8000055303,-2.5385821599
H,0,0.2448817678,3.5727292772,-3.672815833
H,0,-1.104804764,2.3923191161,3.9044463141
H,0,-2.7308671182,2.472395142,3.1945210489
H,0,-0.5920411949,4.270517895,2.4952783169
H,0,-2.0050993871,3.9686469902,1.4612953241
H,0,-0.8215063186,0.1797289531,-1.3523377016
H,0,-1.6122736179,-2.7608190354,-1.1307053887
H,0,-3.9223253928,-3.4246929176,-1.4725664851
O,0,-3.0339999345,1.5500377453,-0.3109315451
O,0,-5.2266858928,0.9043250318,-0.6102073945
H,0,-5.7977014347,-1.7567938574,-1.2381176142
C,0,0.7440374204,-1.0315065973,3.4874166788
C,0,-1.501793533,-2.325415009,2.3161703667
C,0,3.0966348179,-1.8798148061,-1.3947894205
C,0,0.7746524366,-2.6756353539,-2.8141301573
H,0,1.8592457898,-4.2401264422,-0.2580689957
H,0,0.1237930554,-3.9327877139,-0.2014090032
H,0,2.2377584173,-2.7197815942,1.6780783041
H,0,0.9860715433,-3.8848958668,2.1310680351
H,0,-1.3780979231,-3.0442829114,3.1326939475
H,0,-2.1511194961,-1.508503896,2.640113381
H,0,-1.9732182581,-2.8110544753,1.4604681217
H,0,0.7285975551,-1.8533970161,4.2106005251
H,0,1.760438911,-0.6555653379,3.3687870729
H,0,0.0955029905,-0.2247128012,3.8347331974
H,0,1.3126662463,-3.5987444727,-3.0541114959
H,0,-0.3006286288,-2.8579778567,-2.8561252481
H,0,1.0199679554,-1.9139573718,-3.5590419475
H,0,3.5156626915,-2.8067930585,-1.80003579
H,0,3.281271534,-1.0544486381,-2.0861498395
H,0,3.5660753136,-1.6431113114,-0.4383315118
C,0,-4.3840524394,1.9374891124,-0.0891095701
H,0,-4.5877787142,2.8743181375,-0.6145350968
H,0,-4.5687316228,2.0446174265,0.9924409371

dmpeBpin3BisMetaCF3CHactTSA

Ir dmpw bpin3 meta cf3 2
B3LYP/gen
E(RB+HF-LYP) = -2693.82652564

Zero-point correction= 0.530189 (Hartree/Particle)
Thermal correction to Energy= 0.573021

Thermal correction to Enthalpy= 0.573965

Thermal correction to Gibbs Free Energy= 0.450356

Sum of electronic and ZPE= -2693.296336

Sum of electronic and thermal Energies= -2693.253504

Sum of electronic and thermal Enthalpies= -2693.252560

Sum of electronic and thermal Free Energies= -2693.376170

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 359.576	155.042	260.158

C,0,2.7182068847,-1.5717999916,0.7355272891
 C,0,2.1466913907,-0.304088183,0.5509461074
 C,0,3.0479428848,0.7755383247,0.4890631366
 C,0,4.4319124849,0.5836350788,0.5363612056
 C,0,4.9793104735,-0.6926510238,0.670575119
 C,0,4.1030856691,-1.7693954124,0.7760004514
 Ir,0,-0.0826710857,-0.0714910433,0.098082419
 P,0,0.1647201366,-1.1991560388,-2.0325285185
 C,0,-0.6110344247,-2.8943570457,-1.8718666968
 C,0,-0.3656212067,-3.517335893,-0.4884777491
 P,0,-0.788990408,-2.2999306742,0.8707582355
 B,0,-2.0666961817,0.4285683849,-0.4784964149
 O,0,-2.8807270881,-0.3602452452,-1.3108471847
 C,0,-4.0964248059,0.3471058456,-1.6024247972
 C,0,-4.1092893171,1.512119086,-0.5954136296
 O,0,-2.7677704429,1.5720698003,-0.0995679587
 B,0,-0.8913419865,0.8350189356,1.8511339425
 O,0,-1.6843294295,0.1160589331,2.7553394251
 C,0,-1.9956173966,0.9673880877,3.8700314689
 C,0,-1.5833628108,2.3742717585,3.3954649785
 O,0,-0.7202197295,2.1347524857,2.2801768827
 B,0,0.2764555522,1.8230262266,-0.7497122176
 O,0,0.8987097905,2.8997108748,-0.1277091937
 C,0,1.104778037,3.9561689931,-1.0724764983
 C,0,0.2382853476,3.5581087437,-2.2811796932
 O,0,-0.0413720149,2.1656949433,-2.0740978239
 H,0,-4.0674309471,0.6981055404,-2.6416071758
 H,0,-4.9505617424,-0.3281400775,-1.4893959072
 H,0,-4.3750475926,2.469539424,-1.053973631
 H,0,-4.7948696968,1.3274111867,0.2413564264
 H,0,-3.0612223862,0.8886645541,4.1074038354
 H,0,-1.4201923829,0.6385126927,4.7448853818
 H,0,-2.4455132858,2.9637969728,3.0598394177
 H,0,-1.0465388089,2.9448461505,4.159377122
 H,0,-0.707689006,4.1132710393,-2.311065023
 H,0,0.749893889,3.6934494168,-3.2396674326
 H,0,0.8058516904,4.9095679362,-0.6265583266
 H,0,2.1723714452,4.0093487377,-1.3230075131
 H,0,0.8586525014,0.2325988399,1.3962283819
 H,0,2.0869100313,-2.4458695438,0.8229125478
 C,0,4.608471164,-3.1801635267,0.8583572717
 H,0,2.6581004739,1.7822608411,0.3965185069
 C,0,5.3297856289,1.7902191136,0.4848750952
 H,0,6.05160692,-0.8413018969,0.6948429708
 C,0,-0.6039666729,-0.5584983799,-3.5784926829
 C,0,1.8830130216,-1.563424815,-2.6115003472
 C,0,-2.6017170366,-2.5683191965,1.1002349226
 C,0,-0.1493109792,-3.1149427444,2.406858743
 H,0,-0.945578972,-4.4399908458,-0.3679852967
 H,0,0.6905414985,-3.7884945029,-0.3752967269
 H,0,-1.683469278,-2.74393313,-2.0348137827
 H,0,-0.2430239983,-3.5494613852,-2.670253337
 H,0,1.8578734831,-2.1284003598,-3.5487971194
 H,0,2.4096887387,-0.6198262466,-2.7777615424
 H,0,2.4402179482,-2.1303683385,-1.8640671901
 H,0,-0.4060664417,-1.2325359885,-4.4179740131
 H,0,-1.6783019575,-0.4660159836,-3.4175871218

H,0,-0.1989430364,0.4337734589,-3.7813948929
H,0,-0.5506632051,-4.1279339591,2.5145869398
H,0,0.9412027363,-3.1619986419,2.4191507204
H,0,-0.4761809131,-2.5093142674,3.2562444152
H,0,-2.8225896206,-3.6156446979,1.3310391456
H,0,-2.9278366377,-1.9290684014,1.9234890392
H,0,-3.1271758783,-2.2622579494,0.1945847924
F,0,6.595864557,1.4694064338,0.1323534865
F,0,4.8860199992,2.7083251014,-0.4067190252
F,0,5.4007612395,2.4162944897,1.6822626315
F,0,5.9345177781,-3.2513086817,1.0878593895
F,0,3.9878570169,-3.8809777028,1.8393875459
F,0,4.3660033913,-3.8562106177,-0.297300926

methiophenebpylrBeg3TS

bpy thiophene Ir Beg3 TS

B3LYP/gen

E(RB+HF-LYP) = -1954.18593360

Zero-point correction= 0.463139 (Hartree/Particle)

Thermal correction to Energy= 0.496714

Thermal correction to Enthalpy= 0.497658

Thermal correction to Gibbs Free Energy= 0.393446

Sum of electronic and ZPE= -1953.722795

Sum of electronic and thermal Energies= -1953.689220

Sum of electronic and thermal Enthalpies= -1953.688276

Sum of electronic and thermal Free Energies= -1953.792488

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 311.693	122.401	219.333

C,0,3.8466959359,-0.3785875286,-2.0572882733
C,0,4.181687224,-1.4086480586,-1.2191926145
S,0,2.7901978439,-1.8530622409,-0.2565602572
C,0,1.7583703844,-0.6235471041,-0.9719276389
C,0,2.4888721087,0.0515601296,-1.9277116416
Ir,0,-0.2379320778,-0.182051258,-0.1402480847
N,0,0.0662936392,1.988913724,-0.8112903554
C,0,0.7456870591,2.7864981448,0.0424467057
C,0,1.038076939,4.1160252221,-0.2917649336
C,0,0.6209742009,4.6222215758,-1.5180358799
C,0,-0.0882226307,3.7921236204,-2.3835068514
C,0,-0.3459667869,2.4814983354,-1.9890342467
C,0,1.1328902444,2.1823944659,1.3414770366
N,0,0.7634625703,0.8948509694,1.5503149733
C,0,1.0502533834,0.3034719824,2.7226114059
C,0,1.7337990328,0.9621776956,3.7408596248
C,0,2.1321006246,2.280735161,3.5371687382
C,0,1.8248138281,2.8959296151,2.3285556783
B,0,-2.0628714386,0.3780419147,0.8116800936
O,0,-2.8976522128,1.3949683242,0.3385846374
C,0,-3.9492052714,1.6253047201,1.2845773342
C,0,-3.8054870697,0.48228637,2.3130308297
O,0,-2.5377603589,-0.1153734619,2.018164532
B,0,-1.7590819371,-0.7058996344,-1.4539587581
O,0,-2.8377349532,-1.5505515207,-1.2239243299
C,0,-3.5813581647,-1.7027172392,-2.43646592
C,0,-3.0880527905,-0.5523468373,-3.3331908861
O,0,-1.8365519702,-0.1684083058,-2.7482370101
B,0,-0.4132377688,-2.0671266772,0.6524582607
O,0,-0.2788218845,-2.3700083503,2.0145694577
C,0,-0.234102667,-3.7912541005,2.1824470282
C,0,-0.673047862,-4.3510093861,0.8138217171
O,0,-0.5564406622,-3.2432458957,-0.080020862
H,0,0.2704922189,-0.9739987184,-1.4590694202

H,0,-0.8975500418,1.785208267,-2.6123855776
H,0,1.5843995361,4.7524200343,0.3932416884
H,0,-0.4388226767,4.1446536652,-3.3475686551
H,0,0.8445560164,5.649647641,-1.7887842353
H,0,2.1225979837,3.9228588003,2.1580743439
H,0,2.6702730812,2.8267150773,4.306036616
H,0,1.9443906755,0.4419176555,4.668864228
H,0,0.7058234745,-0.7204483356,2.8218148314
H,0,-3.7730104015,0.3054533655,-3.3163834334
H,0,-2.9305331849,-0.8536019314,-4.3734978729
H,0,-4.6535559929,-1.6485856407,-2.2225321657
H,0,-3.3625877049,-2.6863920671,-2.8713066913
C,0,5.5032417025,-2.1042612296,-1.0792563267
H,0,4.5517184733,0.0599485723,-2.7578995741
H,0,2.061117524,0.8383204767,-2.5406803782
H,0,-3.8144877668,2.6152440527,1.7394220272
H,0,-4.9162088754,1.6156734893,0.7703339998
H,0,-3.8126754366,0.8379950365,3.3488839107
H,0,-4.5920858669,-0.2744580078,2.2042720151
H,0,0.7892015044,-4.0928564285,2.4425467021
H,0,-0.9005246363,-4.0864432927,2.999657702
H,0,-0.0388356843,-5.1740917757,0.4681659507
H,0,-1.7145023265,-4.6981224982,0.8265170293
H,0,5.4275102325,-3.1778700003,-1.2896471201
H,0,6.2250582326,-1.6773973551,-1.7823573529
H,0,5.9203740875,-2.001026921,-0.0700363755

methiophenedmpelrBcat3TS

Ir Bcat3 methylthiophene ts for C-H at 2 position
B3LYP/gen
E(RB+HF-LYP) = -2837.14350495

Zero-point correction= 0.584504 (Hartree/Particle)
Thermal correction to Energy= 0.627135
Thermal correction to Enthalpy= 0.628080
Thermal correction to Gibbs Free Energy= 0.506774
Sum of electronic and ZPE= -2836.559000
Sum of electronic and thermal Energies= -2836.516370
Sum of electronic and thermal Enthalpies= -2836.515425
Sum of electronic and thermal Free Energies= -2836.636731

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 393.533	163.097	255.308

C,0,3.5338098577,-1.7612203261,0.8903882682
C,0,2.6496154902,-0.7017400094,0.8729173579
S,0,3.4484480522,0.6788396558,1.6165610042
C,0,4.9455564771,-0.1790003051,1.8837290471
C,0,4.8201832705,-1.4690967682,1.4427352315
Ir,0,0.642804688,-0.4881276917,-0.1124527646
P,0,1.7577074739,-0.115329038,-2.2420897733
C,0,1.6677238236,-1.7103816706,-3.2153758801
C,0,1.7676683623,-2.9516861749,-2.3137811589
P,0,0.5548265504,-2.8257307966,-0.8974787798
B,0,-1.1971330423,-0.0046298335,-1.0467413656
O,0,-1.5403874544,-0.2930699632,-2.3998260209
C,0,-2.8056009707,0.2113471295,-2.6146083139
O,0,-2.2930878777,0.6726766991,-0.4688055024
B,0,-0.7908421446,-0.9082495039,1.3873694931
O,0,-1.4716263803,-2.1519681896,1.4655890502
C,0,-2.3535290502,-2.0473627645,2.5202834607
O,0,-1.2473882134,-0.0832792597,2.4211892777
B,0,0.6011545138,1.5571986262,0.3382696186
O,0,0.577617945,2.1390908104,1.6194860326
C,0,0.5918490293,3.5001843333,1.4509473185

O,0,0.6328379037,2.6099951502,-0.6189913015
H,0,1.0936381429,-0.8364094968,1.4210789636
H,0,3.2897497487,-2.7426203812,0.5043419366
C,0,6.1324823339,0.4752762737,2.5268900949
H,0,5.6218305971,-2.1983151856,1.516154709
C,0,1.1663832589,1.1368666594,-3.4546778478
C,0,3.5603266525,0.2641841176,-2.1581413158
C,0,-1.0214293116,-3.4054591768,-1.6673123511
C,0,0.9374207026,-4.2864407655,0.170790168
H,0,1.58948906,-3.8667176178,-2.8909857413
H,0,2.770685281,-3.0273970859,-1.8794384751
H,0,0.6988141485,-1.6931025732,-3.726361105
H,0,2.4454365515,-1.7187165388,-3.9876381565
H,0,3.9968736161,0.2780859624,-3.1618525553
H,0,3.6905962412,1.2449686598,-1.6939651245
H,0,4.0746444013,-0.4692526006,-1.5351977528
H,0,1.7897337359,1.1283698926,-4.3543091806
H,0,0.1302561179,0.9221611043,-3.71772031
H,0,1.2080460498,2.1180411638,-2.9789759456
H,0,0.9741074723,-5.207884467,-0.4192357541
H,0,1.8804880052,-4.1591837707,0.7031094946
H,0,0.1385990558,-4.3661805554,0.9123203847
H,0,-0.9058175786,-4.4107337286,-2.0856653235
H,0,-1.7927726408,-3.4201303434,-0.893925524
H,0,-1.3335256398,-2.7096828989,-2.4469086271
C,0,-3.2582912359,-2.9786383979,2.9997157302
C,0,-4.035829645,-2.5907748007,4.1024084013
C,0,-3.8964450723,-1.3247566131,4.6813105895
C,0,-2.974418952,-0.39051185,4.1847807801
C,0,-2.2142479901,-0.7845553188,3.0967913898
H,0,-3.3593423988,-3.9579197137,2.5435555292
H,0,-4.7595809357,-3.2890084984,4.511806004
H,0,-4.5144675941,-1.0569827298,5.5329990099
H,0,-2.8572256615,0.5938644892,4.6246256269
C,0,-3.5730576076,0.1860184859,-3.7665058166
C,0,-4.8417222803,0.7826590218,-3.6909794054
C,0,-5.2990003389,1.3712090716,-2.5069967061
C,0,-4.5096510037,1.3896727229,-1.3466661602
C,0,-3.2610052612,0.798123127,-1.4348185789
H,0,-3.2101275894,-0.2734677868,-4.6801168143
H,0,-5.4784792649,0.7860915335,-4.5704248033
H,0,-6.2851839734,1.824753313,-2.4831109699
H,0,-4.8528416351,1.8435017177,-0.423392632
C,0,0.5808004673,4.4985039791,2.410507339
C,0,0.6018333702,5.8226588827,1.9451886521
C,0,0.6324771052,6.1140793702,0.5772679012
C,0,0.6437462449,5.0926366108,-0.3859340288
C,0,0.6237702714,3.7916485968,0.086659503
H,0,0.5560756383,4.2602964415,3.4683740454
H,0,0.5935949793,6.6366938562,2.6639243928
H,0,0.646861522,7.1498301009,0.2513270011
H,0,0.6652270185,5.3081217623,-1.449215253
H,0,6.9568331396,-0.2401349003,2.6022092938
H,0,6.4892726533,1.3381071931,1.9522711903
H,0,5.9049067236,0.8313835763,3.5383808281

veratroleIrBeg3orthoTSPSBA

tempveraorthoPSBA veratrole + dmpe Ir Beg3 TS first try at ortho
B3LYP/gen
E(RB+HF-LYP) = -2248.79264138

Zero-point correction= 0.585590 (Hartree/Particle)
Thermal correction to Energy= 0.626207
Thermal correction to Enthalpy= 0.627151
Thermal correction to Gibbs Free Energy= 0.511898
Sum of electronic and ZPE= -2248.207051

Sum of electronic and thermal Energies= -2248.166434

Sum of electronic and thermal Enthalpies= -2248.165490

Sum of electronic and thermal Free Energies= -2248.280744

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	392.951	148.140	242.572

C,0,2.8941142726,0.1041748247,0.2307900614
C,0,1.7766769204,-0.6479297165,0.6282864544
C,0,2.0345876349,-1.8496886634,1.3230168192
C,0,3.3243896174,-2.3242961686,1.5384070704
C,0,4.4236825451,-1.6155929873,1.0507034908
C,0,4.2075874322,-0.4093290291,0.3831236122
Ir,0,-0.3709409166,-0.0887564892,0.0655581879
P,0,0.1358776761,-0.0152740837,-2.3169937412
C,0,-0.7765995299,-1.4319686894,-3.118612211
C,0,-0.6031919187,-2.7135961791,-2.2907757905
P,0,-1.0541417377,-2.4163260322,-0.4994774346
B,0,-2.3254685391,0.6079072469,-0.3995829311
O,0,-3.2110996156,1.2412372682,0.473645636
C,0,-4.4582235719,1.4907184923,-0.1806411382
C,0,-4.1787385487,1.2052087156,-1.6678209033
O,0,-2.9394554079,0.4824234745,-1.662023106
B,0,-1.3427057983,-0.2696908504,1.9457435865
O,0,-1.9633717572,-1.4626940242,2.348179833
C,0,-2.4576255022,-1.2953670032,3.686075501
C,0,-2.3711667035,0.2230330897,3.930656382
O,0,-1.465132137,0.6920387401,2.9309659525
B,0,-0.1100443226,1.9722742848,0.3312286716
O,0,0.4106277258,2.5711776682,1.4756006011
C,0,0.2160642055,3.9840101813,1.4068005751
C,0,-0.1594757143,4.2511045662,-0.0650028605
O,0,-0.4890316768,2.9602605725,-0.5902358942
H,0,-5.2243228485,0.8211645358,0.2318936824
H,0,-4.7706480819,2.5237018292,0.0029831835
H,0,-4.9571983986,0.5992681103,-2.1432371984
H,0,-4.055021595,2.1274448732,-2.2494355369
H,0,-3.4786983612,-1.6844556068,3.7542893339
H,0,-1.8225795863,-1.8642288573,4.3775377536
H,0,-3.342396507,0.715727048,3.7945651171
H,0,-1.9877996133,0.4759270051,4.9242242214
H,0,-1.018197815,4.922586003,-0.1707227789
H,0,0.6775020444,4.6736694283,-0.6370914854
H,0,-0.5872713698,4.2703126966,2.097105452
H,0,1.1328516106,4.5010877949,1.7118602292
H,0,0.4469491763,-0.0537587525,1.4599119341
O,0,2.7309947867,1.3137103238,-0.4208986173
O,0,5.214209216,0.3382096405,-0.1777070091
H,0,1.1980923819,-2.4112489316,1.7228294189
H,0,3.4826692297,-3.2495034493,2.0868739389
H,0,5.4262538275,-2.0009290939,1.1923813408
C,0,-0.3244360277,1.4276371239,-3.3628534382
C,0,1.8693108882,-0.3422311568,-2.8685321146
C,0,-2.8767186136,-2.7360956307,-0.5073521667
C,0,-0.4518968614,-3.9789443535,0.293303778
H,0,-1.2020123094,-3.5357154681,-2.7007967545
H,0,0.4444747696,-3.0382308931,-2.3059193278
H,0,-1.8286071615,-1.1349265865,-3.1536185588
H,0,-0.4237890558,-1.5736739226,-4.1472181181
H,0,1.9064766872,-0.4432481157,-3.9583581869
H,0,2.5073501594,0.4807119742,-2.5447747555
H,0,2.2443622092,-1.2578046723,-2.4059763822
H,0,-0.0925095631,1.2349105686,-4.4153594634
H,0,-1.3908738881,1.6174460709,-3.2410738791
H,0,0.2213871873,2.3044331212,-3.0118590918
H,0,-0.888564389,-4.855678424,-0.1964704925
H,0,0.636725973,-4.0385772291,0.2376040404

H,0,-0.7488952742,-3.9734871538,1.3451690446
H,0,-3.1034715142,-3.7343648733,-0.8966229264
H,0,-3.2404113913,-2.6467652661,0.5181508537
H,0,-3.3702245377,-1.9802119086,-1.1216512577
C,0,3.2964470692,2.459055206,0.2296802479
H,0,2.9842166918,3.3223260813,-0.3632456741
H,0,2.8959399229,2.554352943,1.2430445059
H,0,4.3875143285,2.4092478857,0.2494250242
C,0,6.5447927183,-0.1293998435,-0.0494316945
H,0,7.1721734522,0.6001163233,-0.5650556635
H,0,6.8568065729,-0.1931733985,1.0015313904
H,0,6.6775433269,-1.1130076152,-0.5190520791

veratroleIrBeg3TSPSBA

tempveraPSBA veratrole + dmpe Ir Beg3 TS first try at
B3LYP/gen
E(RB+HF-LYP) = -2248.79302370

Zero-point correction= 0.585794 (Hartree/Particle)
Thermal correction to Energy= 0.626595
Thermal correction to Enthalpy= 0.627539
Thermal correction to Gibbs Free Energy= 0.511001
Sum of electronic and ZPE= -2248.207230
Sum of electronic and thermal Energies= -2248.166429
Sum of electronic and thermal Enthalpies= -2248.165485
Sum of electronic and thermal Free Energies= -2248.282022

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 393.194	147.986	245.274

C,0,2.4253564039,-1.4879509184,0.3744802336
C,0,1.7788992403,-0.2545144973,0.2010009803
C,0,2.6269157892,0.8584257278,0.0279940671
C,0,4.0142831805,0.7466110441,-0.0283462041
C,0,4.6328471989,-0.5123484664,0.112327299
C,0,3.8200207438,-1.626825663,0.3218207727
Ir,0,-0.4996204094,-0.0771897569,0.0166008976
P,0,-0.4117289829,-1.0801560065,-2.1795937614
C,0,-1.037582109,-2.8399870932,-2.0297696694
C,0,-0.6195822388,-3.4999669941,-0.7055204302
P,0,-1.0109046424,-2.3733135573,0.738599383
B,0,-2.5580803444,0.3495540483,-0.3171703248
O,0,-3.4186463126,-0.4261414483,-1.1168988323
C,0,-4.6855246958,0.2362598558,-1.2442937179
C,0,-4.6495402666,1.3377966916,-0.1685119808
O,0,-3.2724368333,1.4274062494,0.2079457429
B,0,-1.1442029864,0.6858363447,1.8969795594
O,0,-1.760881759,-0.1355914493,2.8536477859
C,0,-2.0015889964,0.6409786053,4.0366733311
C,0,-1.7852129189,2.095961429,3.5799537215
O,0,-1.0359815406,1.9792207129,2.3686583112
B,0,-0.3351049763,1.8689061329,-0.7619057728
O,0,0.2919672811,2.9530370613,-0.1570425229
C,0,0.307047601,4.0691732191,-1.0513663735
C,0,-0.6775640253,3.67659802,-2.1677924926
O,0,-0.8359609778,2.2597977758,-2.0174873617
H,0,-4.77529957,0.6497265462,-2.2569014448
H,0,-5.4951991353,-0.4852428962,-1.0933313109
H,0,-4.9932617625,2.3079943279,-0.5411580964
H,0,-5.2494799182,1.0750340445,0.7123466314
H,0,-3.0154312048,0.4512590056,4.4036481398
H,0,-1.2887574696,0.340814588,4.8159101843
H,0,-2.734236791,2.6041658399,3.3668012733
H,0,-1.2241448146,2.6944907353,4.3044154472
H,0,-1.6541209285,4.1625009866,-2.0451195201

H,0,-0.3018330445,3.9034119515,-3.1711815908
H,0,0.0064607456,4.9744033834,-0.5145605551
H,0,1.3270827282,4.2142919178,-1.4314246405
H,0,0.5344983376,0.2689900981,1.2253361433
H,0,1.8512335658,-2.3925487277,0.5318626844
H,0,2.2134078353,1.8561485075,-0.058803206
O,0,4.7609545806,1.8794314248,-0.2749847867
O,0,6.0008451163,-0.5387105704,0.030768787
C,0,-1.3906309184,-0.4429114756,-3.6044280128
C,0,1.2585673331,-1.2637752129,-2.9463268417
C,0,-2.7863985629,-2.7655875804,1.0711874992
C,0,-0.2344693453,-3.2141694604,2.1955351906
H,0,-1.1153426235,-4.470274475,-0.5800927829
H,0,0.460765228,-3.6837485801,-0.6973036999
H,0,-2.1291760962,-2.7652518418,-2.0840295515
H,0,-0.7031588103,-3.4320003872,-2.8899026111
H,0,1.1944978767,-1.8207027661,-3.8866673956
H,0,1.6631572628,-0.2674558531,-3.1431426931
H,0,1.9416649581,-1.7664418308,-2.2603226497
H,0,-1.2139774446,-1.0477688505,-4.4996514946
H,0,-2.4477813385,-0.4663874123,-3.3386105459
H,0,-1.1021391661,0.5943881786,-3.7811578826
H,0,-0.5317018961,-4.2662410408,2.258505421
H,0,0.8538516188,-3.1455538897,2.1644845573
H,0,-0.582582535,-2.687776901,3.08798224
H,0,-2.9320500259,-3.8355319365,1.2541517995
H,0,-3.0906997518,-2.1952120674,1.9518854054
H,0,-3.3915790971,-2.4408364227,0.2237265915
C,0,5.5344345894,2.3492452378,0.8279999969
H,0,6.0292332199,3.2631735994,0.4904304964
H,0,4.8914754837,2.5855384115,1.6865334766
H,0,6.2914982447,1.6178890827,1.1302347085
H,0,4.2572148053,-2.6122476484,0.4439313021
C,0,6.6460387435,-1.7917587062,0.1641405484
H,0,7.7148205172,-1.5955000768,0.0607202572
H,0,6.4570101737,-2.2470445856,1.1457890315
H,0,6.3327727381,-2.49557827,-0.6185670644

veratroleIrBeg3TSSSB1

tempveraSSBA veratrole + dmpe Ir Beg3 TS SSB try 1
B3LYP/gen
E(RB+HF-LYP) = -2248.79403969

Zero-point correction= 0.586125 (Hartree/Particle)
Thermal correction to Energy= 0.626771
Thermal correction to Enthalpy= 0.627715
Thermal correction to Gibbs Free Energy= 0.512079
Sum of electronic and ZPE= -2248.207915
Sum of electronic and thermal Energies= -2248.167268
Sum of electronic and thermal Enthalpies= -2248.166324
Sum of electronic and thermal Free Energies= -2248.281961

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 393.305	147.908	243.377

C,0,2.6820032959,-0.7103021873,0.1671341014
C,0,1.75082083,0.3461472186,0.2244138333
C,0,2.3026094132,1.6353969669,0.2911876596
C,0,3.6841900475,1.8625228904,0.2320041433
C,0,4.5811674209,0.7996644099,0.1178325104
C,0,4.0605520612,-0.509568556,0.1003777672
Ir,0,-0.5037629752,-0.0081698522,0.0122884539
P,0,-0.2124607157,-0.6112669214,-2.3079608749
C,0,-0.3886650535,-2.4706957385,-2.4433138886
C,0,0.1945112689,-3.205569711,-1.2251610071

P,0,-0.4395070182,-2.4394149695,0.3620448726
B,0,-2.6091552292,-0.0404255296,-0.3035869672
O,0,-3.2718223256,-0.8806893804,-1.217695936
C,0,-4.6637083794,-0.5348468768,-1.2701088776
C,0,-4.8731214256,0.3914556267,-0.0572128194
O,0,-3.5509905653,0.7564235098,0.3493091776
B,0,-1.2914710436,0.2695200558,1.9716842594
O,0,-1.7012083382,-0.8196834502,2.7572716255
C,0,-2.1022942524,-0.3316843048,4.0459180251
C,0,-2.2142633919,1.1923725987,3.8513736703
O,0,-1.4715958889,1.4539394984,2.6588573043
B,0,-0.8184091266,2.0202133053,-0.4457379542
O,0,-0.4922680183,3.1113588013,0.3549185075
C,0,-0.7781391763,4.3296402792,-0.3352460613
C,0,-1.6122077589,3.8931636436,-1.5541838831
O,0,-1.3937488996,2.4800280015,-1.644958099
H,0,-4.8731363164,-0.0270328334,-2.2202073295
H,0,-5.2710524846,-1.4448257802,-1.2247992976
H,0,-5.4446027327,1.2921284547,-0.3031877336
H,0,-5.3782941126,-0.1207927033,0.7717811335
H,0,-3.0479901212,-0.7984110039,4.3398345311
H,0,-1.3382494156,-0.6003413002,4.7872487863
H,0,-3.2538033783,1.5115438347,3.7038013208
H,0,-1.7893870259,1.7633842393,4.6829012006
H,0,-2.6834012149,4.0828755721,-1.4082453194
H,0,-1.2992858558,4.3779381673,-2.4851411516
H,0,-1.3179235065,5.0112435742,0.3298655925
H,0,0.1645104654,4.811055577,-0.629937582
H,0,0.4309643188,0.3658231734,1.2917384097
H,0,2.371480446,-1.7475339544,0.1360688653
O,0,4.8738642219,-1.6137846976,-0.0551707568
H,0,1.6475224581,2.4909700607,0.4026255538
H,0,4.0484497681,2.8834435448,0.2750218735
O,0,5.9432326911,0.9226719963,0.0179138405
C,0,-1.3486877678,-0.0148088641,-3.6303679968
C,0,1.4350717086,-0.2662576967,-3.0684024106
C,0,-2.0535070881,-3.3087150895,0.60057587
C,0,0.5537297986,-3.2616755916,1.6909858746
H,0,-0.0512508423,-4.2737069905,-1.261173492
H,0,1.2873694248,-3.1259845691,-1.2193417399
H,0,-1.4655948274,-2.6573796358,-2.5142826825
H,0,0.0700561994,-2.8225865458,-3.3748810186
H,0,1.4881839167,-0.6807330198,-4.0803157885
H,0,1.5787921661,0.8164962803,-3.1143595218
H,0,2.2356202947,-0.6807974151,-2.4543037587
H,0,-1.0550024157,-0.4139188975,-4.6065140748
H,0,-2.362638247,-0.3317809582,-3.3849114844
H,0,-1.3197532701,1.0758710719,-3.6386618636
H,0,0.5338074649,-4.3520951676,1.5922383555
H,0,1.5882103841,-2.9154835406,1.6837781335
H,0,0.1044941233,-2.9781230509,2.6462616651
H,0,-1.9180437104,-4.3951136103,0.6289825879
H,0,-2.4762724546,-2.9648307434,1.5471027774
H,0,-2.7380593707,-3.035218993,-0.2035527517
C,0,5.7575718169,-1.8892089173,1.0312683807
H,0,6.2825884038,-2.812134096,0.7730747344
H,0,6.4844248332,-1.0840129261,1.1736035146
H,0,5.1981181766,-2.0434994971,1.964230712
C,0,6.4885585182,2.2302703828,0.0038673505
H,0,7.5677629579,2.1070770237,-0.1043147384
H,0,6.1067446387,2.8193986248,-0.8402025921
H,0,6.2792432114,2.7708758782,0.9365254562

veratroleIrBeg3TSSSBout

tempveraSSBA veratrole + dmpe Ir Beg3 TS SSB try 2 with OMe's out
B3LYP/gen

E(RB+HF-LYP) = -2248.79345867

Zero-point correction= 0.586295 (Hartree/Particle)
Thermal correction to Energy= 0.626800
Thermal correction to Enthalpy= 0.627744
Thermal correction to Gibbs Free Energy= 0.512314
Sum of electronic and ZPE= -2248.207163
Sum of electronic and thermal Energies= -2248.166659
Sum of electronic and thermal Enthalpies= -2248.165715
Sum of electronic and thermal Free Energies= -2248.281145

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	393.323	147.788	242.944

C,0,2.7080327393,-0.6842685526,0.3060320674
C,0,1.7664047602,0.3728613541,0.3008703791
C,0,2.2940616099,1.6681157737,0.3499045299
C,0,3.6771056282,1.9093854856,0.3486206907
C,0,4.5879492622,0.8592879128,0.318481918
C,0,4.0872271245,-0.4632504491,0.3038773902
Ir,0,-0.4867553436,0.0083658027,0.0405813257
P,0,-0.1476511276,-0.6118171926,-2.2715559184
C,0,-0.3333589381,-2.4719411331,-2.3917150821
C,0,0.2180047666,-3.1974763581,-1.1535268347
P,0,-0.4425782175,-2.4137126728,0.4142430915
B,0,-2.5845671438,-0.0283791553,-0.3248668757
O,0,-3.2202116554,-0.8708388048,-1.2565402354
C,0,-4.6104254271,-0.5263058621,-1.3492409185
C,0,-4.8553490557,0.4002113702,-0.1432200216
O,0,-3.5457010161,0.7659004456,0.3016776489
B,0,-1.3185218969,0.2975341456,1.9791006692
O,0,-1.7271430068,-0.7879004089,2.7719925073
C,0,-2.1663192962,-0.2854353182,4.0433149067
C,0,-2.3060844827,1.2319946496,3.8184881864
O,0,-1.5370424752,1.488541091,2.641874825
B,0,-0.8042114054,2.0276879542,-0.4517138278
O,0,-0.519404499,3.1352020321,0.3408808115
C,0,-0.7884241978,4.3375471717,-0.3838143822
C,0,-1.5821760029,3.8712307747,-1.617966503
O,0,-1.3449136026,2.4593625473,-1.677649858
H,0,-4.7927520447,-0.0190195236,-2.3051652927
H,0,-5.2179790399,-1.4368528806,-1.3211083607
H,0,-5.4195745839,1.3007556592,-0.4058110328
H,0,-5.3842019176,-0.1120412161,0.6707901625
H,0,-3.1080218222,-0.7671734795,4.3255300193
H,0,-1.4126808012,-0.5238373782,4.8052460514
H,0,-3.3478947819,1.525226966,3.6369154321
H,0,-1.916446368,1.8268287933,4.6504751125
H,0,-2.6592525654,4.0503914089,-1.5055667353
H,0,-1.2483932745,4.3437152459,-2.5479853223
H,0,-1.3508486259,5.0309389059,0.2494363341
H,0,0.1612979808,4.8159883132,-0.6598901299
H,0,0.4099239265,0.4126314399,1.3377321628
H,0,2.3670724996,-1.7097294005,0.2929396588
O,0,5.0413152673,-1.4470992703,0.2860014774
H,0,1.626285779,2.518352618,0.4115823687
H,0,4.0299294275,2.9344410206,0.3834621684
O,0,5.9495224084,0.9857464988,0.3140335735
C,0,-1.2410944437,-0.0289603693,-3.6359724563
C,0,1.5211213706,-0.2814219051,-2.9912385494
C,0,-2.0670515023,-3.270816891,0.6251504129
C,0,0.5101009382,-3.2404497013,1.7710376472
H,0,-0.0305206286,-4.2652928498,-1.1833911237
H,0,1.3107825002,-3.1197136487,-1.1261983323
H,0,-1.4098448575,-2.6516720455,-2.4853796241
H,0,0.1434594878,-2.8379856674,-3.3087478464
H,0,1.6032303392,-0.7120520009,-3.994483398

H,0,1.6658760759,0.8005620541,-3.0502603206
H,0,2.3032882705,-0.6835959484,-2.3460608983
H,0,-0.9223446334,-0.4506265563,-4.594743008
H,0,-2.2650018938,-0.3317595327,-3.4153721396
H,0,-1.2007581236,1.0607799157,-3.6669978708
H,0,0.5031634168,-4.330391827,1.6639345603
H,0,1.5400950081,-2.8830885301,1.8087199888
H,0,0.0235832787,-2.9680014963,2.7111358771
H,0,-1.938339588,-4.3571622233,0.6784669309
H,0,-2.5121559641,-2.9057655335,1.5536005357
H,0,-2.728193527,-3.0101160787,-0.2023117119
C,0,4.6171045921,-2.7924494426,0.3280705204
H,0,5.5260897279,-3.3973758947,0.3240187794
H,0,4.0436506441,-3.0145772331,1.2388613062
H,0,4.0074501863,-3.0613554778,-0.5468349317
C,0,6.4850114237,2.2948375917,0.3502717526
H,0,7.5704086034,2.1779192444,0.3429358044
H,0,6.1809825247,2.8857924822,-0.5246212012
H,0,6.1870660169,2.8335152193,1.2600551739

bpyIrBcat3HPhts

bpy Ir(Bcat)3(H)(Ph) ts

B3LYP/gen

E(RB+HF-LYP) = -2051.41870759

Zero-point correction= 0.539081 (Hartree/Particle)

Thermal correction to Energy= 0.576683

Thermal correction to Enthalpy= 0.577627

Thermal correction to Gibbs Free Energy= 0.464430

Sum of electronic and ZPE= -2050.879626

Sum of electronic and thermal Energies= -2050.842025

Sum of electronic and thermal Enthalpies= -2050.841081

Sum of electronic and thermal Free Energies= -2050.954278

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 361.874	147.990	238.243

B,0,1.0887916997,-0.3056111577,1.1585992539
B,0,-0.8043610176,1.7136718819,0.2014233354
B,0,1.1737286661,0.3272211509,-1.2948724501
C,0,0.4727895486,-3.1032850114,-1.4667255209
H,0,1.0317714237,-2.4267474669,-2.1024528224
C,0,0.5608135234,-4.4851884294,-1.6109450124
H,0,1.1993211688,-4.9066780347,-2.3796048657
C,0,-0.1786995051,-5.2943455574,-0.7519149287
C,0,-0.9720775102,-4.6928564624,0.2184302833
C,0,-1.0169456788,-3.2950355783,0.3075821196
C,0,-1.8196455415,-2.587184365,1.3332464702
C,0,-2.6340641429,-3.2624690461,2.2508683122
H,0,-2.7240110952,-4.3405691484,2.2146815786
C,0,-3.3352502191,-2.5448375023,3.2131785753
C,0,-3.2026248028,-1.1593125477,3.2452090409
H,0,-3.7201686827,-0.5547983137,3.9817897494
C,0,-2.3850035627,-0.5430968611,2.3030001719
H,0,-2.2401294354,0.5301292792,2.2860174024
C,0,2.3839839768,0.1033193605,2.9349065595
C,0,2.9175838687,-0.9932997522,2.2562954307
C,0,-1.011169835,3.9377783631,-0.0014613294
C,0,-1.4648643503,3.5807901849,1.2694995329
C,0,2.8078711889,0.2721722779,-2.8341519012
C,0,3.0431896649,1.3480131527,-1.9778322389
Ir,0,-0.5140736988,-0.2573092299,-0.2460010583
N,0,-0.2990011996,-2.5190515943,-0.5364052586
N,0,-1.7169601696,-1.2349485057,1.3632188324
O,0,1.2570449436,0.5331586008,2.2765746561

O,0,2.1294093624,-1.2660589937,1.1622229413
O,0,-0.6119135974,2.8097973913,-0.6700991326
O,0,-1.3524887913,2.2168999607,1.4129542827
O,0,1.6558001858,-0.3691831395,-2.4347654952
O,0,2.0512314411,1.3948347328,-1.0294674985
H,0,-1.5438840917,-5.3094346074,0.900398824
H,0,-3.969320487,-3.0623066164,3.9262658985
H,0,-0.1368717617,-6.376309804,-0.8296935636
H,0,-0.8076918184,0.2911142752,-1.7288032608
C,0,-2.3721863394,-0.3346887692,-1.4834503908
C,0,-3.4701074162,0.4832178208,-1.1599479052
H,0,-3.3642460674,1.2704454393,-0.418895815
C,0,-4.7175169454,0.2996796975,-1.763419489
H,0,-5.5493234396,0.9402656455,-1.4803656263
C,0,-4.8947599247,-0.6907909517,-2.7308317359
H,0,-5.8619691067,-0.8278743097,-3.2065894011
C,0,-3.8098101706,-1.4900945201,-3.0920878652
H,0,-3.925358732,-2.2529545198,-3.8585304404
C,0,-2.5661566276,-1.3077998943,-2.4797477518
H,0,-1.7348186978,-1.9327809482,-2.793979738
C,0,4.0609407129,-1.6404195336,2.6938842464
C,0,4.662459682,-1.1394316748,3.858887781
C,0,4.1274201036,-0.0399651672,4.5394058098
C,0,2.9674218416,0.6065913201,4.0855269884
C,0,3.6482397746,-0.0215902597,-3.8936240048
C,0,4.760012234,0.8182493905,-4.0666382022
C,0,4.9976724889,1.8961338576,-3.2073413888
C,0,4.1353629525,2.1833984052,-2.137694783
C,0,-1.9354252952,4.5186768779,2.1719516544
C,0,-1.9382580663,5.8572689919,1.7473973762
C,0,-1.4847541921,6.2162573475,0.4739546072
C,0,-1.0089494977,5.2542050531,-0.431008223
H,0,2.5454671201,1.4617818495,4.6025421038
H,0,4.6199455475,0.3237410241,5.4362522495
H,0,5.5628300616,-1.6146532686,4.2366432293
H,0,4.4690844997,-2.4900296145,2.156659551
H,0,5.4466594467,0.6258639552,-4.8854775374
H,0,3.4524377248,-0.8578532506,-4.5565356925
H,0,5.8669213338,2.5262055095,-3.3698411392
H,0,4.3085748915,3.0169978893,-1.4658758513
H,0,-2.281113413,4.2297995464,3.159071015
H,0,-2.2984016016,6.626783385,2.4236632506
H,0,-1.4997194808,7.2606467918,0.1768671764
H,0,-0.6548070687,5.5212759984,-1.4208959716

dmpeBcat3benzeneTS

Ir dmpw bcat3 benzene
B3LYP/gen
E(RB+HF-LYP) = -2477.06447132

Zero-point correction= 0.590458 (Hartree/Particle)
Thermal correction to Energy= 0.631600
Thermal correction to Enthalpy= 0.632544
Thermal correction to Gibbs Free Energy= 0.514822
Sum of electronic and ZPE= -2476.474013
Sum of electronic and thermal Energies= -2476.432871
Sum of electronic and thermal Enthalpies= -2476.431927
Sum of electronic and thermal Free Energies= -2476.549649

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 396.335	159.270	247.767

C,0,3.3590806599,-2.0391751638,0.7254865706
C,0,2.587121863,-0.8916263472,0.9903557153
C,0,3.1505883774,0.049809317,1.8733013105

C,0,4.4268224749,-0.1240191668,2.4188338156
C,0,5.1818501786,-1.256197322,2.114686041
C,0,4.6369897035,-2.2184106026,1.2644722658
Ir,0,0.6006118999,-0.5078900974,-0.0916255642
P,0,1.7370096487,-0.3434115992,-2.2258542678
C,0,1.3958025668,-1.9244705794,-3.1685656996
C,0,1.3438986124,-3.1616212767,-2.2577126803
P,0,0.2369792083,-2.8481536103,-0.7808558464
B,0,-1.1607353939,0.144480019,-1.0813831016
O,0,-1.5520583633,-0.2076619865,-2.40691311
C,0,-2.735478918,0.4490712493,-2.6706042888
O,0,-2.1484967144,1.0147612473,-0.5693863123
B,0,-0.8790099476,-0.6879812771,1.4147688955
O,0,-1.6822618068,-1.8491809978,1.5659230628
C,0,-2.5533261058,-1.5912288464,2.6020697643
O,0,-1.2555973707,0.2420686984,2.3912461816
B,0,0.7925556455,1.5430354582,0.2787137973
O,0,0.7744356082,2.1926970986,1.5319318887
C,0,0.9358833831,3.535776416,1.3037666431
O,0,0.9871056139,2.5429398612,-0.7177628467
H,0,0.9529728503,-0.9025900569,1.4497851648
H,0,2.9787760064,-2.8083057046,0.0641198831
H,0,5.2027671701,-3.1140876798,1.0180138047
H,0,2.5816219576,0.9287308325,2.1528708906
H,0,4.8242929163,0.6308932293,3.0928117437
H,0,6.1720924831,-1.3925543551,2.5402706075
C,0,1.3001160876,0.9494010809,-3.4634316573
C,0,3.5769730617,-0.2031340576,-2.2011060955
C,0,-1.4298409758,-3.3105696504,-1.4298518155
C,0,0.5493597919,-4.2767519211,0.3522359023
H,0,0.9923697121,-4.0385123416,-2.8140051717
H,0,2.3447228327,-3.3999689563,-1.8823447406
H,0,0.4233590645,-1.7712182417,-3.6484765171
H,0,2.1397119626,-2.0499939004,-3.9638505851
H,0,3.9785787616,-0.2575944874,-3.2178858372
H,0,3.8445892412,0.7606999105,-1.7600351825
H,0,4.0184488806,-0.9856079096,-1.5831007948
H,0,1.9000556553,0.829169029,-4.3710109828
H,0,0.2404148038,0.8729664452,-3.7086544543
H,0,1.4846993309,1.9276627581,-3.0177607502
H,0,0.4614999458,-5.2327885844,-0.1740688404
H,0,1.5333837863,-4.2053285638,0.8178222322
H,0,-0.2054375205,-4.2318154366,1.1417136035
H,0,-1.4345896088,-4.3433829922,-1.7934484064
H,0,-2.1519634236,-3.2063809339,-0.6168415081
H,0,-1.7157509397,-2.6312493778,-2.2335775948
C,0,-3.5490332936,-2.3958146127,3.1282620741
C,0,-4.2893540249,-1.8634439569,4.1955453349
C,0,-4.0267323693,-0.5834609785,4.6955842074
C,0,-3.0133816911,0.2211535252,4.1521332767
C,0,-2.2905742879,-0.3147916552,3.0997691461
H,0,-3.745138569,-3.387003101,2.7328337719
H,0,-5.0813320794,-2.4588174557,4.639686068
H,0,-4.6191552613,-0.2021685937,5.5218217119
H,0,-2.8011404777,1.2150034573,4.5307916524
C,0,-3.5055950184,0.4357284387,-3.82106928
C,0,-4.6763596623,1.2103823538,-3.8038103484
C,0,-5.0386646764,1.9551858235,-2.676305696
C,0,-4.247790431,1.9595567296,-1.5169164029
C,0,-3.0957186072,1.1921242818,-1.5473257514
H,0,-3.2162852357,-0.1455887969,-4.6904852557
H,0,-5.3114307745,1.2300783403,-4.6842760276
H,0,-5.9507740636,2.5438292603,-2.6967221905
H,0,-4.5179584403,2.533562878,-0.6373165174
C,0,0.9783303091,4.5764197134,2.2161730955
C,0,1.1577616166,5.8672922815,1.6945646426
C,0,1.286793794,6.0850159825,0.3188600058
C,0,1.242422702,5.0205969147,-0.595830471

C,0,1.0653121054,3.752933295,-0.0681637466
H,0,0.8744934027,4.3953575608,3.2806621459
H,0,1.1955012433,6.7129330397,2.3747895593
H,0,1.4227718562,7.0965971068,-0.0518131263
H,0,1.3390975307,5.180291167,-1.664737601

dmpeBcat3Ir

Ir dmpe bcat3 starting complex
B3LYP/gen
E(RB+HF-LYP) = -2244.84832552

Zero-point correction= 0.492295 (Hartree/Particle)
Thermal correction to Energy= 0.528341
Thermal correction to Enthalpy= 0.529285
Thermal correction to Gibbs Free Energy= 0.420224
Sum of electronic and ZPE= -2244.356031
Sum of electronic and thermal Energies= -2244.319985
Sum of electronic and thermal Enthalpies= -2244.319041
Sum of electronic and thermal Free Energies= -2244.428101

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 331.539	137.222	229.537

Ir,0,-2.363337727,0.3708583755,2.8870635583
P,0,-2.1557556731,2.5503855885,1.8531894232
C,0,-3.4445474594,2.6361286458,0.499828179
C,0,-3.5073605762,1.3200150562,-0.2937870736
P,0,-3.5766891966,-0.1692899027,0.8494320399
B,0,-3.9782246429,0.8482831251,3.9522039602
O,0,-4.8861251584,1.8866783613,3.5821602909
C,0,-5.8758257356,1.8972072002,4.543338793
O,0,-4.453449116,0.2440549684,5.1301518668
B,0,-2.5971592516,-1.5473911074,3.6808360446
O,0,-3.6613661746,-2.4437426677,3.3749147882
C,0,-3.416143074,-3.6091950524,4.0601078553
O,0,-1.7071744106,-2.2219526649,4.5488893514
B,0,-1.1948902952,0.8287733129,4.5411193639
O,0,0.2218505756,0.7396983971,4.4506320456
C,0,0.7199285286,1.120401339,5.6736381777
O,0,-1.5260348185,1.2985276978,5.8306407869
C,0,-2.4337290222,4.1090176255,2.7970846489
C,0,-0.5675965032,2.9033332451,0.9659497117
C,0,-5.3802590779,-0.5117009845,1.0342962599
C,0,-3.0260752375,-1.5562855899,-0.2419764044
H,0,-4.3616009406,1.3148837755,-0.9804088253
H,0,-2.6053118099,1.205894344,-0.9080294663
H,0,-4.3940496288,2.8120289596,1.0164826888
H,0,-3.2593635776,3.4891579409,-0.1639370577
H,0,-0.6029741066,3.8612444063,0.4366960823
H,0,0.2466034224,2.9248901061,1.6954924684
H,0,-0.3515721041,2.1073355624,0.2477054962
H,0,-2.41827634,4.9855695219,2.1411555603
H,0,-3.3988905656,4.0423506273,3.30288752
H,0,-1.6527875852,4.2122283682,3.5553153248
H,0,-3.6135548346,-1.6093453602,-1.1642842647
H,0,-1.9694563917,-1.4346266797,-0.4969238951
H,0,-3.1387971464,-2.4932101947,0.3096576013
H,0,-5.8637342151,-0.6703971796,0.064818177
H,0,-5.4903618488,-1.403811311,1.6555514082
H,0,-5.8554013064,0.3261656238,1.5494466957
C,0,-4.160968721,-4.7763730062,4.0958421469
C,0,-3.6579985976,-5.823893205,4.8832346945
C,0,-2.4615756394,-5.688046474,5.5959981662
C,0,-1.7158356337,-4.4999874762,5.5516851585
C,0,-2.222682345,-3.4734847908,4.7719137189

H,0,-5.0890273803,-4.8708781285,3.5415141251
H,0,-4.2110231183,-6.7567508697,4.9403117068
H,0,-2.1013149002,-6.517497883,6.1972072786
H,0,-0.788008555,-4.3820702141,6.1011063405
C,0,-6.9861909979,2.7174421809,4.6422055025
C,0,-7.838393395,2.4970522497,5.7367288769
C,0,-7.5703581195,1.4958577755,6.6755910096
C,0,-6.440129173,0.6706007529,6.5632783421
C,0,-5.6079426042,0.8971872596,5.4804312381
H,0,-7.1851926328,3.4923772322,3.9090501888
H,0,-8.7212362293,3.1182198681,5.8538298949
H,0,-8.2491154291,1.3520757661,7.5108341878
H,0,-6.2211602809,-0.1084958492,7.2853395367
C,0,2.0366875908,1.1940833973,6.0958913083
C,0,2.2559857672,1.6322133148,7.4119868191
C,0,1.1906789318,1.975926899,8.2510201217
C,0,-0.1404872726,1.8963772365,7.8109608916
C,0,-0.3440389306,1.4628972096,6.5118064615
H,0,2.8553956669,0.9222613725,5.4374548008
H,0,3.2739093446,1.7033296559,7.7839742776
H,0,1.3945493155,2.3096166968,9.2642006019
H,0,-0.9750476362,2.1575955491,8.453387423

dmpeBcat3IrconfB

Ir dmpe bcat3 starting complex
B3LYP/gen
E(RB+HF-LYP) = -2244.84810528

Zero-point correction= 0.492066 (Hartree/Particle)
Thermal correction to Energy= 0.528227
Thermal correction to Enthalpy= 0.529171
Thermal correction to Gibbs Free Energy= 0.419157
Sum of electronic and ZPE= -2244.356039
Sum of electronic and thermal Energies= -2244.319878
Sum of electronic and thermal Enthalpies= -2244.318934
Sum of electronic and thermal Free Energies= -2244.428948

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 331.468	137.330	231.544

Ir,0,0.2617252314,-0.3510708333,-0.8231520909
P,0,0.8223743873,-2.6839945365,-1.1559088067
C,0,2.6712672899,-2.782830919,-1.4351474242
C,0,3.1624297983,-1.6273619705,-2.3251012239
P,0,2.4685436645,0.0269859066,-1.7661773132
B,0,0.8229625494,-0.2527078469,1.0854937627
O,0,0.610011833,0.7951727209,2.0018115063
C,0,1.2093251624,0.4252238192,3.1798900597
O,0,1.5811813259,-1.2694468741,1.7342817175
B,0,-0.1548687344,1.6916719457,-0.6842554324
O,0,0.8114946447,2.7356000762,-0.8021687072
C,0,0.1324783025,3.9259544701,-0.7077253868
O,0,-1.422377485,2.3014686128,-0.5430273851
B,0,-1.6609171963,-0.7184415427,-0.1318627781
O,0,-2.6858508301,-1.1210794882,-1.0337422077
C,0,-3.8296816105,-1.2777975887,-0.2868614199
O,0,-2.2116840861,-0.6730743781,1.1671107168
C,0,0.5074539806,-3.9900831498,0.1053148379
C,0,0.1183704509,-3.4354811087,-2.6961437706
C,0,3.7447405938,0.6677270756,-0.5952246929
C,0,2.7230102511,1.1046614105,-3.2446826139
H,0,4.2576112713,-1.5924951486,-2.3556440073
H,0,2.8208983909,-1.7778391198,-3.3566438393
H,0,3.1314208341,-2.721495871,-0.4423473148
H,0,2.9471657359,-3.7526586468,-1.8664088502

H,0,0.4848772233,-4.4547897122,-2.8562993789
H,0,-0.9716161332,-3.4506870362,-2.612241811
H,0,0.3784662186,-2.8233818824,-3.5645587828
H,0,0.9588137766,-4.9465406644,-0.1776433523
H,0,0.9113227155,-3.6527737356,1.0618904702
H,0,-0.5724923547,-4.1213651278,0.2169746138
H,0,3.7682694585,1.1090320988,-3.5702605518
H,0,2.0916761803,0.7622608936,-4.0695188232
H,0,2.4189080131,2.1194990962,-2.9779378874
H,0,4.7308110274,0.7277500279,-1.0673598022
H,0,3.43416101,1.6622113356,-0.26599666
H,0,3.7976681455,0.0177320868,0.281132877
C,0,0.623700266,5.220249905,-0.7549185467
C,0,-0.3144599732,6.2576834743,-0.6393632736
C,0,-1.6792106757,5.9897290078,-0.4846425625
C,0,-2.1649532649,4.673997358,-0.4392649936
C,0,-1.2294499045,3.6586200115,-0.5526825763
H,0,1.6841852079,5.4178658074,-0.8733265235
H,0,0.0278513628,7.2878322695,-0.6698642781
H,0,-2.3785104039,6.8159208422,-0.3972744806
H,0,-3.2202204731,4.453824791,-0.3188314466
C,0,1.2723423518,1.1157760247,4.3778509869
C,0,1.9621407403,0.4938366137,5.4307664808
C,0,2.5547029401,-0.7629180888,5.2721333038
C,0,2.4832357936,-1.453764511,4.0515170074
C,0,1.8012064542,-0.8293048657,3.0218798591
H,0,0.8064098953,2.0887720631,4.4897031108
H,0,2.034295715,1.0009456704,6.3881609964
H,0,3.0792676692,-1.2166466935,6.1075322611
H,0,2.9365349983,-2.4308214183,3.9193920104
C,0,-5.0991420968,-1.6447350852,-0.7002939827
C,0,-6.08622817,-1.739320414,0.293959418
C,0,-5.793835157,-1.4733558603,1.6356305536
C,0,-4.5023855633,-1.1009259652,2.0416783391
C,0,-3.5377847637,-1.0106955795,1.0524832223
H,0,-5.3155671658,-1.8457509449,-1.7443828326
H,0,-7.0959953479,-2.0233591608,0.0127562772
H,0,-6.5804508688,-1.55389787,2.3799953311
H,0,-4.2644496023,-0.8892767768,3.0787240916

dmpeBcat3TSBisCF3

Ir dmpw bcat3 bistrifluoromethylbenzene
B3LYP/gen
E(RB+HF-LYP) = -3151.13492865

Zero-point correction= 0.600117 (Hartree/Particle)
Thermal correction to Energy= 0.648618
Thermal correction to Enthalpy= 0.649562
Thermal correction to Gibbs Free Energy= 0.512371
Sum of electronic and ZPE= -3150.534812
Sum of electronic and thermal Energies= -3150.486311
Sum of electronic and thermal Enthalpies= -3150.485367
Sum of electronic and thermal Free Energies= -3150.622558

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	407.014	184.394	288.743

6	2.960881	-1.195177	0.157258
6	2.046434	-0.135399	0.255385
6	2.599651	1.136344	0.492717
6	3.982825	1.335359	0.565349
6	4.873474	0.273070	0.418612
6	4.343814	-0.998544	0.218663
77	-0.171297	-0.465219	-0.180791
15	0.316584	-0.958420	-2.509689

6 0.067032 -2.794061 -2.757203
6 0.550520 -3.613443 -1.549908
15 -0.149411 -2.926068 0.044237
5 -2.228580 -0.491987 -0.685958
8 -2.817863 -1.274250 -1.720602
6 -4.167999 -0.988691 -1.725625
8 -3.261611 0.248683 -0.073806
5 -1.106905 -0.263150 1.713833
8 -1.530552 -1.374687 2.484717
6 -2.123724 -0.858180 3.618246
8 -1.414166 0.910339 2.409553
5 -0.447063 1.579411 -0.550221
8 -0.137430 2.651291 0.313687
6 -0.488113 3.813849 -0.330775
8 -0.979426 2.130518 -1.746969
1 0.676588 -0.196341 1.186575
1 2.614230 -2.208252 0.003816
6 5.227546 -2.195910 0.019513
1 1.944067 1.986782 0.636600
6 4.495704 2.736776 0.768168
1 5.943094 0.430282 0.472118
6 -0.658276 -0.219429 -3.885029
6 2.044991 -0.667893 -3.094048
6 -1.787551 -3.769859 0.166169
6 0.777113 -3.825888 1.370216
1 0.274881 -4.668567 -1.660565
1 1.643295 -3.575354 -1.477829
1 -1.009426 -2.931092 -2.903235
1 0.569887 -3.115009 -3.676779
1 2.139954 -0.959661 -4.144610
1 2.282644 0.394436 -2.994704
1 2.765007 -1.229747 -2.497612
1 -0.313588 -0.607853 -4.848473
1 -1.712971 -0.455885 -3.744076
1 -0.542167 0.864867 -3.854558
1 0.710518 -4.909374 1.228600
1 1.828449 -3.535166 1.402166
1 0.319365 -3.561915 2.327152
1 -1.666190 -4.857788 0.168685
1 -2.263769 -3.453637 1.096668
1 -2.423302 -3.470437 -0.667992
6 -2.712335 -1.525341 4.678451
6 -3.238347 -0.728945 5.707712
6 -3.166522 0.667466 5.656535
6 -2.566237 1.330374 4.575207
6 -2.052067 0.533747 3.566459
1 -2.762725 -2.608684 4.709455
1 -3.709923 -1.208817 6.559844
1 -3.583797 1.252847 6.470204
1 -2.504291 2.411884 4.524059
6 -5.163778 -1.488378 -2.547253
6 -6.465080 -1.014341 -2.317666
6 -6.732397 -0.084078 -1.307437
6 -5.712391 0.413844 -0.482132
6 -4.433917 -0.061519 -0.719421
1 -4.946356 -2.209826 -3.328049
1 -7.278414 -1.378328 -2.937959
1 -7.750391 0.262177 -1.157335
1 -5.907498 1.135847 0.303213
6 -0.381020 5.121937 0.109516
6 -0.820903 6.121376 -0.772420
6 -1.340579 5.804483 -2.032011
6 -1.442203 4.473388 -2.466213
6 -1.004307 3.497828 -1.586955
1 0.023301 5.355684 1.088453
1 -0.755820 7.161647 -0.468215
1 -1.673002 6.602516 -2.689014
1 -1.845618 4.217553 -3.440383

9 6.534947 -1.916096 0.177673
9 4.916725 -3.196513 0.880231
9 5.073554 -2.713863 -1.229327
9 5.820272 2.762847 1.036117
9 4.298200 3.499055 -0.333536
9 3.863404 3.356708 1.788300

hartwigbpylrBcat3

bpyIr(Bcat)3 hartwig
B3LYP/gen
E(RB+HF-LYP) = -1819.20228412

Zero-point correction= 0.441405 (Hartree/Particle)
Thermal correction to Energy= 0.473663
Thermal correction to Enthalpy= 0.474607
Thermal correction to Gibbs Free Energy= 0.371311
Sum of electronic and ZPE= -1818.760879
Sum of electronic and thermal Energies= -1818.728621
Sum of electronic and thermal Enthalpies= -1818.727677
Sum of electronic and thermal Free Energies= -1818.830973

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 297.228	125.818	217.405

B,0,0.2140232189,-0.3130434271,1.3291773425
B,0,-0.7710763176,-1.2432458752,-1.0259161432
B,0,-1.2067297655,1.3920570351,-0.3861946609
C,0,1.883336522,3.1810840756,-0.4677805273
H,0,0.8422894855,3.4630892066,-0.3535042178
C,0,2.9000239094,4.1299737895,-0.549655837
H,0,2.657790633,5.1851938399,-0.4879416938
C,0,4.2106717396,3.6909649066,-0.7162135497
C,0,4.4595862717,2.3234323284,-0.7897405814
C,0,3.3954886073,1.41979132,-0.6898887801
C,0,3.5880420082,-0.0530898838,-0.7436114531
C,0,4.8525320031,-0.6528277674,-0.7781762246
H,0,5.7517641469,-0.0494928709,-0.7656313989
C,0,4.9530656764,-2.040561003,-0.8132511316
C,0,3.7872007664,-2.8026950371,-0.8023161598
H,0,3.8162663779,-3.8865246389,-0.8189764162
C,0,2.5621614772,-2.1434617488,-0.7597421858
H,0,1.6243267025,-2.6859690009,-0.7234818423
C,0,-0.4941203196,-0.5347574825,3.433827689
C,0,0.6556586451,-1.3136842546,3.2803474748
C,0,1.1789019821,-2.0576102221,4.324059128
H,0,2.0718659551,-2.6602307617,4.1945652164
C,0,0.4974344147,-1.994722622,5.5503764041
C,0,-0.6534487579,-1.2151140281,5.7033560498
C,0,-1.1740892953,-0.4639056533,4.6374307823
C,0,-2.1327378862,-2.4928316765,-2.2982070644
C,0,-1.7976732067,-3.236664357,-1.1640577425
C,0,-2.284034315,-4.516105386,-0.9566883867
H,0,-2.0205381094,-5.0810253151,-0.0686536538
C,0,-3.1343719105,-5.0379631159,-1.9449324363
C,0,-3.4690999811,-4.2946624604,-3.0814650041
H,0,-4.1313726619,-4.7264397409,-3.8260395248
C,0,-2.9693240406,-2.9976855384,-3.2798452008
H,0,-3.2254191042,-2.4112238548,-4.1558497001
C,0,-2.5243724741,3.2243973963,-0.3277567144
C,0,-3.327487457,2.094201966,-0.1569120514
C,0,-4.6985789028,2.1953009043,0.0148586555
H,0,-5.3134429124,1.3114011916,0.1461325374
C,0,-5.2447346352,3.4880251005,0.0102703467
C,0,-4.4393746301,4.6191344813,-0.1609776927
C,0,-3.051108622,4.5050499156,-0.3356511308

H,0,-2.4179822242,5.376072443,-0.4702870974
Ir,0,0.4865639038,0.2673349594,-0.5490439236
N,0,2.1206200008,1.8588725039,-0.5340242158
N,0,2.4611781503,-0.8041903949,-0.7400421259
O,0,-0.777971395,0.0917468378,2.2456652596
O,0,1.1155534317,-1.1886594599,1.9913794725
O,0,-1.5129202619,-1.270993562,-2.2364518468
O,0,-0.9513191756,-2.4941045576,-0.3746507135
O,0,-1.219351307,2.8207815375,-0.4755950918
O,0,-2.5442081289,0.9741344521,-0.1951916807
H,0,5.4730177124,1.9688765607,-0.9305395134
H,0,-6.3155835968,3.6108943046,0.1426976714
H,0,-1.1574161004,-1.189445498,6.6648848522
H,0,-2.0667349987,0.1432287204,4.7429442744
H,0,0.8731656397,-2.5647772737,6.3948994155
H,0,-4.8944477005,5.6051374622,-0.1593226297
H,0,5.9285833086,-2.5159410374,-0.8402111908
H,0,-3.5404905033,-6.0374413503,-1.8207937809
H,0,5.0303070072,4.3988256172,-0.7917326556

hartwigbpyIrBcat3HPh

bpyIr(Bcat)3(H)(Ph) hartwig
B3LYP/gen
E(RB+HF-LYP) = -2051.43203115

Zero-point correction= 0.540777 (Hartree/Particle)
Thermal correction to Energy= 0.578465
Thermal correction to Enthalpy= 0.579409
Thermal correction to Gibbs Free Energy= 0.466655
Sum of electronic and ZPE= -2050.891254
Sum of electronic and thermal Energies= -2050.853567
Sum of electronic and thermal Enthalpies= -2050.852622
Sum of electronic and thermal Free Energies= -2050.965376

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 362.992	148.739	237.309

B,0,1.26451076,-0.240499633,0.9001658984
B,0,-0.8921615846,1.7434051895,-0.0218214778
B,0,1.4333020611,0.2915913764,-1.1380333686
C,0,0.218786592,-3.0079018829,-1.9190483655
H,0,0.7545243315,-2.3300967367,-2.5719853104
C,0,0.1207916639,-4.368848451,-2.1957569356
H,0,0.5708277823,-4.7704099392,-3.0970237858
C,0,-0.564993033,-5.1832587379,-1.2976353615
C,0,-1.1102300782,-4.6125379771,-0.152537355
C,0,-0.9655512856,-3.2369693852,0.06795074
C,0,-1.4875106716,-2.557608696,1.276393373
C,0,-2.0751826949,-3.2567016712,2.3374256168
H,0,-2.176291682,-4.3334329502,2.2917675674
C,0,-2.5202545177,-2.5692359592,3.4605871996
C,0,-2.3645657135,-1.1865048616,3.5057283566
H,0,-2.6896053444,-0.6040849672,4.3605682923
C,0,-1.7743300847,-0.5432565727,2.4230913458
H,0,-1.6345336136,0.5304375238,2.4005754803
C,0,2.4327815741,0.1750647783,2.753696516
C,0,2.697290222,-1.1380733812,2.3603754222
C,0,-1.2346688877,3.9393662829,-0.2708030296
C,0,-1.612000893,3.5941869946,1.0281573261
C,0,3.2579266646,0.1216809651,-2.4289968644
C,0,3.1812827308,1.4279687192,-1.9404570428
Ir,0,-0.46608313,-0.2177684248,-0.412337389
N,0,-0.3172075651,-2.4533529311,-0.8225572316
N,0,-1.3488949347,-1.2072559098,1.3320305507
O,0,1.5554068105,0.7411948368,1.861382583

O,0,1.9870392148,-1.4109978754,1.2146854199
O,0,-0.7960119609,2.8186222384,-0.9271826574
O,0,-1.4121881505,2.2432084507,1.2021448143
O,0,2.194433587,-0.602141261,-1.9435140475
O,0,2.0740413343,1.5485968946,-1.1403678428
H,0,-1.6480277955,-5.2335476484,0.5527938914
H,0,-2.9752126381,-3.1074908292,4.2861094907
H,0,-0.6735691783,-6.2475377357,-1.4815870919
H,0,-0.1194037778,0.4077920072,-1.8435149052
C,0,-2.4450179192,-0.3215272128,-1.250514841
C,0,-3.6108479867,0.0300954788,-0.5443724049
H,0,-3.5357326161,0.4190920888,0.4685103177
C,0,-4.8859994552,-0.0851461628,-1.1092279542
H,0,-5.7592847477,0.2018296494,-0.5273436571
C,0,-5.0386909907,-0.5535060478,-2.4138634362
H,0,-6.0268860531,-0.6402699059,-2.8577136921
C,0,-3.9003357108,-0.8979542442,-3.1444279907
H,0,-3.9969071956,-1.254216141,-4.1678029718
C,0,-2.6310539064,-0.7805448737,-2.5702228249
H,0,-1.7674119199,-1.047922237,-3.175539759
C,0,3.5533305803,-1.9599016013,3.0745946118
C,0,4.1444351676,-1.4069951433,4.220542739
C,0,3.8788028531,-0.0902787388,4.6153090921
C,0,3.0107636988,0.7326481312,3.8822886489
C,0,4.2842569455,-0.2902012102,-3.26159254
C,0,5.2496503074,0.67267574,-3.5964782222
C,0,5.1728081178,1.9808676787,-3.1075176095
C,0,4.1279304253,2.3855417408,-2.2620904549
C,0,-2.0964002718,4.528896494,1.9261353881
C,0,-2.1938251475,5.8528667459,1.4681305169
C,0,-1.8172448037,6.2001804027,0.1667868745
C,0,-1.3266552101,5.2411751484,-0.733466395
H,0,2.8006783627,1.7554767481,4.1756316958
H,0,4.356519354,0.3053882599,5.5064581235
H,0,4.8240767788,-2.0139491452,4.8110202771
H,0,3.7552077382,-2.9772769265,2.7568514263
H,0,6.07212365,0.3930941819,-4.2478987471
H,0,4.3367207337,-1.308172518,-3.6330225542
H,0,5.9364026681,2.700540236,-3.3866245827
H,0,4.0570768598,3.3965683733,-1.8761318937
H,0,-2.3845252644,4.2489297881,2.9341086426
H,0,-2.568808671,6.619637179,2.1394326159
H,0,-1.9051331319,7.2332034129,-0.1563524522
H,0,-1.031889353,5.4994527908,-1.7448658086

hartwigdmpelrBcat3

dmpeIr(Bcat)3 hartwig
B3LYP/gen
E(RB+HF-LYP) = -2244.84845641

Zero-point correction= 0.492468 (Hartree/Particle)
Thermal correction to Energy= 0.528457
Thermal correction to Enthalpy= 0.529401
Thermal correction to Gibbs Free Energy= 0.420396
Sum of electronic and ZPE= -2244.355988
Sum of electronic and thermal Energies= -2244.319999
Sum of electronic and thermal Enthalpies= -2244.319055
Sum of electronic and thermal Free Energies= -2244.428060

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 331.612	137.162	229.421

C,0,1.3303722805,-1.4046520237,3.1121660168
C,0,0.934708327,-0.0814328395,3.3184345809
C,0,1.0148023305,0.5174262603,4.5639421573

H,0,0.703583335,1.5455727019,4.7128206979
C,0,1.5142420485,-0.2700503571,5.6134096264
C,0,1.9104677311,-1.5949853146,5.4060982274
H,0,2.2915167896,-2.1764081512,6.2400999286
C,0,1.8243052233,-2.1917665973,4.1375959589
H,0,2.1278284112,-3.2194808178,3.9667378097
C,0,0.2223669076,3.8201139965,-0.7406175478
C,0,1.5591303519,3.5702176398,-0.4237202421
C,0,2.4682350664,4.5963756609,-0.2262825947
H,0,3.5040304094,4.3920065553,0.0241402733
C,0,1.9830806277,5.9064786334,-0.3625878642
C,0,0.6439562904,6.1564469557,-0.6817852682
H,0,0.3005824963,7.1820983694,-0.7778765831
C,0,-0.2679666733,5.1079838879,-0.8789247313
H,0,-1.3089129598,5.2892795527,-1.1240787147
C,0,-4.0070725479,0.1896106536,-0.6469364113
C,0,-3.7886629739,0.2710671981,0.7302553178
C,0,-4.8232517565,0.4992298376,1.6215882557
H,0,-4.6411588601,0.5621402062,2.689137128
C,0,-6.1085506847,0.6468835166,1.0760497322
C,0,-6.3270642231,0.5661630338,-0.3030464989
C,0,-5.2694679922,0.3342146103,-1.1971446458
H,0,-5.4272916487,0.2726284855,-2.2688203047
C,0,2.5297985008,-2.7078952039,-2.0669727212
H,0,2.2372023877,-2.7621802177,-3.1229584468
H,0,3.5668529157,-3.0575044976,-2.007216879
C,0,1.6003843674,-3.5898269843,-1.2145629667
H,0,1.9737188787,-3.6485068039,-0.1864114207
H,0,1.555053793,-4.6110729957,-1.611294186
C,0,3.0938614333,-0.0189349038,-3.0462292634
H,0,4.0839247463,-0.3923792064,-3.3269466367
C,0,3.7662119394,-0.6794629572,-0.3318098669
H,0,3.7826534009,0.3745974873,-0.0435862556
C,0,-0.9415989314,-3.3792371311,-2.6519767724
H,0,-1.9689439534,-3.0052349269,-2.6499199831
B,0,0.6066998773,-0.5582360488,1.1606483493
B,0,0.5004125914,1.5948009917,-0.6322835671
B,0,-1.8151432893,-0.0995563613,-0.257861683
O,0,1.1429960852,-1.7257423394,1.7837662611
O,0,0.4940759979,0.4510307095,2.1334148181
O,0,-0.4379467253,2.6247393273,-0.8748650195
O,0,1.7570962683,2.2119048207,-0.3630085614
O,0,-2.8093243126,-0.0539111883,-1.2758278588
O,0,-2.4518194012,0.0873060999,0.9873527598
P,0,2.4163134095,-0.9001923677,-1.5699773246
P,0,-0.1123995071,-2.8466839725,-1.0835083908
Ir,0,0.1634385755,-0.4620366326,-0.7789920736
C,0,-0.9385693691,-3.8989536077,0.1835580996
H,0,-7.3335180812,0.686509663,-0.6927422146
H,0,-0.4946399414,-3.6790285223,1.1564402233
H,0,2.6618811374,6.7410766317,-0.2148184109
H,0,-6.9481322932,0.8290409667,1.7402184231
H,0,1.592694627,0.1611137212,6.6067858121
H,0,-0.429487891,-2.9455243119,-3.5155985872
H,0,-0.9529836247,-4.4691581697,-2.7555590926
H,0,3.1642174951,1.0448823388,-2.8053484649
H,0,2.4142001914,-0.132918007,-3.8953825481
H,0,4.7408598913,-0.9704171655,-0.7366455468
H,0,3.543345817,-1.274455218,0.5566233798
H,0,-0.8361821036,-4.9655001314,-0.0409571335
H,0,-2.000335209,-3.6411295398,0.2219094458

dmpeBpin3PhHCHactTSParSptBack

Ir Bpin3 benzene CH act parallel to Ps new conf B
B3LYP/gen
E(RB+HF-LYP) = -2019.75310567

Zero-point correction= 0.520791 (Hartree/Particle)
Thermal correction to Energy= 0.556120
Thermal correction to Enthalpy= 0.557065
Thermal correction to Gibbs Free Energy= 0.453312
Sum of electronic and ZPE= -2019.232315
Sum of electronic and thermal Energies= -2019.196985
Sum of electronic and thermal Enthalpies= -2019.196041
Sum of electronic and thermal Free Energies= -2019.299794

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	348.971	129.731	218.366

C,0,2.891351283,1.1939365057,-0.2357381002
C,0,2.1588766654,0.1853664459,0.395665178
C,0,2.7851053326,-0.8391692412,1.1323166771
C,0,4.1827825832,-0.7450497441,1.2641701756
C,0,4.9250363614,0.2640730164,0.6401607978
C,0,4.2826703908,1.2348161196,-0.1269990806
Ir,0,1.5709680628,-2.5960432904,1.9360026943
B,0,-0.1930323796,-1.4645937586,1.954050739
O,0,-1.432243962,-1.89864642,1.4555939839
C,0,-2.4356731769,-0.9311920454,1.7924616027
C,0,-1.638133946,0.3128104328,2.2347990187
O,0,-0.3072905333,-0.1677085991,2.4374487869
H,0,4.8523455333,2.0220506514,-0.6134330793
P,0,1.1971208618,-3.4222835756,-0.3057594867
C,0,1.8795643351,-2.4272927722,-1.7062405151
P,0,3.3959147319,-4.2800169512,1.9084901327
C,0,5.185400071,-4.0211728764,2.3221010264
B,0,0.2091293834,-4.083873952,2.6323975726
O,0,-0.1129267668,-5.2682196919,1.9391550535
C,0,-1.1926207322,-5.9361528884,2.6086716338
C,0,-1.2583544505,-5.2586313042,3.9890768096
O,0,-0.5010789948,-4.0552125072,3.8330329901
B,0,1.7350024811,-2.402420129,4.0473870107
O,0,0.9878649463,-1.588603983,4.8770327293
C,0,1.270047178,-1.9293274913,6.2359533431
C,0,2.5821884467,-2.7338224109,6.1637861747
O,0,2.6724397733,-3.1349237466,4.7877219007
C,0,2.1201113113,-5.0334518799,-0.4878874084
C,0,3.508643087,-4.9464800278,0.1620235804
C,0,-0.4866051164,-3.8374048416,-0.9252689339
C,0,3.0708743637,-5.8106089901,2.8953476817
H,0,-0.802183331,-5.8752398413,4.7745817978
H,0,-2.2804920401,-5.0137282536,4.294631266
H,0,-0.9843899052,-7.0096259929,2.664611476
H,0,-2.1161975855,-5.7913487055,2.0340941912
H,0,2.5788988222,-3.6196844795,6.8069806298
H,0,3.4581714678,-2.1232905502,6.418133745
H,0,0.442456232,-2.5299519111,6.6341218895
H,0,1.3591121931,-1.0169292078,6.8338322397
H,0,-3.06029953,-1.3292659137,2.6019497772
H,0,-3.0757731132,-0.7441721103,0.9234785875
H,0,-2.0157265414,0.7518262706,3.1637814411
H,0,-1.6285223017,1.0959290559,1.464694287
H,0,2.201241262,-1.2903949853,2.6657156462
H,0,1.0775969618,0.2064890539,0.3195496195
H,0,2.3682930908,1.9577040336,-0.8070515843
H,0,4.7082178814,-1.4575692122,1.888937221
H,0,6.0048897642,0.2947461268,0.7681064911
H,0,4.0067839947,-5.9233060383,0.1569203853
H,0,4.1484995977,-4.2556357552,-0.4000909284
H,0,1.5078679552,-5.7881843006,0.014733627
H,0,2.1947375505,-5.3066723924,-1.5472142686
H,0,1.7483395198,-2.9612157952,-2.6532339788
H,0,1.3695387556,-1.4638495276,-1.7613300925

H,0,2.9397513118,-2.2256316042,-1.5405994867
H,0,-0.440818366,-4.2352697101,-1.9441136069
H,0,-0.9257508133,-4.573940385,-0.2523733713
H,0,-1.1066641221,-2.9397365518,-0.8982868226
H,0,5.7363118604,-4.9657012956,2.2631139543
H,0,5.642312612,-3.3041896432,1.6375096736
H,0,5.2556996484,-3.6309994951,3.3406400611
H,0,3.8491039973,-6.5634376827,2.7319962767
H,0,3.0454047115,-5.52786452,3.9496678054
H,0,2.0968423348,-6.2177067341,2.6186813622

dmpeBpin3PhHCHactTSParWrdBack

Ir Bpin3 dmpe C-H activation turning benzene parallel to Ps
B3LYP/gen
E(RB+HF-LYP) = -2019.75100331

Zero-point correction= 0.521093 (Hartree/Particle)
Thermal correction to Energy= 0.556395
Thermal correction to Enthalpy= 0.557339
Thermal correction to Gibbs Free Energy= 0.452880
Sum of electronic and ZPE= -2019.229911
Sum of electronic and thermal Energies= -2019.194608
Sum of electronic and thermal Enthalpies= -2019.193664
Sum of electronic and thermal Free Energies= -2019.298124

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 349.143	129.407	219.854

C,0,-2.6600629804,1.207915644,-0.4011663438
C,0,-1.9444945855,-0.0027490882,-0.5062878704
C,0,-2.6839839291,-1.1351072444,-0.8961299082
C,0,-4.0678791094,-1.0846228657,-1.097596278
C,0,-4.7591346902,0.1151053042,-0.9347018808
C,0,-4.0428674917,1.2644174345,-0.594620048
Ir,0,0.2802631172,-0.0234575698,0.030578203
P,0,-0.0000058687,0.8216853644,2.2703082969
C,0,0.4872488067,-0.5445733975,3.4442821479
C,0,-0.1159275156,-1.8846007672,3.0046606567
P,0,0.1984871758,-2.2177818991,1.1855465691
B,0,2.3537635321,0.3151925144,0.4015178123
O,0,3.0693998163,1.4135838304,-0.0677741608
C,0,4.4573220763,1.256489386,0.2340755266
C,0,4.4925490239,0.1347623739,1.289860475
O,0,3.1965186041,-0.4757958905,1.201716189
B,0,1.2101919549,-1.0012699938,-1.6064945413
O,0,0.8425028948,-2.2978666089,-1.9981052237
C,0,1.7374646734,-2.7441294769,-3.0278243175
C,0,2.477800256,-1.4655736027,-3.463934019
O,0,2.2527173447,-0.5409097326,-2.3941432827
B,0,0.4275007691,1.8773137161,-0.8434145262
O,0,0.4878145079,2.116328103,-2.210702442
C,0,0.404906396,3.522262634,-2.4572896472
C,0,0.5767092536,4.168267459,-1.0685799333
O,0,0.3494842988,3.0927164506,-0.1476466949
H,0,4.9952409132,0.9791950631,-0.6811385518
H,0,4.8668068328,2.2028290219,0.6024032622
H,0,5.2669081596,-0.6140901248,1.094877003
H,0,4.6399962508,0.5233232553,2.3064264742
H,0,2.4204781271,-3.4967162422,-2.6117049395
H,0,1.1647114469,-3.2072783185,-3.8370379372
H,0,3.5531131586,-1.6176120241,-3.6000879832
H,0,2.0661300795,-1.0461944134,-4.3902894817
H,0,1.5912192273,4.5589004758,-0.9194600368
H,0,-0.1386146905,4.9753943742,-0.878243966
H,0,1.1867221823,3.8207464295,-3.1631564082

H,0,-0.5711130049,3.7535702561,-2.9035867639
H,0,-0.5480487945,-0.2238652499,-1.3491973059
H,0,-2.1325987943,2.1258047078,-0.1604203435
H,0,-4.5601091335,2.2152599049,-0.4857972517
H,0,-2.1693576384,-2.0720701998,-1.0779726256
H,0,-4.5996884042,-1.9846941505,-1.3979628275
H,0,-5.8335504439,0.1600540059,-1.0911190647
C,0,1.0101656908,2.2440018826,2.864021341
C,0,-1.6887924315,1.2881216465,2.8617243832
C,0,1.727708229,-3.25800216,1.2070489722
C,0,-1.0607587417,-3.538064276,0.8631640883
H,0,0.2705641903,-2.7104575919,3.6130622142
H,0,-1.2044642965,-1.8707690839,3.1381143958
H,0,1.580713988,-0.5951196973,3.4096381485
H,0,0.1919469834,-0.2891038689,4.4691327601
H,0,-1.6760536993,1.5083513507,3.9341813902
H,0,-2.0347277018,2.1697250272,2.3183734627
H,0,-2.3921268119,0.4777876571,2.6594099495
H,0,0.7925883014,2.4755890771,3.9115711194
H,0,2.0706194627,2.0052635757,2.7573443087
H,0,0.7920467506,3.102187114,2.2262626982
H,0,-0.9335602483,-4.3677281401,1.5666870691
H,0,-2.0712986345,-3.1366038973,0.9577981635
H,0,-0.9273803612,-3.9121804539,-0.1549983008
H,0,1.6098960269,-4.1200606947,1.872166635
H,0,1.9094348541,-3.6121521967,0.1889668226
H,0,2.5758686445,-2.6464101188,1.5149943678

dmpeBpin3PhHCHactTSSptParBack

bpy Ir Bpin3 oxidative addition of benzene looking for third ts
B3LYP/gen
E(RB+HF-LYP) = -2019.75119685

Zero-point correction= 0.520306 (Hartree/Particle)
Thermal correction to Energy= 0.555888
Thermal correction to Enthalpy= 0.556832
Thermal correction to Gibbs Free Energy= 0.452440
Sum of electronic and ZPE= -2019.230891
Sum of electronic and thermal Energies= -2019.195309
Sum of electronic and thermal Enthalpies= -2019.194365
Sum of electronic and thermal Free Energies= -2019.298757

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 348.825	129.864	219.712

C,0,-2.9679686767,-1.3176188993,-0.6004005485
C,0,-2.0930665967,-0.2725223462,-0.955803379
C,0,-2.6145730063,0.7064440687,-1.8257081452
C,0,-3.9383639691,0.6683241174,-2.2731866144
C,0,-4.7910839054,-0.3628760953,-1.8789421279
C,0,-4.2950654495,-1.3604955511,-1.0395688897
Ir,0,-0.0064117173,-0.0774396752,-0.0178992983
P,0,-0.8584822208,0.0511522216,2.2255733243
C,0,-0.5415948128,-1.6009257374,3.0558816852
C,0,-0.6763555679,-2.7873885353,2.0882660609
P,0,0.2696442277,-2.4662205796,0.5000284875
B,0,1.8968429124,0.5300713091,0.7331327522
O,0,2.1840171823,1.8052482052,1.2242769739
C,0,3.5947387524,1.9384414271,1.4266626881
C,0,4.1308189048,0.4951966747,1.3559253086
O,0,3.0526774143,-0.26008951,0.7887186403
B,0,1.3759963507,-0.2510967816,-1.626230436
O,0,1.6798297635,-1.4858302155,-2.2162726641
C,0,2.7740216109,-1.3061761558,-3.1256389989
C,0,2.8677929108,0.2213019288,-3.3071296457

O,0,2.1198992308,0.7591090735,-2.2116089181
B,0,-0.2644465269,1.9905349593,-0.2681056554
O,0,-0.0307720713,2.7337202863,-1.4206213887
C,0,-0.5014388261,4.0714229018,-1.2335325872
C,0,-0.7720033695,4.1780914409,0.2792785267
O,0,-0.8167858481,2.8174346824,0.724341897
H,0,4.0115014477,2.5727792568,0.6349214229
H,0,3.786210904,2.4198804871,2.3915931144
H,0,5.0191208984,0.4008200434,0.7229422366
H,0,4.373673885,0.0913912903,2.3478163684
H,0,3.6853964997,-1.7254543755,-2.6801397358
H,0,2.5675991298,-1.8386031148,-4.0594934734
H,0,3.896566707,0.5933362511,-3.268824932
H,0,2.414280549,0.5554925087,-4.2488102822
H,0,0.0354297535,4.7040942414,0.8051117502
H,0,-1.7196125339,4.6757892255,0.5110382369
H,0,0.2543746656,4.7816191427,-1.5839177469
H,0,-1.414408535,4.2197397825,-1.8263715841
H,0,-0.5557046257,-0.4182410347,-1.5135168975
H,0,-2.6255888038,-2.1102467542,0.0548925324
H,0,-4.9387888149,-2.178541621,-0.7234985925
H,0,-1.9673775447,1.5075383413,-2.1680246779
H,0,-4.2987748993,1.4468859577,-2.941550282
H,0,-5.8197437727,-0.395176564,-2.227333602
C,0,-0.1515392188,1.2335201778,3.449437165
C,0,-2.6649842108,0.3531670624,2.4495664256
C,0,1.945078122,-3.1361773663,0.9006745741
C,0,-0.3331578146,-3.7882079376,-0.6456372038
H,0,-0.3295279476,-3.7155188092,2.5582497912
H,0,-1.7285113834,-2.9386760197,1.8215249179
H,0,0.4841230525,-1.5484243908,3.4406956283
H,0,-1.2025753605,-1.7190006412,3.9227906291
H,0,-2.9500076371,0.2851169741,3.5043768936
H,0,-2.8728545865,1.3590179278,2.0761413588
H,0,-3.2498160817,-0.3522440693,1.8576930553
H,0,-0.6022244886,1.0896656762,4.4368450636
H,0,0.9300736568,1.1052492366,3.5107898963
H,0,-0.3510934501,2.2419145355,3.0843605829
H,0,-0.2600475655,-4.7822026115,-0.1917845265
H,0,-1.3645407567,-3.5995233908,-0.94816147
H,0,0.2949022424,-3.748138381,-1.5391339894
H,0,1.8845701688,-4.1854462115,1.2092342564
H,0,2.5671996508,-3.0481540641,0.0077630231
H,0,2.4134081549,-2.5369910652,1.6819189921

dmpeBpin3PhHCHactTSSptSptBack11

Ir Bpin3 dmpe C-H activation for benzene split on top, split on bottom
B3LYP/gen
E(RB+HF-LYP) = -2019.75362566

Zero-point correction= 0.520806 (Hartree/Particle)
Thermal correction to Energy= 0.556124
Thermal correction to Enthalpy= 0.557069
Thermal correction to Gibbs Free Energy= 0.453517
Sum of electronic and ZPE= -2019.232820
Sum of electronic and thermal Energies= -2019.197501
Sum of electronic and thermal Enthalpies= -2019.196557
Sum of electronic and thermal Free Energies= -2019.300108

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 348.973	129.740	217.942

C,0,3.0590310152,-1.1722052726,0.7278761158
C,0,2.2224844971,-0.046916182,0.865985636
C,0,2.8164881658,1.1042022645,1.4204950026

C,0,4.1714772967,1.1427353768,1.7649149776
C,0,4.9839638341,0.0235016275,1.5844389562
C,0,4.4159438976,-1.1403282781,1.0664428275
Ir,0,0.0677090561,-0.0340407579,0.0608750295
P,0,0.8459503376,-0.2146060172,-2.2173248726
C,0,0.5159163445,-1.9672143978,-2.7864256439
C,0,0.7208602502,-3.0030501218,-1.6692385575
P,0,-0.1743204978,-2.4719549637,-0.1117248334
B,0,-1.8904136592,0.2870915673,-0.7107434801
O,0,-2.3927714439,-0.2949912123,-1.8910013748
C,0,-3.6877340946,0.250777151,-2.1836220329
C,0,-4.0939437931,0.9806332961,-0.8900629651
O,0,-2.877587168,1.094881794,-0.1453586736
B,0,-1.1389420278,-0.0137202848,1.8166720049
O,0,-1.8210076815,-1.1612347589,2.2526155861
C,0,-2.4622954756,-0.8653476993,3.5025622907
C,0,-2.3893702518,0.6696928142,3.6066740872
O,0,-1.367479787,1.0400095305,2.6785279372
B,0,0.0892517052,2.0687648063,-0.0102979827
O,0,0.25534787,2.9381384697,1.0624430334
C,0,0.3250989932,4.286988793,0.5952465976
C,0,-0.1181959351,4.2075391453,-0.878134726
O,0,-0.0381067875,2.8127378529,-1.1978905529
H,0,-3.6055116167,0.9360867799,-3.0370411439
H,0,-4.3752470338,-0.5567884166,-2.4555039425
H,0,-4.5081746086,1.9768512417,-1.0744987341
H,0,-4.8237961183,0.4070282943,-0.3043436724
H,0,-3.4879301341,-1.2480012498,3.4915648676
H,0,-1.9151553448,-1.3621362148,4.3144496838
H,0,-3.332526872,1.1462683685,3.310661759
H,0,-2.1214972097,1.0197149632,4.6084340666
H,0,-1.1517494489,4.5499430693,-1.0167020068
H,0,0.5280244079,4.7800739602,-1.5521226916
H,0,-0.3276671195,4.9209395323,1.2037803298
H,0,1.3551317778,4.6545847628,0.6980421404
H,0,0.69777474,-0.071555093,1.5624813343
H,0,2.665333049,-2.0983126218,0.3252363608
H,0,5.0255518851,-2.0302551044,0.9248971784
H,0,2.2031572325,1.9802416449,1.5980872602
H,0,4.5884146372,2.0548245412,2.1860843923
H,0,6.0365009872,0.0527503393,1.8530459516
C,0,0.1208038977,0.7675981578,-3.5978535306
C,0,2.6522130673,0.029537755,-2.5165306839
C,0,-1.8740970339,-3.1468961188,-0.3790812596
C,0,0.4307235667,-3.6516146831,1.1812206091
H,0,0.3768320202,-3.9937649983,-1.9898204617
H,0,1.7852363618,-3.0956097486,-1.4251663189
H,0,-0.5312014016,-1.9686063456,-3.1071807588
H,0,1.1322953909,-2.2010603739,-3.6625558446
H,0,2.9104885073,-0.1983666961,-3.5557798338
H,0,2.8998535303,1.0731843814,-2.3046529101
H,0,3.24078341,-0.5922515559,-1.8408536294
H,0,0.5840939043,0.4942942982,-4.5513944467
H,0,-0.9514313521,0.5729107682,-3.6343938835
H,0,0.2764131436,1.8263912234,-3.3874261751
H,0,0.3416690941,-4.6921846005,0.8516987214
H,0,1.4665880306,-3.4428953936,1.4531206043
H,0,-0.1912655768,-3.5017500172,2.0675180759
H,0,-1.8509323249,-4.2292124971,-0.5449480405
H,0,-2.4600838641,-2.9215101958,0.5147220427
H,0,-2.3361442424,-2.6444956997,-1.2300217964

dmpeBpin3PhHCHactTSSptSptFrnt

C-H act ts bringing Ph in axial
B3LYP/gen
E(RB+HF-LYP) = -2019.75161969

Zero-point correction= 0.520550 (Hartree/Particle)
Thermal correction to Energy= 0.556183
Thermal correction to Enthalpy= 0.557127
Thermal correction to Gibbs Free Energy= 0.451442
Sum of electronic and ZPE= -2019.231069
Sum of electronic and thermal Energies= -2019.195437
Sum of electronic and thermal Enthalpies= -2019.194492
Sum of electronic and thermal Free Energies= -2019.300177

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	349.010	129.835	222.433

C,0,-0.3450394906,-3.4871937447,0.010675699
C,0,0.7905237207,-3.2170102301,1.0096381213
P,0,0.684876834,-1.4778419057,1.6941851808
Ir,0,0.0394794169,-0.0267468695,-0.1161052507
B,0,0.2551081677,1.6240939733,1.1708030244
O,0,0.5196450645,2.9464197731,0.8446960715
C,0,0.4678483561,3.7594111319,2.0187107259
C,0,0.4822466329,2.7538863821,3.1864400256
O,0,0.1776663165,1.4945913603,2.5736984024
P,0,-0.4986714744,-2.1309492135,-1.2751363649
B,0,-0.9639222067,1.1925575946,-1.5581248928
O,0,-1.8230221053,0.6543740557,-2.5243121702
C,0,-2.4185350877,1.7237346908,-3.2714705689
C,0,-1.6471038071,2.9864774862,-2.8259716627
O,0,-0.856330524,2.5602251015,-1.7148046269
B,0,-1.9564277613,0.043902379,0.6254265364
O,0,-2.6950968716,-1.0740328881,1.0593085259
C,0,-3.9411740647,-0.6374440891,1.6228778123
C,0,-4.0571021133,0.8377314613,1.1951064754
O,0,-2.7397175723,1.1897103396,0.7606156449
C,0,-2.2120597946,-2.4256495053,-1.9009704332
C,0,0.464556149,-2.7761951472,-2.7273832361
H,0,-0.2249601235,-4.4640984761,-0.4722892802
H,0,-1.3056621644,-3.4939363563,0.5367618731
C,0,-0.398167317,-1.6691815918,3.1747734526
C,0,2.3317076436,-1.2213618103,2.4805858299
H,0,0.7745839957,-3.9438824146,1.8307028068
H,0,1.7664156721,-3.3088902778,0.5189888401
H,0,-0.2632121865,2.9814232156,3.9557254198
H,0,1.4671831265,2.6937384051,3.6686448803
H,0,-0.4517638224,4.35770288,2.0002055396
H,0,1.3234115501,4.4429425135,2.0337760087
H,0,-2.3115577055,3.798193183,-2.512093596
H,0,-0.9844161659,3.3693402054,-3.6117949568
H,0,-3.486348771,1.7814837078,-3.0273706493
H,0,-2.3214871789,1.5199060285,-4.3432377239
H,0,-4.3631936015,1.4962127078,2.0141276846
H,0,-4.7600168238,0.9727092594,0.3631118031
H,0,-3.900740294,-0.7498861223,2.714023811
H,0,-4.757080909,-1.2605980068,1.2426117266
H,0,-2.3296570468,-3.4539339593,-2.2592006271
H,0,-2.91476286,-2.2309837843,-1.0897497649
H,0,-2.4105682646,-1.7189267182,-2.7079547502
H,0,0.0932092875,-3.75760254,-3.040946322
H,0,0.3471881489,-2.0720111719,-3.556326208
H,0,1.5295023643,-2.8509715677,-2.504076596
H,0,2.5611930301,-2.0272806153,3.1850979118
H,0,3.1061364724,-1.1653909119,1.7139728319
H,0,2.2995390988,-0.2694242897,3.0153146309
H,0,0.0199353663,-2.4033511546,3.8711143394
H,0,-0.4664919355,-0.6929252622,3.6592771421
H,0,-1.3955613698,-1.9741294086,2.8563008387
H,0,0.7711373351,0.6055100575,-1.4218688747
C,0,2.2409970682,0.2018068572,-0.7102976822

C,0,3.0511548132,-0.9105596868,-1.0110444122
C,0,4.4306039491,-0.7944719181,-1.2139191348
C,0,5.0478519574,0.4547446913,-1.1505092988
C,0,4.2641658295,1.5780542421,-0.8853409516
C,0,2.887253683,1.4538826766,-0.6745455463
H,0,2.6154088646,-1.9016696346,-1.06748327
H,0,5.0189302634,-1.6850449002,-1.4246182028
H,0,6.1178310278,0.5510813871,-1.3139851137
H,0,4.7224056515,2.5637075948,-0.846343622
H,0,2.3031602448,2.3453191212,-0.4743158764

IrDMPE_Bpin2_n2BpinH_Ph_goodgs

Ir(dmpe)(Bpin)₃(H)(Ph)
E(RB+HF-LYP) = -2019.76522987

Zero-point correction= 0.524049 (Hartree/Particle)
Thermal correction to Energy= 0.559197
Thermal correction to Enthalpy= 0.560142
Thermal correction to Gibbs Free Energy= 0.456709
Sum of electronic and ZPE= -2019.241181
Sum of electronic and thermal Energies= -2019.206032
Sum of electronic and thermal Enthalpies= -2019.205088
Sum of electronic and thermal Free Energies= -2019.308521

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 350.902	129.474	217.693

C,0,-3.2669007519,0.5502560795,-0.1985304741
C,0,-2.2305549621,-0.3297706726,-0.5741570041
C,0,-2.6184846537,-1.3667303948,-1.452089677
C,0,-3.9366474852,-1.5408555036,-1.886696065
C,0,-4.9398195865,-0.6684426682,-1.4636152366
C,0,-4.5913331082,0.3865301821,-0.621140956
Ir,0,-0.0930588267,-0.0489670331,-0.0760815658
P,0,-0.4654747645,0.2754135432,2.2319387089
C,0,0.0920060863,-1.2529957299,3.1408004948
C,0,-0.365312609,-2.5134202447,2.3969697851
P,0,0.1959013068,-2.4428413328,0.6155021261
B,0,1.9047732148,0.626314487,0.4068995346
O,0,2.2989371955,1.9586563175,0.347051849
C,0,3.6941943691,2.0642819458,0.6423081728
C,0,4.0553078383,0.7042326785,1.2710534227
O,0,2.9492570686,-0.1481856529,0.9345113349
B,0,1.2787199413,-0.4232325442,-1.7165731946
O,0,1.5769723612,-1.7330401453,-2.1188824881
C,0,2.73772895,-1.6895728338,-2.9586331195
C,0,2.842038619,-0.2111574715,-3.3756707638
O,0,2.0802645124,0.490508986,-2.3882534873
B,0,-0.4670085079,1.9580164366,-0.5066387862
O,0,-0.3759377839,2.5338488392,-1.7629386201
C,0,-0.6373998808,3.9359354011,-1.6620096697
C,0,-1.2329209056,4.1209029881,-0.2503006771
O,0,-0.9312955884,2.8937000289,0.4298775047
H,0,4.2446116915,2.249026349,-0.288506127
H,0,3.8673837366,2.9076211678,1.3188090321
H,0,4.9822966962,0.2788504288,0.8736764953
H,0,4.1462955609,0.761244876,2.3639166983
H,0,3.6134338939,-2.017187026,-2.3826659017
H,0,2.6037000748,-2.3688130879,-3.8059298433
H,0,3.870920503,0.1617680465,-3.3831013178
H,0,2.3996732125,-0.0296565694,-4.3634530234
H,0,-0.7884760153,4.9615378305,0.2928056483
H,0,-2.3213113,4.2598870226,-0.2750550675
H,0,0.3026618998,4.4876128952,-1.7875432556
H,0,-1.3271414404,4.2391895711,-2.456190559

H,0,-0.103016567,-0.1637373864,-1.7414110117
H,0,-3.037886236,1.4104543392,0.4221989823
H,0,-5.3492021011,1.0975141759,-0.2972910673
H,0,-1.8681551085,-2.0537625713,-1.8323349659
H,0,-4.1748061827,-2.3566665157,-2.566590265
H,0,-5.9661313048,-0.7981681326,-1.7972198107
C,0,0.4292240131,1.6303819781,3.1015745693
C,0,-2.1777829293,0.5176337065,2.8790391144
C,0,1.8940060796,-3.1677607012,0.7262351
C,0,-0.7348519211,-3.8642393068,-0.1163371132
H,0,0.0147361918,-3.419883664,2.8822874497
H,0,-1.4598161745,-2.5796516943,2.3923251761
H,0,1.1861764728,-1.2133355758,3.180778203
H,0,-0.2809959193,-1.2301077121,4.171274161
H,0,0.1173108357,1.6873840631,4.1490354937
H,0,1.5059072888,1.4594621173,3.0536479103
H,0,0.2009715215,2.5645242245,2.5861162356
H,0,-2.1696625143,0.4450135954,3.9714104292
H,0,-2.5323403478,1.5084605302,2.5898012964
H,0,-2.8576934197,-0.2250701682,2.4596154903
H,0,1.8813277731,-4.1264986244,1.255640329
H,0,2.2685928057,-3.3143471469,-0.2882591542
H,0,2.5552936123,-2.4590905783,1.226673482
H,0,-0.54439246,-4.783169542,0.4480120532
H,0,-1.8051890432,-3.6506475612,-0.1182461092
H,0,-0.408934453,-4.0085347605,-1.1497249755

IrDMPE_Bpin2_n2BpinH_Ph_goodgsB

bpy Ir Bpin2 Ph HBpin eq in front (Chads ground state - alternative)
B3LYP/gen

E(RB+HF-LYP) = -2019.76581535

Zero-point correction= 0.524278 (Hartree/Particle)

Thermal correction to Energy= 0.559388

Thermal correction to Enthalpy= 0.560332

Thermal correction to Gibbs Free Energy= 0.457159

Sum of electronic and ZPE= -2019.241537

Sum of electronic and thermal Energies= -2019.206428

Sum of electronic and thermal Enthalpies= -2019.205483

Sum of electronic and thermal Free Energies= -2019.308656

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 351.021	129.525	217.146

C,0,0.0971959426,-3.4025972688,-0.5524615203
C,0,-0.8340632009,-2.8699107831,-1.6519633416
P,0,-0.6217604278,-1.0292014401,-1.9285832193
Ir,0,-0.1408126507,-0.0086467919,0.1288168813
B,0,-0.3655637124,1.8580683971,-0.8012489138
O,0,-0.6926597728,3.0481422969,-0.1707946887
C,0,-0.6033425419,4.1266353761,-1.1041266675
C,0,-0.5487418616,3.438725748,-2.4822892959
O,0,-0.2264316428,2.0730923172,-2.1838272985
P,0,0.125080414,-2.3181374514,0.9777246835
B,0,1.1771652825,0.9124006255,1.6301906924
O,0,1.9686580782,0.1478798383,2.4950579236
C,0,2.7645584082,1.0504598083,3.2771293181
C,0,2.6553914304,2.391034349,2.5269230862
O,0,1.4651248776,2.2597510412,1.749037409
B,0,1.9276872041,0.0257257862,-0.5125864378
O,0,2.6514654639,-1.1345090691,-0.8389472111
C,0,3.9492410563,-0.7854492228,-1.341148323
C,0,4.0229795413,0.7512438632,-1.2014494017
O,0,2.7243983058,1.1425226478,-0.7454915445
C,0,1.6822367186,-2.8972698172,1.7845328509

C,0,-1.1310503616,-3.0673732667,2.113690151
H,0,-0.1644092342,-4.4337071307,-0.2873219922
H,0,1.1310493586,-3.404933838,-0.9118578448
C,0,0.6161974341,-0.9383815685,-3.2914894051
C,0,-2.1520401126,-0.5315371045,-2.8242467391
H,0,-0.6639518117,-3.3958215897,-2.5988634744
H,0,-1.881753895,-3.0363652772,-1.3824684332
H,0,0.2157184605,3.86200192,-3.1419224452
H,0,-1.5150193358,3.4778887819,-3.0026969386
H,0,0.3052064193,4.7058701588,-0.8966028563
H,0,-1.4696882591,4.7863362701,-0.9909341978
H,0,3.5071580279,2.5546810851,1.8539143617
H,0,2.5653592073,3.2530306159,3.1947486633
H,0,3.7902527997,0.6743597109,3.3445580445
H,0,2.3480388677,1.1096020887,4.2910681326
H,0,4.2417436152,1.2521756611,-2.1504144982
H,0,4.7742587387,1.0678119921,-0.4681080618
H,0,4.0343593674,-1.1150141529,-2.3841010844
H,0,4.7171302028,-1.3031755532,-0.7565109711
H,0,1.67171609,-3.9831998215,1.9273232445
H,0,2.5232363605,-2.6084756524,1.1531270463
H,0,1.7896871572,-2.3951772696,2.7471548932
H,0,-0.9746034493,-4.14528154,2.2273963447
H,0,-1.0276771489,-2.59018109,3.092957635
H,0,-2.1432382223,-2.8714626129,1.7589309149
H,0,-2.3281209237,-1.1917432223,-3.6797270118
H,0,-3.0089210855,-0.55248094,-2.1509281148
H,0,-2.0035554063,0.4915820632,-3.1751933552
H,0,0.2285602907,-1.4289528768,-4.1897569142
H,0,0.8028170441,0.1174284517,-3.4994260032
H,0,1.5436963197,-1.4172013057,-2.9770285659
H,0,-0.1867034372,0.6785320039,1.6555526272
C,0,-2.3049406549,0.0656552947,0.6122020769
C,0,-3.2520954623,-0.9539126664,0.3788474387
C,0,-4.5956719016,-0.8605308026,0.7654063996
C,0,-5.057726279,0.2762196737,1.4248207414
C,0,-4.1525227524,1.3070397825,1.681753632
C,0,-2.8170173648,1.2020942198,1.281698076
H,0,-2.954822514,-1.8725008702,-0.1209970439
H,0,-5.275117999,-1.6833424355,0.5506291006
H,0,-6.0971065296,0.3571909308,1.7320411678
H,0,-4.48503384,2.2063685649,2.1963715938
H,0,-2.1593296932,2.0412760666,1.4823926841

IrDMPE_Bpin2_n2BpinH_Ph_goodgsC

bpy Ir Bpin2 Ph HBpin eq in back with bottom Bpin split - gs alternati
B3LYP/gen
E(RB+HF-LYP) = -2019.76524937

Zero-point correction= 0.524029 (Hartree/Particle)
Thermal correction to Energy= 0.559180
Thermal correction to Enthalpy= 0.560124
Thermal correction to Gibbs Free Energy= 0.456708
Sum of electronic and ZPE= -2019.241220
Sum of electronic and thermal Energies= -2019.206069
Sum of electronic and thermal Enthalpies= -2019.205125
Sum of electronic and thermal Free Energies= -2019.308541

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 350.891	129.482	217.657

C,0,-4.5085209495,0.5984562211,-0.7243304511
C,0,-3.2012559851,0.6296480109,-0.2246578457
C,0,-2.223509312,-0.3221890556,-0.5817575985
C,0,-2.647496307,-1.2865601803,-1.5235440866

C,0,-3.9486257811,-1.3281495674,-2.0354202596
C,0,-4.8967691432,-0.3888314175,-1.6290528298
Ir,0,-0.1020143753,-0.2511605662,0.0441444351
B,0,-0.2755411531,1.7952799817,-0.326213911
O,0,-0.6908626553,2.7400208556,0.6244987775
C,0,-0.8674206802,4.0053652268,-0.0297902913
C,0,-0.2061831923,3.8175463653,-1.4100102687
O,0,-0.080987357,2.4005018847,-1.5572515772
P,0,-0.5779562199,0.0262224958,2.3383165355
C,0,-2.2937592455,0.4140686399,2.8988417457
P,0,-0.0652771697,-2.6817878967,0.6515663279
C,0,-1.0701241291,-3.9865110927,-0.1912994303
B,0,1.9147247177,0.2317284044,0.6604182226
O,0,2.4229380254,1.5259878746,0.6728863926
C,0,3.8016281614,1.5026532947,1.0517488901
C,0,4.0149637455,0.0914607899,1.6349649548
O,0,2.8585957994,-0.6480274909,1.2120096724
B,0,1.3243950285,-0.6920257931,-1.5339238898
O,0,2.2477203982,0.1665563103,-2.1156751461
C,0,3.007858877,-0.5659300966,-3.0813844479
C,0,2.7321906919,-2.0436197458,-2.74585903
O,0,1.5234448275,-2.007319147,-1.9763548903
C,0,-0.2196478577,-1.5798857209,3.2131264032
C,0,-0.7389217342,-2.7664552071,2.3926564785
C,0,0.390028253,1.2533269974,3.3134334016
C,0,1.5531196164,-3.5602534327,0.8259511055
H,0,4.0584026455,0.0956495956,2.7321497566
H,0,4.9206117262,-0.3960898349,1.2602601542
H,0,4.0000010501,2.2987111233,1.7769909288
H,0,4.420774359,1.6819402436,0.1641186974
H,0,3.534423585,-2.4842813158,-2.1392088295
H,0,2.5833081113,-2.6670203507,-3.6326782754
H,0,4.0657864195,-0.2977902395,-2.9991885828
H,0,2.6597458556,-0.299717058,-4.0874475764
H,0,-0.3995519108,4.7970786442,0.5644787928
H,0,-1.940795172,4.2198268791,-0.1120430105
H,0,0.7912247379,4.2730520518,-1.4530931323
H,0,-0.8094502244,4.2216680168,-2.2291029832
H,0,-0.0249372923,-0.309697713,-1.6232626274
H,0,-2.9360034466,1.4428526297,0.4431937472
H,0,-5.2205276405,1.3597473488,-0.4109282856
H,0,-1.9378136209,-2.0211465734,-1.8927578451
H,0,-4.2155857506,-2.0929437801,-2.762271742
H,0,-5.9096833815,-0.4156058818,-2.0222935492
H,0,-0.4696782452,-3.7201235955,2.8613438482
H,0,-1.8326660073,-2.7344669868,2.3216943644
H,0,0.8693855407,-1.6409810291,3.3175260771
H,0,-0.6511744962,-1.560836324,4.2205969997
H,0,0.0224732849,1.3009229003,4.343215481
H,0,1.4457946092,0.9776013137,3.320085887
H,0,0.2844319762,2.2245585898,2.8277348821
H,0,-2.3582514821,0.3005677749,3.985816684
H,0,-2.5305343739,1.4457470635,2.6327989784
H,0,-3.016878335,-0.2400634074,2.4099993575
H,0,1.4267434519,-4.5288289298,1.3214088918
H,0,1.9660926903,-3.7107947271,-0.1730747613
H,0,2.2472379902,-2.9297714317,1.3831172939
H,0,-0.9996118761,-4.9371628865,0.3476928654
H,0,-2.1146042344,-3.6755429927,-0.2508402395
H,0,-0.6920214385,-4.1258350597,-1.2074356363

IrDMPE_Bpin2_n2BpinH_Ph_goodgsD12

Ir Bpin2 Ph HBpin n2-equatorial good gs #4
B3LYP/gen
E(RB+HF-LYP) = -2019.76645866

Zero-point correction= 0.523481 (Hartree/Particle)
 Thermal correction to Energy= 0.558886
 Thermal correction to Enthalpy= 0.559830
 Thermal correction to Gibbs Free Energy= 0.455908
 Sum of electronic and ZPE= -2019.242978
 Sum of electronic and thermal Energies= -2019.207573
 Sum of electronic and thermal Enthalpies= -2019.206629
 Sum of electronic and thermal Free Energies= -2019.310550

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	350.706	129.851	218.721

C,0,-3.2063514808,0.6379839503,-0.2106440361
 C,0,-2.2214901851,-0.2741166439,-0.6595356643
 C,0,-2.7065574068,-1.2776513687,-1.5251371943
 C,0,-4.0496754895,-1.3810893155,-1.9098666684
 C,0,-4.9863364115,-0.4619724986,-1.4422114942
 C,0,-4.5496961224,0.5523096929,-0.5891397101
 Ir,0,-0.1029773035,0.0423630361,-0.0705850803
 P,0,0.2748398386,-2.2381027367,0.3510312864
 C,0,1.1334782303,-2.9929455427,-1.1324280721
 C,0,0.6925783531,-2.3673369496,-2.4644414776
 P,0,0.6686762214,-0.4946287558,-2.3577188111
 B,0,1.8372195462,0.3023687125,0.8484770215
 O,0,2.0260503725,0.4559263069,2.2177493198
 C,0,3.4099813754,0.6882687185,2.4920273561
 C,0,4.1302306674,0.2996295171,1.1853231709
 O,0,3.0813695658,0.2290035818,0.2071856733
 B,0,0.6676699701,2.0568850894,-0.3310501371
 O,0,1.0315753583,2.5453038205,-1.5924240773
 C,0,1.814875596,3.7302011034,-1.4061749865
 C,0,1.51914215,4.1501002512,0.0458699908
 O,0,1.017175736,2.9617302823,0.6643838792
 B,0,-0.8380114116,0.2970634064,1.8751832027
 O,0,-1.337166455,1.4905409205,2.3790152844
 C,0,-1.6746383722,1.3220400999,3.7588528358
 C,0,-1.6322585395,-0.2034439248,3.9868126474
 O,0,-0.9583106855,-0.7202956742,2.8311307007
 H,0,3.5527192082,1.7464787037,2.7437672777
 H,0,3.7247562202,0.0841462999,3.3493507929
 H,0,4.8771544008,1.0355702831,0.8709707412
 H,0,4.6238735314,-0.6786287802,1.2560367432
 H,0,2.8758946754,3.4904901736,-1.55632619
 H,0,1.5199400825,4.4843337855,-2.1421388488
 H,0,2.4080113168,4.4982377592,0.5812571192
 H,0,0.7526604534,4.9336907543,0.1005586728
 H,0,-1.0811230274,-0.4830973899,4.8908890794
 H,0,-2.6365046989,-0.6421632309,4.0432300446
 H,0,-0.938973995,1.8527895795,4.3757535255
 H,0,-2.6630713566,1.752015543,3.9515585298
 H,0,-0.6586457103,1.5991337863,-0.319585965
 H,0,-2.9210450043,1.4409090395,0.4621864019
 H,0,-5.2577353706,1.2874669348,-0.2116369015
 H,0,-2.0267328927,-2.0204504959,-1.9344142916
 H,0,-4.3565838042,-2.182424576,-2.5795093019
 H,0,-6.0301417804,-0.5322999627,-1.7366509689
 C,0,1.3960731148,-2.7273014227,1.7306539534
 C,0,-1.1748626026,-3.3164748151,0.7129254309
 C,0,2.3737464966,-0.0642114973,-2.9315407866
 C,0,-0.3350040445,0.001220099,-3.8266127461
 H,0,1.3548276429,-2.6869067928,-3.2775234098
 H,0,-0.3162917838,-2.6994007286,-2.7272528656
 H,0,2.2024398125,-2.8090107853,-0.9748083947
 H,0,0.9890980926,-4.0796311762,-1.1323508893
 H,0,1.4429858582,-3.8178906922,1.8120767921
 H,0,2.4001551002,-2.3352684166,1.5598392518
 H,0,1.0003455379,-2.2974216859,2.6520856194

H,0,-0.8642739254,-4.363041237,0.7951556101
H,0,-1.5861144192,-2.9751337184,1.6656486662
H,0,-1.9460126216,-3.2096959973,-0.0486971449
H,0,2.583828373,-0.5131873497,-3.9082685269
H,0,2.444237746,1.0224748854,-3.0030449096
H,0,3.1044542969,-0.3989675692,-2.1940683932
H,0,0.0240330111,-0.4767079896,-4.7442610774
H,0,-1.3828720273,-0.254443418,-3.6587727912
H,0,-0.2581351084,1.0865364037,-3.9334619163

bpybeg3veratroleOrthoTSBtoprod

temp bpybeg3veratroleOrthoTSBtoprod
B3LYP/gen
E(RB+HF-LYP) = -1823.15954079

Zero-point correction= 0.536465 (Hartree/Particle)
Thermal correction to Energy= 0.573591
Thermal correction to Enthalpy= 0.574536
Thermal correction to Gibbs Free Energy= 0.464428
Sum of electronic and ZPE= -1822.623075
Sum of electronic and thermal Energies= -1822.585949
Sum of electronic and thermal Enthalpies= -1822.585005
Sum of electronic and thermal Free Energies= -1822.695113

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 359.934	137.262	231.741

C,0,4.1741485574,0.4078844297,-2.1701603821
C,0,4.028200511,-0.2380555941,-0.9426811526
C,0,2.7358024286,-0.4935745743,-0.4216334781
C,0,1.5736085458,-0.0461464171,-1.0652664373
C,0,1.765824513,0.6062423947,-2.3057346027
C,0,3.0269671891,0.8186245311,-2.8541882476
Ir,0,-0.460234895,-0.1416342702,-0.279887049
N,0,-0.4011907753,2.1567006932,-0.4414229917
C,0,0.2477690851,2.7687943647,0.5726843383
C,0,0.5248618503,4.1418553326,0.5303158515
C,0,0.1074248835,4.8895446591,-0.5653340169
C,0,-0.5870318377,4.2518927526,-1.590825786
C,0,-0.8174733828,2.8822198277,-1.4887508444
C,0,0.6139918182,1.9097662972,1.7223347267
N,0,0.3459684393,0.5838356586,1.6061526623
C,0,0.6063922736,-0.2375141582,2.6395496133
C,0,1.1494132824,0.221722281,3.8342892357
C,0,1.4447910132,1.5758013867,3.9643204782
C,0,1.1712420378,2.4253178846,2.8989655738
B,0,-2.296260809,-0.0514142683,0.8676851622
O,0,-3.1692042662,1.0374332716,0.8855348229
C,0,-4.0720743193,0.8983934446,1.9916084719
C,0,-3.8308224004,-0.5354731587,2.5089442846
O,0,-2.6176610296,-0.9505447338,1.8710433076
B,0,-2.2236955008,-0.4195653971,-1.372219524
O,0,-3.0687401405,-1.5286510131,-1.3834638831
C,0,-4.0432492267,-1.346271151,-2.4154437123
C,0,-3.9906862347,0.1613914274,-2.7181538919
O,0,-2.6919630261,0.5563695345,-2.2659598475
B,0,-0.3187575482,-2.1709724519,-0.0130293123
O,0,-0.2397873415,-2.8307976947,1.2180017095
C,0,-0.1368986216,-4.241199644,1.002318926
C,0,-0.3736153863,-4.4191860353,-0.5142340538
O,0,-0.2877865555,-3.0990768231,-1.0521670992
H,0,-0.7051553215,-0.6559988495,-1.7815936151
H,0,-1.3661863765,2.333346871,-2.2450423746
H,0,1.0656717362,4.6232673591,1.3356093881
H,0,-0.9425112403,4.7962151742,-2.4591225902

H,0,0.3194385051,5.9533351301,-0.6129207454
H,0,1.3778856484,3.4843255183,2.986730891
H,0,1.8749063499,1.9689928794,4.8804223619
H,0,1.3389571706,-0.4810618477,4.6380263972
H,0,0.3627615523,-1.2800094899,2.4789703237
H,0,-4.753532765,0.7180238412,-2.1579073863
H,0,-4.0975856053,0.3923224312,-3.7826835959
H,0,-5.0233346497,-1.6804185951,-2.0610101963
H,0,-3.7632802808,-1.9504235547,-3.2884699856
O,0,2.6421864466,-1.1514277799,0.7989038157
O,0,5.0861539491,-0.6523250379,-0.1657516234
H,0,5.1553914083,0.594250802,-2.5904966031
H,0,0.8990568773,0.9504090381,-2.8645672101
H,0,3.1281973354,1.3115518188,-3.8184350994
H,0,-3.8351337681,1.6595967824,2.7457431568
H,0,-5.0993500554,1.0638393999,1.6505828289
H,0,-3.7099008813,-0.5824824574,3.5961572816
H,0,-4.6380068224,-1.2211697187,2.2227659586
H,0,0.8588160806,-4.5852260072,1.3100045419
H,0,-0.884079176,-4.7593656948,1.6126045965
H,0,0.376159161,-5.0621025655,-0.9882485425
H,0,-1.3669684787,-4.8329073602,-0.7290705573
C,0,3.0469831528,-2.5180928967,0.7886266899
H,0,2.748825684,-2.9351294424,1.7540538519
H,0,2.5388534778,-3.0689697269,-0.0125888105
H,0,4.1300891551,-2.6162030967,0.6673183472
C,0,6.3939867968,-0.4135788043,-0.6477341581
H,0,7.0742674206,-0.8042242842,0.1120378902
H,0,6.5825892189,-0.9306027432,-1.5986328254
H,0,6.5884477282,0.658674053,-0.7862584083

dmpeBpin3BisMetaCF3CHacttoprod

tempdmpeBpin3BisMetaCF3CHacttoprod
B3LYP/gen
E(RB+HF-LYP) = -2693.84170491

Zero-point correction= 0.533738 (Hartree/Particle)
Thermal correction to Energy= 0.576324
Thermal correction to Enthalpy= 0.577269
Thermal correction to Gibbs Free Energy= 0.455152
Sum of electronic and ZPE= -2693.307967
Sum of electronic and thermal Energies= -2693.265381
Sum of electronic and thermal Enthalpies= -2693.264436
Sum of electronic and thermal Free Energies= -2693.386553

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 361.649	154.914	257.015

C,0,2.2493612801,-1.1191747453,-0.1827443599
C,0,1.4201682385,-0.0238172385,0.1142288236
C,0,2.1131449651,1.1270016151,0.5509784412
C,0,3.5076555352,1.1799551046,0.6520341065
C,0,4.2977621383,0.0752488863,0.3353204234
C,0,3.6463742258,-1.0812123783,-0.081327373
Ir,0,-0.7926124822,-0.0336689762,0.0372859786
P,0,-0.8280076197,-0.9554406141,-2.1305568172
C,0,-1.2534057502,-2.7694692071,-1.9764772442
C,0,-0.6280020708,-3.4288822782,-0.7379687354
P,0,-0.9088508915,-2.3894406439,0.7975425525
B,0,-2.932994221,0.1021876058,-0.2384263014
O,0,-3.7231494632,-0.9919830493,-0.6343834632
C,0,-5.0708625576,-0.5611462638,-0.8792234779
C,0,-5.1043445932,0.901099265,-0.3893522179
O,0,-3.7331594054,1.2361248229,-0.1464449765
B,0,-1.7778869657,0.7482612896,1.8473267777

O,0,-2.3974807625,-0.1143963984,2.7565158155
C,0,-3.0336766026,0.69206325,3.7623079659
C,0,-3.0437643963,2.1079183599,3.1544115851
O,0,-2.0209144508,2.068677432,2.1578386232
B,0,-0.6332458984,1.8988460952,-0.7680192554
O,0,-0.285986539,3.028416652,-0.0425013179
C,0,-0.0226946678,4.1149193877,-0.9369452742
C,0,-0.5842650508,3.6390550968,-2.2904795805
O,0,-0.747249138,2.2208019568,-2.1280853527
H,0,-5.2875362857,-0.6459639778,-1.9518095663
H,0,-5.7661483569,-1.2106273038,-0.3381004056
H,0,-5.5224262653,1.5895183811,-1.1303436729
H,0,-5.6723511939,1.0138438799,0.5421131209
H,0,-4.0354146875,0.301661358,3.966138629
H,0,-2.4440992278,0.6413167144,4.6863068041
H,0,-4.0017554641,2.3409068642,2.6724725702
H,0,-2.8165879836,2.8916764215,3.8827732925
H,0,-1.5599021359,4.0881396925,-2.5144724671
H,0,0.0909116545,3.8374295208,-3.1289353629
H,0,-0.5111111564,5.0216056342,-0.5672799556
H,0,1.05989241,4.2912543783,-0.9724914216
H,0,-0.4373687565,0.5523040901,1.5658618258
H,0,1.8161765273,-2.057578989,-0.511509666
C,0,4.4090982779,-2.3190631098,-0.4477996231
H,0,1.5505404894,2.0189272306,0.8048453378
C,0,4.1362737703,2.4631178953,1.119307263
H,0,5.3768085819,0.1157952373,0.4104168877
C,0,-2.0572958453,-0.3680966645,-3.3702893322
C,0,0.7123211163,-0.8862923171,-3.1431976369
C,0,-2.4832414448,-3.0836184598,1.4688653166
C,0,0.3151172897,-3.0759450512,2.0031602728
H,0,-1.0403416904,-4.4335177401,-0.588216096
H,0,0.4524646372,-3.5490810078,-0.8701986815
H,0,-2.3449195202,-2.7916245937,-1.8987006487
H,0,-0.9692922672,-3.2961813779,-2.8949786917
H,0,0.5483925381,-1.3877502015,-4.1022231084
H,0,0.9450295319,0.1663804109,-3.3216373069
H,0,1.5593799164,-1.3436412539,-2.633839529
H,0,-1.9409844103,-0.9209691341,-4.3076988494
H,0,-3.0652207769,-0.5175514771,-2.9840232609
H,0,-1.884137745,0.696030855,-3.5362715793
H,0,0.202926327,-4.1600506558,2.1082722474
H,0,1.3356449088,-2.8468512501,1.6916394869
H,0,0.1396845928,-2.6076094089,2.9759315044
H,0,-2.3858253144,-4.1546787462,1.6742583615
H,0,-2.7265209478,-2.5449103089,2.3865080717
H,0,-3.2834326926,-2.9062506824,0.7491067307
F,0,5.4871544128,2.4314050365,1.0603564598
F,0,3.7315430397,3.5201761219,0.3705938226
F,0,3.8017434424,2.7527259014,2.3989812057
F,0,5.7404920703,-2.1909952759,-0.2781520869
F,0,4.0113464247,-3.3891497874,0.2904298836
F,0,4.2021093526,-2.6672948756,-1.7461044917

methiophenebpyIrBeg3toprod

tempmethiophenebpyIrBeg3toprod
B3LYP/gen
E(RB+HF-LYP) = -1954.20206887

Zero-point correction= 0.465752 (Hartree/Particle)
Thermal correction to Energy= 0.499194
Thermal correction to Enthalpy= 0.500138
Thermal correction to Gibbs Free Energy= 0.397527
Sum of electronic and ZPE= -1953.736317
Sum of electronic and thermal Energies= -1953.702875
Sum of electronic and thermal Enthalpies= -1953.701931

Sum of electronic and thermal Free Energies= -1953.804542

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	313.249	122.934	215.963

C,0,-3.3511052279,2.188268514,-2.0279971362
C,0,-4.1532840585,1.6082799423,-1.0848936518
S,0,-3.1618555284,0.6629634248,0.0072292471
C,0,-1.6480428215,1.0477084291,-0.8217942721
C,0,-1.9604884135,1.8783181586,-1.8772244754
Ir,0,0.2557691387,0.2459357403,-0.2441797698
N,0,-0.4868251856,-1.8161259524,-0.937221584
C,0,-1.1880551809,-2.5086710444,-0.0147018615
C,0,-1.8078125403,-3.7236386297,-0.3372565907
C,0,-1.6966877638,-4.2235959811,-1.6298458908
C,0,-0.9672013115,-3.5011308286,-2.5716768222
C,0,-0.3787101489,-2.3009108547,-2.181949719
C,0,-1.2674074126,-1.900993264,1.3337057686
N,0,-0.7212164346,-0.6655396816,1.4869715356
C,0,-0.7822051744,-0.0588362701,2.688623785
C,0,-1.3813431627,-0.654551088,3.7928692349
C,0,-1.9343322818,-1.9251291405,3.6552549488
C,0,-1.8745304364,-2.5499515731,2.4156619163
B,0,1.9722229883,-0.5664750736,0.7925408657
O,0,2.4466428256,-1.8702273434,0.6614330509
C,0,3.3287226936,-2.1586252665,1.7563445579
C,0,3.5592909049,-0.7923550116,2.4369697883
O,0,2.5459892263,0.0585237726,1.8877117194
B,0,2.0588855935,0.1656734451,-1.3123072316
O,0,3.2087203876,0.9321718086,-1.1401347965
C,0,4.0961255145,0.672144914,-2.2320943598
C,0,3.5714776095,-0.6417638692,-2.8383812485
O,0,2.2102937527,-0.7039309875,-2.4015061968
B,0,0.6452839212,2.1336408322,0.4558749075
O,0,0.3916488293,2.5706667066,1.7607334808
C,0,0.5784290866,3.9902740897,1.8218803773
C,0,1.3220349458,4.3292614026,0.5147180881
O,0,1.1188956404,3.1861107872,-0.318686627
H,0,0.6865566036,0.9694263875,-1.608477349
H,0,0.2179921869,-1.7072971729,-2.8631912074
H,0,-2.3822231203,-4.2681911133,0.4017604184
H,0,-0.8537057637,-3.8519871942,-3.5917029835
H,0,-2.1759496167,-5.1608155896,-1.8956504979
H,0,-2.2958263329,-3.5391330468,2.2904495631
H,0,-2.4059355267,-2.4238015749,4.4964806711
H,0,-1.4071947296,-0.121589728,4.7368559766
H,0,-0.3398977863,0.9296172625,2.7347264697
H,0,4.1142761999,-1.5156671189,-2.4547811098
H,0,3.6097408076,-0.6579328889,-3.9321580046
H,0,5.123345725,0.5959287025,-1.862264646
H,0,4.0438440978,1.5048615596,-2.9456106374
C,0,-5.6403841472,1.7166260326,-0.9235259929
H,0,-3.7417545005,2.8279827894,-2.8150488649
H,0,-1.1993396805,2.274491147,-2.5420656867
H,0,2.8444480797,-2.8814172381,2.4251162645
H,0,4.2509682889,-2.6092157455,1.3757424698
H,0,3.4542468332,-0.8343618941,3.5258328951
H,0,4.5448492018,-0.3725668581,2.2008747392
H,0,-0.4022449835,4.4796332972,1.8780117459
H,0,1.1495539628,4.2485556951,2.7195240818
H,0,0.9266279777,5.2226974901,0.0207774709
H,0,2.3983179062,4.4702388555,0.6786979148
H,0,-5.9226825598,2.15199871,0.0433201797
H,0,-6.0529768253,2.3585628812,-1.7082811525
H,0,-6.1397121823,0.742089084,-0.9960804851

dmpeBcat3BisCF3toprod

tempdmpeBcat3BisCF3toprod
B3LYP/gen
E(RB+HF-LYP) = -3151.15044882

Zero-point correction= 0.603162 (Hartree/Particle)
Thermal correction to Energy= 0.651525
Thermal correction to Enthalpy= 0.652470
Thermal correction to Gibbs Free Energy= 0.516521
Sum of electronic and ZPE= -3150.547287
Sum of electronic and thermal Energies= -3150.498923
Sum of electronic and thermal Enthalpies= -3150.497979
Sum of electronic and thermal Free Energies= -3150.633928

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 408.838	184.364	286.128

C,0,3.0379932897,-0.9948259295,-0.5161307105
C,0,2.0692451134,-0.130292567,0.0168353094
C,0,2.5943526705,0.9653278372,0.7392470386
C,0,3.9677492536,1.1697611092,0.907198022
C,0,4.9004023586,0.2907789795,0.355019908
C,0,4.4160945586,-0.7975008185,-0.3615746175
Ir,0,-0.1092356915,-0.4375020483,-0.1069037581
P,0,-0.0419413006,-0.9706745815,-2.4099416827
C,0,-0.1716093516,-2.8265620486,-2.583789654
C,0,0.5715268388,-3.5855739596,-1.4740862398
P,0,0.1597639013,-2.8955663077,0.2214432865
B,0,-2.2319586713,-0.4903185173,-0.4450138707
O,0,-3.0202505196,-1.6550144212,-0.6354068903
C,0,-4.2821783609,-1.2329475171,-0.9989830014
O,0,-3.0460688308,0.6280634335,-0.7063284385
B,0,-1.2572513289,-0.2593299314,1.7251051474
O,0,-1.47964117,-1.3453362323,2.6061990822
C,0,-2.3810033964,-0.8981188942,3.5471045571
O,0,-1.9967566154,0.8487692738,2.1689812471
B,0,-0.2237247934,1.5980743502,-0.5519026206
O,0,-0.1826438433,2.6429204967,0.389600145
C,0,-0.2263883042,3.822830203,-0.3144836455
O,0,-0.2752073736,2.1700138316,-1.8484151286
H,0,0.0924615571,0.0066214748,1.501305244
H,0,2.7349186628,-1.8699810611,-1.0788563487
C,0,5.3412197907,-1.8104569628,-0.9683390109
H,0,1.9193184673,1.6854585594,1.1887460702
C,0,4.4393291262,2.3943962623,1.6442296815
H,0,5.9635772316,0.4477770979,0.4857462766
C,0,-1.3990726709,-0.3760910488,-3.5050014844
C,0,1.4310278341,-0.4604640267,-3.3936521129
C,0,-1.2606660349,-3.9546664011,0.7423564962
C,0,1.5116284761,-3.5615111549,1.290061226
H,0,0.3234346185,-4.6523791079,-1.5079315213
H,0,1.6545751976,-3.5115109581,-1.6162229904
H,0,-1.2433212601,-3.0485855499,-2.5329878587
H,0,0.1788485345,-3.1281254453,-3.5775376686
H,0,1.2986663559,-0.759017472,-4.4381434205
H,0,1.5047382628,0.6279731011,-3.3331952179
H,0,2.353966913,-0.8906874052,-3.0076113028
H,0,-1.2241111748,-0.7179985589,-4.5296872412
H,0,-2.3648331927,-0.7538752352,-3.1655519726
H,0,-1.4134047454,0.7143324857,-3.4763124476
H,0,1.5757849195,-4.6514516861,1.210239837
H,0,2.4713433111,-3.1209817679,1.0150681581
H,0,1.2944567766,-3.2943991387,2.3279988582
H,0,-0.9905547422,-5.0143568311,0.6909521077
H,0,-1.5316856016,-3.6911161186,1.7658829373
H,0,-2.1209729896,-3.751091733,0.1041943161

C,0,-2.9345444916,-1.5810536668,4.6161769532
C,0,-3.8313377128,-0.8634182649,5.422746491
C,0,-4.1445018889,0.4734420919,5.1530402842
C,0,-3.576153835,1.1538370746,4.0655233919
C,0,-2.6926281651,0.4356274573,3.2778218753
H,0,-2.6828881997,-2.6165773803,4.819023885
H,0,-4.2893448485,-1.3580618875,6.2737087314
H,0,-4.8420522191,0.9980983497,5.7986001396
H,0,-3.8097433797,2.1899109534,3.8468482029
C,0,-5.406304941,-1.9865772331,-1.2931326994
C,0,-6.5657516373,-1.2756952053,-1.6381454291
C,0,-6.5769988472,0.1235426529,-1.6799185845
C,0,-5.4311491365,0.8745472557,-1.3789492174
C,0,-4.2927714483,0.1612745319,-1.0405993107
H,0,-5.3888608592,-3.0706551537,-1.2536615166
H,0,-7.4720891556,-1.8241908044,-1.8754720569
H,0,-7.4926021429,0.6408966854,-1.9495648979
H,0,-5.4289622396,1.9587815551,-1.4052304193
C,0,-0.2184251146,5.1224768226,0.1618335301
C,0,-0.2706367096,6.1459386372,-0.7971362207
C,0,-0.327749956,5.8604665843,-2.1652968972
C,0,-0.3346700166,4.5374651902,-2.6350853843
C,0,-0.2827934186,3.5382984807,-1.6787479293
H,0,-0.1726212078,5.3317011847,1.2250648911
H,0,-0.2653549779,7.1804739584,-0.4675798243
H,0,-0.3667325373,6.6765022793,-2.8804767526
H,0,-0.3779171844,4.306253378,-3.6943224348
F,0,6.6402855268,-1.4717502576,-0.8594936616
F,0,5.1940632978,-3.0316447978,-0.3894646721
F,0,5.0797498472,-1.9922892415,-2.290241647
F,0,5.7079819424,2.2604044081,2.0957734194
F,0,4.4193947208,3.4922127132,0.8511599709
F,0,3.6592608795,2.6730725904,2.7124826942

methiophenedmpelrBcat3toprod

tempmethiophenedmpeIrBcat3toprod
B3LYP/gen
E(RB+HF-LYP) = -2837.15936253

Zero-point correction= 0.587418 (Hartree/Particle)
Thermal correction to Energy= 0.629963
Thermal correction to Enthalpy= 0.630907
Thermal correction to Gibbs Free Energy= 0.510480
Sum of electronic and ZPE= -2836.571944
Sum of electronic and thermal Energies= -2836.529400
Sum of electronic and thermal Enthalpies= -2836.528455
Sum of electronic and thermal Free Energies= -2836.648882

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 395.308	163.163	253.459

C,0,3.5327301352,-1.8656701728,-0.2590226723
C,0,2.6040068454,-0.9981161557,0.279589821
S,0,3.3783970439,-0.2130271389,1.655652137
C,0,4.8963623569,-1.0624147586,1.4691060536
C,0,4.8080397508,-1.9045116612,0.3963389949
Ir,0,0.5054711625,-0.5392458779,-0.150528976
P,0,0.9644316066,-0.320801737,-2.4575999096
C,0,0.5088560641,-1.9255631438,-3.2988635885
C,0,0.8122437292,-3.1565035588,-2.4319785585
P,0,0.1227835627,-2.9359575173,-0.7044163825
B,0,-1.4305199231,0.17764783,-0.7249719266
O,0,-2.4482066394,-0.5738141462,-1.3687288558
C,0,-3.4506642391,0.3101263565,-1.7067455096
O,0,-1.8466903203,1.5238302263,-0.6918913151

B,0,-0.9309633526,-0.6818992631,1.4613203317
O,0,-1.5259176265,-1.9136932269,1.8367505012
C,0,-2.5258596089,-1.6003708391,2.730107864
O,0,-1.5536948467,0.3595799369,2.1704170525
B,0,0.9724864922,1.4727343652,0.1601448174
O,0,0.925984253,2.1542909297,1.3879592796
C,0,1.3421149867,3.4402615016,1.1504944538
O,0,1.4326317211,2.3755366149,-0.8351697083
H,0,0.4575770658,-0.6773932827,1.5285052715
H,0,3.3307641748,-2.4900026784,-1.1240132723
C,0,6.057669648,-0.8377387159,2.3915597529
H,0,5.628143331,-2.5417769604,0.0768971897
C,0,0.0242061159,0.9248936032,-3.4360182545
C,0,2.6902234936,0.0576760658,-2.9660856709
C,0,-1.5818263319,-3.6268520691,-0.8839192287
C,0,0.9572255035,-4.2512689716,0.2820751884
H,0,0.3930022904,-4.0608937132,-2.8874674794
H,0,1.8921426235,-3.3109282784,-2.3482740805
H,0,-0.5685275264,-1.8607528666,-3.4882341168
H,0,1.008283062,-1.9876024211,-4.2725582509
H,0,2.7732706222,0.047170368,-4.0573654232
H,0,2.9281969924,1.0536332365,-2.5863976366
H,0,3.3893833915,-0.6492813967,-2.5221309229
H,0,0.3691079325,0.9240532947,-4.4746019272
H,0,-1.0448813256,0.7052180325,-3.4167734963
H,0,0.1942228769,1.9069170145,-2.9918317813
H,0,0.890625296,-5.2270821758,-0.2098101795
H,0,2.0024675587,-3.9789652933,0.4384242708
H,0,0.4656015863,-4.3091345061,1.2570975194
H,0,-1.5475289698,-4.650102705,-1.2723601507
H,0,-2.0630560786,-3.6203736253,0.0954908295
H,0,-2.1679913479,-2.9895676047,-1.5475267983
C,0,-3.4157322878,-2.4437411659,3.3726176435
C,0,-4.3403265825,-1.8399399575,4.2391967245
C,0,-4.3550888221,-0.4551983877,4.4385326733
C,0,-3.4466679232,0.3885957085,3.7814113464
C,0,-2.5396287865,-0.2186051857,2.9296966395
H,0,-3.3948172798,-3.5167426603,3.2140068424
H,0,-5.0573256803,-2.4630026062,4.7649571609
H,0,-5.0841944673,-0.021708386,5.1161828758
H,0,-3.4472936843,1.4631094287,3.927425579
C,0,-4.6522932097,0.0665063473,-2.3509806424
C,0,-5.4844223759,1.1751482701,-2.5690109648
C,0,-5.1115536566,2.4585518299,-2.1530887728
C,0,-3.8914670294,2.6912402606,-1.5008299745
C,0,-3.0787267448,1.5891023057,-1.2917530206
H,0,-4.9342375001,-0.9327705573,-2.6657968892
H,0,-6.4371646185,1.0317556041,-3.0695070213
H,0,-5.7806609575,3.2935572525,-2.3371613205
H,0,-3.5930753941,3.6807336582,-1.1718698873
C,0,1.4668104381,4.4942576428,2.0394767741
C,0,1.9198722904,5.7145696604,1.5140727749
C,0,2.2292371156,5.8536724579,0.1570805309
C,0,2.0989151042,4.7768230308,-0.7345391095
C,0,1.6513167978,3.5798089237,-0.2032249835
H,0,1.2241395036,4.3743764275,3.0897832392
H,0,2.0322120917,6.5672500739,2.1770582528
H,0,2.5777747172,6.8118029301,-0.2166665671
H,0,2.3377146039,4.8741362044,-1.7885817013
H,0,6.8985787424,-1.472451354,2.095422272
H,0,6.402425485,0.2031050489,2.373703407
H,0,5.808823972,-1.0776427205,3.4323048618

bypbpin3methylenedioxyOrthotoprod

tempbypbpin3methylenedioxyOrthotoprod
B3LYP/gen

E(RB+HF-LYP) = -1782.65107661

Zero-point correction= 0.487409 (Hartree/Particle)
Thermal correction to Energy= 0.521295
Thermal correction to Enthalpy= 0.522239
Thermal correction to Gibbs Free Energy= 0.419462
Sum of electronic and ZPE= -1782.163668
Sum of electronic and thermal Energies= -1782.129782
Sum of electronic and thermal Enthalpies= -1782.128837
Sum of electronic and thermal Free Energies= -1782.231615

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	327.118	126.983	216.313

C,0,4.2473697763,0.5664221219,-2.33000612
C,0,4.0941598379,-0.0298011374,-1.0943285876
C,0,2.8372248873,-0.2850765527,-0.5457738854
C,0,1.6306523408,0.0379143204,-1.1481625691
C,0,1.8061461237,0.6326869915,-2.426905406
C,0,3.0547120267,0.8909905146,-2.9990748272
Ir,0,-0.3416653506,-0.2214445996,-0.2809859026
N,0,-0.6207122556,2.0118321329,-0.7435470612
C,0,0.067353505,2.8319243998,0.0812801751
C,0,0.1916221908,4.1991913984,-0.1976510599
C,0,-0.4224879608,4.7233477753,-1.3301237989
C,0,-1.1605088693,3.873963635,-2.151621767
C,0,-1.2315353211,2.5224236457,-1.8221894123
C,0,0.6401802425,2.2005882674,1.2931070916
N,0,0.4756417364,0.8572890052,1.4194271415
C,0,0.9023803963,0.2380215451,2.5346844112
C,0,1.5382924042,0.9228822524,3.5654887928
C,0,1.7476301119,2.2926793193,3.4363316345
C,0,1.2863813571,2.9360522516,2.2930111093
B,0,-2.1317716642,-0.2566548236,0.9418317315
O,0,-3.2558161015,0.5550116747,0.7769570516
C,0,-4.1803254898,0.2974954368,1.8430274513
C,0,-3.3761675816,-0.5428115305,2.8570947087
O,0,-2.1988169628,-0.9410541156,2.1445769312
B,0,-2.0607742267,-0.937578613,-1.2402526063
O,0,-2.6903702312,-2.1669734619,-1.0601033276
C,0,-3.7258957956,-2.2926167257,-2.0408899296
C,0,-3.9518121938,-0.8524214619,-2.5343406699
O,0,-2.7241300722,-0.1862624227,-2.2215356349
B,0,0.1608390644,-2.1439807463,0.2365180791
O,0,0.3653522815,-2.6061578758,1.5399955169
C,0,0.9208236266,-3.9233864324,1.4792857298
C,0,0.6488969537,-4.3792302328,0.0332106562
O,0,0.4036038713,-3.1644178948,-0.6790317949
H,0,-0.5506984161,-0.9515952335,-1.696925879
H,0,-1.7963251773,1.8111699367,-2.4146024162
H,0,0.7655997433,4.8483078571,0.4520208171
H,0,-1.6686752692,4.2416750629,-3.0365493428
H,0,-0.3277002706,5.7796664688,-1.5623972986
H,0,1.4235516636,4.004242368,2.1830281325
H,0,2.2554606556,2.8566195401,4.2127950241
H,0,1.8694415166,0.3773538986,4.4422587329
H,0,0.7293992707,-0.8309418134,2.5679131275
H,0,-4.7753098471,-0.3613989512,-1.9995869827
H,0,-4.1425782317,-0.7895928884,-3.6102071136
H,0,-4.6159418593,-2.7357740118,-1.5835486735
H,0,-3.3817003039,-2.9539375407,-2.8468086131
O,0,3.0280394231,-0.859923644,0.7169760014
O,0,5.0880007123,-0.4225151431,-0.2163527774
H,0,5.2271137564,0.7633880393,-2.7508995465
H,0,0.923082634,0.8991570932,-3.002510561
H,0,3.1073304009,1.3442611086,-3.9857329724
H,0,-4.5373311002,1.2459288075,2.257207405

H,0,-5.0437040868,-0.2495645579,1.4437211689
H,0,-3.083668397,0.0394006368,3.7402412156
H,0,-3.916307806,-1.4323850874,3.1965554481
H,0,1.9961714251,-3.8715275122,1.6975609804
H,0,0.4427407578,-4.5611120732,2.2298323727
H,0,1.4966393664,-4.9077641538,-0.4149051999
H,0,-0.2368472962,-5.0246112609,-0.0333602889
C,0,4.4047638819,-1.2098335028,0.7591379416
H,0,4.5255843368,-2.279432745,0.5149377363
H,0,4.8110338593,-0.9924707595,1.7513217097

bybpin3methylenedioxyMetatoprod

tempbybpin3methylenedioxyMetatoprod
B3LYP/gen
E(RB+HF-LYP) = -1782.64712051

Zero-point correction= 0.486766 (Hartree/Particle)
Thermal correction to Energy= 0.520989
Thermal correction to Enthalpy= 0.521933
Thermal correction to Gibbs Free Energy= 0.417244
Sum of electronic and ZPE= -1782.160354
Sum of electronic and thermal Energies= -1782.126131
Sum of electronic and thermal Enthalpies= -1782.125187
Sum of electronic and thermal Free Energies= -1782.229877

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	326.926	127.399	220.338

C,0,4.4570065275,-0.1747267573,-1.2844552875
C,0,4.0169229638,-0.5200109056,-0.0132422315
C,0,2.6750348609,-0.5674095011,0.3195550878
C,0,1.7130366735,-0.2489269871,-0.6730783926
C,0,2.1920640244,0.0886375015,-1.9541277641
C,0,3.5615747479,0.1362246778,-2.2871177209
Ir,0,-0.4183485264,-0.2432447664,-0.268334475
N,0,-0.3976247,1.9578160443,-0.9088476716
C,0,0.080527976,2.8104156045,0.0239948225
C,0,0.3356675198,4.1534403389,-0.283801239
C,0,0.07767721,4.6211633177,-1.5676112307
C,0,-0.4385838949,3.7386941201,-2.5139158062
C,0,-0.6595923248,2.4149887165,-2.1420075048
C,0,0.2961979356,2.2408587082,1.3732195904
N,0,0.093647585,0.9042198191,1.5161173157
C,0,0.2441256246,0.3411916895,2.7309824093
C,0,0.611355919,1.0755618624,3.8536703138
C,0,0.8275375476,2.4446517474,3.721670202
C,0,0.6640012823,3.0283210245,2.4711410484
B,0,-2.3849776782,-0.1037834678,0.6324148249
O,0,-3.2995503979,0.9286740616,0.4347029681
C,0,-4.2953002174,0.8759375295,1.4670059603
C,0,-4.0459481754,-0.47210858,2.1767095427
O,0,-2.7573893159,-0.8911202471,1.7111156546
B,0,-2.0529397194,-0.812588868,-1.4524271926
O,0,-2.8482643255,-1.9515880033,-1.3585688479
C,0,-3.676787699,-2.0260595096,-2.5226111124
C,0,-3.6361582623,-0.6020549804,-3.1051992367
O,0,-2.4357298383,-0.0426336695,-2.562771157
B,0,-0.1552257237,-2.1623951257,0.4014132049
O,0,0.1555646743,-2.5032712896,1.7245842346
C,0,0.4670934104,-3.90079461,1.7894433741
C,0,-0.0053785092,-4.4569695618,0.4307507188
O,0,-0.162412585,-3.3017839152,-0.3946429985
H,0,-0.4374794675,-1.041052984,-1.6573138993
H,0,-1.0778354144,1.6873054381,-2.8269945113
H,0,0.7403134998,4.8263863066,0.4619499763

H,0,-0.6647222481,4.0600800584,-3.5249203953
H,0,0.2757911985,5.658036767,-1.8211507895
H,0,0.8145366422,4.0935999002,2.3510959911
H,0,1.1150087194,3.0509252407,4.5751004401
H,0,0.7235255605,0.5708665657,4.8069377779
H,0,0.0734377159,-0.7279939554,2.7740431345
H,0,-4.4954276479,-0.0009907798,-2.7795407899
H,0,-3.5910091727,-0.5846881141,-4.1987384818
H,0,-4.6839882519,-2.3467449283,-2.2387920447
H,0,-3.2580023521,-2.7663837539,-3.2167227085
O,0,5.1130999104,-0.7559688789,0.8019973096
O,0,5.8419283343,-0.1747538273,-1.3159790685
H,0,2.3828665184,-0.8627605014,1.3226275749
H,0,1.4811794178,0.315416309,-2.7447031019
H,0,3.898061701,0.4012405207,-3.2846021913
H,0,-4.1591461174,1.7323923154,2.1394063596
H,0,-5.2919564232,0.9470647123,1.0196542468
H,0,-4.0324759296,-0.383847238,3.2679091349
H,0,-4.7893225203,-1.2302065686,1.9010357971
H,0,1.5485594039,-4.0218999739,1.933377365
H,0,-0.0499887485,-4.3544391899,2.6412720532
H,0,0.7193568422,-5.1406710938,-0.0232095769
H,0,-0.9685540909,-4.9771738163,0.5128697839
C,0,6.2298035117,-0.7921228618,-0.088099064
H,0,6.5157445721,-1.8404631249,-0.2766857629
H,0,7.0652902469,-0.2381825624,0.3506960373

bpyBcat3methiophenetoprod

Ir Bcat3 bpy methylthiophene for C-H at 2 position opt to product
B3LYP/gen
E(RB+HF-LYP) = -2411.51199178

Zero-point correction= 0.535017 (Hartree/Particle)
Thermal correction to Energy= 0.574342
Thermal correction to Enthalpy= 0.575286
Thermal correction to Gibbs Free Energy= 0.457858
Sum of electronic and ZPE= -2410.976975
Sum of electronic and thermal Energies= -2410.937650
Sum of electronic and thermal Enthalpies= -2410.936705
Sum of electronic and thermal Free Energies= -2411.054134

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 360.405	152.663	247.149

B,0,1.4167394741,-0.3139580297,0.750909213
B,0,-0.6870494969,1.7798913939,0.1583292087
B,0,1.4659110464,0.2608041722,-1.2956028822
C,0,-0.0618140281,-2.8328413087,-2.2327549465
H,0,0.3031257794,-2.0984035865,-2.9389538519
C,0,-0.1665274067,-4.1795255783,-2.5687844634
H,0,0.1040329165,-4.5102795672,-3.5654609737
C,0,-0.623364916,-5.0727149272,-1.6023988496
C,0,-0.9620583415,-4.588420658,-0.3436633933
C,0,-0.8351560401,-3.2191800976,-0.0759893846
C,0,-1.2044319441,-2.6187707178,1.2272383003
C,0,-1.6221540502,-3.3893712004,2.3183819681
H,0,-1.6634422704,-4.4680716057,2.2402960696
C,0,-1.9825890493,-2.7697007595,3.5089655959
C,0,-1.9209105615,-1.3812214698,3.5887685947
H,0,-2.1955568201,-0.8493930051,4.4927144023
C,0,-1.4917566289,-0.6650414037,2.4769874938
H,0,-1.42443067,0.4158252214,2.4836990258
C,0,2.7713426615,0.0004578034,2.493627336
C,0,2.9136941571,-1.3214270772,2.067856183
C,0,-0.9054927652,4.0039616398,0.1085885875

C,0,-1.2691729009,3.567057474,1.3834513093
C,0,3.1664413409,0.0119027274,-2.7298496755
C,0,3.2318325307,1.2964143436,-2.1855947503
Ir,0,-0.3920439792,-0.1581434551,-0.4252326018
N,0,-0.3833348542,-2.3645549659,-1.0192516556
N,0,-1.1361437812,-1.2649709414,1.325090157
O,0,1.8562508314,0.6337920151,1.6885601202
O,0,2.0873241123,-1.532226657,0.9880756513
O,0,-0.5480597995,2.9215873772,-0.6548870275
O,0,-1.1402703387,2.1975127295,1.4354191772
O,0,2.087625783,-0.6496292502,-2.1912788328
O,0,2.1997220559,1.46486787,-1.2974633897
H,0,-1.3322583021,-5.2699622214,0.411699426
H,0,-2.3062091288,-3.3639581073,4.357739016
H,0,-0.7208354387,-6.1308860025,-1.8241249179
H,0,-0.1078156725,0.5696737703,-1.8201549326
C,0,-2.4021777961,-0.0306757691,-1.121961476
S,0,-3.7387523836,-0.9513910628,-0.4246444209
C,0,-4.9173999384,-0.3483182333,-1.571107468
C,0,-6.3578940816,-0.762944545,-1.5243037022
C,0,-4.3040978808,0.5175274164,-2.4332366371
H,0,-4.8381972407,1.0246491925,-3.2318857109
C,0,-2.9061225634,0.6962757848,-2.1792109238
H,0,-2.2858046601,1.3629716956,-2.7693914885
C,0,3.7745331504,-2.2063559554,2.6953895783
C,0,4.4998378889,-1.7084695093,3.7883168739
C,0,4.3564336249,-0.3831143164,4.2160076654
C,0,3.4822735357,0.5040272426,3.5704156699
C,0,4.0896275576,-0.4390717371,-3.6573351621
C,0,5.100257382,0.4615738011,-4.0297690939
C,0,5.1656894503,1.7481756779,-3.484894941
C,0,4.2243793787,2.192795504,-2.5434269921
C,0,-1.678504003,4.444581161,2.3718580333
C,0,-1.7122516914,5.8066583608,2.0319681654
C,0,-1.3477181017,6.2460179006,0.7552981983
C,0,-0.9340322601,5.3440637514,-0.2378529192
H,0,3.3655618587,1.5338475647,3.8900207108
H,0,4.9357861361,-0.0313088766,5.0642240962
H,0,5.1884087263,-2.3658203178,4.3105001315
H,0,3.8811732381,-3.2299128904,2.3522747856
H,0,5.8456136933,0.1501027892,-4.7552822541
H,0,4.031693917,-1.4399730674,-4.0716979164
H,0,5.9607078902,2.419304372,-3.7953936279
H,0,4.2641616677,3.1876440145,-2.1135221206
H,0,-1.9592017563,4.0935142589,3.3593686398
H,0,-2.0278876224,6.5307899076,2.7770804342
H,0,-1.3849768884,7.3065771888,0.5249815879
H,0,-0.6491007452,5.6734502565,-1.2312860228
H,0,-6.9122230327,-0.2667448354,-2.3268034576
H,0,-6.483208841,-1.8451489123,-1.6537177129
H,0,-6.8358771138,-0.4929527566,-0.5745838294

methiophenedmpeBeg3toprod

Ir Beg3 dmpe methylthiophene for C-H at 2 position opt to product
B3LYP/gen
E(RB+HF-LYP) = -2379.84830966

Zero-point correction= 0.518189 (Hartree/Particle)
Thermal correction to Energy= 0.554849
Thermal correction to Enthalpy= 0.555793
Thermal correction to Gibbs Free Energy= 0.449301
Sum of electronic and ZPE= -2379.330120
Sum of electronic and thermal Energies= -2379.293460
Sum of electronic and thermal Enthalpies= -2379.292516
Sum of electronic and thermal Free Energies= -2379.399009

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	348.173	133.558	224.133

C,0,2.9410687263,-1.4646500484,0.0471190044
C,0,2.1163652228,-0.374075294,0.2417576935
S,0,3.1425733193,0.9333822154,0.8382262392
C,0,4.6140555232,-0.0127929812,0.8048866856
C,0,4.3286643772,-1.2707996338,0.3538180024
Ir,0,-0.0523920513,-0.0699556953,0.0594326004
P,0,-0.0102081986,-0.9118682792,-2.1426702895
C,0,-0.5666494728,-2.6959258471,-2.0902778408
C,0,-0.0918641615,-3.4350518858,-0.8291521649
P,0,-0.4538675642,-2.4271772032,0.7096031442
B,0,-2.1224160277,0.3405533501,-0.3768801354
O,0,-3.0338799481,-0.6429999875,-0.8038221624
C,0,-4.3298403013,-0.0507334638,-0.9810129456
C,0,-4.0554349683,1.4639154056,-0.9708233165
O,0,-2.7460457965,1.5842209742,-0.4049350656
B,0,-1.0961527031,0.6943845484,1.8294952723
O,0,-1.7964886421,-0.1754016241,2.6754879367
C,0,-2.4264923866,0.6149826748,3.6954790296
C,0,-2.3624546258,2.0516754714,3.1445045912
O,0,-1.3059241306,2.0117111371,2.1856343128
B,0,0.3541757601,1.8650238277,-0.6433898817
O,0,0.7158235095,2.9349342404,0.1561845927
C,0,1.1174999219,4.0334885986,-0.6649443132
C,0,0.6487042266,3.6484575563,-2.0823713762
O,0,0.3741003116,2.2419784676,-1.995280448
H,0,-4.7719073355,-0.4023042708,-1.9190300823
H,0,-4.9817540945,-0.3611078175,-0.1547843353
H,0,-4.0512203956,1.8914099433,-1.9815154568
H,0,-4.7728108486,2.0259167955,-0.3645783754
H,0,-3.4483261806,0.2586006854,3.8588279828
H,0,-1.8641543192,0.5061595637,4.6317192962
H,0,-3.2945652468,2.3392396345,2.6402373281
H,0,-2.135514681,2.7980972562,3.9114412003
H,0,-0.2687522834,4.1759936172,-2.3729825374
H,0,1.4097979592,3.8278601668,-2.8488469542
H,0,0.6543147535,4.9554702059,-0.2994509431
H,0,2.2078012055,4.1429928802,-0.606020465
H,0,0.2603677343,0.4675153935,1.6140254707
H,0,2.5786752153,-2.4199470566,-0.3199377242
C,0,5.9388914746,0.5513448605,1.2258530582
H,0,5.0829275401,-2.0455730938,0.2431451571
C,0,-1.1154997872,-0.1915607946,-3.4291642227
C,0,1.5975913212,-0.9043570535,-3.0394156181
C,0,-2.143119477,-3.0173002369,1.1688979138
C,0,0.575259923,-3.2317146724,2.014769362
H,0,-0.5735063721,-4.4172421705,-0.7550148397
H,0,0.9877761192,-3.6101654659,-0.868949289
H,0,-1.6606644721,-2.6494332672,-2.1009625031
H,0,-0.2457413951,-3.2130242493,-3.0021730415
H,0,1.4969431671,-1.4203408901,-3.9996162631
H,0,1.8696476443,0.1399492815,-3.2111363657
H,0,2.3801748758,-1.3627602819,-2.4367279961
H,0,-0.9548465453,-0.6892945025,-4.3906831226
H,0,-2.1560448108,-0.3100429649,-3.1263128098
H,0,-0.8756892826,0.8699263818,-3.5108938631
H,0,0.4428204917,-4.3187340228,2.0247121205
H,0,1.6257078317,-2.9826252473,1.8563214276
H,0,0.2687514344,-2.8280377205,2.9839996418
H,0,-2.1632135659,-4.1054553734,1.2912660355
H,0,-2.4302615903,-2.5313287208,2.1030859771
H,0,-2.8473513594,-2.7068431009,0.3959475331
H,0,6.7188461016,-0.2102060243,1.1264550546
H,0,6.2350694269,1.4125790853,0.6143007941
H,0,5.9316637628,0.886140449,2.27038821

bypbeg3veratroleMetaCtoprod

bpy beg3 ir veratrole meta C opt to prod
B3LYP/gen
E(RB+HF-LYP) = -1823.16063540

Zero-point correction= 0.536003 (Hartree/Particle)
Thermal correction to Energy= 0.573398
Thermal correction to Enthalpy= 0.574342
Thermal correction to Gibbs Free Energy= 0.462764
Sum of electronic and ZPE= -1822.624632
Sum of electronic and thermal Energies= -1822.587238
Sum of electronic and thermal Enthalpies= -1822.586294
Sum of electronic and thermal Free Energies= -1822.697872

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	359.812	137.530	234.836

C,0,4.4345930815,-0.7879897112,-0.0456232761
C,0,3.6376048601,-1.2142149735,1.0169288419
C,0,2.2434702371,-1.0605934006,0.9659943158
C,0,1.5857336921,-0.4780349474,-0.1279377507
C,0,2.4182022193,-0.0763535169,-1.193176073
C,0,3.804387226,-0.216525555,-1.16933818
Ir,0,-0.5524727826,-0.1525621921,-0.223203524
N,0,-0.0511696047,2.0652920803,-0.500036465
C,0,0.2641359936,2.7151951255,0.6424549808
C,0,0.7689581341,4.0220228873,0.6172895746
C,0,0.939929792,4.6651350813,-0.6036906177
C,0,0.5965473651,3.9908763758,-1.7731437315
C,0,0.1056516817,2.6914253597,-1.6752787918
C,0,0.042252622,1.9659691206,1.9002726831
N,0,-0.3517156451,0.6703179913,1.7840774497
C,0,-0.5808596466,-0.052992977,2.8974481738
C,0,-0.4262086241,0.4749598389,4.1746559411
C,0,-0.0249211788,1.8016663098,4.3104625214
C,0,0.2075551607,2.54973268,3.1626483185
B,0,-2.6440903398,0.2015664515,0.2285249921
O,0,-3.3151768087,1.4091489706,0.0453600885
C,0,-4.5300171369,1.388600946,0.8092741705
C,0,-4.676098426,-0.0795036229,1.2614124728
O,0,-3.3878966221,-0.6587512613,1.0218899992
B,0,-1.9152132408,-0.2630011929,-1.8140355254
O,0,-2.8537323153,-1.2511668954,-2.101697488
C,0,-3.3585263194,-1.0294902213,-3.4217587263
C,0,-2.9836285154,0.4315536534,-3.7277110855
O,0,-1.9020873695,0.7044103118,-2.8316418664
B,0,-0.7219396138,-2.1563511405,0.1688833993
O,0,-0.7996360357,-2.7068882945,1.456717847
C,0,-0.6971016445,-4.1330045164,1.3632556676
C,0,-0.8968724476,-4.4284192514,-0.1366416245
O,0,-0.6823637544,-3.1715692362,-0.7803442565
H,0,-0.3442791628,-0.7572706416,-1.692615473
H,0,-0.1956918801,2.1245897926,-2.5477195823
H,0,1.0392772904,4.5304110884,1.5344769704
H,0,0.7090343003,4.4530113779,-2.7478846147
H,0,1.3364362187,5.6751674583,-0.6381250763
H,0,0.5098151475,3.5857225436,3.2476869083
H,0,0.1031935941,2.2500285334,5.290876459
H,0,-0.6210045114,-0.1520361639,5.0378562591
H,0,-0.8832298427,-1.0801344222,2.7297782611
H,0,-3.8120718249,1.120807244,-3.5166479174
H,0,-2.6560766446,0.5854285823,-4.7608339145
H,0,-4.4378098133,-1.2104469523,-3.4396733751
H,0,-2.8763283561,-1.73110411,-4.1150604488

H,0,1.6692732687,-1.4276996787,1.8135582487
H,0,4.088604453,-1.6684849815,1.8932855925
O,0,5.8067518685,-0.8739399485,-0.0890461439
H,0,2.0024932082,0.3741347133,-2.0912080832
O,0,4.5415054454,0.2665686765,-2.2336341964
H,0,-4.4312778033,2.0777760131,1.6576837377
H,0,-5.3621644282,1.7306011768,0.1855904597
H,0,-4.9330624393,-0.1769975581,2.3211682443
H,0,-5.4266309064,-0.6217622285,0.6729115158
H,0,0.2934891941,-4.4471906577,1.7175408798
H,0,-1.4575430213,-4.6005069408,1.997341459
H,0,-0.1877502213,-5.1683642171,-0.5220252052
H,0,-1.9148435068,-4.7775736518,-0.3536603946
C,0,5.164551429,-0.7308764636,-3.0393080302
H,0,5.6635513026,-0.2021976584,-3.8558050522
H,0,5.9060449103,-1.302950875,-2.4717016537
H,0,4.4194480976,-1.41974698,-3.4606403086
C,0,6.4634312265,-1.4420252764,1.0267097105
H,0,7.5314411859,-1.4090914671,0.8014047063
H,0,6.2730280807,-0.871735083,1.9462004188
H,0,6.1631761472,-2.4859385212,1.1926331835

bypbeg3veratroleMetaBtoprod

bpy beg3 ir veratrole meta B opt to prod
B3LYP/gen
E(RB+HF-LYP) = -1823.16111386

Zero-point correction= 0.536455 (Hartree/Particle)
Thermal correction to Energy= 0.573669
Thermal correction to Enthalpy= 0.574613
Thermal correction to Gibbs Free Energy= 0.463402
Sum of electronic and ZPE= -1822.624659
Sum of electronic and thermal Energies= -1822.587445
Sum of electronic and thermal Enthalpies= -1822.586500
Sum of electronic and thermal Free Energies= -1822.697712

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 359.983	137.305	234.063

C,0,4.4657399,-0.7679473828,-0.0543218918
C,0,3.6735257102,-1.2931842125,0.960843332
C,0,2.2750409332,-1.1552895158,0.9231218556
C,0,1.619054076,-0.4856628348,-0.1154212105
C,0,2.4441475276,0.0306756622,-1.1420760248
C,0,3.8337223712,-0.0989082479,-1.128272397
Ir,0,-0.5301177025,-0.1899674899,-0.1816877605
N,0,-0.0777080578,2.0568688606,-0.2514924395
C,0,0.2632306232,2.5962584523,0.9396152254
C,0,0.7685953311,3.9005013812,1.0274147352
C,0,0.9051556952,4.6594964942,-0.1294609934
C,0,0.524168979,4.1024391027,-1.348563167
C,0,0.0392945856,2.7972381067,-1.3639312019
C,0,0.0565217924,1.7336654699,2.1243266502
N,0,-0.3338940353,0.4525269659,1.8916097219
C,0,-0.5617623003,-0.3669157668,2.9362854795
C,0,-0.4087646844,0.0460182089,4.2555998129
C,0,-0.0099913177,1.355703058,4.5097484839
C,0,0.2207852228,2.2034801206,3.433096459
B,0,-2.6261724129,0.071276469,0.3009726768
O,0,-3.3610916751,1.247834954,0.1643709542
C,0,-4.5743137327,1.13336365,0.9221529683
C,0,-4.6377331674,-0.3540208921,1.3283551591
O,0,-3.322032182,-0.8558508116,1.0632733762
B,0,-1.8787976492,-0.1972827969,-1.7859630448
O,0,-2.8072403306,-1.1717926271,-2.1455022612

C,0,-3.3352086303,-0.8457218286,-3.4342584455
C,0,-2.9817060145,0.6402289063,-3.6201696286
O,0,-1.8834407764,0.8465506601,-2.7263291706
B,0,-0.6637566537,-2.2226530595,0.0427837576
O,0,-0.7080539263,-2.8789967712,1.2809168462
C,0,-0.5887987041,-4.2907013373,1.0671308153
C,0,-0.8116859312,-4.4638105745,-0.4488190708
O,0,-0.6339800695,-3.1535395068,-0.9889951823
H,0,-0.3103661816,-0.6649209783,-1.6976344923
H,0,-0.2919460274,2.3167421466,-2.2769453426
H,0,1.0646536269,4.3175217313,1.9820175133
H,0,0.6009751821,4.660829795,-2.275386195
H,0,1.3004881617,5.6692456706,-0.076868599
H,0,0.5178961319,3.229424053,3.6096351145
H,0,0.1164642045,1.7152825338,5.5262819545
H,0,-0.6028415282,-0.6558078966,5.0592834883
H,0,-0.859737786,-1.376085464,2.6784419459
H,0,-3.8117953278,1.298388313,-3.3314221443
H,0,-2.6779916331,0.8867849457,-4.6425536336
H,0,-4.4126230638,-1.0375454936,-3.4513886122
H,0,-2.8563616819,-1.4801188468,-4.1917141782
H,0,1.70279564,-1.6075775802,1.7291736844
H,0,4.1317328151,-1.8218753799,1.7902898566
O,0,5.8345221193,-0.8446742055,-0.1154302811
H,0,1.9847446837,0.5424436113,-1.9807888377
O,0,4.6771016797,0.3807119049,-2.0978571532
H,0,-4.517874772,1.8008964522,1.7913334279
H,0,-5.4233021145,1.4455943407,0.3054696113
H,0,-4.8809451726,-0.4980466861,2.3861350613
H,0,-5.3626780027,-0.9174758444,0.7280760555
H,0,0.4117434598,-4.6187853427,1.3776683486
H,0,-1.3320168751,-4.8197478772,1.6726742256
H,0,-0.0955655507,-5.1536521483,-0.9071221663
H,0,-1.8265764143,-4.8149718545,-0.6767400502
C,0,4.100644999,1.0223699421,-3.216267057
H,0,4.9323859154,1.3020234957,-3.8667257687
H,0,3.4211181087,0.3574092268,-3.7669818771
H,0,3.5482877499,1.9292349439,-2.9314133398
C,0,6.4940560865,-1.5352903353,0.9246184565
H,0,7.5598103748,-1.4944680181,0.6894695629
H,0,6.325189028,-1.0647207525,1.9038568037
H,0,6.17965356,-2.5868607591,0.9839811225

bypbeg3veratroleMetaAtoprod

bpy beg3 ir veratrole meta A opt to prod
B3LYP/gen
E(RB+HF-LYP) = -1823.16074622

Zero-point correction= 0.536013 (Hartree/Particle)
Thermal correction to Energy= 0.573449
Thermal correction to Enthalpy= 0.574394
Thermal correction to Gibbs Free Energy= 0.462346
Sum of electronic and ZPE= -1822.624733
Sum of electronic and thermal Energies= -1822.587297
Sum of electronic and thermal Enthalpies= -1822.586353
Sum of electronic and thermal Free Energies= -1822.698400

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 359.845	137.533	235.824

C,0,4.458357912,-0.5738505454,0.5334763334
C,0,3.5920126091,-0.8656832248,1.5798094953
C,0,2.2035355963,-0.7930656125,1.4095886329
C,0,1.6288010141,-0.4264214671,0.1824727521
C,0,2.5249526431,-0.1443302814,-0.8721599567

C,0,3.914148239,-0.2069262149,-0.7143482267
Ir,0,-0.5070470777,-0.23281341,-0.1286824009
N,0,-0.0911706971,1.9581821398,-0.6610685733
C,0,0.135542306,2.7609812818,0.4018210746
C,0,0.5942439365,4.0744035363,0.2335008506
C,0,0.801571598,4.5665395969,-1.0502306947
C,0,0.5363692643,3.7387404823,-2.1392649562
C,0,0.0931450854,2.4406592407,-1.8988134836
C,0,-0.1476322455,2.172401724,1.7303033468
N,0,-0.5039597394,0.8610812294,1.7575816322
C,0,-0.8040820673,0.2834366233,2.9369235839
C,0,-0.7563720574,0.9783023339,4.1408733137
C,0,-0.3887671801,2.3212122655,4.1296479032
C,0,-0.0857687501,2.9200732472,2.9125857785
B,0,-2.6410060797,0.0889172465,0.0906129335
O,0,-3.3492303647,1.1970671811,-0.3706340555
C,0,-4.6255653127,1.2416180245,0.2847438187
C,0,-4.7403031796,-0.1213269301,0.9991003658
O,0,-3.4102531722,-0.6535418004,0.9734458782
B,0,-1.7121218795,-0.6589177392,-1.7908578035
O,0,-2.5879505115,-1.7242670239,-1.9860927054
C,0,-2.9978589354,-1.7324142282,-3.3566505819
C,0,-2.6508215722,-0.3206678779,-3.8617589019
O,0,-1.6473987953,0.134342208,-2.9484931036
B,0,-0.6420937571,-2.1681075719,0.5339509297
O,0,-0.8390290458,-2.5383273193,1.8705621412
C,0,-0.6889394332,-3.9582818328,1.9924528327
C,0,-0.7079497432,-4.4666445973,0.5366634871
O,0,-0.4698841769,-3.3009081784,-0.2537132148
H,0,-0.1455808699,-1.0278767425,-1.4729162705
H,0,-0.1498449032,1.7569349689,-2.7036385536
H,0,0.7983350796,4.704800284,1.0900727551
H,0,0.6702603581,4.0835668297,-3.1590114754
H,0,1.1613664119,5.5805595199,-1.194835497
H,0,0.1909264984,3.9662109811,2.8817293093
H,0,-0.3405396402,2.8960925526,5.0492895954
H,0,-1.0041880359,0.4639395898,5.0628905906
H,0,-1.0721621778,-0.7654152418,2.8866037779
H,0,-3.5150885986,0.355160828,-3.8174185952
H,0,-2.2531940124,-0.313605888,-4.8816399612
H,0,-4.0659177268,-1.9624654359,-3.4213120919
H,0,-2.440795818,-2.5100955571,-3.8954683889
H,0,1.5702626657,-1.0476775862,2.255575251
H,0,4.0280808499,-1.1463779027,2.5353405124
O,0,5.822130896,-0.5941677839,0.7530215432
H,0,2.1253561001,0.1342003253,-1.8414493379
O,0,4.8253659709,0.0776941705,-1.7038456705
H,0,-4.6370926129,2.0834100401,0.988667253
H,0,-5.4138045865,1.4049090642,-0.4571890671
H,0,-5.0823292931,-0.0334138457,2.035385472
H,0,-5.4108232636,-0.8108343123,0.471445356
H,0,0.2614218994,-4.1785728027,2.4957431906
H,0,-1.5054965357,-4.364239,2.5984634212
H,0,0.0673133293,-5.2137829753,0.3377966346
H,0,-1.6812736339,-4.8954028382,0.2648605631
C,0,4.3309795557,0.4419847411,-2.9778621361
H,0,5.2081219038,0.6185038768,-3.604175178
H,0,3.7225356391,-0.3553278922,-3.4256657577
H,0,3.7299372533,1.3605085407,-2.9345236918
C,0,6.5229067638,-1.6509224331,0.1022591656
H,0,7.570749585,-1.5569975364,0.3996470614
H,0,6.1459657421,-2.632232253,0.4227312543
H,0,6.44710233,-1.5741890259,-0.9873842563

bpyBcat3methiopheneTS

Ir Bcat3 bpy methylthiophene ts for C-H at 2 position

B3LYP/gen

E(RB+HF-LYP) = -2411.49694718

Zero-point correction= 0.533105 (Hartree/Particle)

Thermal correction to Energy= 0.572287

Thermal correction to Enthalpy= 0.573231

Thermal correction to Gibbs Free Energy= 0.456009

Sum of electronic and ZPE= -2410.963842

Sum of electronic and thermal Energies= -2410.924660

Sum of electronic and thermal Enthalpies= -2410.923716

Sum of electronic and thermal Free Energies= -2411.040938

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 359.115	151.862	246.714

B,0,1.3594146206,-0.427819549,1.0005771737
B,0,-0.5652333991,1.6957756528,0.3372928054
B,0,1.2168287746,0.3534803486,-1.3990606179
C,0,0.3701969959,-3.0668415657,-1.6781819902
H,0,0.907764965,-2.3779783578,-2.3193504345
C,0,0.3579933149,-4.4383083362,-1.9190934319
H,0,0.8927358499,-4.8401317839,-2.7727517278
C,0,-0.346488383,-5.262593549,-1.0452878441
C,0,-1.0044556297,-4.6882797724,0.0369039801
C,0,-0.9525011357,-3.3002729079,0.221272783
C,0,-1.6026782851,-2.6212120268,1.3689568194
C,0,-2.3390503607,-3.3148164934,2.3371827846
H,0,-2.4812201716,-4.3849645064,2.2571507995
C,0,-2.8925197244,-2.6247231639,3.410170165
C,0,-2.6911143507,-1.2503493081,3.5016502437
H,0,-3.0944517028,-0.6692136071,4.323418863
C,0,-1.9539527553,-0.6147527163,2.5069260608
H,0,-1.7582996109,0.4504376415,2.5302402311
C,0,2.786369216,-0.246630592,2.7116523956
C,0,3.3036963221,-1.1847174574,1.8173266157
C,0,-0.7900289577,3.9223905738,0.2520301245
C,0,-0.9693255696,3.5236098394,1.5778186876
C,0,2.7331249456,0.3307107548,-3.0523998853
C,0,3.0126294565,1.4077991526,-2.2110022219
Ir,0,-0.3733728709,-0.2625545454,-0.2224635021
N,0,-0.2728129104,-2.5096584098,-0.640324466
N,0,-1.4314344893,-1.2792992686,1.4623422578
O,0,1.5897570266,0.224510791,2.2259483565
O,0,2.4352021707,-1.3159738596,0.7587026896
O,0,-0.5472183889,2.8167073485,-0.5213513078
O,0,-0.8374971766,2.1563273358,1.6519044648
O,0,1.6222616096,-0.3298037026,-2.5744903787
O,0,2.090377117,1.4366425904,-1.1935190197
H,0,-1.5482420646,-5.3186941993,0.7290037684
H,0,-3.4662526831,-3.1561824022,4.1630297585
H,0,-0.3813305628,-6.3368678581,-1.1975870406
H,0,-0.7783159568,0.288888452,-1.6853057119
C,0,-2.2922169066,-0.2508804899,-1.3004644755
S,0,-3.5739311444,0.8657968898,-0.8638060079
C,0,-4.7467212721,0.104535565,-1.9150853898
C,0,-6.1615695882,0.5926037222,-2.0135388816
C,0,-4.1582903368,-0.9407269766,-2.5760268488
H,0,-4.6934737296,-1.5568486023,-3.2927413302
C,0,-2.7810465883,-1.132292088,-2.2413797591
H,0,-2.1670115951,-1.9010414737,-2.6992000262
C,0,4.5058260769,-1.8321713102,2.047438658
C,0,5.1845934909,-1.4994094748,3.2299948025
C,0,4.6660255125,-0.5589904279,4.1270952245
C,0,3.4460209846,0.0899225831,3.8818015654
C,0,3.4995223137,0.0533638959,-4.170592495
C,0,4.582780345,0.9111965345,-4.4196152595
C,0,4.8645881808,1.9905250801,-3.5755790194

C,0,4.0769055149,2.2611722399,-2.4457218247
C,0,-1.2319570222,4.431749829,2.5886722294
C,0,-1.3125860062,5.7836486175,2.2176778034
C,0,-1.1341023668,6.1842101301,0.8895092086
C,0,-0.8671658001,5.2522225,-0.1258506178
H,0,3.0361573099,0.8233094853,4.5679650796
H,0,5.2187713671,-0.3230285864,5.0315151663
H,0,6.1326654949,-1.9809493508,3.4501036081
H,0,4.8999873189,-2.5572148223,1.3432556677
H,0,5.2118823045,0.7318332298,-5.2862400356
H,0,3.269915336,-0.7842310436,-4.8208164871
H,0,5.7099562442,2.6347626652,-3.7975614906
H,0,4.2844881216,3.0957625283,-1.7849794963
H,0,-1.3649962664,4.110148062,3.6163584167
H,0,-1.5160585351,6.5308096961,2.9789901049
H,0,-1.2023209611,7.2379779858,0.6360914182
H,0,-0.7270460742,5.5516256056,-1.1589608107
H,0,-6.7165864357,-0.0188395704,-2.7313759332
H,0,-6.6855919232,0.5366986703,-1.0518544292
H,0,-6.2134872714,1.6344417331,-2.350922356

methiophenedmpeBeg3TS

Ir Beg3 dmpe methylthiophene ts for C-H at 2 position
B3LYP/gen
E(RB+HF-LYP) = -2379.83322682

Zero-point correction= 0.514656 (Hartree/Particle)
Thermal correction to Energy= 0.551566
Thermal correction to Enthalpy= 0.552510
Thermal correction to Gibbs Free Energy= 0.445092
Sum of electronic and ZPE= -2379.318571
Sum of electronic and thermal Energies= -2379.281661
Sum of electronic and thermal Enthalpies= -2379.280717
Sum of electronic and thermal Free Energies= -2379.388135

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	346.113	133.701	226.080

C,0,3.1172307231,-0.8739173227,1.0621806285
C,0,2.2211423765,0.1016000195,0.6731674916
S,0,3.1290813717,1.5889384447,0.4126588765
C,0,4.6710302048,0.8527634005,0.7747257079
C,0,4.4862476034,-0.4620945514,1.1082054616
Ir,0,0.0472641381,-0.0680577938,0.1270999705
P,0,0.6818965328,-0.9058601392,-2.0601297774
C,0,0.4205934726,-2.7602134536,-2.0576806741
C,0,0.7391114504,-3.3908158872,-0.6909074613
P,0,-0.1315224767,-2.4551208613,0.6760375698
B,0,-1.9637212359,0.0218358253,-0.5549343203
O,0,-2.5202544153,-0.8525629915,-1.5070712482
C,0,-3.8421260926,-0.4117606338,-1.8504238017
C,0,-4.1857233574,0.638148494,-0.7765162104
O,0,-2.9330791592,0.9409778972,-0.1555939912
B,0,-1.0525202699,0.4472074156,1.8741522883
O,0,-1.6977185516,-0.5243432202,2.6549643683
C,0,-2.2750678283,0.1197721491,3.8011557703
C,0,-2.2044824903,1.6214673599,3.4640139317
O,0,-1.240517713,1.704269764,2.4120940729
B,0,0.0114562946,1.9266938372,-0.5336782837
O,0,0.3652761439,3.0372269265,0.217092184
C,0,0.3695850994,4.1997760541,-0.6150187352
C,0,-0.3562459116,3.7540791788,-1.8983265702
O,0,-0.3302777125,2.320677948,-1.8394528081
H,0,-3.8271648914,0.018453409,-2.8598634301
H,0,-4.5269059541,-1.2661524797,-1.8496996727

H,0,-4.6177742685,1.5515354155,-1.1974282151
H,0,-4.8784129857,0.2455584296,-0.0211298646
H,0,-3.2981921348,-0.2400062211,3.9499772608
H,0,-1.6848860025,-0.1331594689,4.6915538677
H,0,-3.1657130103,2.0063835807,3.1005880842
H,0,-1.8804423444,2.2361607198,4.3095684551
H,0,-1.3998577343,4.0932833265,-1.9202514322
H,0,0.1384404995,4.0960983605,-2.8135513982
H,0,-0.1375220834,5.0222286919,-0.1009134355
H,0,1.4079761399,4.4992895362,-0.8093677197
H,0,0.8322021124,0.3919642257,1.4857585692
H,0,2.817368798,-1.8871420026,1.2991980404
C,0,5.9540705006,1.6288807457,0.7246784713
H,0,5.3036062126,-1.1216274873,1.3862550602
C,0,-0.1575590738,-0.38131605,-3.6135653691
C,0,2.459732721,-0.7152851762,-2.5179309931
C,0,-1.8268559288,-3.1907552574,0.6482919652
C,0,0.504463365,-3.229204907,2.2335991987
H,0,0.455268963,-4.4500945731,-0.6752891687
H,0,1.8147917428,-3.336824733,-0.4871506757
H,0,-0.6358603191,-2.9130727292,-2.3038406993
H,0,1.0148469288,-3.2231381721,-2.85424258
H,0,2.686510053,-1.2694921892,-3.4344821145
H,0,2.6673213765,0.345774557,-2.6773535939
H,0,3.0987621093,-1.0584671539,-1.7022440482
H,0,0.2741845642,-0.8893513999,-4.4818897967
H,0,-1.2191453139,-0.6153373196,-3.5299745157
H,0,-0.047434497,0.7000925827,-3.7126604747
H,0,0.4010856007,-4.3191124304,2.2082046211
H,0,1.5477026793,-2.9693395793,2.4168861516
H,0,-0.0943139943,-2.830747363,3.0567484616
H,0,-1.7925848165,-4.2761338507,0.7908264882
H,0,-2.3957526118,-2.7292876649,1.4587384847
H,0,-2.3161934164,-2.9482563615,-0.2959341249
H,0,6.7937657103,0.9798022218,0.9912994106
H,0,6.1514377551,2.0362374499,-0.2742711326
H,0,5.9502563524,2.4740094581,1.4233414247

bypbeg3veratroleMetaTSC

bpy beg3 ir ts veratrole meta C
B3LYP/gen
E(RB+HF-LYP) = -1823.14654571

Zero-point correction= 0.533698 (Hartree/Particle)
Thermal correction to Energy= 0.571228
Thermal correction to Enthalpy= 0.572172
Thermal correction to Gibbs Free Energy= 0.458790
Sum of electronic and ZPE= -1822.612848
Sum of electronic and thermal Energies= -1822.575318
Sum of electronic and thermal Enthalpies= -1822.574374
Sum of electronic and thermal Free Energies= -1822.687756

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 358.451	137.008	238.633

C,0,4.4073052404,-0.9304469711,-0.1167287702
C,0,3.5573362868,-1.8253170611,0.5365303941
C,0,2.1666586828,-1.6855400363,0.4400461862
C,0,1.5738235128,-0.6406006268,-0.2832591882
C,0,2.4500536122,0.2263522454,-0.9636559489
C,0,3.8353488598,0.1030437541,-0.886886178
Ir,0,-0.6126244105,-0.2070322898,-0.1014661917
N,0,-0.1468948641,2.0218319149,-0.3877053631
C,0,0.2274727785,2.7001180984,0.7202258686
C,0,0.5551328942,4.0615410667,0.6578711882

C,0,0.4963037986,4.7258245387,-0.5620070172
C,0,0.1030633258,4.0173411375,-1.6950002933
C,0,-0.2120693592,2.6675529089,-1.5626572075
C,0,0.2438874539,1.9309624112,1.9881431974
N,0,-0.1611302424,0.6384354929,1.9222807063
C,0,-0.2129782021,-0.0963372116,3.0471432052
C,0,0.1551964027,0.4133766474,4.2887684597
C,0,0.5934997988,1.7327885774,4.3693199631
C,0,0.6335637296,2.4973523044,3.2089403999
B,0,-2.6466635135,0.3011469743,0.3188841292
O,0,-3.2983241636,1.4059342473,-0.2382259457
C,0,-4.5921828861,1.5476130367,0.3614918976
C,0,-4.7720524187,0.2680152753,1.2065693537
O,0,-3.4727769686,-0.3334486586,1.2368072488
B,0,-1.6578656241,-0.5121785341,-1.8692219467
O,0,-2.7720581937,-1.3162100866,-2.0808381361
C,0,-3.1060233407,-1.3025249651,-3.4709192432
C,0,-2.3325900754,-0.0978360768,-4.0374460785
O,0,-1.3187438136,0.1571004811,-3.0563920713
B,0,-1.0287823653,-2.1543219592,0.3728985352
O,0,-1.2661239468,-2.6212804718,1.6759285636
C,0,-1.347154416,-4.050109717,1.6676394716
C,0,-1.4124574707,-4.4200293957,0.1711252699
O,0,-1.0015298965,-3.2344962981,-0.5094603664
H,0,0.2522612476,-0.9172579363,-1.2604012276
H,0,-0.5301675951,2.0631931387,-2.4056809368
H,0,0.8518957906,4.6014936034,1.5483680178
H,0,0.0392257779,4.4931931946,-2.6676592373
H,0,0.7516935946,5.7792948532,-0.6230567956
H,0,0.969718321,3.5255257173,3.2547592687
H,0,0.8966092051,2.1642937601,5.3184015821
H,0,0.0971385198,-0.2206154892,5.1668886291
H,0,-0.5684642782,-1.1131812505,2.920483969
H,0,-2.9702489571,0.7902812435,-4.1382336084
H,0,-1.8643437749,-0.3024633521,-5.0053677287
H,0,-4.1901685964,-1.2084518415,-3.5904629296
H,0,-2.7870592796,-2.2482655871,-3.9277782338
H,0,1.546461722,-2.4099122769,0.9591179833
H,0,3.96635035,-2.6383983539,1.1267919961
O,0,5.7777571013,-0.9727189085,-0.0729690576
H,0,2.0724690439,1.0369696437,-1.579193814
O,0,4.6220331302,1.0377448787,-1.5283202745
H,0,-4.6075464288,2.4578513953,0.9749751985
H,0,-5.3519441563,1.6512705646,-0.4206403316
H,0,-5.1053275982,0.4762056215,2.2289639875
H,0,-5.4814075295,-0.4335409288,0.7503409036
H,0,-0.4582025482,-4.4682428446,2.1596943107
H,0,-2.231918956,-4.3724000342,2.2265404821
H,0,-0.7471671169,-5.2495589955,-0.0917617555
H,0,-2.4312853806,-4.6836793648,-0.141427249
C,0,5.3606696709,0.5476045561,-2.6463966839
H,0,5.8878052157,1.407123374,-3.0680291448
H,0,6.088549205,-0.2131577033,-2.3466723059
H,0,4.6895667748,0.1288750652,-3.4086715102
C,0,6.3822570996,-1.9928697265,0.7005929374
H,0,7.4598980769,-1.8429765468,0.6112077109
H,0,6.0960551362,-1.9240116541,1.7585679443
H,0,6.1259358848,-2.9943105572,0.3294987562

bypbeg3veratroleMetaTSB

bpy beg3 ir ts veratrole meta B
B3LYP/gen
E(RB+HF-LYP) = -1823.14743311

Zero-point correction= 0.534253 (Hartree/Particle)
Thermal correction to Energy= 0.571552

Thermal correction to Enthalpy= 0.572496

Thermal correction to Gibbs Free Energy= 0.460257

Sum of electronic and ZPE= -1822.613180

Sum of electronic and thermal Energies= -1822.575882

Sum of electronic and thermal Enthalpies= -1822.574937

Sum of electronic and thermal Free Energies= -1822.687176

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 358.654	136.779	236.226

C,0,4.3891596088,-1.0805766026,-0.3737871688
 C,0,3.5343331905,-1.9638697385,0.2800757501
 C,0,2.1442506461,-1.7700780037,0.2545982615
 C,0,1.5729152429,-0.6738821963,-0.3981184139
 C,0,2.44840963,0.2010997272,-1.0768502738
 C,0,3.8310645953,0.0174487538,-1.0708092597
 Ir,0,-0.5923373769,-0.1957629289,-0.1086434761
 N,0,-0.0298419253,2.0324848582,-0.0537228806
 C,0,0.3863750208,2.5152119006,1.1382898751
 C,0,0.7867179937,3.8517130037,1.2770589566
 C,0,0.7550078515,4.695802439,0.1728681347
 C,0,0.314938982,4.1886877479,-1.0481555022
 C,0,-0.0699789786,2.8521721628,-1.115664066
 C,0,0.3700466531,1.5632132181,2.2749763498
 N,0,-0.0855319156,0.3127012595,2.0152755194
 C,0,-0.159053642,-0.5832534421,3.015577284
 C,0,0.2306331734,-0.282765226,4.3174830746
 C,0,0.7155898573,0.9925654727,4.595895585
 C,0,0.7819175135,1.9227338028,3.5649094398
 B,0,-2.6058632441,0.2914246016,0.4189586387
 O,0,-3.199346576,1.5276491401,0.1446691767
 C,0,-4.4981391107,1.5735125937,0.749706035
 C,0,-4.7563307738,0.1278473968,1.2238765534
 O,0,-3.4785078325,-0.5133997236,1.1405388895
 B,0,-1.652972523,-0.1562512754,-1.892208646
 O,0,-2.8313523314,-0.8180526654,-2.2140977478
 C,0,-3.1478068999,-0.5787392424,-3.5875219732
 C,0,-2.2699547777,0.624548566,-3.9772390227
 O,0,-1.2484180329,0.6494911807,-2.9714983833
 B,0,-1.085400108,-2.17660392,0.0688417565
 O,0,-1.2014367122,-2.8557772592,1.2934461839
 C,0,-1.3787254505,-4.2556905069,1.051490083
 C,0,-1.6417704427,-4.350005213,-0.465673014
 O,0,-1.2364816103,-3.0818094382,-0.9799594773
 H,0,0.2143597274,-0.8007411772,-1.3622853504
 H,0,-0.4249207884,2.3974394865,-2.0345354432
 H,0,1.1189112983,4.2337333049,2.2342732285
 H,0,0.2651700044,4.8103131115,-1.9358157388
 H,0,1.0648032066,5.732041361,0.2683547031
 H,0,1.1543009952,2.9195379322,3.7647191092
 H,0,1.0349683821,1.2632736725,5.5976462862
 H,0,0.1526557915,-1.0417420664,5.088399384
 H,0,-0.5463965471,-1.5574331756,2.737794496
 H,0,-2.8293657636,1.5690985829,-3.9490950418
 H,0,-1.8105833098,0.5209980605,-4.9652576848
 H,0,-4.2189345824,-0.3779952042,-3.691647601
 H,0,-2.9032808477,-1.4734987734,-4.1742860192
 H,0,1.5159869955,-2.4895082497,0.7714119801
 H,0,3.9387207165,-2.8188017982,0.8113369009
 O,0,5.7531707642,-1.1853816542,-0.4174532229
 H,0,2.0341944488,1.035510831,-1.6301985234
 O,0,4.7317463116,0.8285526147,-1.7078675309
 H,0,-4.4830154655,2.2883722313,1.5828961179
 H,0,-5.234778986,1.919353028,0.0167539487
 H,0,-5.1294014725,0.076000074,2.2522625629
 H,0,-5.4648016098,-0.3997810907,0.5732015696
 H,0,-0.4682098359,-4.7934924977,1.3485534783

H,0,-2.2124165496,-4.6312613823,1.6539187246
H,0,-1.0663177814,-5.1474026887,-0.947870258
H,0,-2.704970737,-4.508993087,-0.688068542
C,0,4.2252956981,1.9079132592,-2.4679265285
H,0,5.094857071,2.4049853896,-2.9028802117
H,0,3.5643665908,1.5647465582,-3.275419763
H,0,3.6747231121,2.6266491868,-1.8449590008
C,0,6.3458416575,-2.2911087265,0.2344433119
H,0,7.4213774298,-2.1987237151,0.0709286546
H,0,6.1453767141,-2.2861602219,1.3149600739
H,0,5.9991059116,-3.2463422667,-0.1831401721

bypbeg3veratroleMetaTSA

bpy beg3 ir ts veratrole meta A
B3LYP/gen
E(RB+HF-LYP) = -1823.14646219

Zero-point correction= 0.533763 (Hartree/Particle)
Thermal correction to Energy= 0.571251
Thermal correction to Enthalpy= 0.572195
Thermal correction to Gibbs Free Energy= 0.459041
Sum of electronic and ZPE= -1822.612699
Sum of electronic and thermal Energies= -1822.575211
Sum of electronic and thermal Enthalpies= -1822.574267
Sum of electronic and thermal Free Energies= -1822.687421

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 358.466	136.987	238.153

C,0,4.3449608436,-1.2960655014,0.1309205897
C,0,3.3934560373,-2.0724826026,0.7841341034
C,0,2.0256205793,-1.8209224538,0.6325646231
C,0,1.5736786482,-0.762795081,-0.1690707633
C,0,2.5422415437,0.0041818746,-0.8458769892
C,0,3.9117654034,-0.24134122,-0.6994587415
Ir,0,-0.5788603456,-0.1540888046,-0.0846838646
N,0,0.0989548882,2.0414323642,-0.1673429411
C,0,0.4483316693,2.6047662677,1.0107017553
C,0,0.898091735,3.9313895778,1.0722015875
C,0,0.986178491,4.6814196673,-0.0949320246
C,0,0.6167610943,4.0915594795,-1.302031523
C,0,0.1773636572,2.7702841454,-1.2918291556
C,0,0.307345522,1.75197247,2.2156802656
N,0,-0.1922269049,0.505657162,2.0254070712
C,0,-0.3773511889,-0.299169559,3.0868118869
C,0,-0.0609734949,0.0914268043,4.3847833353
C,0,0.4682181142,1.3622552258,4.5934813547
C,0,0.6499996312,2.199076454,3.4983158576
B,0,-2.5944434717,0.4633021129,0.2607679203
O,0,-3.1029621249,1.7033791601,-0.1369434057
C,0,-4.4384172205,1.8494185992,0.3638123836
C,0,-4.8042248001,0.4510052833,0.9032527623
O,0,-3.5565692745,-0.2492075439,0.965665393
B,0,-1.5047524334,-0.2049976114,-1.9415522306
O,0,-2.7040429963,-0.8108300191,-2.2940979209
C,0,-2.9119161097,-0.6690678281,-3.7012488004
C,0,-1.9170102754,0.4269804187,-4.126049046
O,0,-0.9691365481,0.4728011759,-3.0511213681
B,0,-1.198034248,-2.0852860985,0.2083786848
O,0,-1.4229226689,-2.6556868061,1.4716954927
C,0,-1.6678752612,-4.059127817,1.327797455
C,0,-1.8522429865,-4.2597498845,-0.1906502716
O,0,-1.3441980388,-3.0605334488,-0.7758549408
H,0,0.2898968205,-0.9006886374,-1.2166939462
H,0,-0.1275538159,2.255680339,-2.1971259559

H,0,1.1754433113,4.3787535937,2.0184874773
H,0,0.6619343998,4.6382605312,-2.2379572788
H,0,1.33393071,5.7093433806,-0.0587005394
H,0,1.0590784537,3.1909340187,3.6434006375
H,0,0.7341775493,1.7008612571,5.5901197089
H,0,-0.2277535637,-0.5965795717,5.2064749143
H,0,-0.792844013,-1.2754366594,2.8623867403
H,0,-2.4011397978,1.4076893804,-4.2240731678
H,0,-1.3993552088,0.1992108663,-5.0631110555
H,0,-3.9545316942,-0.3981172605,-3.8960735681
H,0,-2.7042826547,-1.6273750816,-4.1943291009
H,0,1.3146494631,-2.4507142583,1.1585808618
H,0,3.7486596895,-2.878719793,1.420358694
O,0,5.6836318044,-1.5423100328,0.3496989832
H,0,2.2159151585,0.8053187402,-1.4984683541
O,0,4.9017295014,0.484139025,-1.3137948813
H,0,-4.4468823152,2.6144682939,1.1512637969
H,0,-5.1006343389,2.18191016,-0.4425427107
H,0,-5.2604917733,0.4827194718,1.8982843531
H,0,-5.4824867065,-0.0866883023,0.2290454914
H,0,-0.8076423698,-4.6191081198,1.7185004652
H,0,-2.5537780292,-4.3399378043,1.9067537568
H,0,-1.2996352697,-5.1234621641,-0.575376421
H,0,-2.9091380386,-4.3766287774,-0.4632830773
C,0,4.517088171,1.5402967871,-2.1746921001
H,0,5.4447670822,1.9741304993,-2.5533197597
H,0,3.9152334014,1.1807116574,-3.0199755984
H,0,3.9491285803,2.314602468,-1.6417326735
C,0,6.3949903959,-2.0806827807,-0.7636900903
H,0,7.417401497,-2.2562071342,-0.4198830557
H,0,5.9565800687,-3.0343697523,-1.088012474
H,0,6.4101174422,-1.3836974652,-1.6076251076

bypbeg3veratroleOrthoTSB

bpy beg3 ir ts veratrole ortho B

B3LYP/gen

E(RB+HF-LYP) = -1823.14565005

Zero-point correction= 0.534163 (Hartree/Particle)

Thermal correction to Energy= 0.571333

Thermal correction to Enthalpy= 0.572277

Thermal correction to Gibbs Free Energy= 0.461637

Sum of electronic and ZPE= -1822.611487

Sum of electronic and thermal Energies= -1822.574317

Sum of electronic and thermal Enthalpies= -1822.573373

Sum of electronic and thermal Free Energies= -1822.684013

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 358.517	136.870	232.862

C,0,4.0857515807,0.8680362331,-2.1449237054
C,0,4.0167548099,0.0396989608,-1.0235325297
C,0,2.759139579,-0.3859080744,-0.5296963059
C,0,1.5672695942,0.0721203392,-1.1051791391
C,0,1.6685416433,0.8954794587,-2.2453834759
C,0,2.901216851,1.2848171732,-2.7584916132
Ir,0,-0.4255417321,-0.1846616819,-0.095710863
N,0,-0.6492898413,2.1097908735,-0.3576114975
C,0,-0.1289720684,2.8740754477,0.6270664743
C,0,-0.1962811754,4.2731921428,0.568859836
C,0,-0.8101375533,4.8859292942,-0.5177221278
C,0,-1.3494004237,4.086840338,-1.5226850291
C,0,-1.247301957,2.7033915785,-1.4008927344
C,0,0.4839212156,2.1518981498,1.7687130705
N,0,0.4113779918,0.7988430909,1.7415423314

C,0,0.9046217254,0.0907210661,2.7721554724
C,0,1.510072292,0.6950038713,3.8699952778
C,0,1.6129071232,2.0829078001,3.9010180822
C,0,1.0904938552,2.8169109506,2.8420833589
B,0,-2.3181745376,-0.2066655406,0.8971384675
O,0,-3.2718671294,0.7990253903,0.6915956115
C,0,-4.3768576241,0.5906328264,1.5802977511
C,0,-4.1406577602,-0.8180157487,2.1615642187
O,0,-2.7805474531,-1.1187621727,1.8349944538
B,0,-1.7952765842,-0.7508742092,-1.5420531429
O,0,-2.6952860341,-1.8101279856,-1.5102715817
C,0,-3.3723423276,-1.8918119622,-2.7671571511
C,0,-3.0954048538,-0.5343918737,-3.4385576944
O,0,-1.9550937512,-0.0243342108,-2.7345534597
B,0,-0.2248961397,-2.1500807539,0.4421766659
O,0,-0.1308231491,-2.6130734094,1.7602430639
C,0,0.0619576594,-4.0287342933,1.763167987
C,0,-0.1473637516,-4.4509367705,0.2925975859
O,0,-0.1118694141,-3.2274471681,-0.4429147159
H,0,0.2187971957,-0.8513068413,-1.407302323
H,0,-1.6493379595,2.029665362,-2.149746024
H,0,0.2193643636,4.8808591129,1.3628448392
H,0,-1.8427458184,4.5177898363,-2.3873593699
H,0,-0.8682218128,5.9687873067,-0.573275684
H,0,1.1579685647,3.8974522956,2.852461057
H,0,2.087045033,2.5900113994,4.7359118808
H,0,1.8942758018,0.0787770669,4.6754730909
H,0,0.789621357,-0.9832086714,2.6941021316
H,0,-3.935462434,0.1627835483,-3.3199089684
H,0,-2.8615395287,-0.6200730364,-4.5043062233
H,0,-4.4384523401,-2.0778894178,-2.6023571966
H,0,-2.9593347533,-2.7284511387,-3.3452711547
O,0,2.7266357211,-1.1891316756,0.5956682428
O,0,5.1161230415,-0.4011006975,-0.3278372897
H,0,5.0423472067,1.1879479101,-2.5408571691
H,0,0.7597694649,1.2173141472,-2.7444034649
H,0,2.9510034374,1.9143854876,-3.6434551088
H,0,-4.3680240032,1.3674208036,2.3564266387
H,0,-5.3179718746,0.6726750106,1.0261385947
H,0,-4.2787254293,-0.8615810006,3.2471309254
H,0,-4.7947298221,-1.5691698807,1.7005440286
H,0,1.0741311717,-4.2603851611,2.1210499976
H,0,-0.6569725523,-4.4954084969,2.4449811276
H,0,0.6349127774,-5.1266887344,-0.0710991182
H,0,-1.1195363449,-4.9364163602,0.1395716815
C,0,3.19822056,-2.5252870698,0.4033717546
H,0,3.121030821,-3.017686522,1.3759096691
H,0,2.5684004554,-3.0536597542,-0.321688361
H,0,4.242060018,-2.5384472244,0.0770558916
C,0,6.394660951,0.0007478434,-0.7833216384
H,0,7.115531347,-0.4466059073,-0.096202282
H,0,6.5980841546,-0.3573787943,-1.8015693077
H,0,6.5091589452,1.0927690844,-0.7634231995

dmpelrBcat3HPhprodfromts

dmpeIr(Bcat)3 H Ph product from initial ts
B3LYP/gen
E(RB+HF-LYP) = -2477.07743077

Zero-point correction= 0.593612 (Hartree/Particle)
Thermal correction to Energy= 0.634531
Thermal correction to Enthalpy= 0.635475
Thermal correction to Gibbs Free Energy= 0.519065
Sum of electronic and ZPE= -2476.483818
Sum of electronic and thermal Energies= -2476.442900
Sum of electronic and thermal Enthalpies= -2476.441956

Sum of electronic and thermal Free Energies= -2476.558365

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	398.174	159.140	245.005

C,0,3.8620835884,-1.2325432962,0.1844027081
C,0,2.7856778945,-0.5225013165,0.7543779766
C,0,3.0812126696,0.1120839156,1.9836747256
C,0,4.3416657512,0.0457394158,2.5853205204
C,0,5.3815103098,-0.6625667454,1.982601111
C,0,5.1314219323,-1.3049545175,0.7719604135
Ir,0,0.7140744968,-0.4285371624,-0.0326731364
P,0,1.4322975928,-0.025306976,-2.2440524825
C,0,1.3645640142,-1.6362437186,-3.1924058444
C,0,1.7207788033,-2.8569480536,-2.330701268
P,0,0.8029733109,-2.8163104567,-0.6975743067
B,0,-1.2338808571,0.0046038599,-0.8367452593
O,0,-2.0663758078,-0.8687670779,-1.5835648084
C,0,-3.1407367064,-0.126489484,-2.0242688872
O,0,-1.8310203967,1.2824810213,-0.8521235659
B,0,-0.8835809916,-0.8766233131,1.3538904833
O,0,-1.301533864,-2.2040940026,1.6341397901
C,0,-2.4417310075,-2.0962233667,2.3972426341
O,0,-1.760087077,0.0188280776,1.9949468536
B,0,0.8047258365,1.6112117931,0.3895518964
O,0,0.5083865558,2.2129793384,1.6283629925
C,0,0.7240733249,3.561206779,1.4845922185
O,0,1.2219041156,2.6305671934,-0.5079507395
H,0,0.4682220423,-0.6598999956,1.6136223548
H,0,3.729064815,-1.7611931135,-0.7548761789
H,0,5.9204783597,-1.8685667919,0.2781306672
H,0,2.3100529895,0.6813053123,2.4938662904
H,0,4.5068104457,0.5546007547,3.5323960986
H,0,6.3627102115,-0.7136323112,2.4465320092
C,0,0.436814218,1.0971298067,-3.3148624607
C,0,3.1196979046,0.6609700171,-2.515028824
C,0,-0.7335098523,-3.7585688576,-1.1055072662
C,0,1.7096039987,-4.0337852532,0.3519109664
H,0,1.4873170258,-3.7849880188,-2.8648584026
H,0,2.7930475238,-2.8756263233,-2.1146351978
H,0,0.3312511609,-1.7218218906,-3.5472062906
H,0,2.0066736499,-1.5696686148,-4.0781443194
H,0,3.3430840349,0.6993976682,-3.5858773337
H,0,3.1289307075,1.6717095517,-2.1009740483
H,0,3.8738301656,0.0736582251,-1.9935404399
H,0,0.902139627,1.1812654346,-4.3019535478
H,0,-0.5804864172,0.7191683718,-3.4326873945
H,0,0.3986180033,2.0790612261,-2.8405062205
H,0,1.8311611868,-4.9948672362,-0.1582797267
H,0,2.6864635804,-3.6310571923,0.6257881948
H,0,1.1313379412,-4.1866848014,1.2673093856
H,0,-0.4871003588,-4.7450394188,-1.5120163049
H,0,-1.3227314094,-3.8714133103,-0.1942688815
H,0,-1.3321008763,-3.1936482828,-1.8211382003
C,0,-3.2433442867,-3.100856973,2.910975912
C,0,-4.3551118927,-2.6945514803,3.665572679
C,0,-4.6321640334,-1.3405577842,3.8827723615
C,0,-3.8107783316,-0.3317098818,3.3565084042
C,0,-2.717044957,-0.7449022414,2.614910264
H,0,-3.0183747921,-4.148216783,2.7395703865
H,0,-5.0114278027,-3.4488426147,4.088704383
H,0,-5.5009321868,-1.0617051834,4.471166841
H,0,-4.0144328411,0.7210917991,3.518002932
C,0,-4.2261399359,-0.5254819056,-2.7863006177
C,0,-5.1780849323,0.4601425555,-3.0887606067
C,0,-5.0303655066,1.7772928938,-2.6387183111
C,0,-3.9257291642,2.1678584042,-1.8669339476

C,0,-2.9929593925,1.1860709711,-1.5751290024
H,0,-4.3336842341,-1.5502041679,-3.1262177742
H,0,-6.0468371312,0.1927892788,-3.6825625667
H,0,-5.7872527498,2.5141357462,-2.8898459034
H,0,-3.8026983881,3.1847037689,-1.5101170997
C,0,0.5635981206,4.5738389192,2.4149221735
C,0,0.8606636282,5.8778964372,1.988245085
C,0,1.2974392528,6.1357792181,0.6848648018
C,0,1.4558848366,5.0997009445,-0.249576331
C,0,1.159190775,3.8192042021,0.1840322545
H,0,0.2230640851,4.3620366552,3.4227788516
H,0,0.7479444133,6.7019646779,2.6863768844
H,0,1.5188950164,7.1562588213,0.387015511
H,0,1.7941502639,5.289643859,-1.2629615182

hartwigdmpelrBcat3HPh

dmpeIr(Bcat)3(H)(Ph) hartwig
B3LYP/gen
E(RB+HF-LYP) = -2477.07696407

Zero-point correction= 0.593711 (Hartree/Particle)
Thermal correction to Energy= 0.634560
Thermal correction to Enthalpy= 0.635504
Thermal correction to Gibbs Free Energy= 0.519402
Sum of electronic and ZPE= -2476.483253
Sum of electronic and thermal Energies= -2476.442404
Sum of electronic and thermal Enthalpies= -2476.441460
Sum of electronic and thermal Free Energies= -2476.557562

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	398.192	159.074	244.357

C,0,3.1370943876,-0.2304676149,-2.0742809283
C,0,2.8371019429,1.1218231087,-1.9096516362
C,0,3.6381473354,2.1186106587,-2.442056117
H,0,3.3975100379,3.1672223716,-2.3046344294
C,0,4.7698277153,1.7011554918,-3.1585531897
C,0,5.0700029013,0.3440790858,-3.3239533479
H,0,5.9556475165,0.0571546737,-3.8826013979
C,0,4.2506326586,-0.6563859005,-2.7789771603
H,0,4.4776481379,-1.7107674105,-2.8972311245
C,0,-1.632598678,3.519374989,-0.6339013347
C,0,-1.4363980732,3.5626806431,0.7470757039
C,0,-1.5850596339,4.7347018762,1.4688467883
H,0,-1.4298778381,4.757376551,2.5421441757
C,0,-1.9433403563,5.882603845,0.7443894583
C,0,-2.1394021003,5.8386233157,-0.6397233086
H,0,-2.4152296879,6.7452154424,-1.1699520538
C,0,-1.9857697675,4.643301888,-1.360383165
H,0,-2.1339093736,4.5993909008,-2.434456086
C,0,2.8173653807,-0.7403451647,2.706611629
C,0,2.6494440558,0.645103355,2.6581740478
C,0,3.5246029288,1.5108811638,3.2918704778
H,0,3.3830341488,2.5850975469,3.2470730859
C,0,4.5925344576,0.9267471665,3.9900877486
C,0,4.7601314357,-0.4613925683,4.0391741889
C,0,3.8665686795,-1.3288464251,3.3916824693
H,0,3.9867148493,-2.4064124034,3.4257583934
C,0,-1.56970298,-2.5615046569,-2.5845728765
H,0,-2.5398504753,-2.9294903433,-2.2355394528
H,0,-1.5696174991,-2.6523553976,-3.6770806392
C,0,-0.4285682853,-3.3774707712,-1.9626243554
H,0,0.5229214912,-3.1087385552,-2.4344728525
H,0,-0.5831126594,-4.4507340716,-2.123503084
C,0,-3.1374145111,-0.0892467494,-2.5071498027

H,0,-3.4333723512,-0.3799507598,-3.5201223911
C,0,-0.4660041148,-0.0141875299,-3.4847340369
H,0,-0.3409001589,1.050339341,-3.2773931887
C,0,-1.2569325549,-4.2448746761,0.7338642032
H,0,-1.008693509,-4.2126334361,1.7989331196
B,0,1.2456084792,-0.0642243938,-0.863326198
B,0,-1.0682350044,1.4617971281,0.0690989939
B,0,1.0060328363,-0.288159872,1.4789636761
O,0,2.1693671467,-0.978263123,-1.4389816694
O,0,1.6845773985,1.2379944955,-1.1742917303
O,0,-1.417412503,2.2324866393,-1.0726366028
O,0,-1.0968480028,2.309690234,1.1927165817
O,0,1.8026965504,-1.339330441,1.9968849782
O,0,1.5312989953,0.9401526126,1.9208485913
P,0,-1.4652492313,-0.7525884004,-2.123132335
P,0,-0.1824204132,-3.0189113277,-0.1407630934
Ir,0,-0.6244265561,-0.5766443729,0.0769055913
C,0,1.4760840305,-3.7855084485,0.1327371707
H,0,5.5974719457,-0.8790880396,4.5897981678
H,0,2.2330050456,-3.1974991008,-0.3869543379
H,0,5.3027456948,1.5679829748,4.5031242436
H,0,5.4271503922,2.4488864299,-3.5917389171
H,0,-2.0700266553,6.8233077212,1.2718265915
H,0,1.7046078895,-3.7737659472,1.1991092103
H,0,1.4828625165,-4.8172861396,-0.2345691112
H,0,-1.0834577472,-5.2592442455,0.3600528971
H,0,-2.31067585,-3.984612811,0.635107841
H,0,-3.0866054272,0.9982066829,-2.4340229406
H,0,-3.865968738,-0.4545238358,-1.7834599182
H,0,-0.9780986558,-0.1441989116,-4.4431791029
H,0,0.5186497775,-0.4830687944,-3.5374575144
H,0,-0.3521167599,-0.4712607684,1.7300805164
C,0,-2.6548879851,-0.8815568493,0.8965181396
C,0,-3.6294772515,-1.7767727523,0.4084498227
H,0,-3.4284816254,-2.3792583977,-0.4736171826
C,0,-4.8816738074,-1.951471839,1.0111375504
H,0,-5.5900446212,-2.6575114924,0.5823603025
C,0,-5.2167698794,-1.2285692369,2.1537574233
H,0,-6.1849835528,-1.3585373714,2.6294352196
C,0,-4.2797781354,-0.3341171161,2.6719546888
H,0,-4.5142465549,0.2439827275,3.5630147492
C,0,-3.0366600566,-0.1652909393,2.0548174105
H,0,-2.3526527029,0.5579217519,2.4872657872

hartwigbpyIrBeg3

hartwig bpyIr(Beg)3
B3LYP/gen
E(RB+HF-LYP) = -1361.88631332

Zero-point correction= 0.371311 (Hartree/Particle)
Thermal correction to Energy= 0.398039
Thermal correction to Enthalpy= 0.398983
Thermal correction to Gibbs Free Energy= 0.308834
Sum of electronic and ZPE= -1361.515002
Sum of electronic and thermal Energies= -1361.488274
Sum of electronic and thermal Enthalpies= -1361.487330
Sum of electronic and thermal Free Energies= -1361.577479

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 249.773	96.371	189.734

B,0,1.67694854,12.9510099861,5.5912064143
B,0,2.0308433634,11.0231739558,3.6035548599
B,0,2.5460925209,10.4635067942,6.2713140169
C,0,-0.0995353648,11.4148848888,8.3190147456

H,0,0.9736699163,11.3427448301,8.4547571223
C,0,-0.9684680193,11.6042682512,9.3895403846
H,0,-0.5769670278,11.6643996932,10.3992038549
C,0,-2.3325153689,11.7219713918,9.1286838615
C,0,-2.7755352092,11.652243633,7.8113802978
C,0,-1.8472711224,11.4525923143,6.7818762834
C,0,-2.2323080371,11.393787351,5.3478207894
C,0,-3.565736618,11.3694617642,4.9217991874
H,0,-4.3748585202,11.3603497409,5.6419870773
C,0,-3.8508321891,11.3444393388,3.5594939227
C,0,-2.7964227886,11.3422546461,2.6493665629
H,0,-2.9715198707,11.326088023,1.5790137843
C,0,-1.4911700944,11.3521666364,3.1373159621
H,0,-0.6223161996,11.339532657,2.4856169055
C,0,2.7231192817,14.9680892337,5.2611758898
C,0,2.1506459674,14.9087271678,6.6925857056
C,0,3.7716715516,10.7292470963,2.109345094
C,0,2.5090310207,11.1621921135,1.3345533947
C,0,4.4181450398,10.2571429428,7.6014025428
C,0,3.9622278914,8.8590233168,7.1375456141
Ir,0,0.8965058488,11.1381348413,5.3084678905
N,0,-0.525700241,11.3291779651,7.0481806113
N,0,-1.2130623919,11.3744159022,4.452823366
O,0,2.5408377359,13.6467408459,4.7478808082
O,0,1.3303456722,13.7372882328,6.6992331327
O,0,3.4053768768,10.8278849437,3.4838986315
O,0,1.4644282664,11.1294330405,2.3121935246
O,0,3.351415926,11.1283520656,7.2101765907
O,0,2.9264887545,9.1174053621,6.1873498373
H,0,-3.8297787786,11.767944348,7.5906099621
H,0,-4.8815536823,11.3245110916,3.2185830692
H,0,-3.0422636997,11.8762879,9.9356293819
H,0,3.7858713399,15.2310135199,5.2385334593
H,0,1.5478811709,15.7868007759,6.9490748561
H,0,2.1779593424,15.6827126696,4.6291999825
H,0,2.9430638413,14.7999077932,7.4448307424
H,0,4.5723122258,10.3206725608,8.6843754949
H,0,3.5594961214,8.2609480423,7.9672786275
H,0,4.0604082261,9.6941257594,1.8814111523
H,0,2.2643119358,10.4885102722,0.5054818826
H,0,4.6323552636,11.3760843343,1.906539341
H,0,2.5998512743,12.1809600379,0.935271539
H,0,5.3437761481,10.5722703728,7.1027004781
H,0,4.76640616,8.2860565561,6.6635283649

hartwigbpyIrBeg3HPh

bpyIr(Beg)3(H)(Ph) hartwig

B3LYP/gen

E(RB+HF-LYP) = -1594.12059163

Zero-point correction= 0.470966 (Hartree/Particle)

Thermal correction to Energy= 0.502262

Thermal correction to Enthalpy= 0.503206

Thermal correction to Gibbs Free Energy= 0.405423

Sum of electronic and ZPE= -1593.649626

Sum of electronic and thermal Energies= -1593.618330

Sum of electronic and thermal Enthalpies= -1593.617386

Sum of electronic and thermal Free Energies= -1593.715169

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 315.174	117.182	205.802

B,0,-0.0067260837,-0.00881875,-0.0224370136
B,0,-0.0110226838,0.0056130903,3.0004175269
B,0,2.0518459949,-0.0002246659,0.8224633405

C,0,2.386567924,3.4104784376,-0.2146259034
H,0,3.1621549466,2.6993947864,0.0421942425
C,0,2.6611143143,4.5859823686,-0.9088728316
H,0,3.682593601,4.8229618481,-1.1862696193
C,0,1.6044260584,5.4364884929,-1.2262839441
C,0,0.315023131,5.0730590207,-0.8541317835
C,0,0.1102715573,3.8703570398,-0.1648368041
C,0,-1.2317868447,3.399540757,0.2453688297
C,0,-2.4081314089,4.0583907904,-0.1337419835
H,0,-2.3598509811,4.9508641456,-0.7445003321
C,0,-3.6426063926,3.5606375755,0.2655036463
C,0,-3.6787526647,2.4030797601,1.0389025739
H,0,-4.6153874515,1.9737179169,1.3772443262
C,0,-2.4805576052,1.7865975457,1.3829075312
H,0,-2.447285452,0.8906919955,1.9914378805
C,0,-1.2729448353,-1.6155721423,-1.0706899913
C,0,-0.6361845698,-0.6920998136,-2.130699774
C,0,0.0302646068,-1.5930716313,4.6518082845
C,0,-1.3903631048,-1.003920597,4.5511790861
C,0,4.0659453496,-0.5973180882,-0.1357886034
C,0,3.3190823596,-1.862413864,0.3482477038
Ir,0,0.6078991036,1.3312299849,1.5642055769
N,0,1.1456714342,3.0635893138,0.1570718002
N,0,-1.2829438234,2.2696742146,0.9985721716
O,0,-0.9655430963,-0.9908547736,0.1814898753
O,0,0.241627796,0.1618802656,-1.3826381991
O,0,0.8243153128,-0.7557917832,3.8094047732
O,0,-1.3481052887,-0.1854190813,3.3757053848
O,0,3.1480037985,0.4756486153,0.0904072571
O,0,2.160062505,-1.3719887471,1.0232395718
H,0,-0.5161226773,5.7263254073,-1.0892365228
H,0,-4.5571973838,4.0681668566,-0.0252684564
H,0,1.7777769892,6.3680803883,-1.7561392153
H,0,4.9837856798,-0.4144011881,0.43704592
H,0,3.0062070798,-2.5016469982,-0.4869276771
H,0,-0.0615756485,-1.237933449,-2.8859356165
H,0,-2.3584553229,-1.7069203787,-1.1802182972
H,0,0.4268665051,-1.5744699081,5.6720919018
H,0,-2.1658186429,-1.769006204,4.4411385485
H,0,0.0737579966,-2.6256718398,4.2813826622
H,0,-1.6387984662,-0.3762994553,5.4169179167
H,0,4.3260985829,-0.6398993007,-1.1988848164
H,0,3.9154772957,-2.4683249153,1.0383265505
H,0,-0.8390957141,-2.6231054956,-1.0834169494
H,0,-1.3818671914,-0.0747088464,-2.6475045721
H,0,2.0049504327,0.9168699064,2.2222058424
C,0,0.6696865235,2.7951012961,3.1607749149
C,0,-0.438402099,3.1046144626,3.9731660526
H,0,-1.3679926199,2.5541255504,3.84612392
C,0,-0.3866957232,4.0932633223,4.9626572807
H,0,-1.2690083601,4.2981997833,5.5661046616
C,0,0.790337736,4.8085146228,5.1833479945
C,0,1.9118867491,4.5155822713,4.4052587469
H,0,0.8361032511,5.5749910031,5.952848726
H,0,2.8432598001,5.0545197408,4.568212431
C,0,1.8472740736,3.5275035091,3.4181604852
H,0,2.7450126469,3.3229298311,2.8379529678

Ir_bpy_Bpin3_PhH_CHact_ts_lit

E(RB+HF-LYP) = -1594.10718476

Zero-point correction=	0.468878 (Hartree/Particle)
Thermal correction to Energy=	0.500951
Thermal correction to Enthalpy=	0.501896
Thermal correction to Gibbs Free Energy=	0.401240
Sum of electronic and zero-point Energies=	-1593.638306

Sum of electronic and thermal Energies=	-1593.606233
Sum of electronic and thermal Enthalpies=	-1593.605289
Sum of electronic and thermal Free Energies=	-1593.705944

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	314.352	118.627	211.847
C,0,-3.1488959587,3.0024722008,-2.6260586062			
C,0,-2.3480037554,3.5389683806,-1.6160863832			
C,0,-1.3401889858,2.768909144,-1.0283888314			
C,0,-1.1209579837,1.432658029,-1.4116503175			
C,0,-1.9217123737,0.9217277399,-2.4484893358			
C,0,-2.9261751663,1.6900488548,-3.044818907			
Ir,0,0.2261427672,0.1380044766,-0.1778117126			
N,0,-1.242776276,-1.5986742643,-0.4876133999			
C,0,-2.2728811956,-1.6760772232,0.384446917			
C,0,-3.2249212868,-2.7009870847,0.290367618			
C,0,-3.119338244,-3.6526130077,-0.7165265914			
C,0,-2.0458511843,-3.5627336789,-1.6085800733			
C,0,-1.1341061112,-2.5216951479,-1.4563289667			
C,0,-2.3216235924,-0.6354449741,1.4390374084			
N,0,-1.3107312616,0.268604591,1.4511937031			
C,0,-1.288703656,1.2193363967,2.4025150771			
C,0,-2.2752424935,1.3233249279,3.3785458513			
C,0,-3.3259176944,0.4094792961,3.371305914			
C,0,-3.3458066751,-0.5784385261,2.3935516679			
B,0,1.3483984575,-1.0422182173,1.2055543175			
O,0,1.3274923845,-2.43973934,1.2259065046			
C,0,2.0779808414,-2.9072587986,2.3545229381			
C,0,2.7810371991,-1.6472946948,2.9022339125			
O,0,2.1230984264,-0.554813676,2.2506506593			
B,0,1.7928176349,-0.6679371611,-1.2768925149			
O,0,3.1470813853,-0.6855771368,-0.9694285559			
C,0,3.8727651748,-1.2720162611,-2.0525224081			
C,0,2.7947728107,-1.9696891993,-2.9031369838			
O,0,1.5673692119,-1.3627576365,-2.4778397744			
B,0,1.4459151553,1.7141537658,0.3030835297			
O,0,1.2734042805,2.5231674366,1.4397262099			
C,0,2.1741190307,3.6348962142,1.3767412255			
C,0,3.1396962035,3.2758513669,0.2298533396			
O,0,2.4792884373,2.2267367833,-0.4783374996			
H,0,0.3990761114,0.8017565506,-1.6348834681			
H,0,-0.2803017765,-2.4018284297,-2.114788313			
H,0,-4.0455958862,-2.7610373646,0.9942322719			
H,0,-1.9138671768,-4.2824862649,-2.4093401278			
H,0,-3.8440124818,-4.4501443878,-0.7991605351			
H,0,-4.1552354099,-1.2969726914,2.3728784919			
H,0,-4.1170665913,0.4604817714,4.1130924232			
H,0,-2.2108718583,2.1094183014,4.1230667215			
H,0,-0.4442983701,1.898325419,2.3607196091			
H,0,2.7511055005,-3.0497174461,-2.7096309889			
H,0,2.9273499307,-1.814488161,-3.9783956369			
H,0,4.6234331426,-1.9664981728,-1.6616968462			
H,0,4.3896171364,-0.4803524588,-2.6098567591			
H,0,-0.7281025644,3.2122379404,-0.2477276784			
H,0,-2.5024618292,4.564010079,-1.2862611959			
H,0,-3.9272173276,3.6035088449,-3.0886952254			
H,0,-1.7558834075,-0.0911825463,-2.8054510837			
H,0,-3.5289588904,1.2626905232,-3.8430852301			
H,0,1.3902726393,-3.3512702769,3.0861794694			
H,0,2.7820968814,-3.6823096418,2.0337539432			
H,0,2.6837352699,-1.5422679451,3.9880295761			
H,0,3.8480614098,-1.6260056595,2.6480246366			
H,0,1.6046803421,4.5503574623,1.1667609878			
H,0,2.6797398668,3.7556755328,2.3403111745			
H,0,3.3305898835,4.1169563479,-0.4449271614			
H,0,4.1034499582,2.9086185741,0.6059368903			

Ir(bpy)_Bpin3_H_Ph

Ir(bpy)(Bpin)3(H)(Ph)
E(RB+HF-LYP) = -1594.12080695

Zero-point correction= 0.471227 (Hartree/Particle)
Thermal correction to Energy= 0.503172
Thermal correction to Enthalpy= 0.504117
Thermal correction to Gibbs Free Energy= 0.404809
Sum of electronic and ZPE= -1593.649580
Sum of electronic and thermal Energies= -1593.617635
Sum of electronic and thermal Enthalpies= -1593.616690
Sum of electronic and thermal Free Energies= -1593.715998

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	315.745	119.135	209.011

C,0,-2.8055939266,-1.5654994903,2.4395703342
C,0,-1.9674507461,-1.2412593949,1.3654448844
N,0,-1.1043043185,-0.1949118581,1.4528452027
C,0,-1.0599186721,0.5306890804,2.5870491932
C,0,-1.8719332165,0.2546096338,3.6819767746
C,0,-2.7609885167,-0.8144420679,3.6079648709
C,0,-1.9599648627,-2.0134074594,0.1019760715
N,0,-1.0932292629,-1.5940520281,-0.8458858954
C,0,-1.0348776378,-2.2482634842,-2.0149770712
C,0,-1.8287369307,-3.3567343177,-2.2967121671
C,0,-2.7172683722,-3.805785948,-1.3225407446
C,0,-2.784809909,-3.126206337,-0.1115433821
Ir,0,0.1699583868,0.2300914453,-0.2755238175
B,0,1.1002911323,1.9612372229,0.3079599847
O,0,1.9255583611,2.7434093229,-0.4918603698
C,0,2.4448802825,3.8260592638,0.2817699474
C,0,1.5561291062,3.8606249752,1.5404433207
O,0,0.9238100162,2.5744368002,1.5569689499
C,0,-1.4333741744,1.5034759703,-0.9770183579
C,0,-2.0567817002,2.4819363796,-0.178630972
C,0,-3.1056100229,3.2778654964,-0.6536656539
C,0,-3.5675627196,3.1276376222,-1.9612204114
C,0,-2.9648851428,2.1728172694,-2.7822178582
C,0,-1.9205345062,1.3808204499,-2.294874265
B,0,1.4967721579,-0.9875930755,0.9318836037
O,0,2.1931867735,-0.4835235952,2.0182372354
C,0,2.8181123705,-1.5655706549,2.718810281
C,0,2.1618798432,-2.834893184,2.135730671
O,0,1.5002829515,-2.3818519365,0.9455381669
B,0,1.9246193461,-0.4804029163,-1.1802005825
O,0,1.8624519557,-1.4393151938,-2.2037310442
C,0,3.198676525,-1.7933283541,-2.5720873132
C,0,4.0539862527,-0.6421727623,-2.0143312777
O,0,3.2408990321,-0.0696487982,-0.985904356
H,0,0.8178391,0.6951343233,-1.661930176
H,0,-0.3008759923,-1.8805688281,-2.7202501894
H,0,-3.4698513802,-3.4648981112,0.6555315759
H,0,-1.739170917,-3.8547322535,-3.2561016801
H,0,-3.3467888802,-4.6726322766,-1.498452787
H,0,-3.488807091,-2.4017745454,2.3647009845
H,0,-3.4082038589,-1.0634517369,4.443260231
H,0,-1.7972611403,0.8723948842,4.5701554199
H,0,-0.3449834724,1.3456717922,2.5900841949
H,0,3.4573877893,-2.7569061966,-2.1131292913
H,0,3.2681452577,-1.8947065534,-3.6598168152
H,0,5.0045610179,-0.9785263018,-1.5887904029
H,0,4.2630749682,0.1208541082,-2.7753924568
H,0,-1.7079413166,2.6485169381,0.8382715492

H,0,-3.5544524246,4.023690986,-0.0001942852
H,0,-4.3767795579,3.7485957337,-2.3371358154
H,0,-1.4705004944,0.6547561257,-2.9694042339
H,0,-3.3034666416,2.0461324437,-3.8087294842
H,0,1.4175017618,-3.268905596,2.8155805134
H,0,2.8865628535,-3.6140866148,1.8789741318
H,0,2.6497685924,-1.4533134301,3.7946996358
H,0,3.8988034908,-1.5350106172,2.5331294094
H,0,0.7853134962,4.6400369823,1.480239655
H,0,2.125555311,4.003912433,2.464511364
H,0,2.3966343269,4.7531122895,-0.2985746593
H,0,3.4957084233,3.6243148649,0.5276774728

IrDMPE_Bpin3

Ir(dmpe)(Bpin)₃
E(RB+HF-LYP) = -1787.53406933

Zero-point correction= 0.422265 (Hartree/Particle)
Thermal correction to Energy= 0.452674
Thermal correction to Enthalpy= 0.453618
Thermal correction to Gibbs Free Energy= 0.358714
Sum of electronic and ZPE= -1787.111805
Sum of electronic and thermal Energies= -1787.081396
Sum of electronic and thermal Enthalpies= -1787.080451
Sum of electronic and thermal Free Energies= -1787.175355

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 284.057	107.871	199.742

C,0,-0.0998131177,3.2568065064,-1.1552701002
C,0,-1.53510628,3.1758412935,-0.6082769419
P,0,-1.7485392914,1.6962272453,0.5346572546
Ir,0,-0.2754951103,-0.0662230201,-0.2156894707
B,0,-1.0755465087,-1.5239398737,1.0484418065
O,0,-0.5839766411,-2.1808422998,2.1700741798
C,0,-1.5817699311,-3.0809984012,2.6641008626
C,0,-2.6302920835,-3.154014752,1.5381042893
O,0,-2.367316897,-1.9907671463,0.7418762704
P,0,0.4736036486,1.5923924697,-1.7936993464
B,0,0.9400309886,-1.5958866449,-0.968973738
O,0,2.2844852697,-1.4788362592,-1.3532793715
C,0,2.7765585758,-2.7735430525,-1.7219486515
C,0,1.50588777,-3.6156850644,-1.9375677668
O,0,0.4758978209,-2.8812307237,-1.265874026
B,0,1.2320940715,0.3337536033,1.0443468917
O,0,1.6275225251,1.6592903401,1.3417142442
C,0,2.6258908048,1.6099369763,2.3715706276
C,0,3.0842310265,0.1384932015,2.3833864848
O,0,2.0324245486,-0.5677467169,1.7263975732
C,0,2.2715409997,1.8610427246,-2.1014058035
C,0,-0.2111595926,1.5393848358,-3.5177571117
H,0,-0.0140308356,4.0293683758,-1.9290731359
H,0,0.5956993026,3.5068778012,-0.3468481106
C,0,-1.5040128154,2.4169878822,2.2185331801
C,0,-3.5782536981,1.4229436078,0.4933314916
H,0,-1.8154924832,4.1036590793,-0.0959002577
H,0,-2.2468426843,3.0397804773,-1.4324692408
H,0,-3.6612726232,-3.1259977852,1.9070436487
H,0,-2.5075725048,-4.0522133236,0.9194475068
H,0,-2.0046701925,-2.6804337317,3.5959039472
H,0,-1.1253471235,-4.0513280443,2.8854031672
H,0,1.5810985793,-4.6207370518,-1.5099032033
H,0,1.2493634305,-3.7128679146,-3.0013258492
H,0,3.3983946246,-3.168895203,-0.9083818245
H,0,3.3957994676,-2.69353832,-2.6219543291

H,0,3.2211567115,-0.2568616815,3.3949771746
H,0,4.0197590543,-0.0032257885,1.826003086
H,0,2.1730819854,1.9059851991,3.3273378541
H,0,3.4335706585,2.312132087,2.1402564159
H,0,2.4531376452,2.6749743011,-2.8109826595
H,0,2.7489630116,2.0899345681,-1.1462137224
H,0,2.6986286922,0.9281862065,-2.4760307203
H,0,0.0927100535,2.4119639534,-4.105965506
H,0,0.1482361305,0.6332850918,-4.0136237471
H,0,-1.3035550198,1.4928816315,-3.487511442
H,0,-4.1375945339,2.3230439508,0.7695239
H,0,-3.8767789712,1.1061538315,-0.5098568302
H,0,-3.8249025403,0.609818897,1.1804060133
H,0,-2.146742446,3.2876280983,2.3861495683
H,0,-1.7307528906,1.6511895897,2.9655268481
H,0,-0.4542820861,2.6973650053,2.3246329488

Irbpy_Bpin3

Ir(bpy)(Bpin)₃
E(RB+HF-LYP) = -1361.88604005

Zero-point correction= 0.371266 (Hartree/Particle)
Thermal correction to Energy= 0.398025
Thermal correction to Enthalpy= 0.398970
Thermal correction to Gibbs Free Energy= 0.308975
Sum of electronic and ZPE= -1361.514774
Sum of electronic and thermal Energies= -1361.488015
Sum of electronic and thermal Enthalpies= -1361.487070
Sum of electronic and thermal Free Energies= -1361.577065

E	CV	S
KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total 249.765	96.398	189.409

Ir,0,0.1635529963,-0.0019094733,-0.3550644187
N,0,-1.6842220373,-1.3242024742,-0.3021789652
C,0,-1.6256370623,-2.6645757355,-0.3534373128
C,0,-2.7634429459,-3.4671133061,-0.3567002198
C,0,-4.0120662192,-2.850196709,-0.3178834255
C,0,-4.0771453459,-1.460367922,-0.2837350353
C,0,-2.8927170904,-0.7133997067,-0.2741108335
C,0,-2.8769697537,0.7727534562,-0.2485551209
C,0,-4.0399715543,1.5393847251,-0.1068660274
C,0,-3.9501671081,2.9283665343,-0.0957830814
C,0,-2.6970568276,3.5234925114,-0.220905321
C,0,-1.577029354,2.7050171787,-0.350527355
N,0,-1.6619781442,1.3631004046,-0.3661778484
H,0,-0.6272553316,-3.0831748911,-0.4117908427
H,0,-2.6644566116,-4.5465073703,-0.3943192874
H,0,-4.9243368776,-3.4388223782,-0.3231714212
H,0,-5.0417444668,-0.9677926489,-0.2744218921
H,0,-5.0060173682,1.0622849603,0.0048971541
H,0,-4.8459147062,3.5319721479,0.0146066334
H,0,-2.5781267236,4.6016437793,-0.2128689361
H,0,-0.5689868252,3.1020477523,-0.429607818
B,0,1.6178556436,-1.421365855,-0.4417094845
O,0,1.5694137791,-2.409250205,-1.4468809594
C,0,2.655211665,-3.3264759146,-1.2670842422
C,0,3.5114341307,-2.704496194,-0.1410901345
O,0,2.7010996382,-1.6632724251,0.4036356553
H,0,3.7678717277,-3.4257634036,0.6432478285
H,0,4.4434804406,-2.2720535592,-0.5269004419
H,0,3.2067247901,-3.4364883299,-2.2070309954
H,0,2.2560693642,-4.3119243577,-0.9898754063
H,0,2.5546383656,-0.1494755472,3.7241725914
H,0,1.7241588098,1.3376963939,4.2393296195

C, 0, 0.3660479798, -0.360954298, 3.8267241368
H, 0, 0.5421253971, -1.270617768, 4.410605262
H, 0, -0.410655612, 0.2283672293, 4.3337189737
O, 0, -0.0833650325, -0.7068422912, 2.5122959171
B, 0, 0.6163648935, 0.0787194677, 1.5840153612
O, 0, 1.5629434267, 0.8714867851, 2.2239470178
B, 0, 1.6601240438, 1.349395882, -0.6708013671
O, 0, 2.9000269003, 1.1053276589, -1.2698762643
C, 0, 3.6766342648, 2.3031729144, -1.2779826212
C, 0, 2.6664399321, 3.4230846142, -0.9548401305
O, 0, 1.5254329132, 2.7345559308, -0.4363748757
H, 0, 4.4640426897, 2.2296571702, -0.5162487195
H, 0, 4.1557006179, 2.4313683395, -2.2550353844
H, 0, 3.0419319346, 4.1335178567, -0.2102943564
H, 0, 2.3766735708, 3.9880415964, -1.8521626357
C, 0, 1.6510621992, 0.4591371613, 3.5894623135

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