Supporting Information for:

Mechanistic Investigations of Cu-Catalyzed Fluorination of Diaryliodonium Salts: Elaborating the Cu^{I}/Cu^{III} Manifold in Copper Catalysis

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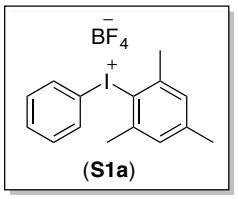
I. General Procedures and Materials and Methods

General Procedures. NMR spectra were obtained on a Varian MR400 (400.52 MHz for ^{1}H; 100.71 MHz for ^{13}C; 376.87 MHz for ^{19}F), a Varian vnmrs 500 (500.10 MHz for ^{1}H), or a Varian vnmrs 700 (699.76 MHz for ^{1}H; 175.95 MHz for ^{13}C) spectrometer. ^{1}H and ^{13}C NMR chemical shifts are reported in parts per million (ppm) relative to TMS, with the residual solvent peak used as an internal reference. ^{19}F NMR spectra are referenced based on the internal standard 1-fluoro-3-nitrobenzene (–109.03 ppm). UV-Vis spectra for Cu trapping experiments were obtained on Shimadzu UV-1601 UV-VIS Spectrometer. Slow addition experiments with $NBu_4F•H_2O$ were performed using a Fisher Scientific syringe pump (90-120V/60 Hz).

Materials and Methods. Diaryliodonium substrates **S1a-S5a** were prepared according to literature procedures and stored in a drybox under N_2 until use.[1] $MesI(OAc)_2$ was obtained from TCI America. *m*-CPBA was obtained from Sigma Aldrich. Aryl boronic acids were obtained from Frontier Scientific and Oakwood Products. Anhydrous KF, anhydrous DMF $BF_3•OEt_2$ and $NBu_4F•H_2O$ were obtained from Alfa Aesar and used as received. $Cu(OTf)_2$ was obtained from Strem. $(CH_3CN)_4CuOTf$ was purchased from Sigma Aldrich. 2,2'-biquinoline, 4-iodonitrobenzene and 18-crown-6 were obtained from Acros. TfOH and 1-fluoro-3-nitrobenzene were obtained from Oakwood Products. All reactions were conducted in a nitrogen atmosphere glovebox or using standard Schlenk techniques unless otherwise stated.

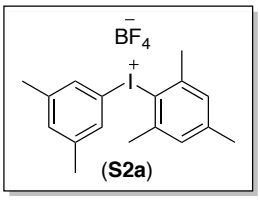
[1] Ichiishi, N.; Canty, A. J.; Yates, B. F.; Sanford, M. S. *Org. Lett.* **2013**, *15*, 5134–5137.

II. Synthesis of Diaryliodonium Substrates



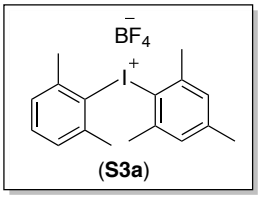
(**S1a**)

(*Mesityl)(phenyl)iodonium tetrafluoroborate* **S1a.** [Ph–I–Mes]BF_4 was prepared using a literature procedure[2] and was obtained as an off-white solid (2.79 g, 68% yield). The ^1H, ^{13}C, and ^{19}F NMR spectroscopic data for this compound were identical to that reported previously in the literature.[3] HRMS $[M\text{-}BF_4]^+$ Calcd for $C_{15}H_{16}I^+$: 323.0291; Found: 323.0301.



(**S2a**)

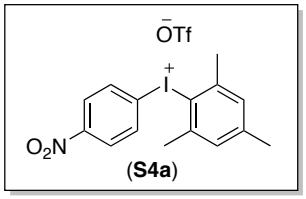
(*Mesityl)(3,5-dimethylphenyl)iodonium tetrafluoroborate* **S2a.** [3,5-MePh–I–Mes]BF_4 was prepared using a literature procedure[2] and was obtained as a white solid (479 mg, 73% yield). The ^1H, ^{13}C, and ^{19}F NMR spectroscopic data were identical to that reported previously in the literature.[1] HRMS $[M\text{-}BF_4]^+$ Calcd for $C_{17}H_{20}I^+$: 351.0604; Found: 351.0603.



(**S3a**)

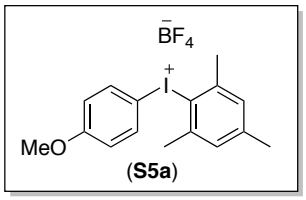
(*Mesityl)(2,6-dimethylphenyl)iodonium tetrafluoroborate* **S3a.** [2,6-MePh–I–Mes]BF_4 was prepared using a literature procedure[2] and was obtained as a white solid (331 mg, 72% yield). The ^1H, ^{13}C, and ^{19}F NMR spectroscopic data were identical to that reported previously in the literature.[1] HRMS $[M\text{-}BF_4]^+$ Calcd for $C_{17}H_{20}I^+$: 351.0604; Found: 351.0613.

[2] Chen, D.-W.; Ochiai, M. *J. Org. Chem.* **1999**, *64*, 6804.
[3] Kieffer, M. E.; Chuang, K. V.; Reisman, S. E. *Chem. Sci.* **2012**, *3*, 3170.



(**S4a**)

(*Mesityl)(4-nitrophenyl)iodonium trilfate* **S4a.**[4] To an oven-dried round-bottom flask equipped with a stir bar was added *m*-CPBA (950 mg, 5.5 mmol, 1.10 equiv), CH_2Cl_2 (0.20 M), 4-iodonitrobenzene (1.25 g, 5.0 mmol, 1.00 equiv), and mesitylene (0.77 mL, 5.5 mmol, 1.10 equiv). The mixture was cooled to 0 ºC and TfOH (0.90 mL, 10 mmol, 2.0 equiv) was added dropwise while stirring. The reaction was then warmed to room temperature and stirred for 2 h. The solvent was removed under vacuum, and Et_2O was added to provide a heterogeneous mixture, which was cooled to –20 ºC for 30 min. The product was collected on a fritted glass funnel, washed with Et_2O to afford **S4a** as a beige solid (1.55 g, 60% yield). The ^1H, ^{13}C, and ^{19}F NMR spectroscopic data were identical to that reported previously in the literature.[5] HRMS [M-OTf]$^+$ Calcd for $C_{15}H_{15}INO_2^+$: 368.0142; Found 368.0143.



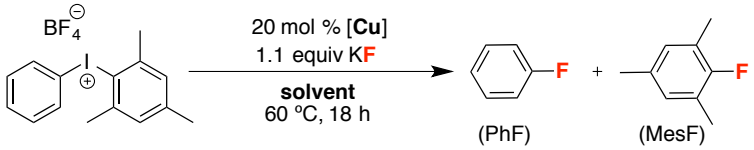
(**S5a**)

(*Mesityl)(4-methoxyphenyl)iodonium tetrafluoroborate* **S5a.** [4-OMePh–I–Mes]BF_4 was prepared using a literature procedure[2] and was obtained as an off-white solid (1.01 g, 76% yield). The ^1H, ^{13}C, and ^{19}F NMR spectroscopic data for this compound were identical to that reported previously in the literature.[2] HRMS [M-BF_4]$^+$ Calcd for $C_{16}H_{18}IO^+$: 353.0397; Found: 353.0404

[4] Bielawski, M.; Zhu, M.; Olofsson, B. *Adv. Synth. Catal.* **2007**, *349*, 2610.
[5] Bigot, A.; Williamson, A. E.; Gaunt, M. J. *J. Am. Chem. Soc.* **2011**, *133*, 13778.

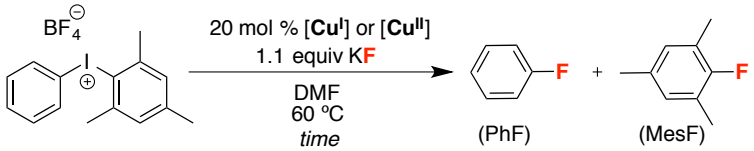
III. Experimental Details

A. Procedure for Experiments in Table 1



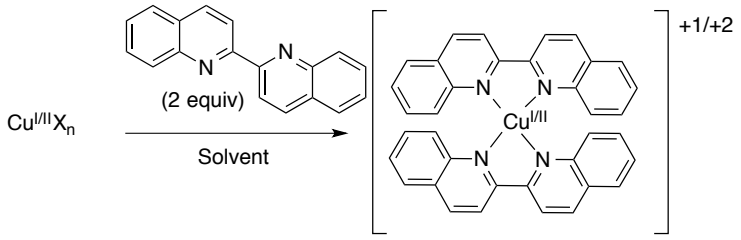
In a glovebox, [Ph-I-Mes]BF_4 (20.5 mg, 0.05 mmol, 1 equiv), [Cu] (0.01 mmol, 0.2 equiv), KF (3.2 mg, 0.055 mmol, 1.1 equiv) and 18-crown-6 (5.3 mg, 0.02 mmol, 0.4 equiv) were combined in DMF (0.5 mL) in a 4 mL vial. The vial was sealed with a Teflon-lined cap, and the reaction mixture was stirred at 60 ºC for 18 h. After cooling to room temperature, the reaction was quenched with sat. aqueous $NaHCO_3$ (0.5 mL), and 1-fluoro-3-nitrobenzene (5.3 µl, 0.05 mmol, 1 equiv) was added as an internal standard. After cooling, the reaction mixture was diluted with CH_2Cl_2 (2 mL), and was analyzed by ^{19}F NMR spectroscopy and GC-MS. The ^{19}F NMR data for PhF and MesF matched that of corresponding authentic samples and GC-MS analysis was used for further confirming the identity of products. All characterization data matched to the previous literature.[1]

B. Procedure for Experiments in Figure 1



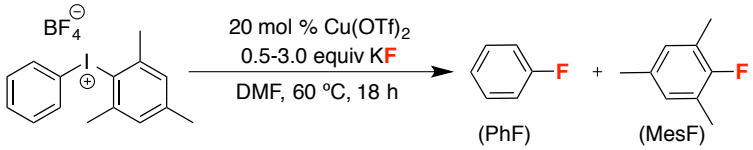
In a glovebox, [Ph-I-Mes]BF_4 (41.0 mg, 0.1 mmol, 1 equiv), $Cu(OTf)_2$ or $(CH_3CN)_4CuOTf$ (7.2 mg or 7.5 mg, 0.02 mmol, 0.2 equiv), KF (6.4 mg, 0.11 mmol, 1.1 equiv) and 18-crown-6 (5.3 mg, 0.02 mmol, 0.4 equiv) were combined in DMF (1.0 mL) in a 4 mL vial. The vial was sealed with a Teflon-lined cap, and the reaction mixture was stirred at 60 ºC for corresponding time in Figure 1. A reaction was quenched immediately at each time point by immersing the vial into liquid N_2 followed by adding sat. aqueous $NaHCO_3$ (0.1 mL), and 1-fluoro-3-nitrobenzene (5.3 µl, 0.05 mmol, 0.5 equiv) was added as an internal standard. The reaction was analyzed by ^{19}F NMR spectroscopy and GC-MS. The ^{19}F NMR data for PhF and MesF matched that of corresponding authentic samples and GC-MS analysis was used for further confirming the identity of products. All characterization data matched to the previous literature.[1]

C. Procedure for Experiments in Table 2



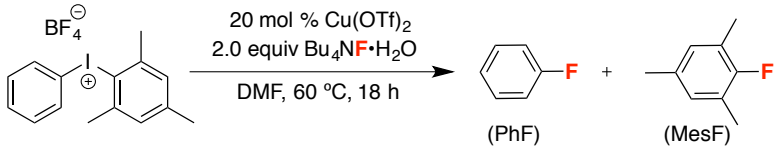
To a 4 mL vial charged with a stir bar was added $Cu(OTf)_2$ or $(CH_3CN)_4CuOTf$ (0.05 mmol, 1 equiv). The appropriate solvent (1.5 mL) was added via a syringe, and the reaction mixture was stirred until the Cu dissolved completely. To the mixture, 2,2'-biquinoline (25.6 mg, 0.10 mmol, 2 equiv) was added. The resulting mixture was stirred at rt for 1 h and then the color was recorded. The reaction was then diluted with 3.0 mL of the corresponding solvent to analyze via UV-Vis spectrometry.

D. Procedure for Experiments in Table 4



In a glovebox, $[Ph\text{-}I\text{-}Mes]BF_4$ (41.0 mg, 0.1 mmol, 1 equiv), $Cu(OTf)_2$ (7.2 mg, 0.02 mmol, 0.2 equiv), KF (0.5 -3.0 equiv), and 18-crown-6 (5.3 mg, 0.02 mmol, 0.4 equiv) were combined DMF (1.0 mL) in a 4 mL vial. The vial was sealed with a Teflon-lined cap, and the reaction mixture was stirred at 60 ºC for 18h. After cooling to room temperature, the reaction was quenched with sat. aqueous $NaHCO_3$ (0.5 mL), and 1-fluoro-3-nitrobenzene (10.6 µl, 0.05 mmol, 1.0 equiv) was added as an internal standard. The reaction was analyzed by ^{19}F NMR spectroscopy and GC-MS. The ^{19}F NMR data for PhF and MesF matched that of corresponding authentic samples and GC-MS analysis was used for further confirming the identity of products. All characterization data matched to the previous literature.[1]

E. Procedure for Experiments in Scheme 2



Single addition of $NBu_4F•H_2O$. In a glovebox, [Ph-I-Mes]BF_4 (41.0 mg, 0.1 mmol, 1 equiv), $Cu(OTf)_2$ (7.2 mg, 0.02 mmol, 0.2 equiv), and $NBu_4F•H_2O$ (2.0 equiv) were combined in DMF (1.0 mL) in a 4 mL vial. The vial was sealed with a Teflon-lined cap, and the reaction mixture was stirred at 60 ºC for 18h. After cooling to room temperature, the reaction was quenched with sat. aqueous $NaHCO_3$ (0.5 mL), and 1-fluoro-3-nitrobenzene (10.6 µl, 0.05 mmol, 1.0 equiv) was added as an internal standard. The reaction was analyzed by ^{19}F NMR spectroscopy and GC-MS.

Slow addition of $NBu_4F•H_2O$. In a glovebox, [Mes-I-Ph]BF_4 (20.5 mg, 0.05 mmol, 1.0 equiv) and $Cu(OTf)_2$ (3.6 mg, 0.01 mmol, 0.2 equiv) were combined in DMF (150 µL) in a 4 mL vial equipped with a stir bar. The vial was sealed with a cap containing a PTFE/silicone septum, removed from the glovebox, and heated to 60 ºC. $Bu_4NF•3H_2O$ (0.1 mmol, 2.0 equiv) were added dropwise over 7 h as a stock solution (350 µL of a 0.2 M solution with respect to $Bu_4NF•3H_2O$, prepared under inert atmosphere in dry DMF) via syringe pump using a 1 mL plastic syringe with an air-tight needle. The reaction mixture was stirred for an additional 11 h at 60 ºC. After cooling to room temperature, the reaction was quenched with saturated aqueous $NaHCO_3$ (0.5 mL), and 1-fluoro-3-nitrobenzene (5.3 µL, 0.05 mmol, 1 equiv) was added as an internal standard. The reaction mixture was diluted with CH_2Cl_2 (2.0 mL), and the reaction was analyzed by ^{19}F NMR spectroscopy and GC-MS.

F. Procedure for experiments in Table 5-6

Cu-catalyzed reactions in Table 5. Reactions were performed according to the literature procedure.[1] Selectivities of ArF and MesF were determined by crude ^{19}FNMR using 1-fluoro-3-nitrobenzene as an internal standard.

Cu-free reactions in Table 6. Reactions were conducted analogously to Cu-catalyzed reactions, but in the absence of Cu.

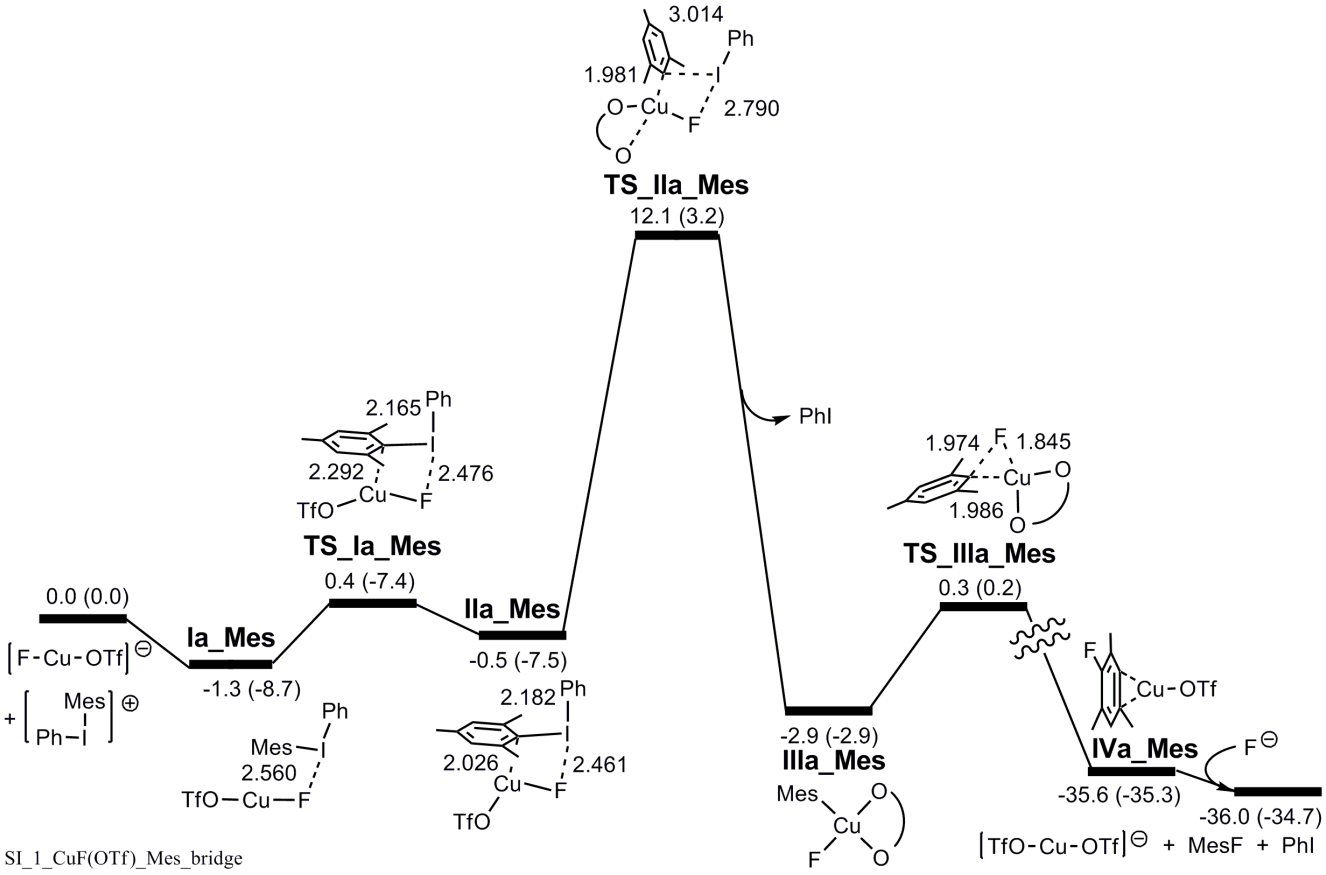
IV. DFT Calculations

A. Computational Details

Gaussian 09[1] was used for DFT calculations at the BP86 level.[2,3] All calculations were carried out for *N*,*N*-dimethylformamide as solvent with the IEFPCM (SCRF) model and utilized the quadruple-ξ valence polarised def2-QZVP[4-7]basis set on Cu and I along with the corresponding ECP and the 6-311+G(2d,p) basis set on other atoms. All thermodynamic data were calculated at the standard state (298.15 K and 1 atm) and entropy calculations were adjusted by the method proposed by Okuno.[8] All transition structures contained one imaginary frequency (except for **TS_1** showing a low additional value of -6*i* cm^{-1}), exhibiting atom displacements consistent with the anticipated reaction pathway. The nature of transition structures was confirmed by intrinsic reaction coordinate (IRC) searches, vibrational frequency calculations, and potential energy surface scans.

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B. Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr. J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.
2. Lee, C., Yang, W.; Parr, R. G. *Phys. Rev. B***1988**, *37*, 785. (c) Becke, A. D.; *J. Chem. Phys*. **1993**, *98*, 5648.
3. Becke, A. D.; *J. Chem. Phys*. **1993**, *98*, 5648.
4. Miertus, S.; Scrocco, E.; Tomasi, J. *J.Chem. Phys*. **1981**, *55*, 117.
5. Miertus, S, Tomasi, J. *J. Chem. Phys*. **1982**, *65*, 239.
6. Cramer, C. J.; Truhlar, D. G. *Chem. Rev*. **1999**, *99*, 2161.
7. Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev*. **2005**, *105*, 2999.
8. Weigend, F.; Furche, F.; Ahlrichs, R. *J. Chem. Phys*. **2003**, *119*, 12753.
9. Okuno, Y. *Chem.,Eur. J*. **1997**, *3*, 212.

Figure S1. Computed pathway for oxidation of $[CuF(OTf)]^-$ by $[Ph(Mes)I]^+$ with transfer of a mesityl group to copper, together with direct reductive elimination from the Cu^{III} product **IIIa_Mes**. Energies ΔG (ΔH) are in kcal/mol.



B. Energies of calculated species, Gaussview diagrams, and Cartesian coordinates

a. Copper species for reaction of $[Mes(Ph)I]^+$ with $[CuF(OTf)]^-$ (Figure 2)

$[CuF(OTf)]^-$

Zero-point correction= 0.027853 (Hartree/Particle)
Thermal correction to Energy= 0.039012
Thermal correction to Enthalpy= 0.039956
Thermal correction to Gibbs Free Energy= -0.012205
Sum of electronic and zero-point Energies= -1258.234887
Sum of electronic and thermal Energies= -1258.223729
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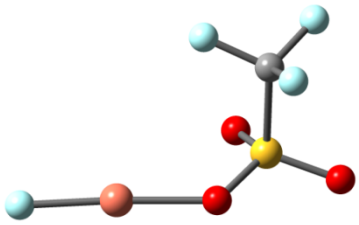
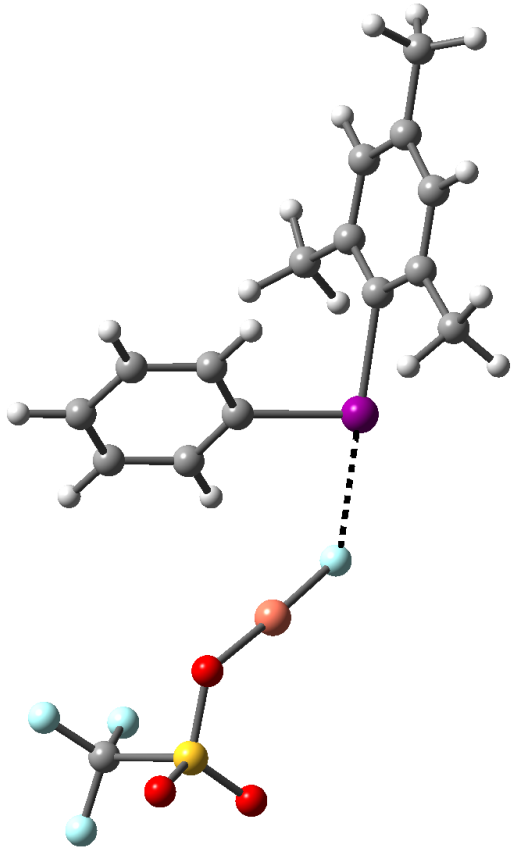


Cu	-2.005613	-0.005373	-0.173231
C	1.701857	-0.781858	-0.005940
S	0.832099	0.896690	0.084963
O	1.785170	1.830892	-0.524163
O	0.501188	1.065908	1.506140
O	-0.375528	0.678777	-0.821596
F	2.004237	-1.094124	-1.284664
F	0.917219	-1.759452	0.499083
F	2.849665	-0.744741	0.708123
F	-3.620963	-0.635538	0.346001

Ia

Zero-point correction= 0.283077 (Hartree/Particle)
Thermal correction to Energy= 0.313419
Thermal correction to Enthalpy= 0.314363
Thermal correction to Gibbs Free Energy= 0.213314
Sum of electronic and zero-point Energies= -1850.580372
Sum of electronic and thermal Energies= -1850.550031
Sum of electronic and thermal Enthalpies= -1850.549086
Sum of electronic and thermal Free Energies= -1850.650135
E(RB-P86) = -1850.86344914 A.U

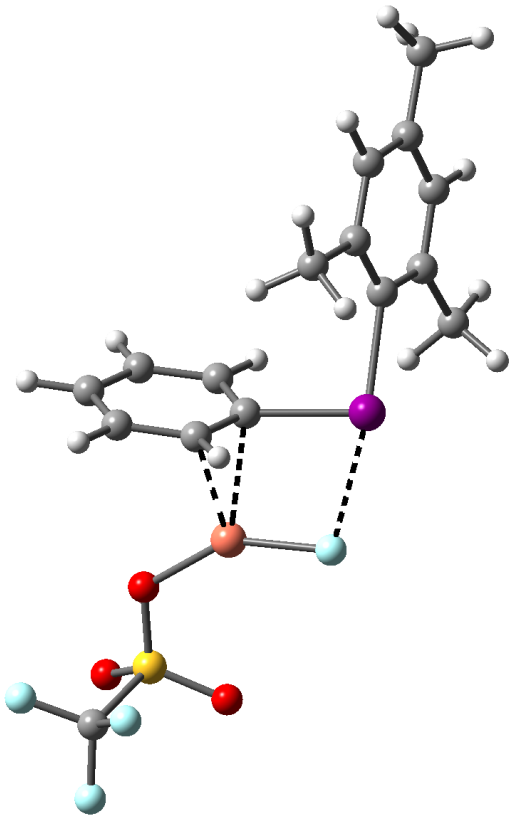


C	3.775490	-0.363879	-0.127685
C	4.477872	0.576801	-0.909262
C	4.351608	-1.049157	0.962877
C	5.805825	0.842195	-0.541409
C	5.685564	-0.739863	1.271315
C	6.424875	0.202499	0.541992
H	6.371773	1.570380	-1.129575
H	6.157129	-1.259053	2.110742
I	1.759751	-0.846718	-0.663997
C	0.898135	0.996788	0.024798
C	1.396179	1.570755	1.191601
C	-0.135703	1.557106	-0.725094
C	0.824975	2.775711	1.623298
H	2.209427	1.113241	1.756863
C	-0.691048	2.761860	-0.271161
H	-0.496695	1.079488	-1.636011
C	-0.214480	3.366958	0.896639
H	1.197964	3.243014	2.537061
H	-1.497498	3.223563	-0.844536
H	-0.653096	4.305684	1.241068
Cu	-2.068514	-0.951738	-0.178211
F	-0.676600	-1.393368	-1.294458
C	-5.407778	0.765611	-0.265561
S	-4.894417	-0.757161	0.734960

F	-5.237401	1.892801	0.457848
F	-6.710792	0.669751	-0.610155
F	-4.672914	0.866703	-1.395696
O	-5.107855	-1.888641	-0.176793
O	-5.701915	-0.680962	1.956472
O	-3.425336	-0.461272	1.032122
C	7.846072	0.532877	0.926012
H	7.863729	1.304941	1.713767
H	8.370056	-0.348868	1.322537
H	8.412864	0.923635	0.069094
C	3.623676	-2.088162	1.783937
H	2.686078	-1.698243	2.209566
H	3.364865	-2.974203	1.182348
H	4.256176	-2.424342	2.616248
C	3.872816	1.292840	-2.090929
H	3.500305	0.584182	-2.847557
H	3.023414	1.927236	-1.790921
H	4.620039	1.938775	-2.570504

TS_Ia

Zero-point correction= 0.281818 (Hartree/Particle)
Thermal correction to Energy= 0.311688
Thermal correction to Enthalpy= 0.312632
Thermal correction to Gibbs Free Energy= 0.212830
Sum of electronic and zero-point Energies= -1850.577685
Sum of electronic and thermal Energies= -1850.547815
Sum of electronic and thermal Enthalpies= -1850.546871
Sum of electronic and thermal Free Energies= -1850.646673
E(RB-P86) = -1850.85950285 A.U.

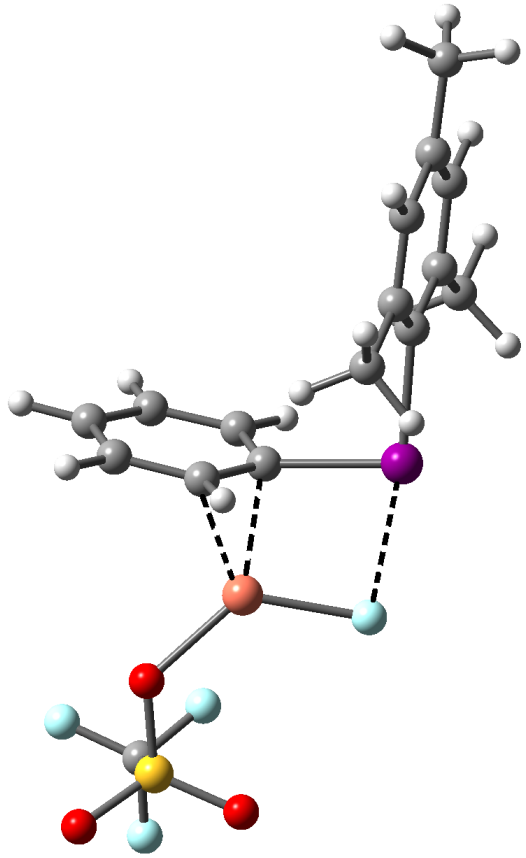


C	3.582101	-0.348878	-0.097522
C	4.202956	0.682996	-0.830301
C	4.186125	-0.973208	1.016332
C	5.470845	1.101821	-0.394973
C	5.455487	-0.511004	1.393267
C	6.112494	0.522028	0.707265
H	5.968245	1.906950	-0.943445
H	5.943072	-0.978067	2.254050
I	1.667777	-1.081498	-0.735236
C	0.547685	0.656710	-0.114277
C	0.718791	1.131509	1.194986
C	-0.145036	1.401736	-1.099950
C	0.163994	2.373581	1.528741
H	1.265034	0.553157	1.940652
C	-0.687986	2.646837	-0.729270
H	-0.173560	1.072301	-2.140292
C	-0.529607	3.128312	0.573961
H	0.280932	2.748158	2.547575
H	-1.216711	3.235928	-1.480989
H	-0.944974	4.099901	0.847378
Cu	-1.519056	-0.202056	-0.280733
F	-0.696580	-1.664780	-1.286928
C	-5.520925	0.198852	-0.264572
S	-4.269599	-0.407642	1.016867
F	-5.756590	1.521079	-0.115578

F	-6.691676	-0.461997	-0.118984
F	-5.064140	-0.014265	-1.519047
O	-4.068201	-1.828386	0.695609
O	-4.883076	-0.072875	2.308314
O	-3.069444	0.472329	0.708336
C	7.484297	0.979466	1.138581
H	7.526418	1.138692	2.226919
H	8.243587	0.217987	0.894815
H	7.772353	1.914223	0.637954
C	3.550413	-2.101992	1.795219
H	2.563847	-1.825553	2.198586
H	3.406664	-2.998264	1.170865
H	4.190472	-2.386196	2.641066
C	3.571423	1.349329	-2.027485
H	3.259251	0.613925	-2.785702
H	2.677063	1.927975	-1.745200
H	4.280646	2.042711	-2.498611

IIa

Zero-point correction= 0.282598 (Hartree/Particle)
Thermal correction to Energy= 0.312850
Thermal correction to Enthalpy= 0.313795
Thermal correction to Gibbs Free Energy= 0.214918
Sum of electronic and zero-point Energies= -1850.577876
Sum of electronic and thermal Energies= -1850.547624
Sum of electronic and thermal Enthalpies= -1850.546680
Sum of electronic and thermal Free Energies= -1850.645556
E(RB-P86) = -1850.86047405 A.U

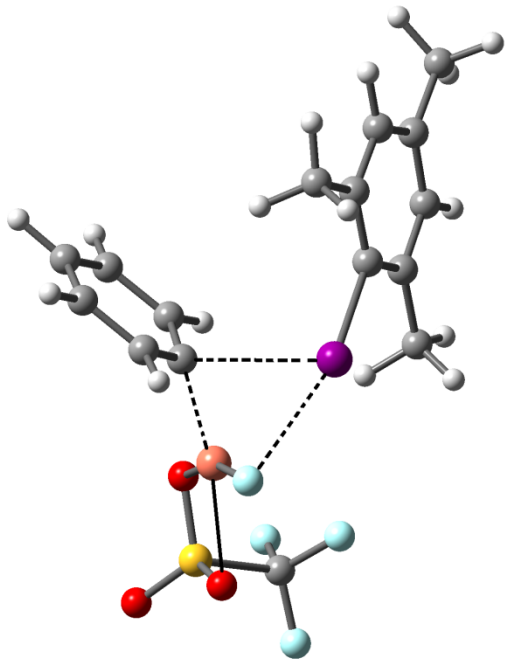


C	-3.514209	-0.385755	0.083036
C	-4.161943	-0.130333	1.310214
C	-4.132760	-0.175408	-1.169109
C	-5.469601	0.377802	1.247885
C	-5.439379	0.333803	-1.158694
C	-6.123473	0.618644	0.032338
H	-5.990043	0.587838	2.186743
H	-5.935718	0.508896	-2.117739
I	-1.544708	-1.249206	0.129078
C	-0.426414	0.605025	-0.026511
C	-0.123997	1.138506	-1.313895
C	-0.302142	1.401500	1.137788
C	0.279339	2.488359	-1.407262
H	-0.310510	0.560700	-2.221267
C	0.111823	2.726833	1.002975
H	-0.513257	0.985440	2.122712
C	0.382861	3.275852	-0.262564
H	0.494124	2.904615	-2.393332
H	0.217434	3.340309	1.900074
H	0.682406	4.321883	-0.346885
Cu	1.432294	-0.142932	-0.435847
F	0.871812	-1.942944	0.165202
C	5.034670	0.259147	0.988640

S	4.546219	-0.314362	-0.747310
F	4.080498	-0.072691	1.888636
F	6.194619	-0.325663	1.363616
F	5.202795	1.599740	1.022862
O	4.383548	-1.769244	-0.621814
O	5.625999	0.183541	-1.609344
O	3.250995	0.443332	-0.973789
C	-3.466680	-0.461416	-2.493758
H	-2.617220	0.214983	-2.675423
H	-3.085469	-1.492435	-2.548962
H	-4.180880	-0.321059	-3.315963
C	-7.537749	1.143219	0.000810
H	-7.664310	1.903472	-0.784494
H	-8.248483	0.329109	-0.219510
H	-7.824829	1.584492	0.965386
C	-3.534263	-0.371842	2.663013
H	-3.181009	-1.408341	2.774086
H	-2.672063	0.290153	2.837818
H	-4.265008	-0.177919	3.459469

TS_IIa

Zero-point correction= 0.281235 (Hartree/Particle)
Thermal correction to Energy= 0.311231
Thermal correction to Enthalpy= 0.312176
Thermal correction to Gibbs Free Energy= 0.213397
Sum of electronic and zero-point Energies= -1850.564996
Sum of electronic and thermal Energies= -1850.535000
Sum of electronic and thermal Enthalpies= -1850.534056
Sum of electronic and thermal Free Energies= -1850.632834
E(RB-P86) = -1850.84623134 A.U

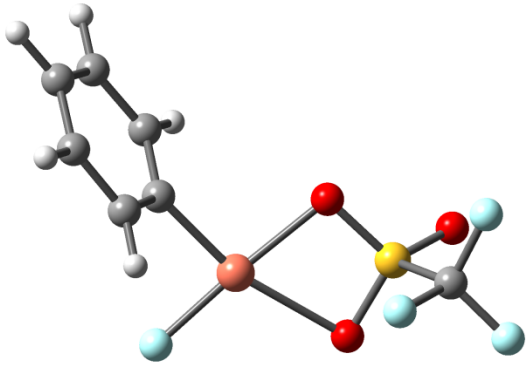


C	-2.625474	-0.739743	-0.439164
C	-2.420606	-2.072069	-0.015380
C	-3.830555	-0.037348	-0.202541
C	-3.482616	-2.701084	0.651522
C	-4.849200	-0.725012	0.470408
C	-4.700042	-2.052252	0.903106
H	-3.347311	-3.734203	0.984554
H	-5.790068	-0.201447	0.663505
I	-1.070254	0.250910	-1.481910
C	-0.048856	1.876435	0.507045
C	-0.241362	3.215828	0.171419
C	-0.402651	1.322179	1.735039
C	-0.684180	4.074587	1.189770
H	-0.016680	3.585751	-0.828895
C	-0.846545	2.205327	2.732255
H	-0.305010	0.256403	1.943842
C	-0.988321	3.570842	2.459896
H	-0.801799	5.137981	0.968280
H	-1.090578	1.804817	3.719011
H	-1.356419	4.243568	3.237389
Cu	1.523778	1.105313	-0.388000
F	1.204642	1.857919	-2.089854
C	3.600574	-2.118675	0.308945
S	3.685252	-0.241330	0.528847
F	2.558493	-2.452941	-0.475680
F	4.737354	-2.557684	-0.266082
F	3.457134	-2.718053	1.507090
O	3.631619	0.311715	-0.856072
O	4.886754	-0.010710	1.325630
O	2.369148	0.105453	1.204019
C	-1.140140	-2.831462	-0.255214
H	-0.922982	-2.927557	-1.330977
H	-0.276927	-2.326103	0.204399
H	-1.209298	-3.841819	0.169525
C	-4.056769	1.388353	-0.640356
H	-3.320570	2.073477	-0.191184
H	-3.970777	1.493132	-1.733809
H	-5.059305	1.725669	-0.344720
C	-5.830010	-2.765518	1.602207
H	-6.573039	-3.124703	0.869967
H	-5.468769	-3.638511	2.163691
H	-6.358874	-2.094627	2.295513

IIIa

Zero-point correction= 0.114895 (Hartree/Particle)
Thermal correction to Energy= 0.131658
Thermal correction to Enthalpy= 0.132602
Thermal correction to Gibbs Free Energy= 0.067156
Sum of electronic and zero-point Energies= -1489.624917

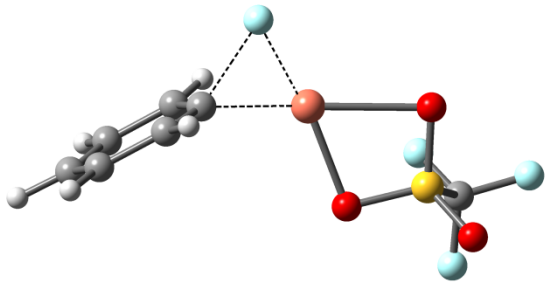
Sum of electronic and thermal Energies= -1489.608155
Sum of electronic and thermal Enthalpies= -1489.607210
Sum of electronic and thermal Free Energies= -1489.672656
E(RB-P86) = -1489.73981207 A.U.



C	-2.187446	0.067700	-0.034341
C	-2.728497	-0.479346	-1.179148
C	-2.716890	0.012024	1.238968
C	-3.912480	-1.222817	-1.002872
H	-2.285054	-0.362216	-2.168120
C	-3.907551	-0.730986	1.374903
H	-2.254797	0.483331	2.107394
C	-4.494332	-1.339566	0.262485
H	-4.370827	-1.688348	-1.878483
H	-4.355970	-0.817703	2.367342
H	-5.420746	-1.905461	0.381715
Cu	-0.500685	0.954680	-0.179164
F	-1.288716	2.222929	-1.140379
C	2.750175	-0.908574	-0.467717
S	1.863611	0.274899	0.720815
F	2.057225	-1.013026	-1.612670
F	3.976404	-0.427922	-0.729316
F	2.855387	-2.118423	0.104578
O	1.640578	1.538559	-0.045730
O	2.665578	0.297433	1.931530
O	0.464957	-0.355535	0.876610

TS_IIIa

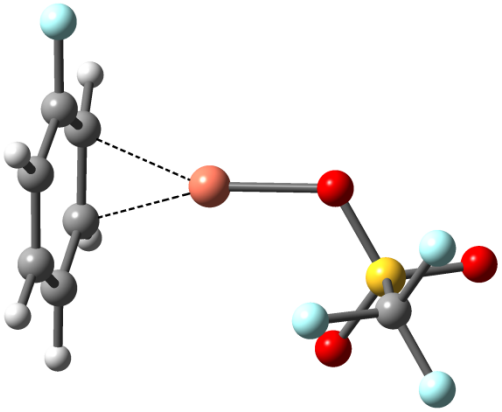
Zero-point correction= 0.113993 (Hartree/Particle)
Thermal correction to Energy= 0.130346
Thermal correction to Enthalpy= 0.131291
Thermal correction to Gibbs Free Energy= 0.066392
Sum of electronic and zero-point Energies= -1489.617973
Sum of electronic and thermal Energies= -1489.601619
Sum of electronic and thermal Enthalpies= -1489.600675
Sum of electronic and thermal Free Energies= -1489.665574
E(RB-P86) = -1489.73196584 A.U.



C	2.379759	-0.184053	-0.273255
C	2.618718	1.015653	-0.919470
C	3.130461	-0.737184	0.748711
C	3.623963	1.818512	-0.353764
H	2.047654	1.344509	-1.787901
C	4.127775	0.094882	1.286240
H	2.945483	-1.735940	1.144698
C	4.372596	1.358682	0.736161
H	3.821488	2.797746	-0.795103
H	4.719349	-0.273638	2.127009
H	5.169938	1.981551	1.145819
Cu	0.522849	-0.808536	-0.370231
F	1.772205	-1.541454	-1.519964
C	-2.862293	0.915813	-0.212132
S	-1.924187	-0.509304	0.609469
O	-2.762765	-0.934296	1.722923
O	-0.588959	0.125363	0.993914
O	-1.637972	-1.478677	-0.490765
F	-2.144927	1.414029	-1.235795
F	-3.085753	1.892497	0.686059
F	-4.042397	0.467065	-0.678397

IVa

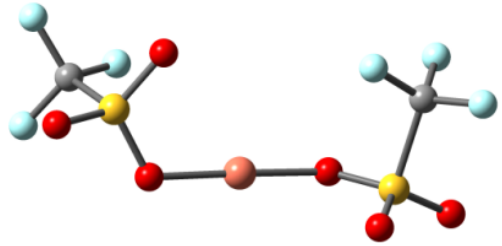
Zero-point correction= 0.116563 (Hartree/Particle)
Thermal correction to Energy= 0.133156
Thermal correction to Enthalpy= 0.134100
Thermal correction to Gibbs Free Energy= 0.067432
Sum of electronic and zero-point Energies= -1489.673869
Sum of electronic and thermal Energies= -1489.657276
Sum of electronic and thermal Enthalpies= -1489.656332
Sum of electronic and thermal Free Energies= -1489.723000
E(RB-P86) = -1489.79043170 A.U.



C	3.246963	0.375895	-0.717101
C	3.097583	1.579391	-0.043784
C	2.928356	-0.870209	-0.134204
C	2.588334	1.560454	1.266752
H	3.372952	2.513640	-0.535176
C	2.433035	-0.870496	1.206648
H	3.211943	-1.795101	-0.641479
C	2.248687	0.358220	1.887632
H	2.460787	2.503704	1.800716
H	2.319746	-1.818066	1.739608
H	1.870097	0.353352	2.910390
Cu	0.839826	-0.881131	-0.111475
F	3.752534	0.378647	-1.976043
C	-2.590229	1.044840	-0.160517
S	-2.129395	-0.778621	0.044110
O	-3.283125	-1.512695	-0.481510
O	-1.787115	-0.926227	1.465694
O	-0.918068	-0.890427	-0.882142
F	-1.570523	1.839339	0.230560
F	-3.672249	1.330759	0.595217
F	-2.879769	1.320081	-1.449282

$[Cu(OTf)_2]^-$

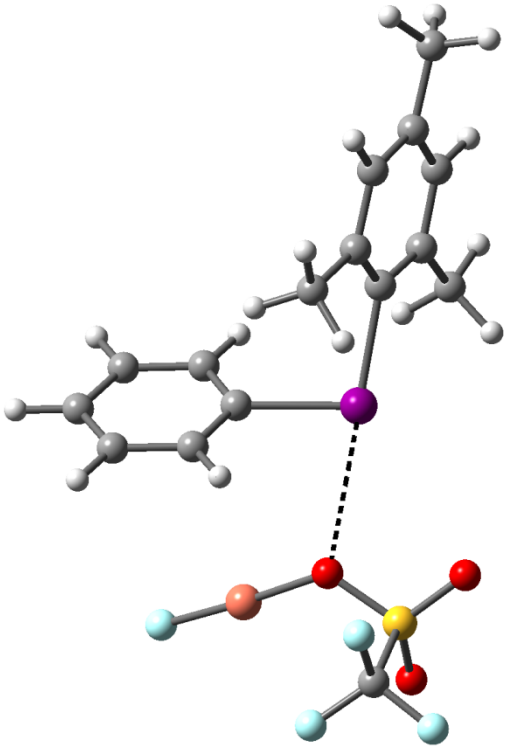
Zero-point correction= 0.052566 (Hartree/Particle)
Thermal correction to Energy= 0.071405
Thermal correction to Enthalpy= 0.072350
Thermal correction to Gibbs Free Energy= -0.001625
Sum of electronic and zero-point Energies= -2120.069001
Sum of electronic and thermal Energies= -2120.050161
Sum of electronic and thermal Enthalpies= -2120.049217
Sum of electronic and thermal Free Energies= -2120.123192



Cu	0.027233	-0.911613	-0.010337
C	3.519451	0.179099	0.787501
C	-3.203469	1.116565	0.089369
S	2.597208	0.275331	-0.862299
S	-2.926753	-0.753773	0.018694
O	3.645582	0.152251	-1.879161
O	1.834285	1.527860	-0.786493
O	-4.083744	-1.322616	0.716231
O	-2.750464	-1.050507	-1.409135
O	1.730473	-0.983814	-0.813686
O	-1.650941	-0.911185	0.847069
F	-3.337247	1.531586	1.367057
F	-4.328157	1.438763	-0.586952
F	-2.164522	1.773874	-0.469565
F	4.227941	-0.966506	0.874009
F	2.650395	0.225716	1.821682
F	4.372206	1.221229	0.897950

Ib

Zero-point correction= 0.282764 (Hartree/Particle)
Thermal correction to Energy= 0.313494
Thermal correction to Enthalpy= 0.314438
Thermal correction to Gibbs Free Energy= 0.211047
Sum of electronic and zero-point Energies= -1850.573581
Sum of electronic and thermal Energies= -1850.542851
Sum of electronic and thermal Enthalpies= -1850.541907
Sum of electronic and thermal Free Energies= -1850.645298
E(RB-P86) = -1850.85634493 A.U

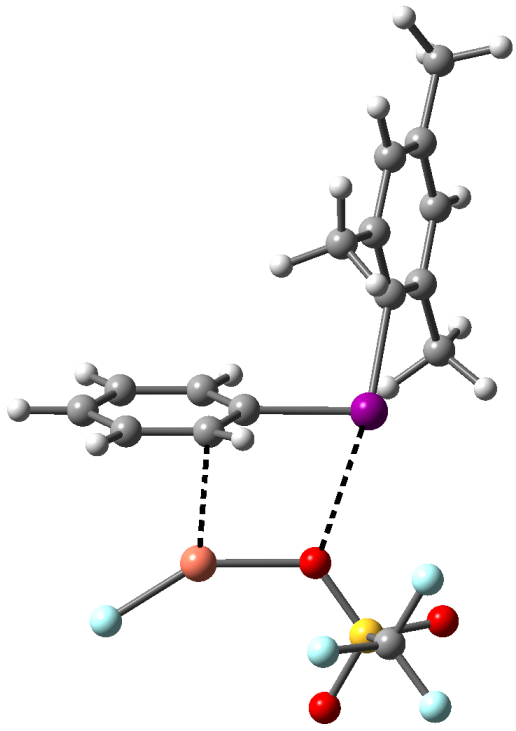


O	-2.091878	-0.230152	-0.310654
C	3.020093	-0.554362	-0.059594
C	3.691148	-0.791005	-1.276151
C	3.662484	-0.442620	1.189010
C	5.088690	-0.898954	-1.203445
C	5.061686	-0.554572	1.181436
C	5.789968	-0.783037	0.005470
H	5.640876	-1.080589	-2.129817
H	5.592232	-0.462127	2.133352
I	0.884452	-0.442108	-0.126074
C	0.589745	1.623465	0.347006
C	-0.158861	1.917671	1.487753
C	1.114385	2.600332	-0.498941
C	-0.384595	3.266797	1.790941
H	-0.556222	1.131388	2.130146
C	0.883421	3.941293	-0.166938
H	1.685926	2.344250	-1.390821
C	0.136807	4.272019	0.969871
H	-0.967662	3.522393	2.677930
H	1.285966	4.725003	-0.811836
H	-0.041199	5.320820	1.215523
Cu	-2.860548	1.406321	-0.847049
C	-3.734250	-1.814435	1.066806
F	-3.517273	3.015984	-1.348964
F	-4.377298	-3.001181	1.048375
F	-2.901181	-1.791486	2.127760
F	-4.646540	-0.831007	1.212151
S	-2.764446	-1.590176	-0.543570

O	-1.761856	-2.661099	-0.530296
O	-3.779090	-1.580018	-1.600453
C	2.937962	-0.204523	2.488904
H	2.469720	0.792313	2.515813
H	2.141553	-0.947604	2.652672
H	3.638286	-0.266441	3.331952
C	3.001427	-0.949062	-2.610053
H	2.330594	-1.822859	-2.620479
H	2.396044	-0.067244	-2.869709
H	3.745426	-1.092111	-3.404495
C	7.290481	-0.932039	0.042952
H	7.569229	-1.991839	0.169510
H	7.751430	-0.582234	-0.891869
H	7.728572	-0.374345	0.882768

TS_Ib

Zero-point correction= 0.282052 (Hartree/Particle)
Thermal correction to Energy= 0.311933
Thermal correction to Enthalpy= 0.312877
Thermal correction to Gibbs Free Energy= 0.213841
Sum of electronic and zero-point Energies= -1850.569077
Sum of electronic and thermal Energies= -1850.539196
Sum of electronic and thermal Enthalpies= -1850.538252
Sum of electronic and thermal Free Energies= -1850.637288
E(RB-P86) = -1850.85112875 A.U.

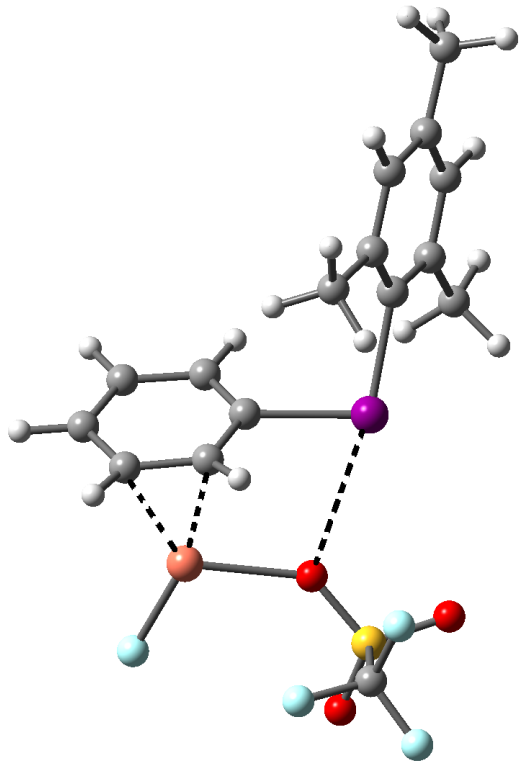


O	-1.984645	-0.290576	-0.265711
C	3.035729	-0.577872	0.039338
C	3.789443	-0.954694	-1.090667

C	3.598148	-0.205377	1.275803
C	5.184651	-0.929942	-0.943051
C	5.000139	-0.197966	1.345704
C	5.807209	-0.555668	0.256959
H	5.799856	-1.214593	-1.801325
H	5.468672	0.096473	2.288928
I	0.903685	-0.645857	-0.129897
C	0.473609	1.444517	-0.038577
C	-0.449524	1.868041	0.936789
C	1.068109	2.307783	-0.953608
C	-0.739541	3.250502	0.997162
H	-0.795396	1.194523	1.723970
C	0.762764	3.675147	-0.863805
H	1.761529	1.950087	-1.715064
C	-0.134494	4.141876	0.101841
H	-1.404896	3.615999	1.781144
H	1.231149	4.369046	-1.564487
H	-0.364950	5.206983	0.161659
Cu	-2.424339	1.657239	-0.166500
C	-3.698488	-1.947448	0.905109
F	-3.642652	3.029735	-0.513273
F	-4.602526	-2.926629	0.685214
F	-2.739584	-2.425211	1.727468
F	-4.319472	-0.919638	1.522860
S	-2.945036	-1.381600	-0.735534
O	-2.219575	-2.554546	-1.237089
O	-4.077946	-0.869152	-1.513344
C	2.786554	0.188463	2.483070
H	2.244630	1.133131	2.315958
H	2.039853	-0.579281	2.740022
H	3.440856	0.329648	3.353167
C	3.187089	-1.386557	-2.406211
H	2.600114	-2.312768	-2.299725
H	2.517844	-0.620226	-2.826679
H	3.980831	-1.578969	-3.139787
C	7.310528	-0.567229	0.379908
H	7.670613	-1.583314	0.613741
H	7.791211	-0.260467	-0.560415
H	7.653050	0.098254	1.184623

IIb

Zero-point correction= 0.282514 (Hartree/Particle)
Thermal correction to Energy= 0.312794
Thermal correction to Enthalpy= 0.313739
Thermal correction to Gibbs Free Energy= 0.214758
Sum of electronic and zero-point Energies= -1850.572726
Sum of electronic and thermal Energies= -1850.542446
Sum of electronic and thermal Enthalpies= -1850.541502
Sum of electronic and thermal Free Energies= -1850.640482
E(RB-P86) = -1850.85524052 A.U

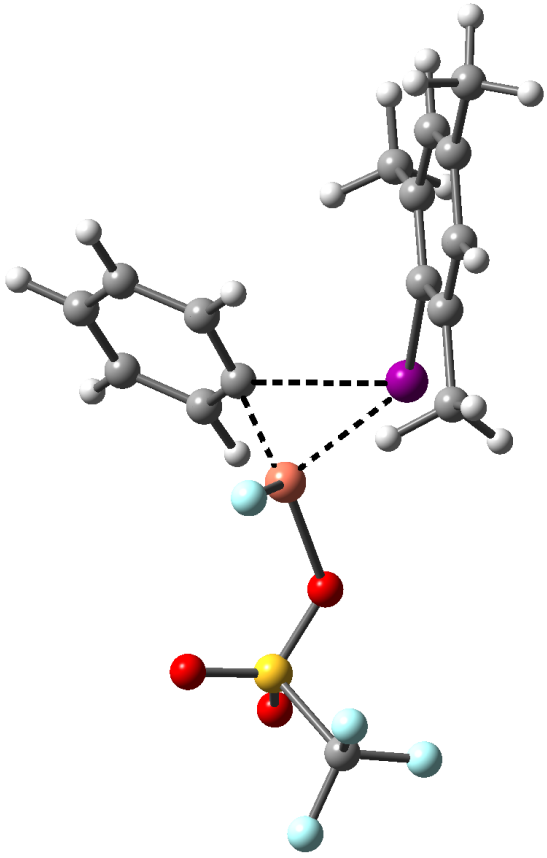


O	-1.995116	-0.313356	-0.488732
C	3.040100	-0.530823	0.032765
C	3.819768	-0.915385	-1.076975
C	3.573783	-0.127898	1.272077
C	5.211358	-0.860829	-0.906226
C	4.974141	-0.092362	1.365498
C	5.806266	-0.452666	0.296875
H	5.846431	-1.150776	-1.748100
H	5.420545	0.226376	2.311545
I	0.913429	-0.638484	-0.180028
C	0.415158	1.434203	-0.049241
C	-0.546866	1.781082	0.933426
C	0.952019	2.338322	-0.948149
C	-1.011596	3.132756	0.936458
H	-0.781280	1.106361	1.759824
C	0.522937	3.683926	-0.878818
H	1.685765	2.038933	-1.696878
C	-0.454882	4.071050	0.028041
H	-1.640230	3.480073	1.759914
H	0.956810	4.411310	-1.567266
H	-0.792841	5.108218	0.061545
Cu	-2.320506	1.819739	-0.087216
C	-3.574586	-1.856097	0.990809
F	-3.951210	2.384017	-0.818971
F	-4.447484	-2.887972	0.949870
F	-2.586727	-2.169464	1.860320
F	-4.223917	-0.767562	1.462501
S	-2.871232	-1.522894	-0.733855

O	-2.083755	-2.727190	-1.044169
O	-4.053964	-1.252831	-1.562033
C	2.734680	0.270012	2.458776
H	2.200141	1.216344	2.277288
H	1.979972	-0.495164	2.699572
H	3.368103	0.411810	3.344095
C	3.248940	-1.393639	-2.390516
H	2.685588	-2.332759	-2.268896
H	2.566272	-0.656937	-2.840640
H	4.058818	-1.583634	-3.106902
C	7.307311	-0.433441	0.444228
H	7.683843	-1.441274	0.687553
H	7.796628	-0.120794	-0.489737
H	7.623559	0.241989	1.251344

TS_IIb

Zero-point correction= 0.282514 (Hartree/Particle)
Thermal correction to Energy= 0.312794
Thermal correction to Enthalpy= 0.313739
Thermal correction to Gibbs Free Energy= 0.214758
Sum of electronic and zero-point Energies= -1850.572726
Sum of electronic and thermal Energies= -1850.542446
Sum of electronic and thermal Enthalpies= -1850.541502
Sum of electronic and thermal Free Energies= -1850.640482
E(RB-P86) = -1850.84586101 A.U.

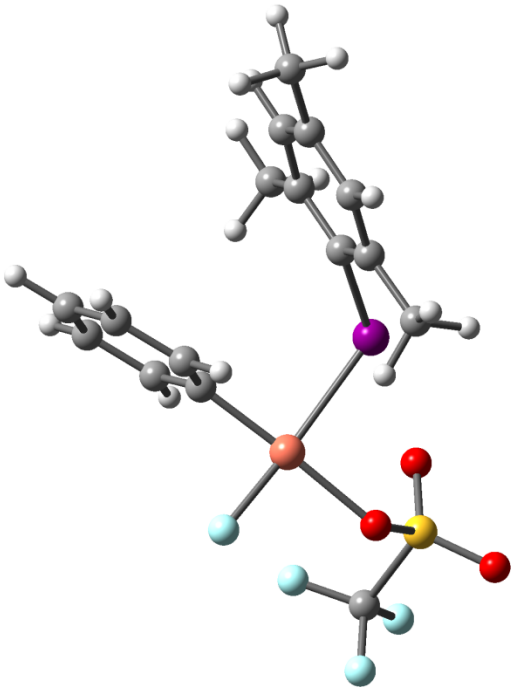


O	-2.406859	-0.066679	-0.571393
C	2.725957	-0.731327	-0.450314
C	3.881918	0.011366	-0.774025
C	2.718559	-1.874920	0.381044
C	5.084151	-0.438501	-0.208951
C	3.959519	-2.260211	0.905201
C	5.145941	-1.561941	0.627971
H	6.000435	0.112110	-0.437892
H	3.993639	-3.140691	1.552601
I	0.906047	-0.132733	-1.349450
C	0.366493	1.795296	0.247968
C	1.382123	2.040331	1.170314
C	-0.405010	2.790285	-0.356554
C	1.526969	3.360142	1.621431
H	2.015602	1.244076	1.565442
C	-0.236980	4.099493	0.119736
H	-1.134271	2.570324	-1.136871
C	0.723184	4.380304	1.097755
H	2.280164	3.578094	2.381546
H	-0.854353	4.895879	-0.301318
H	0.861088	5.407288	1.441691
Cu	-0.713939	0.199771	0.634737
C	-4.508691	-1.546022	0.062336
F	-0.635534	-0.513276	2.380221
F	-5.796475	-1.503894	0.474730
F	-4.463390	-2.195055	-1.123275
F	-3.796534	-2.257993	0.964072
S	-3.820505	0.207296	-0.106550
O	-4.654835	0.821194	-1.149669
O	-3.903728	0.769775	1.250222
C	3.883166	1.220784	-1.673863
H	3.585168	0.961058	-2.702223
H	3.189483	1.997012	-1.314410
H	4.888246	1.659852	-1.716194
C	1.480851	-2.659789	0.727173
H	0.766664	-2.049743	1.309526
H	0.959818	-3.017281	-0.174654
H	1.747521	-3.536606	1.331858
C	6.453610	-2.011610	1.226875
H	6.616827	-3.087044	1.056750
H	7.302721	-1.457678	0.804508
H	6.453269	-1.856337	2.318339

IIIb

Zero-point correction=	0.282739 (Hartree/Particle)
Thermal correction to Energy=	0.312894
Thermal correction to Enthalpy=	0.313838
Thermal correction to Gibbs Free Energy=	0.215430
Sum of electronic and zero-point Energies=	-1850.576582
Sum of electronic and thermal Energies=	-1850.546427
Sum of electronic and thermal Enthalpies=	-1850.545483

Sum of electronic and thermal Free Energies= -1850.643891
E(RB-P86) = -1850.85932126 A.U.

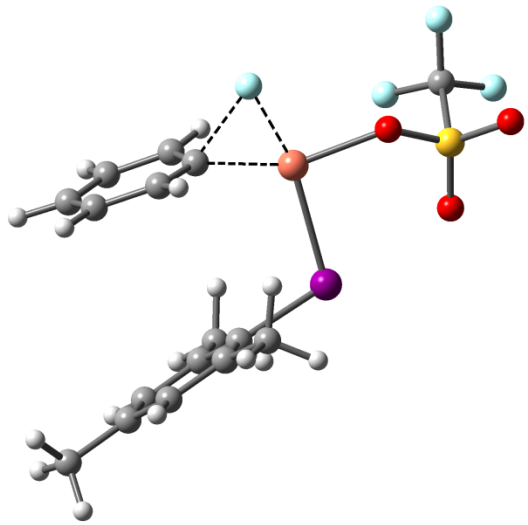


O	2.426748	-0.484939	-1.104619
C	-2.389203	-1.027339	0.236110
C	-3.254273	-0.495317	1.215383
C	-2.836424	-1.587184	-0.980919
C	-4.626494	-0.529467	0.927309
C	-4.220914	-1.582480	-1.203273
C	-5.129090	-1.058141	-0.270761
H	-5.322177	-0.128545	1.669688
H	-4.596934	-2.009094	-2.137521
I	-0.312105	-1.094485	0.670918
C	-0.595616	1.950996	-0.286832
C	-1.656995	2.039141	-1.171639
C	-0.411077	2.784966	0.805324
C	-2.615450	3.040771	-0.929055
H	-1.760850	1.383465	-2.037417
C	-1.385332	3.777074	1.026445
H	0.440909	2.693576	1.480859
C	-2.477913	3.901516	0.163504
H	-3.459314	3.139056	-1.615899
H	-1.272219	4.441370	1.886494
H	-3.226365	4.676549	0.342745
Cu	0.835679	0.731009	-0.692952
C	4.661940	0.190534	0.194824
F	1.518886	2.078014	-1.728251
F	5.570195	-0.250647	1.091653
F	5.295698	0.454032	-0.966444
F	4.119680	1.335898	0.660547

S	3.324594	-1.122552	-0.061884
O	4.048949	-2.284675	-0.582798
O	2.675807	-1.244604	1.259296
C	-2.780679	0.076243	2.527994
H	-2.286910	-0.689949	3.147004
H	-2.057692	0.892732	2.377566
H	-3.629968	0.474287	3.098836
C	-1.916346	-2.177095	-2.019967
H	-1.197262	-1.434707	-2.400345
H	-1.330253	-3.015918	-1.612567
H	-2.496844	-2.551324	-2.873410
C	-6.608691	-1.045235	-0.560636
H	-6.917147	-1.944753	-1.113208
H	-7.199159	-0.978895	0.363920
H	-6.871288	-0.174387	-1.185105

TS_IIIb

Zero-point correction= 0.281504 (Hartree/Particle)
Thermal correction to Energy= 0.311299
Thermal correction to Enthalpy= 0.312243
Thermal correction to Gibbs Free Energy= 0.214406
Sum of electronic and zero-point Energies= -1850.569708
Sum of electronic and thermal Energies= -1850.539913
Sum of electronic and thermal Enthalpies= -1850.538968
Sum of electronic and thermal Free Energies= -1850.636805
E(RB-P86) = -1850.85121151 A.U

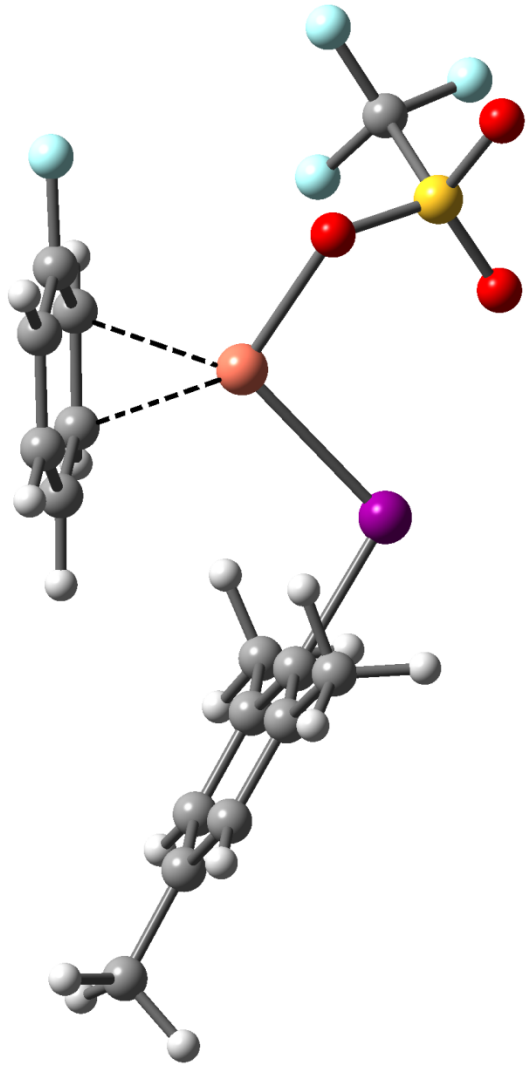


C	0.646917	2.165938	-0.405014
C	0.667218	2.737571	0.858603
C	1.678616	2.222659	-1.329435
C	1.899254	3.261090	1.284159
H	-0.209272	2.758977	1.506986
C	2.894850	2.758364	-0.873994
H	1.570120	1.860915	-2.352253
C	3.002260	3.276033	0.421714

H	1.972284	3.676136	2.291914
H	3.744960	2.786021	-1.559067
H	3.943564	3.718727	0.753183
Cu	-0.787428	0.830607	-0.687781
F	-1.053635	2.596024	-1.300514
C	4.333190	-1.200071	-1.029950
C	2.936202	-1.326759	-1.047462
C	2.262394	-1.128587	0.175926
C	2.922890	-0.835411	1.383796
C	4.322939	-0.725052	1.330029
C	5.044225	-0.900028	0.141944
H	4.878469	-1.344095	-1.967500
H	4.860218	-0.496345	2.254982
I	0.144850	-1.380740	0.218375
C	-4.444416	0.286250	0.768554
F	-5.303391	-0.427951	1.528296
F	-5.139766	1.246602	0.122595
F	-3.546903	0.883552	1.585142
S	-3.566929	-0.848527	-0.463781
O	-4.643010	-1.374888	-1.310003
O	-2.841852	-1.811144	0.389701
O	-2.659674	0.110825	-1.198089
C	2.232971	-1.666243	-2.338108
H	1.703942	-2.630262	-2.266461
H	1.481345	-0.907212	-2.606375
H	2.956120	-1.735280	-3.161667
C	2.212091	-0.649661	2.701631
H	1.670945	-1.561390	3.001227
H	2.933867	-0.409190	3.493715
H	1.473826	0.165941	2.654310
C	6.548919	-0.781607	0.118175
H	7.014800	-1.744906	-0.145952
H	6.877280	-0.049239	-0.636073
H	6.943154	-0.470072	1.095344

IVb

Zero-point correction= 0.283928 (Hartree/Particle)
Thermal correction to Energy= 0.313940
Thermal correction to Enthalpy= 0.314884
Thermal correction to Gibbs Free Energy= 0.215457
Sum of electronic and zero-point Energies= -1850.627902
Sum of electronic and thermal Energies= -1850.597890
Sum of electronic and thermal Enthalpies= -1850.596946
Sum of electronic and thermal Free Energies= -1850.696373
E(RB-P86) = -1850.91183035 A.U



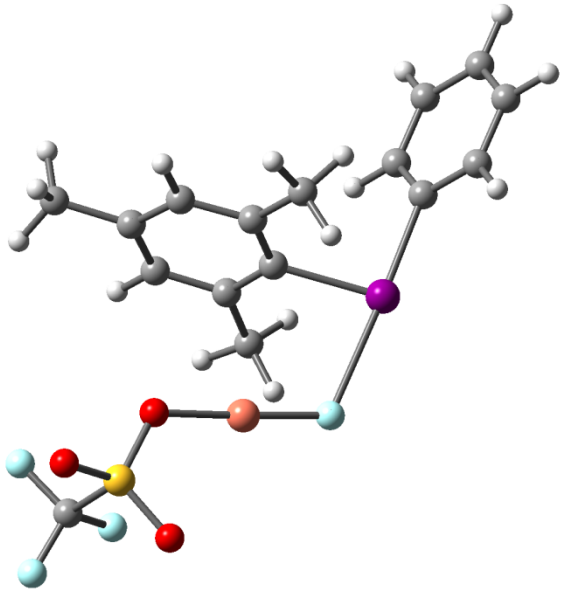
C	-1.341077	3.499115	0.305796
C	-0.918754	2.502973	1.210343
C	-0.484486	4.107777	-0.594986
C	0.458334	2.129929	1.195109
H	-1.592255	2.171676	2.004079
C	0.869616	3.717204	-0.605466
H	-0.861140	4.876719	-1.271014
C	1.342445	2.748298	0.275109
H	0.853875	1.507915	2.001519
H	1.553738	4.195082	-1.309238
H	2.396888	2.468808	0.274868
Cu	-0.657459	0.675779	0.107369
F	-2.646712	3.880149	0.344614
C	4.765167	0.123125	-0.905392
C	3.424259	-0.225009	-1.133709
C	2.743000	-0.874323	-0.084971
C	3.346709	-1.181511	1.147610
C	4.692945	-0.807632	1.310769
C	5.418486	-0.160086	0.303217

H	5.311705	0.631502	-1.705679
H	5.181470	-1.036023	2.262694
I	0.711503	-1.469720	-0.407281
C	-4.090812	-1.015587	0.794897
F	-4.756559	-2.184845	0.918833
F	-4.980507	-0.004169	0.896020
F	-3.212086	-0.914302	1.819216
S	-3.185546	-0.949177	-0.865190
O	-4.256558	-0.957075	-1.868548
O	-2.283783	-2.117009	-0.828555
O	-2.471564	0.381031	-0.784466
C	2.782684	0.100339	-2.459532
H	2.483793	-0.813973	-2.997508
H	1.872563	0.706738	-2.328459
H	3.480096	0.659543	-3.097878
C	2.627419	-1.883728	2.272855
H	2.291455	-2.889340	1.972438
H	3.289410	-1.992310	3.142760
H	1.730872	-1.328100	2.590807
C	6.869257	0.211919	0.499818
H	7.525650	-0.426570	-0.114451
H	7.058816	1.253254	0.196862
H	7.175308	0.095606	1.549013

b. Copper species for reaction of $[Mes(Ph)I]^+$ with $[CuF(OTf)]^-$ with mesityl transfer (Figure 3 and Figure S1)

Ia_Mes

Zero-point correction= 0.282934 (Hartree/Particle)
Thermal correction to Energy= 0.313365
Thermal correction to Enthalpy= 0.314309
Thermal correction to Gibbs Free Energy= 0.213151
Sum of electronic and zero-point Energies= -1850.582163
Sum of electronic and thermal Energies= -1850.551732
Sum of electronic and thermal Enthalpies= -1850.550787
Sum of electronic and thermal Free Energies= -1850.651945
E(RB-P86) = -1850.86509658 A.U.

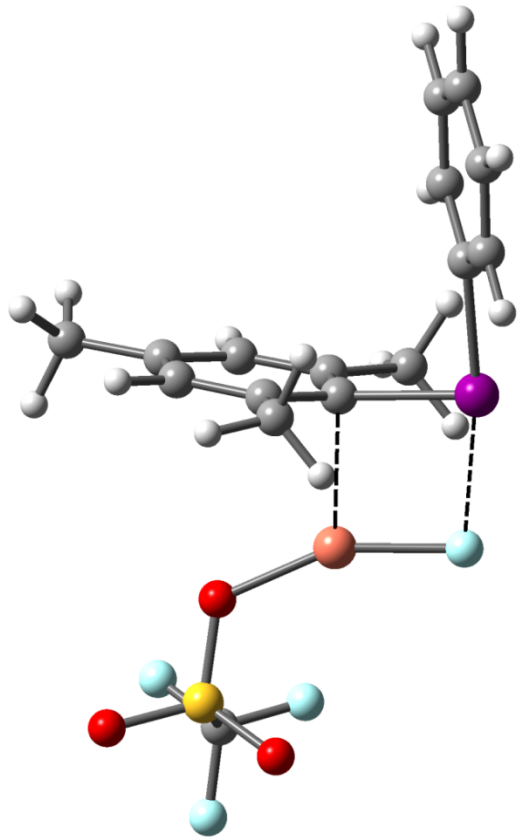


C	4.233300	-0.369430	-0.087343
C	4.652395	0.632121	-0.967504
C	5.075756	-0.894974	0.896514
C	5.956579	1.126016	-0.845104
H	3.986747	1.030957	-1.734885
C	6.382313	-0.397905	0.995109
H	4.730741	-1.672938	1.580376
C	6.819457	0.611119	0.130400
H	6.296768	1.912194	-1.522560
H	7.051759	-0.799202	1.758948
H	7.836576	0.999108	0.216296
I	2.261426	-1.201092	-0.264895
C	1.206183	0.650715	-0.062744
C	1.179738	1.267903	1.201322
C	0.574071	1.162458	-1.211769
C	0.491606	2.489871	1.278513
C	-0.101149	2.383355	-1.054183
C	-0.145964	3.064673	0.170410
H	0.450953	2.997435	2.246472
H	-0.610649	2.806418	-1.924518
Cu	-1.509546	-1.093949	0.214550
F	-0.126961	-2.100342	-0.464529
C	-4.931465	0.128461	-0.771663
S	-4.339315	-0.496657	0.914059
F	-4.802815	1.469807	-0.855526
F	-6.232876	-0.189597	-0.948765
F	-4.213870	-0.433585	-1.769863
O	-4.501748	-1.954897	0.847642
O	-5.143348	0.252259	1.885079
O	-2.885548	-0.028310	0.931159
C	1.831149	0.695363	2.433899
H	1.492779	-0.334107	2.630077
H	2.928463	0.669311	2.337583

H	1.586346	1.307158	3.311867
C	0.566120	0.465929	-2.549746
H	1.580342	0.376997	-2.970922
H	0.153728	-0.551053	-2.460190
H	-0.047898	1.027266	-3.266056
C	-0.851779	4.392705	0.289335
H	-0.151643	5.221080	0.088048
H	-1.675139	4.475861	-0.434260
H	-1.255575	4.543202	1.300702

TS_Ia_Mes

Zero-point correction= 0.282121 (Hartree/Particle)
Thermal correction to Energy= 0.311919
Thermal correction to Enthalpy= 0.312863
Thermal correction to Gibbs Free Energy= 0.212438
Sum of electronic and zero-point Energies= -1850.579459
Sum of electronic and thermal Energies= -1850.549661
Sum of electronic and thermal Enthalpies= -1850.548717
Sum of electronic and thermal Free Energies= -1850.649142
E(RB-P86) = -1850.86158017 A.U.

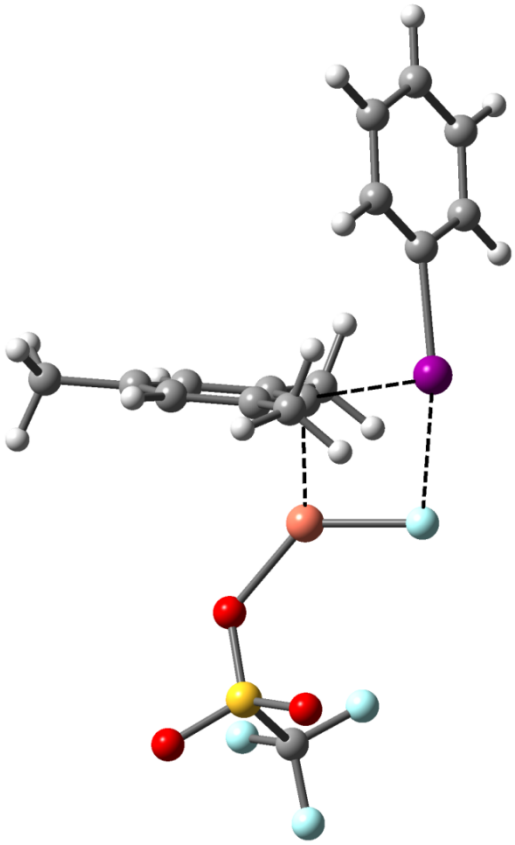


C	-4.026013	-0.323204	0.012151
C	-4.388775	0.686356	0.908918
C	-4.879246	-0.742410	-1.013933
C	-5.639683	1.297142	0.761120
H	-3.719550	1.000812	1.711542

C	-6.134003	-0.131200	-1.137753
H	-4.581491	-1.528727	-1.710534
C	-6.510796	0.887571	-0.256366
H	-5.933374	2.090677	1.451647
H	-6.810015	-0.451193	-1.933549
H	-7.487081	1.365435	-0.361432
I	-2.157145	-1.358992	0.224870
C	-0.927052	0.419364	0.119996
C	-0.886486	1.119867	-1.113078
C	-0.468220	0.968923	1.349193
C	-0.312020	2.400207	-1.084989
C	0.093272	2.253904	1.287342
C	0.172902	2.986042	0.092876
H	-0.251649	2.955417	-2.025316
H	0.472643	2.693504	2.214007
Cu	1.103501	-0.630831	-0.048070
F	0.150000	-2.244655	0.372536
C	4.979335	-0.243442	0.589503
S	3.938447	-0.195366	-0.989411
F	5.166134	1.002482	1.078336
F	6.190523	-0.785724	0.329808
F	4.373980	-0.988719	1.541004
O	3.790527	-1.605496	-1.379111
O	4.685933	0.694268	-1.886827
O	2.653692	0.449172	-0.493040
C	-1.424682	0.564758	-2.406662
H	-1.134796	-0.485867	-2.557047
H	-2.525865	0.609982	-2.430503
H	-1.049269	1.149728	-3.256484
C	-0.567637	0.252503	2.674711
H	-1.605239	0.236405	3.046973
H	-0.226978	-0.790905	2.600551
H	0.048374	0.764272	3.425671
C	0.793783	4.359694	0.070542
H	0.670891	4.871808	1.035576
H	1.876206	4.289703	-0.129791
H	0.354138	4.985045	-0.719561

IIa_Mes

Zero-point correction= 0.282121 (Hartree/Particle)
Thermal correction to Energy= 0.311919
Thermal correction to Enthalpy= 0.312863
Thermal correction to Gibbs Free Energy= 0.212438
Sum of electronic and zero-point Energies= -1850.579459
Sum of electronic and thermal Energies= -1850.549661
Sum of electronic and thermal Enthalpies= -1850.548717
Sum of electronic and thermal Free Energies= -1850.649142
E(RB-P86) = -1850.86236341 A.U.

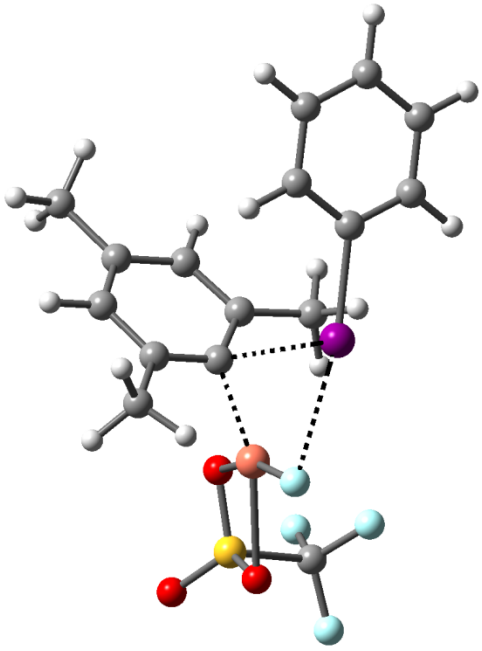


C	-3.855140	-0.661185	0.082952
C	-4.486812	-1.292815	1.160160
C	-4.485165	0.351634	-0.647958
C	-5.784225	-0.896346	1.509656
H	-3.985486	-2.082863	1.722917
C	-5.775679	0.746414	-0.276263
H	-3.992969	0.832534	-1.494871
C	-6.424590	0.122814	0.796878
H	-6.287299	-1.385143	2.346763
H	-6.275586	1.539513	-0.836566
H	-7.433785	0.432436	1.076535
I	-1.904661	-1.371168	-0.467316
C	-0.903490	0.535321	-0.113223
C	-0.731860	1.410817	-1.234720
C	-0.792595	0.989296	1.237743
C	-0.449307	2.756774	-0.950628
C	-0.510253	2.352717	1.426135
C	-0.355523	3.250132	0.359926
H	-0.305191	3.438349	-1.793615
H	-0.418127	2.717905	2.452952
Cu	1.037473	-0.022320	-0.275739
F	0.474162	-1.839460	-0.888555
C	4.707019	-0.924727	0.909499
S	4.109194	0.175529	-0.508821
F	3.806411	-1.897389	1.175360
F	5.880823	-1.510141	0.580449

F	4.893573	-0.198291	2.033896
O	3.909042	-0.748949	-1.634061
O	5.155292	1.198283	-0.636178
O	2.822778	0.748106	0.059041
C	-1.022690	0.099431	2.433754
H	-0.569090	0.544790	3.329084
H	-2.101202	-0.019138	2.631075
H	-0.598885	-0.905296	2.295704
C	-0.049574	4.704015	0.615258
H	-0.466940	5.038216	1.575710
H	1.040752	4.867291	0.654848
H	-0.447856	5.344266	-0.184779
C	-0.887141	0.960247	-2.668258
H	-0.434450	-0.026389	-2.841662
H	-1.950250	0.891772	-2.952121
H	-0.409907	1.683274	-3.342898

TS_IIa_Mes

Zero-point correction= 0.281143 (Hartree/Particle)
Thermal correction to Energy= 0.311175
Thermal correction to Enthalpy= 0.312119
Thermal correction to Gibbs Free Energy= 0.213347
Sum of electronic and zero-point Energies= -1850.562804
Sum of electronic and thermal Energies= -1850.532772
Sum of electronic and thermal Enthalpies= -1850.531828
Sum of electronic and thermal Free Energies= -1850.630600
E(RB-P86) = -1850.84394702 A.U.

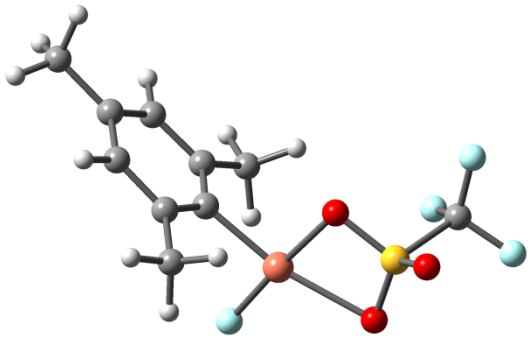


C	-3.730430	-0.945470	0.310916
C	-3.990789	-1.555334	1.546545
C	-4.614840	-0.002835	-0.232447
C	-5.160810	-1.220857	2.237669

H	-3.297324	-2.287127	1.964655
C	-5.778127	0.324681	0.473395
H	-4.404906	0.467493	-1.194464
C	-6.052804	-0.281681	1.705439
H	-5.371457	-1.698122	3.197431
H	-6.471452	1.057101	0.053665
H	-6.962457	-0.021994	2.251167
I	-1.978606	-1.466910	-0.752761
C	-0.218147	0.944890	-0.344546
C	-0.568632	1.780757	-1.403650
C	-0.368287	1.213776	1.022685
C	-0.924575	3.094000	-1.023541
C	-0.734189	2.537612	1.318805
C	-1.012330	3.485481	0.316537
H	-1.156872	3.808363	-1.819859
H	-0.809602	2.820539	2.373574
Cu	1.334520	-0.203877	-0.784200
F	0.584777	-1.502021	-1.848295
C	4.543604	-0.832800	1.273988
S	3.940633	0.199535	-0.193874
F	3.591484	-1.704689	1.656837
F	5.647521	-1.518436	0.919631
F	4.842447	-0.026414	2.310502
O	3.499950	-0.797831	-1.213107
O	5.055424	1.083397	-0.518094
O	2.688114	0.882259	0.330547
C	-0.095348	0.216947	2.118852
H	-0.328690	0.650019	3.100290
H	-0.699758	-0.693066	1.984210
H	0.963225	-0.086467	2.119860
C	-1.419352	4.890328	0.689218
H	-2.166951	4.888643	1.496761
H	-0.549382	5.460663	1.055542
H	-1.835694	5.429918	-0.172322
C	-0.554455	1.384818	-2.860208
H	-0.354369	0.312694	-2.979833
H	-1.523404	1.621845	-3.325249
H	0.217081	1.951124	-3.406111

IIIa_Mes

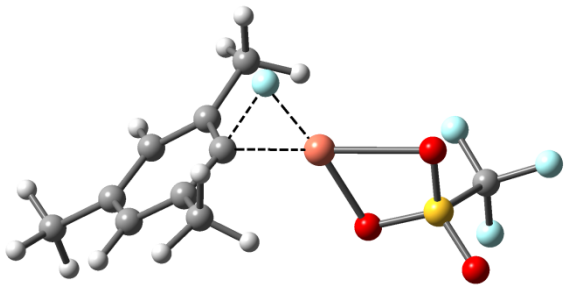
Zero-point correction= 0.194304 (Hartree/Particle)
Thermal correction to Energy= 0.216679
Thermal correction to Enthalpy= 0.217624
Thermal correction to Gibbs Free Energy= 0.139403
Sum of electronic and zero-point Energies= -1607.526803
Sum of electronic and thermal Energies= -1607.504427
Sum of electronic and thermal Enthalpies= -1607.503483
Sum of electronic and thermal Free Energies= -1607.581703
E(RB-P86) = -1607.72110639 A.U.



C	-1.747614	-0.128820	0.273049
C	-2.454933	-1.102688	-0.410368
C	-2.128870	1.161672	0.593443
C	-3.688023	-0.649997	-0.930074
C	-3.374285	1.538005	0.041273
C	-4.154658	0.655116	-0.718186
H	-4.287223	-1.363809	-1.504022
H	-3.726694	2.555410	0.238672
Cu	0.027395	-0.659188	0.808949
F	-0.642948	-1.093776	2.397214
C	3.198249	1.038700	-0.383380
S	2.302554	-0.628323	-0.513965
F	2.618371	1.804847	0.554752
F	4.481144	0.819879	-0.048606
F	3.147287	1.668240	-1.568835
O	2.221331	-1.161322	0.877823
O	3.020272	-1.378411	-1.531484
O	0.862526	-0.233182	-0.893667
C	-1.307557	2.113332	1.426626
H	-1.910325	2.979543	1.729269
H	-0.928627	1.615530	2.331264
H	-0.440822	2.484526	0.857035
C	-5.477085	1.102097	-1.298119
H	-5.955432	1.862512	-0.664596
H	-5.330952	1.548647	-2.295864
H	-6.170072	0.256745	-1.413867
C	-1.969815	-2.516147	-0.616722
H	-1.723798	-2.992078	0.344997
H	-2.739052	-3.120048	-1.115159
H	-1.062491	-2.534364	-1.241166

TS_IIIa_Mes

Zero-point correction= 0.193505 (Hartree/Particle)
Thermal correction to Energy= 0.215501
Thermal correction to Enthalpy= 0.216446
Thermal correction to Gibbs Free Energy= 0.138420
Sum of electronic and zero-point Energies= -1607.521531
Sum of electronic and thermal Energies= -1607.499535
Sum of electronic and thermal Enthalpies= -1607.498591
Sum of electronic and thermal Free Energies= -1607.576616
E(RB-P86) = -1607.71503628 A.U

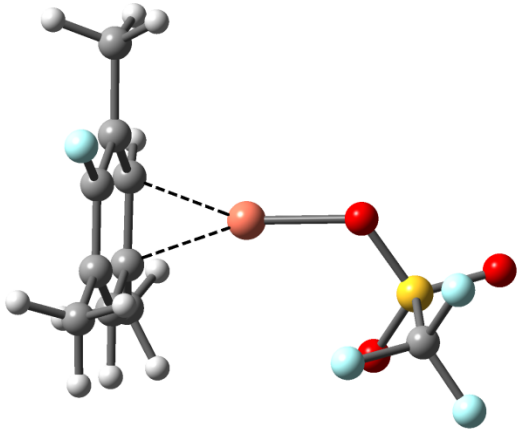


C	-1.910385	-0.211759	0.469032
C	-2.248344	1.102838	0.773436
C	-2.638508	-1.139511	-0.267312
C	-3.338769	1.590634	0.028566
C	-3.715825	-0.574538	-0.977676
C	-4.075034	0.776417	-0.847998
H	-3.621465	2.638292	0.169965
H	-4.292052	-1.233777	-1.633858
Cu	0.014239	-0.668312	0.648056
F	-1.106867	-1.059922	2.060757
C	3.331565	1.012591	-0.284542
S	2.417636	-0.628457	-0.517684
O	3.202300	-1.366806	-1.500602
O	1.030238	-0.191796	-0.987403
O	2.262543	-1.190581	0.853933
F	2.663473	1.799106	0.579268
F	3.440397	1.649432	-1.465440
F	4.564585	0.774543	0.201807
C	-2.303346	-2.606014	-0.354113
H	-1.299048	-2.765093	-0.779545
H	-2.316542	-3.069419	0.643479
H	-3.029005	-3.124757	-0.993912
C	-1.521231	1.956767	1.779152
H	-1.605019	1.524325	2.787437
H	-0.448534	2.037351	1.542941
H	-1.944597	2.969429	1.794087
C	-5.237752	1.342180	-1.625828
H	-5.780009	2.100798	-1.042795
H	-4.882973	1.832010	-2.548456
H	-5.945016	0.554609	-1.921257

IVa_Mes

Zero-point correction= 0.196405 (Hartree/Particle)
Thermal correction to Energy= 0.218415
Thermal correction to Enthalpy= 0.219359
Thermal correction to Gibbs Free Energy= 0.140888
Sum of electronic and zero-point Energies= -1607.578223
Sum of electronic and thermal Energies= -1607.556214
Sum of electronic and thermal Enthalpies= -1607.555270
Sum of electronic and thermal Free Energies= -1607.633741

E(RB-P86) = -1607.77462865 A.U

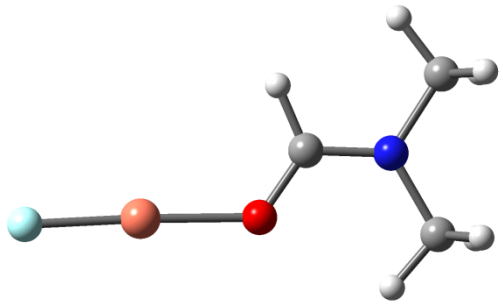


C	2.929421	0.949131	-0.380543
C	2.427492	1.288124	0.889357
C	2.916311	-0.334466	-0.921088
C	1.896695	0.249786	1.660691
C	2.390248	-1.371617	-0.095758
C	1.890608	-1.100497	1.218236
H	1.510064	0.478733	2.657061
H	2.509141	-2.408978	-0.423920
Cu	0.380055	-0.963965	-0.255126
F	3.449087	1.956273	-1.143543
C	-2.941299	1.159237	-0.011519
S	-2.596917	-0.687273	-0.236948
O	-3.743835	-1.185000	-1.001681
O	-2.383203	-1.200255	1.123463
O	-1.325063	-0.656045	-1.082175
F	-1.912320	1.760879	0.623773
F	-4.060018	1.330105	0.726024
F	-3.118262	1.760478	-1.206888
C	3.476203	-0.618874	-2.289007
H	4.558948	-0.417389	-2.317006
H	3.313006	-1.668382	-2.565999
H	3.009732	0.021785	-3.052195
C	2.453171	2.713568	1.371756
H	2.031696	2.787559	2.382538
H	3.481231	3.107339	1.391501
H	1.873146	3.368277	0.702422
C	1.577639	-2.222000	2.186116
H	2.465772	-2.429810	2.805885
H	0.757080	-1.950378	2.864865
H	1.310755	-3.150978	1.664060

c. Copper species for reaction of $[Mes(Ph)I]^+$ with CuF(DMF) (Figure 4)
CuF(DMF)

Zero-point correction= 0.102540 (Hartree/Particle)
Thermal correction to Energy= 0.112242

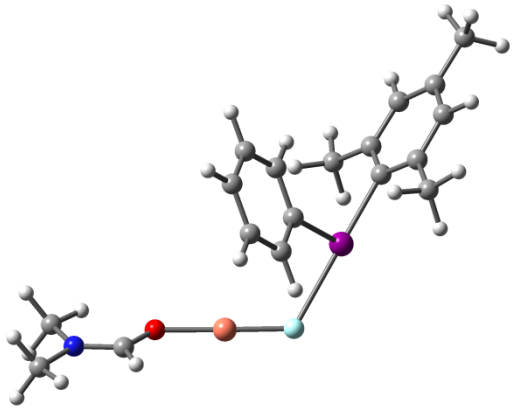
Thermal correction to Enthalpy= 0.113186
Thermal correction to Gibbs Free Energy= 0.066169
Sum of electronic and zero-point Energies= -544.857081
Sum of electronic and thermal Energies= -544.847379
Sum of electronic and thermal Enthalpies= -544.846435
Sum of electronic and thermal Free Energies= -544.893453
E(RB-P86) = -544.959621126 A.U.



Cu	1.706463	0.047923	-0.000081
O	-0.112475	0.438997	-0.000890
F	3.486492	-0.263180	0.000652
C	-1.047374	-0.419325	-0.000437
H	-0.845475	-1.500953	-0.000600
N	-2.335864	-0.085022	0.000023
C	-3.379131	-1.111280	0.000250
H	-4.008616	-1.002426	0.895718
H	-4.008913	-1.002598	-0.895028
H	-2.920131	-2.107479	0.000257
C	-2.770664	1.313157	0.000448
H	-3.379206	1.507990	0.895797
H	-3.379295	1.508550	-0.894742
H	-1.890348	1.963635	0.000472

Ia_DMF

Zero-point correction= 0.357818 (Hartree/Particle)
Thermal correction to Energy= 0.386701
Thermal correction to Enthalpy= 0.387645
Thermal correction to Gibbs Free Energy= 0.290776
Sum of electronic and zero-point Energies= -1137.200629
Sum of electronic and thermal Energies= -1137.171746
Sum of electronic and thermal Enthalpies= -1137.170802
Sum of electronic and thermal Free Energies= -1137.267671
E(RB-P86) = -1137.55844697 A.U.

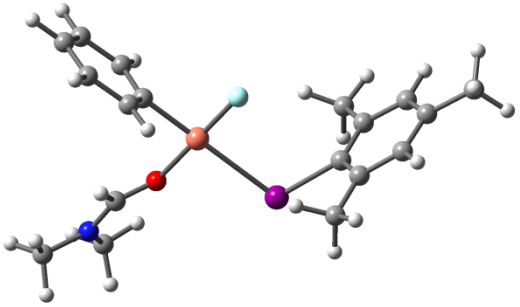


C	-3.028540	-0.424926	0.001567
C	-3.372174	-1.236239	1.102285
C	-3.918502	0.495883	-0.591553
C	-4.669995	-1.085520	1.617667
C	-5.196235	0.598658	-0.022832
C	-5.592189	-0.180446	1.074920
H	-4.961745	-1.698957	2.474873
H	-5.901410	1.312889	-0.457742
I	-1.080579	-0.664491	-0.852607
C	-0.282316	1.199702	-0.140840
C	0.605819	1.889458	-0.964811
C	-0.681006	1.659951	1.111599
C	1.116331	3.107923	-0.495583
H	0.898076	1.493868	-1.937465
C	-0.158491	2.882212	1.556013
H	-1.384425	1.103473	1.732705
C	0.737441	3.601489	0.757542
H	1.809480	3.670132	-1.124950
H	-0.455890	3.261997	2.535750
H	1.138873	4.552955	1.112247
Cu	2.741608	-0.875161	-0.822270
F	1.265345	-0.939064	-1.906264
C	5.241861	-0.140592	0.163468
H	5.345999	0.548131	-0.687743
O	4.211174	-0.867735	0.317756
N	6.267720	-0.154038	1.009312
C	6.282654	-1.015644	2.193232
H	6.370480	-0.394910	3.096985
H	5.354822	-1.595134	2.228711
H	7.146097	-1.694918	2.140910
C	7.436641	0.698525	0.785208
H	7.567253	1.381985	1.636921
H	8.336932	0.074821	0.684798
H	7.297770	1.284591	-0.131445
C	-3.553528	1.358938	-1.773534
H	-2.723773	2.043722	-1.535114
H	-3.238479	0.751279	-2.636780
H	-4.413172	1.967837	-2.082857

C	-2.436046	-2.240149	1.733783
H	-2.164798	-3.043118	1.030167
H	-1.498570	-1.773239	2.074041
H	-2.913849	-2.708234	2.604636
C	-6.986287	-0.062601	1.639768
H	-7.698407	-0.652654	1.038577
H	-7.034416	-0.436691	2.671987
H	-7.336964	0.979863	1.626566

TS_IIa_DMF

Zero-point correction= 0.356193 (Hartree/Particle)
Thermal correction to Energy= 0.384640
Thermal correction to Enthalpy= 0.385584
Thermal correction to Gibbs Free Energy= 0.291548
Sum of electronic and zero-point Energies= -1137.182877
Sum of electronic and thermal Energies= -1137.154430
Sum of electronic and thermal Enthalpies= -1137.153486
Sum of electronic and thermal Free Energies= -1137.247522
E(RB-P86) = -1137.53907002 A.U.

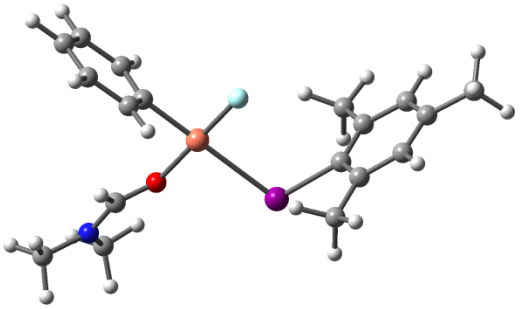


C	2.371760	0.285433	-0.350976
C	2.334280	1.658124	-0.691610
C	3.301164	-0.255857	0.567900
C	3.288323	2.488657	-0.088648
C	4.227342	0.631944	1.131183
C	4.243594	2.000148	0.816561
H	3.281666	3.553533	-0.338256
H	4.958772	0.237448	1.842236
I	0.990865	-1.019165	-1.275638
C	-1.049476	-1.258909	0.783204
C	-1.283450	-2.594348	1.089814
C	-0.737179	-0.273413	1.710439
C	-1.336885	-2.926264	2.455125
H	-1.453705	-3.342106	0.315843
C	-0.795514	-0.640114	3.066592
H	-0.476431	0.746411	1.424311
C	-1.092229	-1.956811	3.433188
H	-1.559346	-3.959080	2.733675
H	-0.589713	0.119995	3.823808
H	-1.112534	-2.233800	4.489279
Cu	-1.833731	-0.750362	-0.933743

F	-1.621167	-2.288516	-1.975368
C	-3.475823	1.235873	0.322422
H	-3.593975	0.558101	1.181453
O	-2.712955	0.938499	-0.651399
N	-4.164461	2.365796	0.384773
C	-4.106834	3.367614	-0.683575
H	-3.799374	4.332588	-0.256115
H	-3.386615	3.047669	-1.442849
H	-5.102906	3.477193	-1.136471
C	-5.037858	2.654151	1.525722
H	-4.708499	3.581701	2.015404
H	-6.072232	2.780378	1.174878
H	-4.995678	1.826867	2.244141
C	3.333674	-1.713370	0.952122
H	2.377480	-2.036169	1.393242
H	3.522166	-2.357620	0.078470
H	4.127945	-1.897280	1.687766
C	1.338337	2.245366	-1.659199
H	1.450787	1.811646	-2.665752
H	0.302001	2.054629	-1.339584
H	1.477178	3.331642	-1.739041
C	5.275825	2.918231	1.418938
H	6.176448	2.954775	0.782157
H	4.896965	3.946539	1.507096
H	5.593004	2.570520	2.412556

IIIa_DMF

Zero-point correction= 0.357590 (Hartree/Particle)
Thermal correction to Energy= 0.386267
Thermal correction to Enthalpy= 0.387211
Thermal correction to Gibbs Free Energy= 0.291981
Sum of electronic and zero-point Energies= -1137.195386
Sum of electronic and thermal Energies= -1137.166709
Sum of electronic and thermal Enthalpies= -1137.165765
Sum of electronic and thermal Free Energies= -1137.260995
E(RB-P86) = -1137.55297617 A.U.



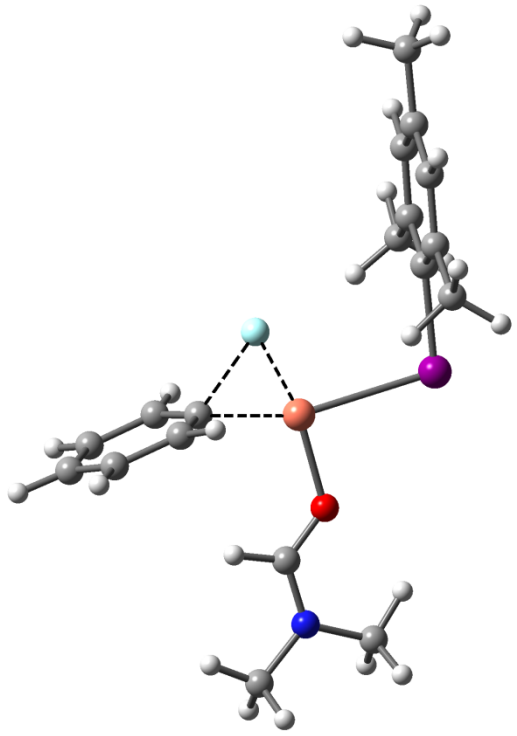
C	2.811902	-0.383868	0.014747
C	3.405706	0.005563	-1.201833
C	3.361126	-0.082884	1.276579
C	4.609725	0.723589	-1.117652

C	4.566548	0.637469	1.287059
C	5.208176	1.044646	0.108770
H	5.089110	1.040743	-2.048397
H	5.012029	0.886448	2.254758
I	1.014292	-1.521873	-0.059687
C	-2.360699	1.773303	-0.077245
C	-2.663958	2.359666	1.137341
C	-2.950043	2.076515	-1.290281
C	-3.700996	3.313468	1.132584
H	-2.137910	2.118573	2.062568
C	-3.977712	3.040069	-1.263608
H	-2.665197	1.598276	-2.228795
C	-4.346928	3.648969	-0.060593
H	-3.975515	3.794559	2.074306
H	-4.479107	3.297310	-2.199641
H	-5.141410	4.398323	-0.054363
Cu	-0.982045	0.418688	-0.082713
F	0.197238	1.760083	0.032411
C	-3.268147	-1.162806	0.372290
H	-3.584483	-0.433049	1.128225
O	-2.185996	-1.004821	-0.298441
N	-4.057858	-2.203302	0.194332
C	-3.759776	-3.252737	-0.787079
H	-4.610342	-3.348823	-1.476182
H	-2.855413	-2.987836	-1.342948
H	-3.611198	-4.207541	-0.262921
C	-5.278588	-2.361524	0.993185
H	-6.147821	-2.407324	0.322414
H	-5.218303	-3.293975	1.571812
H	-5.388226	-1.512492	1.677608
C	2.723680	-0.491166	2.580715
H	1.704696	-0.083906	2.676184
H	2.643258	-1.586662	2.666404
H	3.318822	-0.126152	3.428526
C	2.816652	-0.307998	-2.554093
H	2.735299	-1.394489	-2.718209
H	1.803579	0.111478	-2.659712
H	3.444807	0.110611	-3.351860
C	6.519186	1.791131	0.159132
H	6.594870	2.408343	1.066071
H	7.368107	1.086517	0.170593
H	6.644903	2.440916	-0.718929

TS_IIIa_DMF

Zero-point correction= 0.356464 (Hartree/Particle)
Thermal correction to Energy= 0.384788
Thermal correction to Enthalpy= 0.385733
Thermal correction to Gibbs Free Energy= 0.290373
Sum of electronic and zero-point Energies= -1137.189188
Sum of electronic and thermal Energies= -1137.160864
Sum of electronic and thermal Enthalpies= -1137.159920

Sum of electronic and thermal Free Energies= -1137.255279
E(RB-P86) = -1137.54565243 A.U.

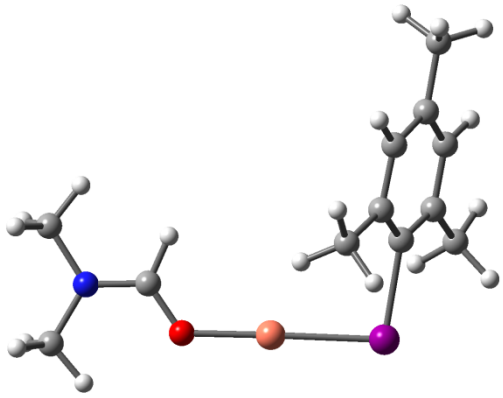


C	-1.867717	1.981685	-0.053152
C	-2.332691	2.418677	-1.282422
C	-2.304017	2.418908	1.186708
C	-3.455932	3.263016	-1.249616
H	-1.884421	2.108882	-2.226965
C	-3.427677	3.264366	1.180475
H	-1.831513	2.111623	2.120314
C	-3.993335	3.686245	-0.028131
H	-3.886120	3.598353	-2.195892
H	-3.833377	3.602401	2.136540
H	-4.847721	4.365617	-0.018527
Cu	-0.936734	0.230290	-0.068735
F	0.069757	1.798959	-0.072287
C	-3.521750	-0.915987	0.132904
H	-3.897643	0.097582	0.339098
O	-2.284582	-1.130275	-0.085340
N	-4.430629	-1.877946	0.130273
C	-5.842154	-1.581550	0.391942
H	-6.447569	-1.883542	-0.474566
H	-6.176442	-2.140906	1.277416
H	-5.970351	-0.507408	0.569900
C	-4.080320	-3.277334	-0.130770
H	-4.630757	-3.628949	-1.015206
H	-4.364776	-3.890188	0.736524
H	-3.003061	-3.356522	-0.305896
C	3.367391	-0.052214	-1.191724

C	4.520837	0.743810	-1.087536
C	5.066196	1.117087	0.148168
C	4.431054	0.669338	1.314387
C	3.274380	-0.128146	1.282831
C	2.770674	-0.466862	0.013278
H	5.004637	1.075839	-2.010979
H	4.844090	0.942109	2.290184
I	1.040345	-1.717466	-0.089848
C	2.644862	-0.581201	2.576170
H	1.602986	-0.233350	2.661335
H	2.624532	-1.680122	2.653535
H	3.207010	-0.188533	3.434204
C	2.838274	-0.425294	-2.553768
H	2.828584	-1.517520	-2.698975
H	1.804325	-0.072390	-2.695420
H	3.461549	0.018264	-3.341938
C	6.289799	1.999493	0.220674
H	6.879493	1.795034	1.126127
H	6.937646	1.859916	-0.656846
H	6.001915	3.064045	0.250184

IVa_DMF

Zero-point correction= 0.268494 (Hartree/Particle)
Thermal correction to Energy= 0.289957
Thermal correction to Enthalpy= 0.290901
Thermal correction to Gibbs Free Energy= 0.212280
Sum of electronic and zero-point Energies= -805.743281
Sum of electronic and thermal Energies= -805.721818
Sum of electronic and thermal Enthalpies= -805.720874
Sum of electronic and thermal Free Energies= -805.799494
E(RB-P86) = -806.011774845 A.U.

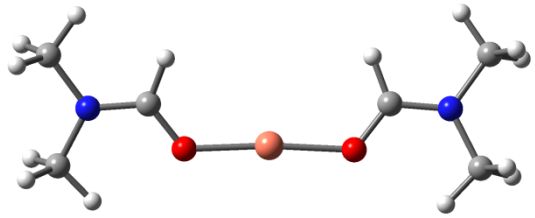


Cu	-1.380811	-0.935740	0.018165
C	-3.446193	0.976336	-0.221852
H	-2.677550	1.762390	-0.267239
O	-3.143755	-0.253638	-0.113951
N	-4.700021	1.409616	-0.288236
C	-4.995755	2.838341	-0.415999

H	-5.556984	3.019230	-1.344254
H	-5.601968	3.168738	0.439913
H	-4.060252	3.410058	-0.440194
C	-5.840474	0.491993	-0.235604
H	-6.428071	0.584960	-1.160520
H	-6.478319	0.752886	0.621396
H	-5.474046	-0.533789	-0.128867
C	2.714934	0.250256	-1.077760
C	3.438920	1.454283	-1.105679
C	3.396927	2.380190	-0.054153
C	2.607044	2.079830	1.063105
C	1.862278	0.891347	1.162603
C	1.939700	0.011280	0.070082
H	4.056467	1.663731	-1.984060
H	2.567214	2.784355	1.898975
I	0.860019	-1.849247	0.179231
C	1.033516	0.629407	2.393584
H	-0.040189	0.559228	2.148610
H	1.315481	-0.317632	2.880116
H	1.160988	1.440695	3.122623
C	2.809284	-0.707361	-2.239266
H	3.239414	-1.674665	-1.933679
H	1.818619	-0.914720	-2.674038
H	3.447458	-0.288761	-3.028905
C	4.168291	3.675905	-0.133475
H	4.382432	4.076801	0.867460
H	5.120263	3.543256	-0.667944
H	3.590936	4.440757	-0.679706

$[Cu(DMF)_2]^+$

Zero-point correction= 0.202354 (Hartree/Particle)
Thermal correction to Energy= 0.218117
Thermal correction to Enthalpy= 0.219062
Thermal correction to Gibbs Free Energy= 0.155855
Sum of electronic and zero-point Energies= -693.309584
Sum of electronic and thermal Energies= -693.293821
Sum of electronic and thermal Enthalpies= -693.292877
Sum of electronic and thermal Free Energies= -693.356084
E(RB-P86) = -693.511938307 A.U.



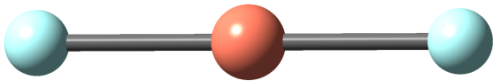
Cu	0.000008	-0.478439	-0.001253
O	1.857967	-0.558594	0.079633
C	2.634575	0.434848	-0.084100

H	2.251074	1.444459	-0.291588
N	3.957578	0.333622	-0.017529
C	4.812055	1.506995	-0.211144
H	5.418129	1.677322	0.690647
H	5.482244	1.340817	-1.067089
H	4.191670	2.390885	-0.402973
C	4.623657	-0.943447	0.248950
H	5.222862	-0.858823	1.167266
H	5.289243	-1.190150	-0.591036
H	3.868631	-1.726729	0.368274
C	-2.634437	0.435307	0.082535
H	-2.250725	1.445275	0.287904
O	-1.857947	-0.558102	-0.081822
N	-3.957554	0.333676	0.018955
C	-4.811911	1.507152	0.212585
H	-4.191328	2.391514	0.401552
H	-5.420081	1.675817	-0.688103
H	-5.480090	1.342154	1.070324
C	-4.623974	-0.943860	-0.244338
H	-3.869196	-1.727724	-0.361390
H	-5.222969	-0.861527	-1.163004
H	-5.289816	-1.188035	0.596175

d. Copper species for reaction of $[Mes(Ph)I]^+$ with $[CuF_2]^-$ (Figure 5)

$[CuF_2]^-$

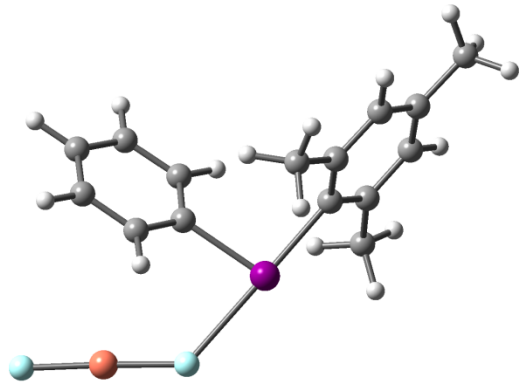
Zero-point correction= 0.003151 (Hartree/Particle)
Thermal correction to Energy= 0.007131
Thermal correction to Enthalpy= 0.008075
Thermal correction to Gibbs Free Energy= -0.021498
Sum of electronic and zero-point Energies= -396.399343
Sum of electronic and thermal Energies= -396.395363
Sum of electronic and thermal Enthalpies= -396.394419
Sum of electronic and thermal Free Energies= -396.423992
E(RB-P86) = -396.402493821 A.U



Cu	0.000000	0.000000	0.000000
F	0.000000	0.000000	-1.817269
F	0.000000	0.000000	1.817270

Ia_F

Zero-point correction= 0.257944 (Hartree/Particle)
Thermal correction to Energy= 0.280885
Thermal correction to Enthalpy= 0.281829
Thermal correction to Gibbs Free Energy= 0.199641
Sum of electronic and zero-point Energies= -988.745245
Sum of electronic and thermal Energies= -988.722304
Sum of electronic and thermal Enthalpies= -988.721359
Sum of electronic and thermal Free Energies= -988.803548
E(RB-P86) = -989.003188677 A.U.

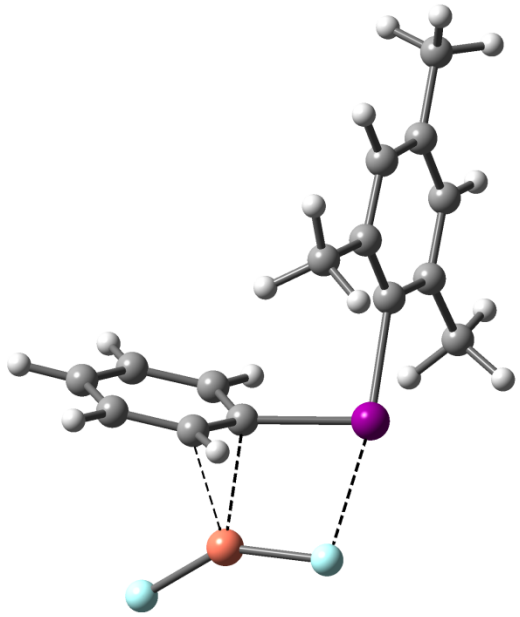


C	-2.154821	-0.383953	-0.130490
C	-2.889170	-0.933911	0.940776
C	-2.720544	0.479406	-1.092096
C	-4.241543	-0.568132	1.036656
C	-4.075403	0.808109	-0.932732
C	-4.851221	0.297854	0.118140
H	-4.831885	-0.977462	1.861636
H	-4.534310	1.484862	-1.659459
I	-0.099445	-0.967136	-0.338019
C	0.742170	0.944982	0.133250
C	1.738387	1.443147	-0.706991
C	0.281222	1.625115	1.258425
C	2.288337	2.694875	-0.397938
H	2.070771	0.891158	-1.586323
C	0.848055	2.873981	1.547250
H	-0.499624	1.211929	1.898140
C	1.847452	3.404998	0.723593
H	3.063776	3.108704	-1.045789
H	0.504391	3.423624	2.425975
H	2.283047	4.378747	0.956545
Cu	3.861282	-0.769917	0.017272
F	5.380696	0.044940	0.578493
F	2.348980	-1.641401	-0.572103
C	-1.944466	1.056793	-2.249362
H	-1.136878	1.722627	-1.905622
H	-1.478245	0.266854	-2.859539
H	-2.606737	1.642237	-2.900786
C	-2.308875	-1.888145	1.959363
H	-1.991419	-2.835536	1.495018
H	-1.430544	-1.465974	2.471673
H	-3.060585	-2.128092	2.722959
C	-6.313637	0.649633	0.239981
H	-6.931154	-0.054156	-0.343391
H	-6.653543	0.596621	1.284150
H	-6.516390	1.659281	-0.145512

TS_Ia_F

Zero-point correction= 0.256903 (Hartree/Particle)

Thermal correction to Energy= 0.279093
Thermal correction to Enthalpy= 0.280037
Thermal correction to Gibbs Free Energy= 0.202143
Sum of electronic and zero-point Energies= -988.739795
Sum of electronic and thermal Energies= -988.717605
Sum of electronic and thermal Enthalpies= -988.716661
Sum of electronic and thermal Free Energies= -988.794555
E(RB-P86) = -988.996698023 A.U

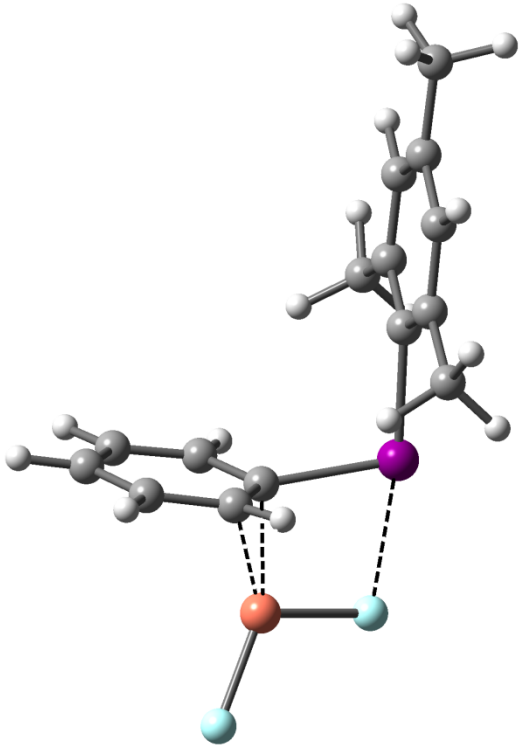


C	-1.960207	-0.349798	-0.138870
C	-2.674797	-0.834748	0.977710
C	-2.493381	0.599501	-1.036309
C	-3.961308	-0.314470	1.187461
C	-3.782633	1.083397	-0.765127
C	-4.529389	0.645675	0.337781
H	-4.535538	-0.680097	2.043855
H	-4.214944	1.822188	-1.446317
I	-0.026688	-1.196843	-0.531238
C	1.120372	0.578665	-0.009510
C	1.797240	1.261152	-1.047926
C	0.848873	1.192669	1.227291
C	2.266587	2.557518	-0.796673
H	1.926660	0.801229	-2.028534
C	1.332023	2.488997	1.444797
H	0.285119	0.675963	2.004591
C	2.031879	3.170003	0.441253
H	2.803579	3.088484	-1.585383
H	1.147138	2.967268	2.408994
H	2.387779	4.186198	0.620994
Cu	3.055768	-0.390076	0.270569
F	4.454070	0.244048	1.336117

F	2.349231	-1.850954	-0.818433
C	-1.748170	1.106120	-2.245923
H	-0.832110	1.647336	-1.960787
H	-1.446503	0.282294	-2.912369
H	-2.377714	1.795901	-2.823678
C	-2.140987	-1.883932	1.926334
H	-1.973155	-2.846315	1.416712
H	-1.182414	-1.585721	2.378558
H	-2.857665	-2.057984	2.739950
C	-5.903201	1.204908	0.615384
H	-5.840265	2.060270	1.309236
H	-6.385067	1.563215	-0.305490
H	-6.554799	0.452833	1.083591

IIa_F

Zero-point correction= 0.257616 (Hartree/Particle)
Thermal correction to Energy= 0.280201
Thermal correction to Enthalpy= 0.281145
Thermal correction to Gibbs Free Energy= 0.203000
Sum of electronic and zero-point Energies= -988.741531
Sum of electronic and thermal Energies= -988.718946
Sum of electronic and thermal Enthalpies= -988.718001
Sum of electronic and thermal Free Energies= -988.796147
E(RB-P86) = -988.999146789 A.U

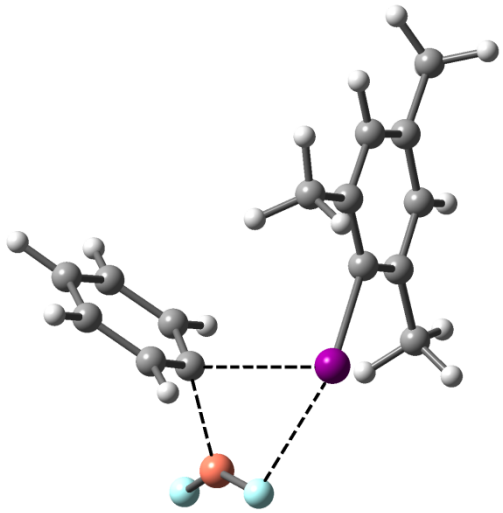


C	-1.960672	-0.364001	-0.000841
C	-2.695712	-0.027304	1.155207
C	-2.489982	-0.240197	-1.304792

C	-3.996460	0.468579	0.967044
C	-3.795244	0.260053	-1.421793
C	-4.563507	0.620432	-0.304892
H	-4.581513	0.740256	1.850550
H	-4.222426	0.367300	-2.423317
I	-0.011816	-1.249557	0.237801
C	1.162738	0.582838	0.201973
C	1.489714	1.193793	-1.048545
C	1.276590	1.313029	1.415396
C	1.889025	2.551871	-1.053385
H	1.291857	0.684439	-1.993725
C	1.695025	2.639968	1.366075
H	1.053875	0.838222	2.371211
C	1.978461	3.266564	0.136250
H	2.109520	3.029990	-2.009911
H	1.795558	3.197154	2.299947
H	2.276165	4.316538	0.119832
Cu	2.957454	-0.157356	-0.230102
F	4.760669	-0.159038	-0.768960
F	2.364968	-1.968852	0.488897
C	-1.733224	-0.611162	-2.558493
H	-0.851114	0.030463	-2.706802
H	-1.381339	-1.653941	-2.535172
H	-2.378201	-0.493223	-3.439394
C	-2.162720	-0.169250	2.561303
H	-1.835250	-1.198269	2.775856
H	-1.301820	0.493573	2.738447
H	-2.939868	0.095881	3.290467
C	-5.972440	1.133568	-0.473560
H	-6.662836	0.304963	-0.704086
H	-6.333906	1.624801	0.440568
H	-6.038881	1.850037	-1.306093

TS_IIa_F

Zero-point correction= 0.256519 (Hartree/Particle)
Thermal correction to Energy= 0.278919
Thermal correction to Enthalpy= 0.279863
Thermal correction to Gibbs Free Energy= 0.201081
Sum of electronic and zero-point Energies= -988.733467
Sum of electronic and thermal Energies= -988.711067
Sum of electronic and thermal Enthalpies= -988.710123
Sum of electronic and thermal Free Energies= -988.788905
E(RB-P86) = -1137.53907002 A.U.

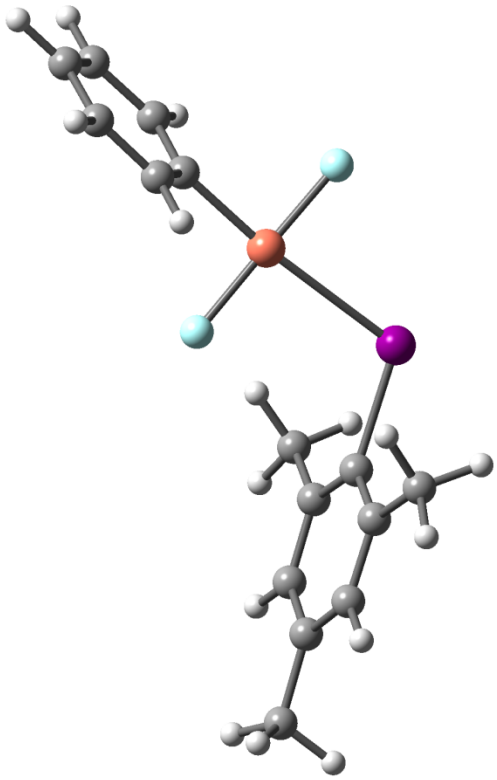


C	2.371760	0.285433	-0.350976
C	2.334280	1.658124	-0.691610
C	3.301164	-0.255857	0.567900
C	3.288323	2.488657	-0.088648
C	4.227342	0.631944	1.131183
C	4.243594	2.000148	0.816561
H	3.281666	3.553533	-0.338256
H	4.958772	0.237448	1.842236
I	0.990865	-1.019165	-1.275638
C	-1.049476	-1.258909	0.783204
C	-1.283450	-2.594348	1.089814
C	-0.737179	-0.273413	1.710439
C	-1.336885	-2.926264	2.455125
H	-1.453705	-3.342106	0.315843
C	-0.795514	-0.640114	3.066592
H	-0.476431	0.746411	1.424311
C	-1.092229	-1.956811	3.433188
H	-1.559346	-3.959080	2.733675
H	-0.589713	0.119995	3.823808
H	-1.112534	-2.233800	4.489279
Cu	-1.833731	-0.750362	-0.933743
F	-1.621167	-2.288516	-1.975368
C	-3.475823	1.235873	0.322422
H	-3.593975	0.558101	1.181453
O	-2.712955	0.938499	-0.651399
N	-4.164461	2.365796	0.384773
C	-4.106834	3.367614	-0.683575
H	-3.799374	4.332588	-0.256115
H	-3.386615	3.047669	-1.442849
H	-5.102906	3.477193	-1.136471
C	-5.037858	2.654151	1.525722
H	-4.708499	3.581701	2.015404
H	-6.072232	2.780378	1.174878
H	-4.995678	1.826867	2.244141

C	3.333674	-1.713370	0.952122
H	2.377480	-2.036169	1.393242
H	3.522166	-2.357620	0.078470
H	4.127945	-1.897280	1.687766
C	1.338337	2.245366	-1.659199
H	1.450787	1.811646	-2.665752
H	0.302001	2.054629	-1.339584
H	1.477178	3.331642	-1.739041
C	5.275825	2.918231	1.418938
H	6.176448	2.954775	0.782157
H	4.896965	3.946539	1.507096
H	5.593004	2.570520	2.412556

IIIa_F

Zero-point correction= 0.257738 (Hartree/Particle)
Thermal correction to Energy= 0.280395
Thermal correction to Enthalpy= 0.281339
Thermal correction to Gibbs Free Energy= 0.200785
Sum of electronic and zero-point Energies= -988.752476
Sum of electronic and thermal Energies= -988.729819
Sum of electronic and thermal Enthalpies= -988.728875
Sum of electronic and thermal Free Energies= -988.809430
E(RB-P86) = -989.010214250 A.U

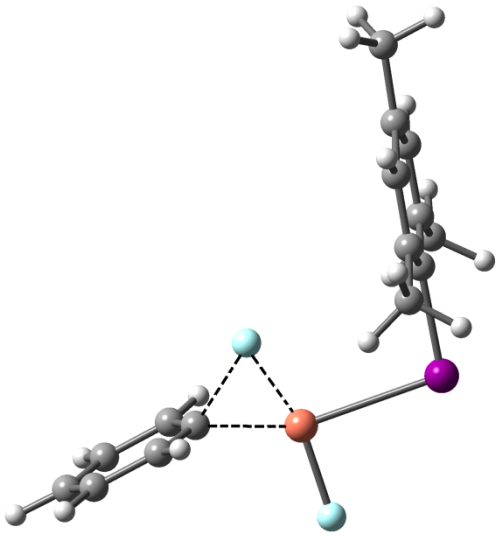


C	-2.381309	-0.167025	-0.019138
C	-2.969604	0.263167	1.187153

C	-2.790153	0.298662	-1.283458
C	-4.014039	1.196168	1.089254
C	-3.840766	1.231847	-1.309784
C	-4.467467	1.688876	-0.143111
H	-4.483862	1.545887	2.013490
H	-4.172646	1.610121	-2.281252
I	-0.810300	-1.603140	0.073041
C	3.374468	0.544531	0.011351
C	3.756162	1.315115	1.094522
C	4.157687	0.282062	-1.097999
C	5.052483	1.863832	1.056544
H	3.097699	1.509663	1.941960
C	5.444442	0.854268	-1.114902
H	3.819523	-0.343260	-1.925190
C	5.885879	1.635631	-0.042758
H	5.389067	2.476999	1.896078
H	6.091531	0.668637	-1.975658
H	6.887316	2.071165	-0.064503
Cu	1.619553	-0.235187	0.045122
F	0.895720	1.401779	-0.001038
F	2.321093	-1.891434	0.090753
C	-2.532522	-0.227689	2.544667
H	-2.646240	-1.319873	2.634823
H	-1.472259	0.002143	2.735509
H	-3.132322	0.244588	3.334455
C	-2.162410	-0.153727	-2.578124
H	-1.082082	0.060818	-2.599874
H	-2.278191	-1.239703	-2.724988
H	-2.630549	0.357272	-3.430376
C	-5.612671	2.670934	-0.207440
H	-6.579401	2.152483	-0.091336
H	-5.546857	3.416220	0.599394
H	-5.634271	3.200680	-1.170341

TS_IIIa_F

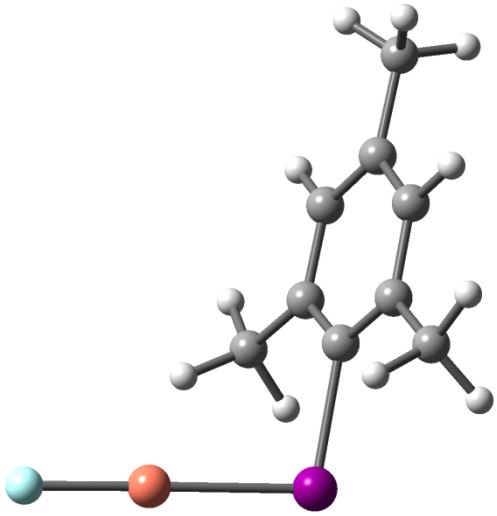
Zero-point correction= 0.256486 (Hartree/Particle)
Thermal correction to Energy= 0.278863
Thermal correction to Enthalpy= 0.279808
Thermal correction to Gibbs Free Energy= 0.198771
Sum of electronic and zero-point Energies= -988.739745
Sum of electronic and thermal Energies= -988.717368
Sum of electronic and thermal Enthalpies= -988.716424
Sum of electronic and thermal Free Energies= -988.797460
E(RB-P86) = -988.996231096 A.U



C	-2.943715	0.869391	-0.000253
C	-3.519500	1.135168	-1.233277
C	-3.519175	1.135733	1.232800
C	-4.856146	1.565310	-1.214443
H	-2.984455	0.986461	-2.171638
C	-4.855829	1.565863	1.214126
H	-2.983880	0.987465	2.171088
C	-5.518790	1.782392	-0.000121
H	-5.362855	1.744859	-2.165402
H	-5.362286	1.745843	2.165137
H	-6.550535	2.138916	-0.000068
Cu	-1.574725	-0.573208	-0.000066
F	-1.111580	1.248465	-0.000566
F	-2.470794	-2.172652	0.000349
C	2.636505	0.416966	1.237425
C	3.493602	1.530209	1.201831
C	3.937829	2.097293	-0.000119
C	3.494155	1.529553	-1.201977
C	2.637072	0.416308	-1.237363
C	2.231282	-0.117749	0.000086
H	3.817776	1.963743	2.152769
H	3.818771	1.962571	-2.153001
I	0.956016	-1.831449	0.000257
C	2.195180	-0.142567	2.566401
H	1.097870	-0.128206	2.664484
H	2.514565	-1.189911	2.689499
H	2.621391	0.444445	3.391316
C	2.196334	-0.143936	-2.566236
H	2.515768	-1.191346	-2.688632
H	1.099067	-0.129620	-2.664815
H	2.622917	0.442633	-3.391274
C	4.883795	3.275147	-0.000253
H	5.933258	2.934929	-0.001314
H	4.742569	3.902593	-0.892297
H	4.744017	3.901654	0.892670

IVa_F

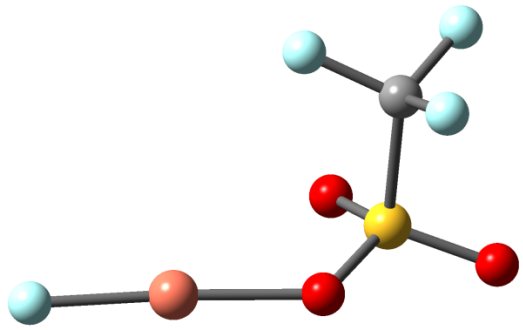
Zero-point correction= 0.169006 (Hartree/Particle)
Thermal correction to Energy= 0.184230
Thermal correction to Enthalpy= 0.185174
Thermal correction to Gibbs Free Energy= 0.123120
Sum of electronic and zero-point Energies= -657.291875
Sum of electronic and thermal Energies= -657.276650
Sum of electronic and thermal Enthalpies= -657.275706
Sum of electronic and thermal Free Energies= -657.337760
E(RB-P86) = -657.460880426 A.U



Cu	-2.304009	0.702500	0.565656
F	-3.295911	1.951872	1.450401
C	1.819768	-1.049630	0.589354
C	3.120715	-0.568407	0.815313
C	3.575634	0.645485	0.282034
C	2.690064	1.400203	-0.498459
C	1.376193	0.978114	-0.768096
C	0.982066	-0.247450	-0.204723
H	3.793264	-1.170745	1.433300
H	3.021649	2.353697	-0.919993
I	-1.009630	-0.968719	-0.606137
C	1.392501	-2.364536	1.192205
H	0.511075	-2.243695	1.841830
H	1.125248	-3.099335	0.415768
H	2.205664	-2.791052	1.794749
C	0.473382	1.837967	-1.614455
H	0.101632	1.290787	-2.495261
H	-0.411948	2.171560	-1.046347
H	1.009332	2.730396	-1.964215
C	4.991617	1.113154	0.520264
H	5.674887	0.686428	-0.233316
H	5.069813	2.207725	0.452239
H	5.357603	0.797600	1.508244

[CuF(OTf)]$^-$

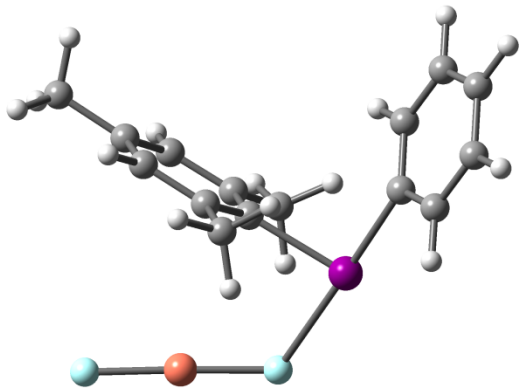
Zero-point correction= 0.027853 (Hartree/Particle)
Thermal correction to Energy= 0.039012
Thermal correction to Enthalpy= 0.039956
Thermal correction to Gibbs Free Energy= -0.012205
Sum of electronic and zero-point Energies= -1258.234887
Sum of electronic and thermal Energies= -1258.223729
Sum of electronic and thermal Enthalpies= -1258.222784
Sum of electronic and thermal Free Energies= -1258.274946
E(RB-P86) = -1258.26274063 A.U



Cu	-2.005613	-0.005373	-0.173231
C	1.701857	-0.781858	-0.005940
S	0.832099	0.896690	0.084963
O	1.785170	1.830892	-0.524163
O	0.501188	1.065908	1.506140
O	-0.375528	0.678777	-0.821596
F	2.004237	-1.094124	-1.284664
F	0.917219	-1.759452	0.499083
F	2.849665	-0.744741	0.708123
F	-3.620963	-0.635538	0.346001

Ia_F_Mes

Zero-point correction= 0.258062 (Hartree/Particle)
Thermal correction to Energy= 0.280908
Thermal correction to Enthalpy= 0.281853
Thermal correction to Gibbs Free Energy= 0.201022
Sum of electronic and zero-point Energies= -988.746919
Sum of electronic and thermal Energies= -988.724072
Sum of electronic and thermal Enthalpies= -988.723128
Sum of electronic and thermal Free Energies= -988.803958
E(RB-P86) = -989.004980176 A.U.

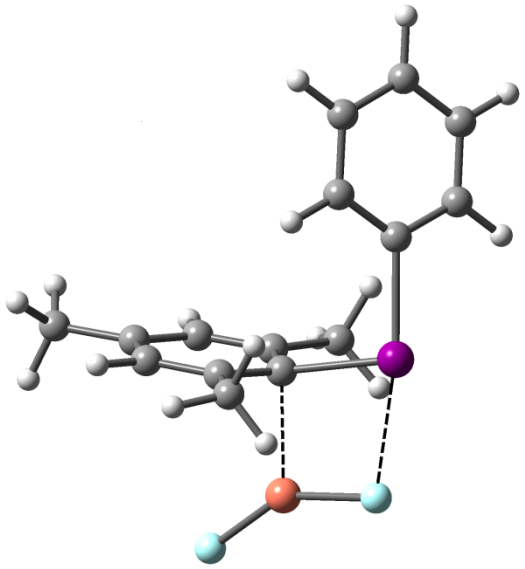


C	-2.751007	-0.237171	0.053609
C	-3.072922	0.815193	0.914596
C	-3.664363	-0.739914	-0.877418
C	-4.349571	1.383625	0.828723
H	-2.351525	1.196428	1.639534
C	-4.942506	-0.168504	-0.939829
H	-3.396042	-1.557629	-1.549493
C	-5.282482	0.891461	-0.092694
H	-4.613331	2.210230	1.492078
H	-5.666120	-0.552217	-1.662267
H	-6.277682	1.337288	-0.150221
I	-0.831339	-1.199106	0.181393
C	0.321719	0.599189	0.078315
C	0.400967	1.264570	-1.158711
C	0.955360	1.034214	1.257246
C	1.147228	2.453917	-1.175157
C	1.687645	2.228421	1.161764
C	1.788646	2.954251	-0.033599
H	1.231197	2.996480	-2.121088
H	2.198922	2.592617	2.057300
Cu	2.990788	-1.422307	-0.212430
F	4.532432	-0.618389	-0.723425
F	1.447213	-2.285455	0.309047
C	0.911293	0.281955	2.563910
H	1.513142	0.800625	3.321622
H	-0.115898	0.191429	2.951917
H	1.311350	-0.737043	2.442659
C	-0.256520	0.774554	-2.423343
H	-1.354920	0.783972	-2.337999
H	0.019480	1.417610	-3.269271
H	0.046981	-0.256319	-2.664494
C	2.558488	4.250891	-0.087161
H	2.975051	4.428812	-1.088871
H	1.898257	5.102115	0.150550
H	3.380622	4.259818	0.642586

TS_Ia_F_Mes

Zero-point correction= 0.257240 (Hartree/Particle)

Thermal correction to Energy= 0.279254
Thermal correction to Enthalpy= 0.280198
Thermal correction to Gibbs Free Energy= 0.203434
Sum of electronic and zero-point Energies= -988.741555
Sum of electronic and thermal Energies= -988.719541
Sum of electronic and thermal Enthalpies= -988.718597
Sum of electronic and thermal Free Energies= -988.795361
E(RB-P86) = -988.998794991 A.U

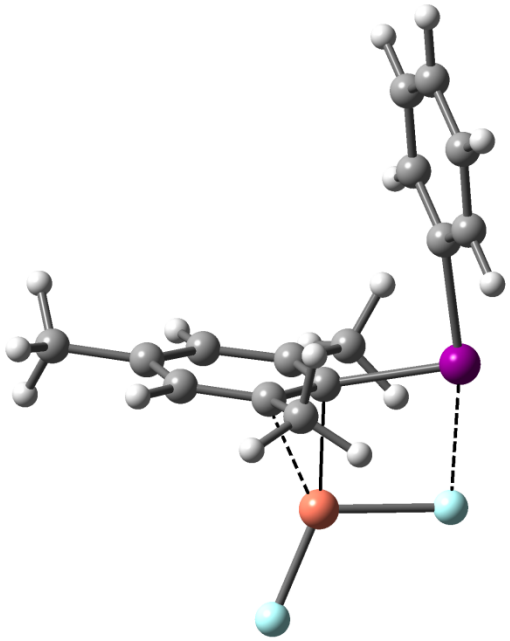


C	2.549054	-0.059382	0.059111
C	3.500314	-0.317627	-0.934148
C	2.708206	0.986347	0.974287
C	4.640526	0.493948	-1.004983
C	3.845815	1.796560	0.881325
C	4.810802	1.549757	-0.103177
H	5.389898	0.299556	-1.775362
H	3.977560	2.618933	1.587887
I	0.861571	-1.380217	0.190009
C	-0.619308	0.219052	0.047784
C	-1.092899	0.763161	1.276086
C	-0.694707	0.914963	-1.190074
C	-1.733174	2.008192	1.204449
C	-1.346552	2.156692	-1.171750
C	-1.863418	2.722869	0.002845
H	-2.133998	2.434187	2.128764
H	-1.442500	2.700059	-2.116354
Cu	-2.402050	-1.049055	-0.224897
F	-4.080082	-0.399119	-0.722496
F	-1.284189	-2.566689	0.228064
H	5.698126	2.183141	-0.166853
H	1.965554	1.181356	1.749946
H	3.364735	-1.134615	-1.646033
C	-0.124044	0.380195	-2.479341

H	-0.524810	0.941758	-3.333618
H	0.974022	0.476914	-2.501991
H	-0.364545	-0.683836	-2.624554
C	-0.951072	0.060771	2.604960
H	0.087254	0.094517	2.974345
H	-1.587247	0.544751	3.357788
H	-1.240079	-0.998870	2.537361
C	-2.564955	4.057520	-0.027347
H	-2.443433	4.596076	0.923637
H	-2.185943	4.691490	-0.841780
H	-3.647481	3.922818	-0.191942

IIa_F_Mes

Zero-point correction= 0.257355 (Hartree/Particle)
Thermal correction to Energy= 0.280162
Thermal correction to Enthalpy= 0.281106
Thermal correction to Gibbs Free Energy= 0.201881
Sum of electronic and zero-point Energies= -988.743031
Sum of electronic and thermal Energies= -988.720223
Sum of electronic and thermal Enthalpies= -988.719279
Sum of electronic and thermal Free Energies= -988.798505
E(RB-P86) = -989.000385633 A.U

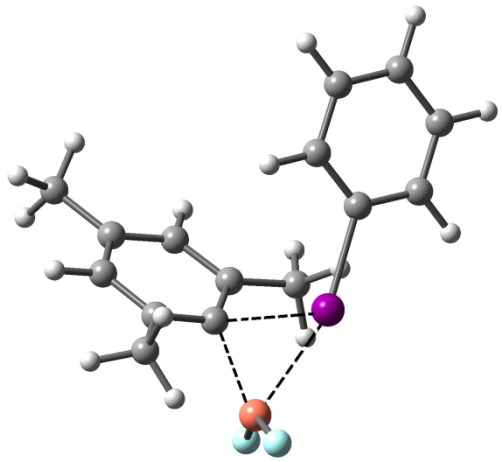


C	-2.541382	-0.075634	-0.030812
C	-3.352559	-0.287540	1.090011
C	-2.849016	0.903638	-0.981580
C	-4.498639	0.500703	1.257122
H	-3.102809	-1.054509	1.826003
C	-3.990728	1.692068	-0.794956
H	-2.219835	1.058725	-1.859316
C	-4.814407	1.490169	0.319602

H	-5.138694	0.340488	2.127539
H	-4.237866	2.461214	-1.530070
H	-5.706056	2.105818	0.456173
I	-0.843791	-1.375414	-0.284034
C	0.643800	0.216713	-0.123856
C	1.083195	0.830425	-1.345664
C	0.856054	0.828152	1.155931
C	1.707678	2.076011	-1.240976
C	1.496367	2.090347	1.161588
C	1.900932	2.733649	-0.008092
H	2.062681	2.550353	-2.160589
H	1.657145	2.574846	2.128773
Cu	2.271906	-0.804456	0.309769
F	4.035091	-1.155258	0.852296
F	1.291135	-2.513202	-0.377359
C	0.897288	0.184360	-2.696556
H	1.534034	0.679418	-3.441757
H	1.154899	-0.884240	-2.673419
H	-0.145207	0.264972	-3.045813
C	0.289987	0.289526	2.450273
H	0.886294	0.647555	3.300347
H	-0.743710	0.647259	2.593185
H	0.269655	-0.808142	2.481952
C	2.568496	4.084959	0.034615
H	2.085486	4.787709	-0.662068
H	2.535464	4.518105	1.043653
H	3.625766	4.007502	-0.268415

TS_IIa_F_Mes

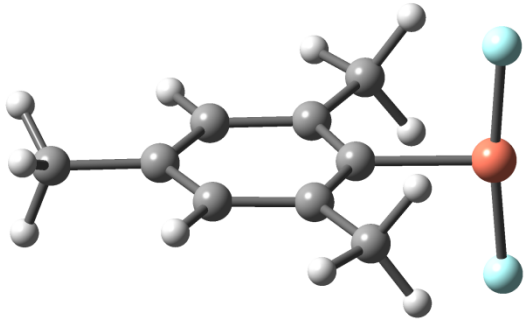
Zero-point correction= 0.256348 (Hartree/Particle)
Thermal correction to Energy= 0.278849
Thermal correction to Enthalpy= 0.279794
Thermal correction to Gibbs Free Energy= 0.200574
Sum of electronic and zero-point Energies= -988.732672
Sum of electronic and thermal Energies= -988.710171
Sum of electronic and thermal Enthalpies= -988.709227
Sum of electronic and thermal Free Energies= -988.788446
E(RB-P86) = -988.989020242 A.U.



C	-2.527177	-0.185936	-0.119410
C	-3.290080	-0.451063	1.026690
C	-2.885578	0.829746	-1.016388
C	-4.438208	0.311276	1.267849
H	-3.001965	-1.244261	1.718938
C	-4.033867	1.586630	-0.756842
H	-2.285802	1.026874	-1.906369
C	-4.809031	1.329300	0.380759
H	-5.041436	0.106671	2.155105
H	-4.321717	2.378956	-1.451399
H	-5.704178	1.923594	0.576066
I	-0.815119	-1.370656	-0.505863
C	1.282344	0.440865	0.036362
C	1.724000	0.912942	-1.203371
C	0.891604	1.227136	1.129297
C	1.971030	2.302050	-1.254920
C	1.153607	2.602150	0.991758
C	1.693038	3.155202	-0.181262
H	2.373362	2.709111	-2.187943
H	0.920945	3.250182	1.842509
Cu	2.062336	-1.330771	0.535531
F	3.039136	-0.926924	2.048687
F	1.647554	-2.607852	-0.771342
C	1.938751	0.065753	-2.432270
H	2.727248	0.498048	-3.063860
H	2.198676	-0.969715	-2.174186
H	1.012373	0.031660	-3.030398
C	0.318954	0.678496	2.409440
H	0.137038	1.488994	3.127677
H	-0.635214	0.158141	2.233156
H	1.021762	-0.042648	2.855006
C	1.959992	4.637952	-0.279724
H	1.990482	4.972055	-1.326335
H	1.192684	5.219654	0.251837
H	2.932819	4.887825	0.176585

IIIa'_F_Mes

Zero-point correction= 0.169406 (Hartree/Particle)
Thermal correction to Energy= 0.184391
Thermal correction to Enthalpy= 0.185336
Thermal correction to Gibbs Free Energy= 0.125006
Sum of electronic and zero-point Energies= -745.702413
Sum of electronic and thermal Energies= -745.687428
Sum of electronic and thermal Enthalpies= -745.686483
Sum of electronic and thermal Free Energies= -745.746814
E(RB-P86) = -745.871819128 A.U

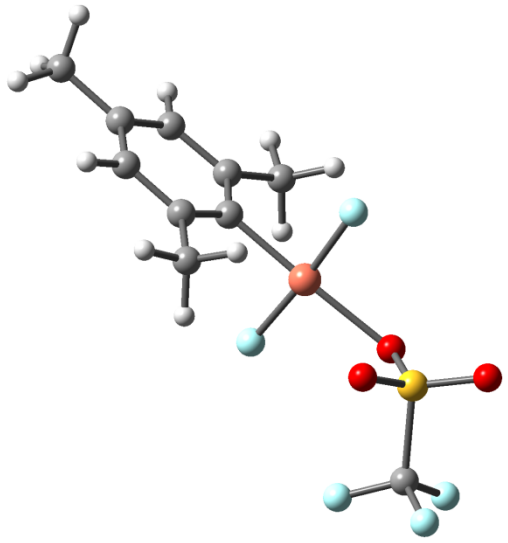


C	0.043797	-0.000055	-0.000036
C	0.634501	-1.249234	-0.005072
C	0.634387	1.249176	-0.005165
C	2.047335	-1.206605	-0.008726
C	2.047234	1.206670	-0.008802
C	2.760289	0.000066	-0.007762
H	2.580567	-2.162449	-0.015230
H	2.580381	2.162561	-0.015369
Cu	-1.876317	-0.000002	0.004729
F	-1.994501	0.000202	1.773628
F	-1.995369	-0.000217	-1.763780
C	-0.126734	-2.550523	-0.009606
H	0.564355	-3.403373	-0.017933
H	-0.767501	-2.632681	0.882155
H	-0.776263	-2.621840	-0.895875
C	-0.126942	2.550407	-0.009813
H	0.564085	3.403307	-0.018199
H	-0.776463	2.621614	-0.896099
H	-0.767726	2.632592	0.881934
C	4.272131	0.000116	0.016984
H	4.680189	-0.891686	-0.479597
H	4.680114	0.892533	-0.478544
H	4.644315	-0.000496	1.054957

IIIa_F_Mes

Zero-point correction= 0.196013 (Hartree/Particle)
Thermal correction to Energy= 0.220072
Thermal correction to Enthalpy= 0.221016
Thermal correction to Gibbs Free Energy= 0.138175

Sum of electronic and zero-point Energies= -1707.599594
Sum of electronic and thermal Energies= -1707.575536
Sum of electronic and thermal Enthalpies= -1707.574592
Sum of electronic and thermal Free Energies= -1707.657433
E(RB-P86) = -1707.79560796 A.U

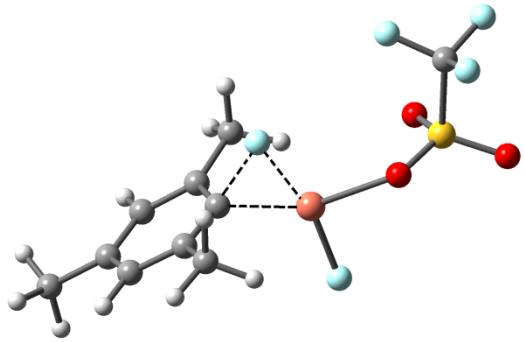


C	-2.171501	0.073042	-0.005842
C	-2.574381	-1.253396	0.013967
C	-2.988723	1.189101	-0.122995
C	-3.967395	-1.459662	-0.091946
C	-4.368175	0.914107	-0.225805
C	-4.871565	-0.395445	-0.209567
H	-4.334848	-2.490987	-0.081331
H	-5.053741	1.762365	-0.323641
Cu	-0.290019	0.402531	0.136134
F	-0.215847	0.352738	-1.665706
C	3.944517	-0.161280	-0.747642
S	2.773388	-0.085668	0.735615
O	3.630081	0.402270	1.827969
O	2.249094	-1.457521	0.850284
O	1.752776	0.923982	0.278012
F	3.305375	-0.609175	-1.851699
F	4.972365	-1.003625	-0.485259
F	4.459295	1.059960	-1.021617
F	-0.498403	0.433862	1.928662
C	-2.459003	2.602263	-0.148091
H	-1.897580	2.828888	0.772090
H	-1.772523	2.749491	-0.996730
H	-3.280086	3.326322	-0.238133
C	-1.610109	-2.407811	0.136007
H	-0.903556	-2.419553	-0.708712
H	-1.015662	-2.326043	1.059212
H	-2.145851	-3.366478	0.151871
C	-6.360387	-0.648461	-0.297641

H	-6.849379	-0.469726	0.674537
H	-6.837597	0.021124	-1.028962
H	-6.573168	-1.686552	-0.590137

TS_IIIa_F_Mes

Zero-point correction= 0.194556 (Hartree/Particle)
Thermal correction to Energy= 0.218505
Thermal correction to Enthalpy= 0.219450
Thermal correction to Gibbs Free Energy= 0.135433
Sum of electronic and zero-point Energies= -1707.586354
Sum of electronic and thermal Energies= -1707.562405
Sum of electronic and thermal Enthalpies= -1707.561461
Sum of electronic and thermal Free Energies= -1707.645478
E(RB-P86) = -1707.78091088 A.U



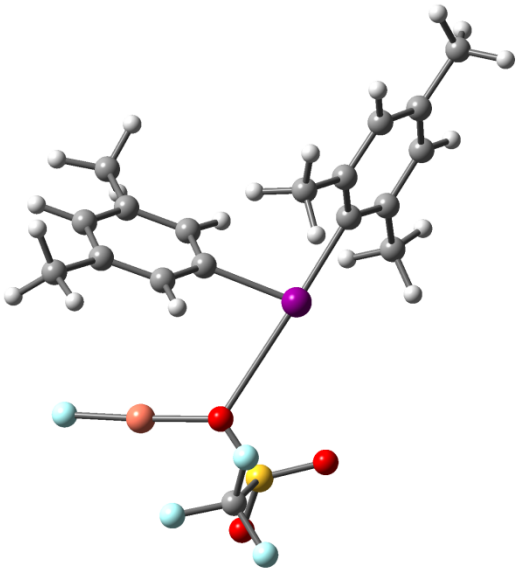
C	2.065090	-0.021504	-0.313496
C	2.489045	1.297016	-0.141169
C	2.881314	-1.126223	-0.561451
C	3.879625	1.458591	-0.006410
C	4.259887	-0.887837	-0.416304
C	4.777448	0.386529	-0.134314
H	4.260800	2.466735	0.185674
H	4.941257	-1.734754	-0.546197
Cu	0.288368	-0.466578	0.484509
F	0.531097	-0.077338	-1.359835
C	-3.810221	0.195133	-0.871633
S	-2.835717	0.056102	0.743340
O	-3.850513	-0.364806	1.724573
O	-2.252425	1.399360	0.925256
O	-1.825104	-1.004283	0.413387
F	-3.007247	0.571441	-1.893849
F	-4.796096	1.116627	-0.750615
F	-4.379765	-0.989662	-1.196994
F	0.608228	-0.778861	2.272547
C	2.344856	-2.486046	-0.930084
H	1.607792	-2.843990	-0.192668
H	1.839456	-2.457956	-1.907786
H	3.160884	-3.219599	-0.981851
C	1.542749	2.468970	-0.086501
H	1.097489	2.656959	-1.076209
H	0.710410	2.287683	0.611930

H	2.072264	3.377031	0.232581
C	6.264634	0.600497	0.022488
H	6.564292	1.603123	-0.316516
H	6.566673	0.509623	1.079942
H	6.839315	-0.144497	-0.546856

e. Copper species for reactions of $[Mes(Ar)I]^+$ with $[CuF_2]^-$, adducts and transition structures not documented above, (Table 3)

Reactions of $[3,5\text{-}Me_2C_6H_4(Ph)I]BF_4$
G-I: adducts

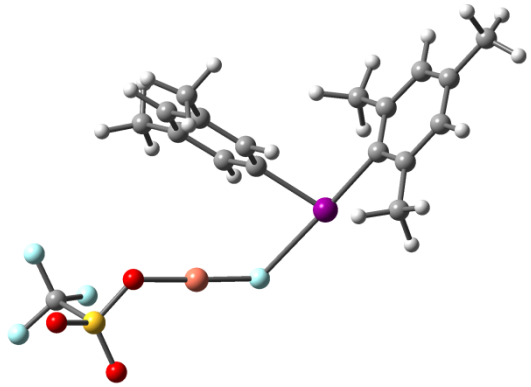
Zero-point correction= 0.335723 (Hartree/Particle)
Thermal correction to Energy= 0.370132
Thermal correction to Enthalpy= 0.371076
Thermal correction to Gibbs Free Energy= 0.260000
Sum of electronic and zero-point Energies= -1929.175668
Sum of electronic and thermal Energies= -1929.141260
Sum of electronic and thermal Enthalpies= -1929.140315
Sum of electronic and thermal Free Energies= -1929.251391
E(RB-P86) = -1929.51139149 A.U.



O	-2.094900	-0.472026	-0.428577
C	2.998845	-0.849009	0.004691
C	3.720560	-1.167364	-1.163207
C	3.589238	-0.648368	1.267367
C	5.113755	-1.266415	-1.024937
C	4.987660	-0.756288	1.326586
C	5.764257	-1.064728	0.201109
H	5.704403	-1.509264	-1.912817
H	5.477616	-0.594102	2.290777
I	0.868208	-0.729980	-0.156287
C	0.588802	1.367466	0.172778
C	-0.216821	1.736554	1.251504
C	1.178474	2.271614	-0.702163

C	-0.442373	3.105111	1.471471
H	-0.654853	0.991045	1.916455
C	0.965811	3.646671	-0.476436
H	1.789917	1.943630	-1.544235
C	0.158869	4.033109	0.602547
H	-0.013014	5.100110	0.773188
Cu	-2.851065	1.188461	-0.910236
C	-3.704830	-2.007506	1.039790
F	-3.501354	2.811762	-1.379612
F	-4.372104	-3.180781	1.063808
F	-2.821277	-1.992791	2.059535
F	-4.589006	-1.004142	1.219943
S	-2.808315	-1.817336	-0.616775
O	-1.831020	-2.911184	-0.640846
O	-3.871900	-1.792398	-1.624206
C	2.808859	-0.324175	2.515349
H	2.280582	0.638194	2.425536
H	2.052665	-1.095972	2.731314
H	3.482036	-0.258767	3.380051
C	3.087525	-1.417854	-2.511055
H	2.434811	-2.305327	-2.495135
H	2.475010	-0.566513	-2.844948
H	3.864887	-1.591200	-3.266671
C	7.262240	-1.205577	0.309650
H	7.540974	-2.263718	0.448959
H	7.764468	-0.854505	-0.603504
H	7.657630	-0.643908	1.167569
C	-1.301977	3.568122	2.622734
H	-0.719424	4.189844	3.320977
H	-2.140013	4.183778	2.260396
H	-1.716402	2.719034	3.182884
C	1.598804	4.666813	-1.392198
H	1.251349	5.681635	-1.155490
H	2.696589	4.650622	-1.298585
H	1.359705	4.455691	-2.445810

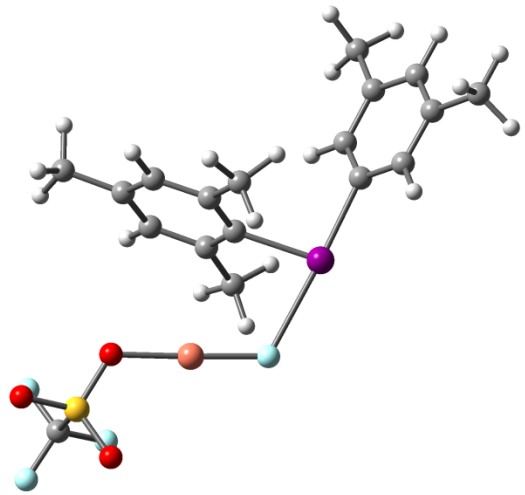
Zero-point correction= 0.335628 (Hartree/Particle)
Thermal correction to Energy= 0.369901
Thermal correction to Enthalpy= 0.370845
Thermal correction to Gibbs Free Energy= 0.260268
Sum of electronic and zero-point Energies= -1929.182523
Sum of electronic and thermal Energies= -1929.148250
Sum of electronic and thermal Enthalpies= -1929.147306
Sum of electronic and thermal Free Energies= -1929.257883
E(RB-P86) = -1929.51815112 A.U.



C	3.815512	-0.499908	-0.163577
C	4.463448	0.470612	-0.954603
C	4.435767	-1.152688	0.922214
C	5.779118	0.805768	-0.598248
C	5.755502	-0.775815	1.217302
C	6.439509	0.201937	0.480968
H	6.301726	1.559538	-1.194438
H	6.261361	-1.270234	2.051707
I	1.813751	-1.087930	-0.670037
C	0.850448	0.746119	-0.127071
C	1.011662	1.230346	1.165096
C	0.078644	1.378605	-1.102998
C	0.359389	2.430769	1.512573
H	1.618358	0.704146	1.903829
C	-0.579021	2.570914	-0.759931
H	-0.014750	0.966039	-2.108380
C	-0.425326	3.072679	0.544903
H	-0.939292	3.999631	0.816441
Cu	-1.959749	-1.053062	-0.154113
F	-0.629207	-1.747634	-1.214479
C	-5.453105	0.309041	-0.394936
S	-4.715962	-0.798648	0.951286
F	-5.327925	1.611944	-0.063675
F	-6.766304	0.030944	-0.552158
F	-4.828617	0.105406	-1.576302
O	-4.891144	-2.165584	0.443449
O	-5.427261	-0.411407	2.173847
O	-3.264553	-0.325313	0.991418
C	7.845838	0.604879	0.850913
H	7.832356	1.396893	1.618733
H	8.409947	-0.242611	1.266571
H	8.391985	0.998791	-0.018025
C	3.772786	-2.229984	1.749023
H	2.822119	-1.890783	2.188274
H	3.552827	-3.127133	1.148202
H	4.432734	-2.535924	2.571728
C	3.816433	1.147243	-2.137266
H	3.448158	0.413334	-2.871787

H	2.955846	1.763985	-1.832711
H	4.536494	1.803049	-2.644332
C	0.510276	2.995460	2.905107
H	1.546778	3.323014	3.086075
H	-0.151051	3.859620	3.055748
H	0.271090	2.239292	3.668593
C	-1.411279	3.309927	-1.780173
H	-1.603207	2.691224	-2.667424
H	-2.378094	3.615421	-1.352739
H	-0.897518	4.227247	-2.111375

Zero-point correction= 0.335693 (Hartree/Particle)
Thermal correction to Energy= 0.369917
Thermal correction to Enthalpy= 0.370861
Thermal correction to Gibbs Free Energy= 0.261071
Sum of electronic and zero-point Energies= -1929.183692
Sum of electronic and thermal Energies= -1929.149468
Sum of electronic and thermal Enthalpies= -1929.148524
Sum of electronic and thermal Free Energies= -1929.258314
E(RB-P86) = -1929.51938499 A.U.

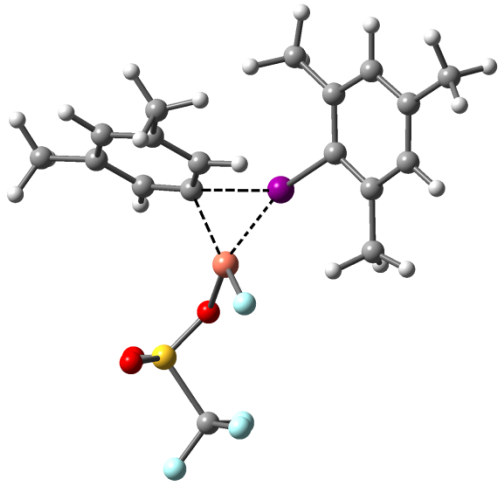


C	3.843780	-0.426391	-0.212771
C	4.174027	0.789367	-0.814752
C	4.767734	-1.197749	0.488728
C	5.490164	1.264345	-0.701896
H	3.430189	1.372783	-1.361129
C	6.097157	-0.740952	0.590994
H	4.478666	-2.141689	0.957358
C	6.430404	0.482368	-0.005522
H	7.460521	0.843438	0.072869
I	1.858625	-1.225450	-0.414868
C	0.826270	0.584634	0.059736
C	0.864098	1.039423	1.391589
C	0.148260	1.240254	-0.985074
C	0.193780	2.244442	1.653706

C	-0.505258	2.436420	-0.643897
C	-0.487843	2.957509	0.656846
H	0.202278	2.626262	2.678630
H	-1.047066	2.969694	-1.429974
Cu	-1.920245	-1.095677	0.135506
F	-0.553359	-2.097142	-0.580753
C	-5.325555	0.178009	-0.819320
S	-4.745350	-0.493587	0.852804
F	-5.178593	1.519098	-0.872518
F	-6.630873	-0.118041	-1.005719
F	-4.613958	-0.370931	-1.829103
O	-4.922879	-1.948004	0.750633
O	-5.545554	0.240043	1.838616
O	-3.287093	-0.041017	0.886937
C	1.566398	0.311610	2.509042
H	1.211123	-0.726854	2.600967
H	2.655404	0.273403	2.346009
H	1.386633	0.818933	3.465801
C	0.072548	0.721944	-2.400175
H	1.065841	0.677677	-2.874732
H	-0.352345	-0.293538	-2.425930
H	-0.563130	1.377213	-3.009921
C	-1.176862	4.260434	0.979594
H	-0.446315	5.086004	1.014903
H	-1.930410	4.514962	0.221460
H	-1.667970	4.219298	1.962983
C	7.122000	-1.554670	1.345095
H	8.125116	-1.116619	1.250416
H	6.872650	-1.605981	2.417302
H	7.160015	-2.590018	0.972259
C	5.885753	2.590275	-1.307000
H	5.960446	3.366724	-0.527563
H	6.869002	2.525804	-1.796580
H	5.149026	2.930738	-2.047847

G-I: TS's

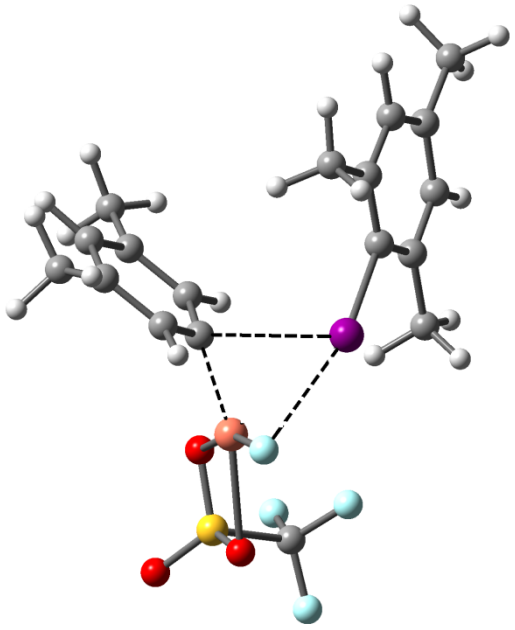
Zero-point correction= 0.333754 (Hartree/Particle)
Thermal correction to Energy= 0.367764
Thermal correction to Enthalpy= 0.368708
Thermal correction to Gibbs Free Energy= 0.259674
Sum of electronic and zero-point Energies= -1929.168034
Sum of electronic and thermal Energies= -1929.134025
Sum of electronic and thermal Enthalpies= -1929.133081
Sum of electronic and thermal Free Energies= -1929.242115
E(RB-P86) = -1929.50178881 A.U.



O	-2.462714	-0.415447	-0.569719
C	2.677889	-1.056416	-0.514953
C	3.832573	-0.350337	-0.919181
C	2.680320	-2.128036	0.405105
C	5.042257	-0.760403	-0.342788
C	3.930031	-2.475909	0.939164
C	5.113942	-1.813619	0.582248
H	5.956635	-0.233750	-0.629380
H	3.970913	-3.297227	1.659790
I	0.841462	-0.505154	-1.413348
C	0.346106	1.531722	0.072624
C	1.386395	1.816941	0.951035
C	-0.425070	2.484107	-0.590306
C	1.566719	3.163611	1.320975
H	2.015486	1.034269	1.380296
C	-0.245952	3.831661	-0.215165
H	-1.163865	2.215296	-1.346712
C	0.751779	4.140773	0.722224
H	0.916931	5.190223	0.983034
Cu	-0.734314	-0.029284	0.573001
C	-4.621314	-1.667067	0.322863
F	-0.688320	-0.669322	2.351613
F	-5.905576	-1.494352	0.712669
F	-4.608379	-2.515055	-0.730912
F	-3.942788	-2.243329	1.340033
S	-3.852671	-0.002882	-0.141917
O	-4.678865	0.472535	-1.261643
O	-3.886009	0.777028	1.105650
C	3.818790	0.786777	-1.908876
H	3.429793	0.467847	-2.888769
H	3.190014	1.621367	-1.559538
H	4.835838	1.171344	-2.058938
C	1.446763	-2.876960	0.835838
H	0.742094	-2.221492	1.379367
H	0.909516	-3.303474	-0.025639

H	1.722868	-3.703209	1.504168
C	6.439019	-2.241956	1.158416
H	6.902125	-3.014657	0.521374
H	7.142813	-1.399463	1.215143
H	6.319528	-2.673587	2.162199
C	2.606493	3.536684	2.349058
H	3.073069	4.501619	2.102333
H	2.144433	3.639273	3.344751
H	3.392892	2.773139	2.423376
C	-1.113294	4.906296	-0.824292
H	-2.013633	5.068524	-0.209060
H	-0.573414	5.862198	-0.882010
H	-1.448089	4.628645	-1.833561

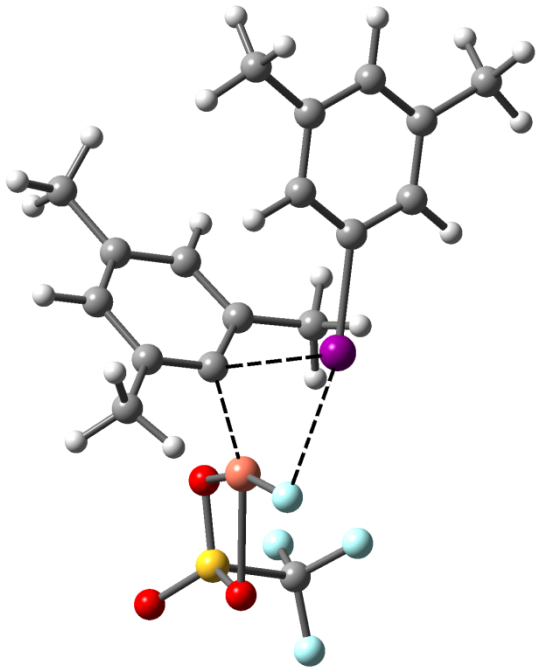
Zero-point correction= 0.333933 (Hartree/Particle)
Thermal correction to Energy= 0.367769
Thermal correction to Enthalpy= 0.368713
Thermal correction to Gibbs Free Energy= 0.260889
Sum of electronic and zero-point Energies= -1929.167091
Sum of electronic and thermal Energies= -1929.133255
Sum of electronic and thermal Enthalpies= -1929.132311
Sum of electronic and thermal Free Energies= -1929.240135
E(RB-P86) = -1929.50102378 A.U.



C	-2.515596	-1.134506	-0.508069
C	-2.260586	-2.394059	0.077856
C	-3.758482	-0.470491	-0.384171
C	-3.311049	-2.992841	0.790509
C	-4.763004	-1.123740	0.341846
C	-4.564511	-2.381680	0.933578
H	-3.136449	-3.970661	1.248630

H	-5.732354	-0.627879	0.448620
I	-0.982490	-0.202222	-1.636436
C	-0.057442	1.729855	0.152695
C	-0.281537	3.002523	-0.358735
C	-0.424339	1.307389	1.425259
C	-0.774336	3.980054	0.530985
H	-0.045536	3.247210	-1.394804
C	-0.920252	2.283642	2.312585
H	-0.299639	0.275386	1.756172
C	-1.093417	3.596820	1.843309
H	-1.512626	4.345389	2.522301
Cu	1.542125	0.893061	-0.626183
F	1.244714	1.414865	-2.417559
C	3.731979	-2.120599	0.571918
S	3.745467	-0.230919	0.488402
F	2.693672	-2.614263	-0.129731
F	4.877596	-2.605195	0.053401
F	3.626639	-2.525598	1.852940
O	3.681688	0.091430	-0.966648
O	4.933588	0.168101	1.238167
O	2.414135	0.168010	1.100541
C	-0.938317	-3.109176	-0.038731
H	-0.694959	-3.339316	-1.088415
H	-0.111799	-2.499199	0.356752
H	-0.962637	-4.054687	0.519589
C	-4.037262	0.881853	-0.991704
H	-3.342096	1.647199	-0.611900
H	-3.929608	0.862033	-2.088145
H	-5.060462	1.204056	-0.756082
C	-5.679807	-3.059461	1.689643
H	-6.437898	-3.455292	0.992966
H	-5.306232	-3.900321	2.290363
H	-6.195920	-2.353140	2.357687
C	-0.948453	5.405217	0.062379
H	-1.739514	5.913404	0.632414
H	-0.016535	5.977266	0.204322
H	-1.201754	5.448000	-1.006505
C	-1.250264	1.912569	3.738925
H	-2.127463	2.471513	4.096795
H	-1.454175	0.837485	3.839053
H	-0.408309	2.156464	4.407761

Zero-point correction= 0.333701 (Hartree/Particle)
Thermal correction to Energy= 0.367659
Thermal correction to Enthalpy= 0.368603
Thermal correction to Gibbs Free Energy= 0.260103
Sum of electronic and zero-point Energies= -1929.164086
Sum of electronic and thermal Energies= -1929.130128
Sum of electronic and thermal Enthalpies= -1929.129184
Sum of electronic and thermal Free Energies= -1929.237684
E(RB-P86) = -1929.49778709 A.U.

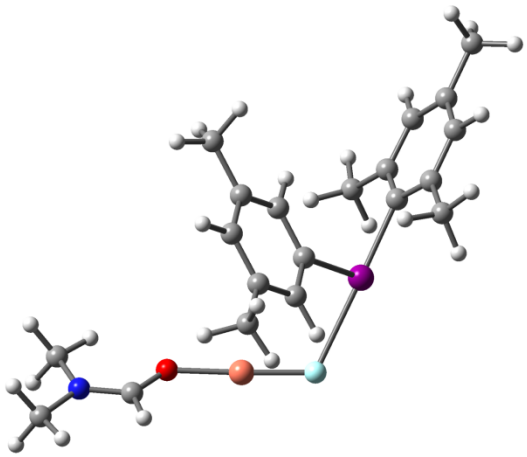


C	-3.410846	-0.913765	-0.154241
C	-3.714876	-1.649154	0.998575
C	-4.284040	0.060788	-0.652747
C	-4.926590	-1.416723	1.668430
H	-3.021245	-2.403095	1.376634
C	-5.499466	0.304949	0.006949
H	-4.029298	0.627164	-1.550907
C	-5.798701	-0.438680	1.160674
H	-6.742555	-0.249613	1.682309
I	-1.594874	-1.283825	-1.170958
C	0.161924	0.992171	-0.205558
C	-0.172590	2.026805	-1.077457
C	-0.050179	0.961099	1.179244
C	-0.593513	3.218255	-0.445718
C	-0.477762	2.180088	1.732074
C	-0.753297	3.310950	0.941081
H	-0.819559	4.079482	-1.082611
H	-0.605510	2.229743	2.818199
Cu	1.740537	-0.034773	-0.814818
F	1.030093	-1.107849	-2.125327
C	4.896868	-1.024567	1.196563
S	4.323194	0.256210	-0.073704
F	3.943479	-1.955803	1.388647
F	6.015581	-1.629435	0.752559
F	5.162116	-0.419638	2.370324
O	3.921213	-0.539167	-1.271171
O	5.437694	1.189854	-0.198039
O	3.049430	0.824836	0.529764
C	0.220197	-0.238138	2.050758

H	-0.090235	-0.041366	3.085303
H	-0.321012	-1.123506	1.683596
H	1.293512	-0.485104	2.055115
C	-1.233188	4.589861	1.583609
H	-1.994876	4.388651	2.351869
H	-0.398581	5.109162	2.083877
H	-1.658604	5.278181	0.840491
C	-0.079586	1.951952	-2.582636
H	0.187436	0.941382	-2.916794
H	-1.042750	2.232252	-3.035763
H	0.676629	2.660269	-2.957012
C	-5.285244	-2.198687	2.910713
H	-4.497570	-2.918077	3.174080
H	-5.436283	-1.526277	3.770207
H	-6.224428	-2.756661	2.768374
C	-6.470318	1.335459	-0.521081
H	-6.014251	1.949340	-1.310117
H	-7.364633	0.850167	-0.945279
H	-6.815398	2.004048	0.282513

J: adduct

Zero-point correction= 0.410564 (Hartree/Particle)
Thermal correction to Energy= 0.443278
Thermal correction to Enthalpy= 0.444222
Thermal correction to Gibbs Free Energy= 0.337933
Sum of electronic and zero-point Energies= -1215.802269
Sum of electronic and thermal Energies= -1215.769554
Sum of electronic and thermal Enthalpies= -1215.768610
Sum of electronic and thermal Free Energies= -1215.874900
E(RB-P86) = -1216.21283262 A.U



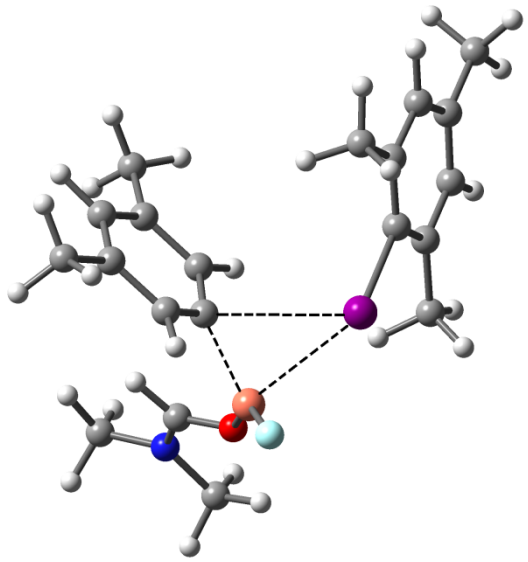
C	-3.080393	-0.536047	0.015951
C	-3.454242	-1.218483	1.191096
C	-3.919791	0.383619	-0.648451
C	-4.727703	-0.931229	1.710694
C	-5.174507	0.626999	-0.071795

C	-5.595675	-0.014270	1.103471
H	-5.045096	-1.448325	2.620696
H	-5.843656	1.338428	-0.564585
I	-1.173740	-1.002739	-0.839779
C	-0.231114	0.878213	-0.400749
C	0.611944	1.413838	-1.373467
C	-0.490224	1.485557	0.820905
C	1.242501	2.639359	-1.101164
H	0.783656	0.898597	-2.318955
C	0.133443	2.719831	1.094938
H	-1.158834	1.034730	1.556822
C	0.990994	3.267929	0.131161
H	1.480020	4.223107	0.345792
Cu	2.578702	-1.314091	-0.695788
F	1.161621	-1.587314	-1.826404
C	5.053848	-0.492548	0.311309
H	5.289607	-0.054877	-0.669930
O	3.959756	-1.099539	0.530930
N	5.993421	-0.341514	1.240307
C	5.827881	-0.864312	2.598167
H	5.893904	-0.036185	3.319001
H	4.851352	-1.351813	2.679879
H	6.626858	-1.589208	2.812439
C	7.244819	0.355595	0.938703
H	7.356503	1.222521	1.606171
H	8.095343	-0.325129	1.090227
H	7.236786	0.698970	-0.102865
C	-3.525677	1.099517	-1.916033
H	-2.657413	1.758765	-1.755588
H	-3.254216	0.390367	-2.714183
H	-4.355607	1.719424	-2.279897
C	-2.579904	-2.232433	1.891253
H	-2.410038	-3.123192	1.265535
H	-1.591579	-1.819646	2.146092
H	-3.057290	-2.565432	2.822333
C	-6.946830	0.290548	1.702021
H	-7.727400	0.325937	0.927113
H	-7.232923	-0.459226	2.452507
H	-6.938712	1.275805	2.197351
C	-0.138037	3.430291	2.399835
H	0.621082	4.199693	2.597790
H	-1.121824	3.927456	2.375097
H	-0.150242	2.726044	3.244906
C	2.163571	3.270356	-2.118169
H	1.801680	4.268828	-2.410251
H	3.175207	3.401769	-1.702574
H	2.242681	2.655133	-3.024779

J: TS

Zero-point correction= 0.409007 (Hartree/Particle)
Thermal correction to Energy= 0.441281

Thermal correction to Enthalpy= 0.442226
Thermal correction to Gibbs Free Energy= 0.338584
Sum of electronic and zero-point Energies= -1215.785545
Sum of electronic and thermal Energies= -1215.753271
Sum of electronic and thermal Enthalpies= -1215.752327
Sum of electronic and thermal Free Energies= -1215.855969
E(RB-P86) = -1216.19455266 A.U

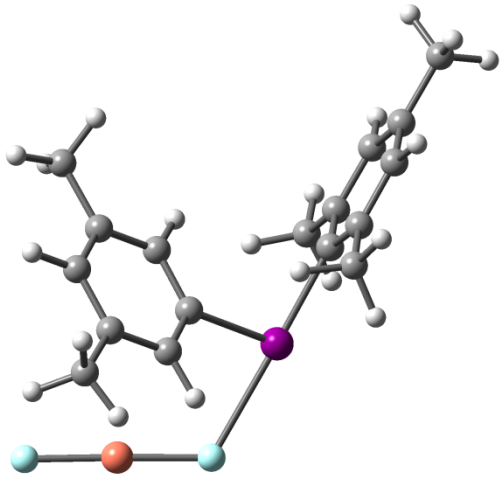


C	-2.531791	-0.377532	-0.352567
C	-2.580639	-1.779764	-0.186620
C	-3.410058	0.507475	0.316893
C	-3.564623	-2.285847	0.676562
C	-4.368426	-0.065626	1.162034
C	-4.464640	-1.453849	1.357173
H	-3.626319	-3.368930	0.815821
H	-5.063158	0.598323	1.684869
I	-1.101150	0.435552	-1.682138
C	1.175198	1.179923	0.171109
C	1.506651	2.513947	0.009218
C	0.810417	0.569732	1.359077
C	1.625587	3.284717	1.188573
H	1.703294	2.947591	-0.971059
C	0.925356	1.344626	2.535506
H	0.461538	-0.462683	1.411014
C	1.323429	2.685478	2.420792
H	1.378050	3.294679	3.327793
Cu	1.743139	0.070291	-1.324033
F	1.587770	1.216470	-2.782713
C	3.258202	-1.581803	0.467400
H	3.339717	-0.733510	1.164364
O	2.513843	-1.513537	-0.562599
N	3.965138	-2.656326	0.781193
C	3.963691	-3.857819	-0.058824

H	3.577624	-4.708258	0.521344
H	3.331779	-3.686320	-0.935651
H	4.992970	-4.078088	-0.376281
C	4.792473	-2.684985	1.990985
H	4.460482	-3.504817	2.643854
H	5.843939	-2.847748	1.714399
H	4.698973	-1.732647	2.525846
C	-3.359030	2.005448	0.151759
H	-2.376784	2.410962	0.441295
H	-3.535329	2.302782	-0.894360
H	-4.124652	2.485511	0.775726
C	-1.646407	-2.729762	-0.891825
H	-1.755830	-2.663452	-1.986191
H	-0.593070	-2.506944	-0.660158
H	-1.851998	-3.765353	-0.589878
C	-5.505500	-2.026583	2.285686
H	-6.510435	-1.654036	2.031948
H	-5.522021	-3.124294	2.244763
H	-5.307775	-1.727086	3.328195
C	0.620370	0.724893	3.878336
H	1.540795	0.334668	4.343101
H	0.194654	1.471017	4.564909
H	-0.086091	-0.111554	3.786072
C	2.076057	4.723183	1.098712
H	1.653793	5.317584	1.921802
H	3.174286	4.790224	1.169211
H	1.776951	5.178942	0.144481

K, L: adducts

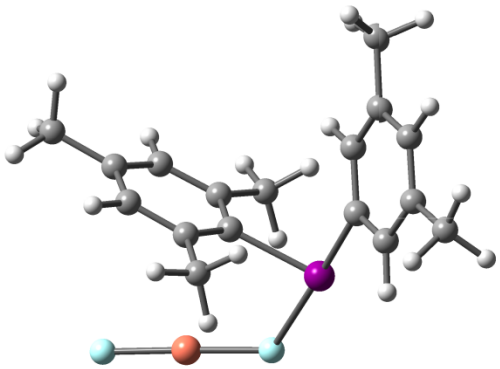
Zero-point correction= 0.310785 (Hartree/Particle)
Thermal correction to Energy= 0.337482
Thermal correction to Enthalpy= 0.338426
Thermal correction to Gibbs Free Energy= 0.247788
Sum of electronic and zero-point Energies= -1067.347265
Sum of electronic and thermal Energies= -1067.320568
Sum of electronic and thermal Enthalpies= -1067.319624
Sum of electronic and thermal Free Energies= -1067.410262
E(RB-P86) = -1067.65805016 A.U



C	-2.283237	-0.491433	-0.168605
C	-2.992267	-0.873536	0.990258
C	-2.840873	0.310756	-1.184169
C	-4.307425	-0.401139	1.114458
C	-4.159985	0.754027	-0.993444
C	-4.907469	0.412224	0.141212
H	-4.877011	-0.681676	2.005414
H	-4.612314	1.385063	-1.763961
I	-0.280773	-1.227308	-0.412499
C	0.693172	0.658833	-0.112877
C	1.653729	1.045696	-1.047916
C	0.339143	1.421961	0.991590
C	2.302395	2.277330	-0.862966
H	1.896765	0.413668	-1.902432
C	0.985074	2.661035	1.181163
H	-0.416783	1.087103	1.704278
C	1.953073	3.061993	0.250999
H	2.456476	4.022391	0.397689
Cu	3.472059	-1.314535	0.325000
F	4.811421	-0.633359	1.339903
F	2.128610	-2.041462	-0.706585
C	-2.094201	0.708379	-2.433092
H	-1.199291	1.307004	-2.199568
H	-1.757606	-0.173960	-3.000734
H	-2.737774	1.308442	-3.089993
C	-2.419689	-1.760248	2.071886
H	-2.215692	-2.776528	1.698252
H	-1.473541	-1.366696	2.474272
H	-3.129522	-1.848668	2.905119
C	-6.329053	0.890186	0.310273
H	-7.037112	0.049798	0.222225
H	-6.482346	1.336611	1.304927
H	-6.595118	1.637164	-0.450277
C	3.350452	2.748907	-1.842360
H	3.093081	3.739872	-2.248034
H	4.330825	2.844930	-1.348778

H	3.459449	2.049910	-2.682866
C	0.629573	3.521326	2.370624
H	1.270830	4.411947	2.421809
H	-0.418571	3.856700	2.315936
H	0.741767	2.961383	3.312090

Zero-point correction= 0.310911 (Hartree/Particle)
Thermal correction to Energy= 0.337522
Thermal correction to Enthalpy= 0.338466
Thermal correction to Gibbs Free Energy= 0.248289
Sum of electronic and zero-point Energies= -1067.348240
Sum of electronic and thermal Energies= -1067.321629
Sum of electronic and thermal Enthalpies= -1067.320685
Sum of electronic and thermal Free Energies= -1067.410862
E(RB-P86) = -1067.65915115 A.U.

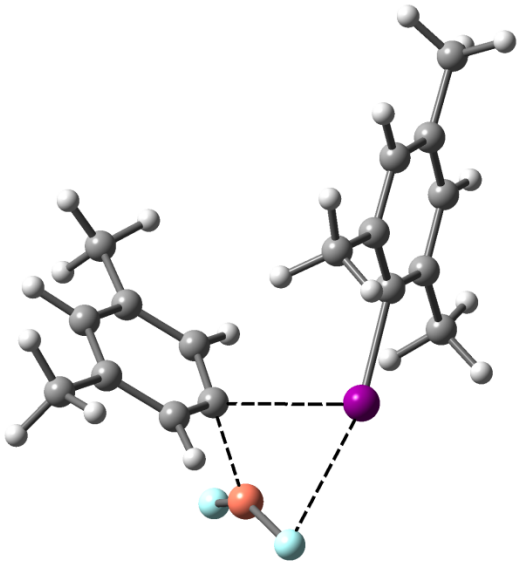


C	2.350584	-0.391590	-0.166783
C	2.662549	0.787433	-0.848754
C	3.279309	-1.077497	0.612489
C	3.959768	1.310650	-0.740683
H	1.916628	1.307749	-1.453020
C	4.591067	-0.570563	0.715963
H	3.005356	-1.991321	1.145644
C	4.903243	0.615301	0.039332
H	5.917544	1.017974	0.122024
I	0.392079	-1.261801	-0.352746
C	-0.687126	0.545057	0.022142
C	-0.681857	1.060658	1.330634
C	-1.359058	1.137261	-1.063364
C	-1.379887	2.263878	1.524953
C	-2.041415	2.333769	-0.790611
C	-2.057542	2.915245	0.485073
H	-1.397453	2.693031	2.530789
H	-2.581839	2.817244	-1.609402
Cu	-3.448697	-1.333458	0.073391
F	-4.945864	-0.476958	0.632233
F	-1.952593	-2.241136	-0.506682
C	-1.401501	0.546599	-2.451019
H	-2.046996	1.151337	-3.101470

H	-0.400941	0.506161	-2.910606
H	-1.798028	-0.480547	-2.428517
C	0.012594	0.398380	2.493103
H	1.101574	0.340439	2.336410
H	-0.165369	0.965072	3.416419
H	-0.352753	-0.629251	2.648088
C	-2.779071	4.217710	0.729875
H	-3.120083	4.297371	1.771909
H	-2.110635	5.073416	0.535239
H	-3.649080	4.324092	0.066160
C	5.621213	-1.296019	1.548994
H	6.572385	-0.746485	1.571502
H	5.273694	-1.424843	2.586124
H	5.817225	-2.302652	1.146269
C	4.339859	2.589452	-1.448830
H	4.641456	3.363788	-0.725373
H	5.195096	2.427150	-2.123630
H	3.503986	2.984503	-2.042427

K, L: TS's

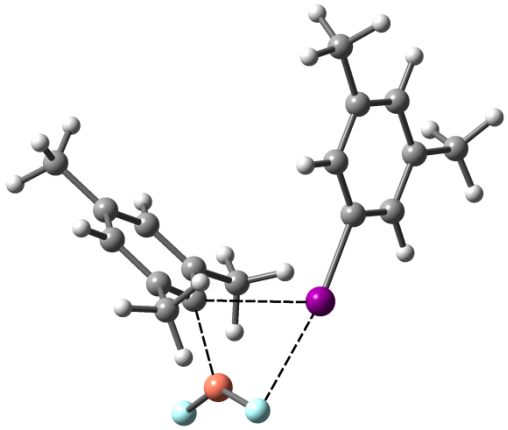
Zero-point correction= 0.309019 (Hartree/Particle)
Thermal correction to Energy= 0.335342
Thermal correction to Enthalpy= 0.336286
Thermal correction to Gibbs Free Energy= 0.247534
Sum of electronic and zero-point Energies= -1067.335500
Sum of electronic and thermal Energies= -1067.309177
Sum of electronic and thermal Enthalpies= -1067.308233
Sum of electronic and thermal Free Energies= -1067.396985
E(RB-P86) = -1067.64451903 A.U.



C	-2.024082	-0.397913	-0.344826
C	-2.766342	-0.902683	0.745375
C	-2.466279	0.686244	-1.137920

C	-3.997363	-0.286413	1.019342
C	-3.703521	1.255791	-0.808446
C	-4.484497	0.786254	0.259634
H	-4.591056	-0.663340	1.857150
H	-4.066159	2.095881	-1.408007
I	-0.174870	-1.317627	-0.832782
C	1.551152	0.417571	0.155246
C	2.297795	1.007742	-0.862837
C	0.965076	1.115070	1.207310
C	2.600464	2.378383	-0.739376
H	2.667661	0.421733	-1.704620
C	1.267217	2.485995	1.327859
H	0.332406	0.625021	1.948044
C	2.070574	3.092073	0.347717
H	2.277058	4.163597	0.425441
Cu	2.365956	-1.346656	0.632749
F	2.615173	-1.397192	2.463290
F	2.529276	-2.043709	-1.113707
C	-2.309632	-2.059838	1.599837
H	-2.197921	-2.980912	1.005756
H	-1.334596	-1.860143	2.070814
H	-3.039350	-2.256055	2.396769
C	-1.677858	1.235475	-2.300819
H	-0.682300	1.586840	-1.987814
H	-1.521256	0.470826	-3.078691
H	-2.208312	2.081441	-2.758278
C	-5.822618	1.411604	0.566025
H	-6.585242	1.068212	-0.153280
H	-6.171449	1.144898	1.573550
H	-5.778064	2.508406	0.488834
C	3.474850	3.054335	-1.769184
H	3.201004	4.113194	-1.884149
H	4.534001	3.017231	-1.464511
H	3.395444	2.562745	-2.749103
C	0.740198	3.273386	2.504350
H	1.457675	3.247351	3.341305
H	0.585556	4.328306	2.234885
H	-0.210574	2.861698	2.871656

Zero-point correction= 0.308958 (Hartree/Particle)
Thermal correction to Energy= 0.335360
Thermal correction to Enthalpy= 0.336304
Thermal correction to Gibbs Free Energy= 0.246679
Sum of electronic and zero-point Energies= -1067.334156
Sum of electronic and thermal Energies= -1067.307754
Sum of electronic and thermal Enthalpies= -1067.306810
Sum of electronic and thermal Free Energies= -1067.396435
E(RB-P86) = -1067.64311362 A.U.



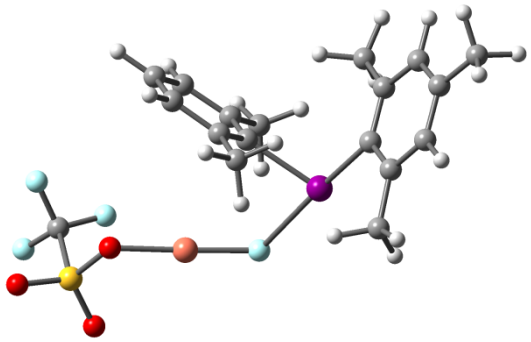
C	-2.118574	-0.561155	-0.292181
C	-2.852041	-1.006884	0.813873
C	-2.588840	0.459186	-1.127884
C	-4.098199	-0.422721	1.095070
H	-2.469684	-1.808347	1.449697
C	-3.833181	1.050932	-0.859101
H	-2.002308	0.791359	-1.986922
C	-4.566270	0.598304	0.251313
H	-5.537259	1.056350	0.465556
I	-0.252768	-1.461342	-0.728647
C	1.619382	0.560339	0.147011
C	2.019210	1.243350	-1.004750
C	1.076506	1.136398	1.303248
C	2.060037	2.649172	-0.874259
C	1.137310	2.541586	1.347803
C	1.628493	3.310460	0.280640
H	2.426117	3.224511	-1.730474
H	0.781605	3.035162	2.257609
Cu	2.568316	-1.166901	0.439367
F	3.375853	-0.915645	2.078284
F	2.415970	-2.252682	-1.073677
C	2.387819	0.604120	-2.319482
H	3.078772	1.249194	-2.879467
H	2.835182	-0.388999	-2.180529
H	1.481868	0.468708	-2.934356
C	0.531728	0.356468	2.470702
H	0.242748	1.035034	3.284324
H	-0.356543	-0.226883	2.181468
H	1.294242	-0.345074	2.842235
C	1.682532	4.816266	0.377874
H	1.688412	5.283339	-0.617073
H	0.828599	5.212870	0.946331
H	2.599597	5.137792	0.900057
C	-4.374842	2.147873	-1.745619
H	-5.334444	1.850946	-2.197985
H	-4.560880	3.066524	-1.166917
H	-3.674965	2.390146	-2.557063

C	-4.906491	-0.867189	2.291434
H	-4.852815	-0.117526	3.098201
H	-5.968797	-0.987660	2.030778
H	-4.537768	-1.820301	2.695535

Reactions of [2,6-$Me_2C_6H_4$(Ph)I]BF_4

H, I: adducts

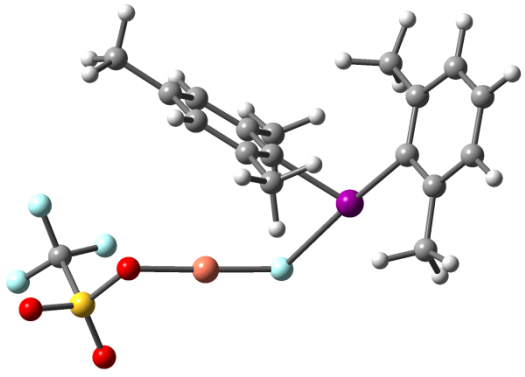
Zero-point correction= 0.336632 (Hartree/Particle)
Thermal correction to Energy= 0.370200
Thermal correction to Enthalpy= 0.371144
Thermal correction to Gibbs Free Energy= 0.264820
Sum of electronic and zero-point Energies= -1929.177522
Sum of electronic and thermal Energies= -1929.143954
Sum of electronic and thermal Enthalpies= -1929.143010
Sum of electronic and thermal Free Energies= -1929.249334
E(RB-P86) = -1929.51415374 A.U.



C	3.775902	-0.268949	-0.221764
C	4.345432	0.960791	-0.609681
C	4.494698	-1.270929	0.461733
C	5.682123	1.184870	-0.245771
C	5.831035	-0.983229	0.786574
C	6.440108	0.232807	0.451240
H	6.141499	2.137434	-0.525775
H	6.408084	-1.743766	1.320577
I	1.744922	-0.744975	-0.771204
C	0.695510	0.855664	0.221737
C	0.763149	0.927335	1.624995
C	-0.029503	1.744690	-0.596313
C	0.072480	1.997618	2.223006
C	-0.704910	2.783229	0.070118
C	-0.646965	2.915401	1.457922
H	0.101966	2.091915	3.311071
H	-1.281205	3.494557	-0.526077
Cu	-2.061631	-1.036652	-0.229904
F	-0.686554	-1.480068	-1.361796
C	-5.373029	0.708821	-0.307092
S	-4.884334	-0.828786	0.683356
F	-5.199112	1.827156	0.429130
F	-6.673477	0.629299	-0.665545

F	-4.625936	0.813909	-1.428764
O	-5.109155	-1.949790	-0.238628
O	-5.697028	-0.752337	1.901502
O	-3.413118	-0.555836	0.990461
C	1.505432	-0.056995	2.490093
H	1.188532	-1.091145	2.281966
H	2.593675	0.000117	2.328871
H	1.312124	0.147962	3.551072
C	-0.135826	1.626196	-2.094973
H	0.847467	1.716653	-2.583175
H	-0.561496	0.651454	-2.379098
H	-0.782938	2.419253	-2.491749
H	-1.176781	3.734820	1.948538
C	3.601869	2.015431	-1.388126
H	3.225288	1.612092	-2.342147
H	2.739177	2.406142	-0.826620
H	4.263618	2.860410	-1.619213
C	3.921956	-2.619100	0.830979
H	3.010609	-2.529920	1.442002
H	3.661534	-3.208763	-0.062743
H	4.657146	-3.197798	1.405695
C	7.882931	0.502367	0.801719
H	8.234152	-0.166956	1.599475
H	8.532041	0.344669	-0.075930
H	8.027056	1.542957	1.128313

Zero-point correction= 0.336520 (Hartree/Particle)
Thermal correction to Energy= 0.370149
Thermal correction to Enthalpy= 0.371093
Thermal correction to Gibbs Free Energy= 0.264553
Sum of electronic and zero-point Energies= -1929.177727
Sum of electronic and thermal Energies= -1929.144099
Sum of electronic and thermal Enthalpies= -1929.143154
Sum of electronic and thermal Free Energies= -1929.249695
E(RB-P86) = -1929.51424737 A.U.



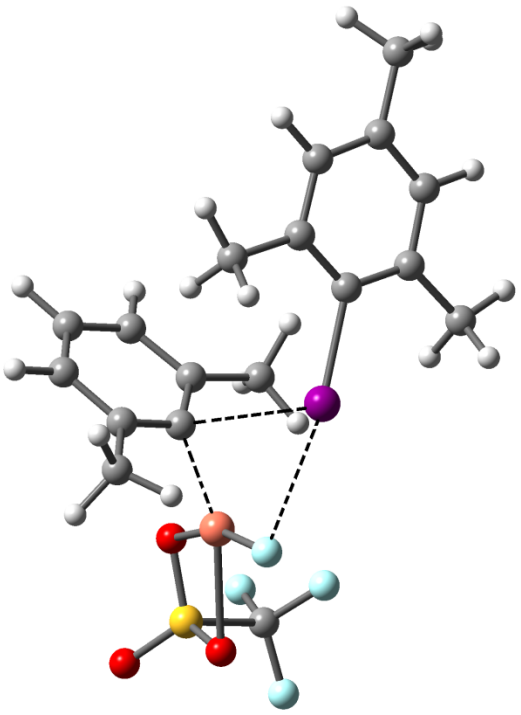
C	4.044736	-0.289834	-0.065658
C	4.600142	0.867145	-0.647077
C	4.738183	-1.124389	0.836407

C	5.904861	1.210267	-0.250228
C	6.042612	-0.732128	1.185198
C	6.616227	0.425513	0.658049
H	6.362015	2.106993	-0.675697
H	6.607466	-1.355764	1.882366
H	7.629161	0.712427	0.949190
I	2.052498	-0.927713	-0.615914
C	0.922691	0.801135	-0.019289
C	0.905422	1.154719	1.341897
C	0.213290	1.484786	-1.026388
C	0.149470	2.290058	1.678392
C	-0.528888	2.602044	-0.610033
C	-0.564717	3.027680	0.725084
H	0.114851	2.591438	2.729166
H	-1.097205	3.151629	-1.365785
Cu	-1.704640	-1.168974	-0.110537
F	-0.339259	-1.846872	-1.135828
C	-5.122850	0.263349	-0.545648
S	-4.512426	-0.871792	0.841008
F	-4.982856	1.560432	-0.198112
F	-6.429732	0.024558	-0.792946
F	-4.425900	0.047259	-1.683773
O	-4.694593	-2.230731	0.314607
O	-5.293153	-0.467235	2.014576
O	-3.053222	-0.445088	0.984567
C	1.621124	0.389017	2.423872
H	1.319438	-0.670617	2.429272
H	2.713907	0.425883	2.293542
H	1.385796	0.811489	3.409258
C	0.184719	1.065928	-2.474052
H	1.191614	1.067495	-2.920504
H	-0.220952	0.047132	-2.574444
H	-0.444202	1.752449	-3.055640
C	-1.343528	4.257171	1.122868
H	-0.713826	5.158412	1.032835
H	-2.219365	4.403223	0.474807
H	-1.683852	4.196768	2.166397
C	3.885378	1.721436	-1.661878
H	3.576100	1.125647	-2.535775
H	2.982426	2.191164	-1.242086
H	4.544699	2.523056	-2.019906
C	4.172112	-2.400786	1.412409
H	3.234862	-2.227085	1.963501
H	3.958044	-3.143428	0.627160
H	4.891575	-2.853225	2.107597

H, I: TS's

Zero-point correction= 0.334400 (Hartree/Particle)
Thermal correction to Energy= 0.367814
Thermal correction to Enthalpy= 0.368759
Thermal correction to Gibbs Free Energy= 0.263249

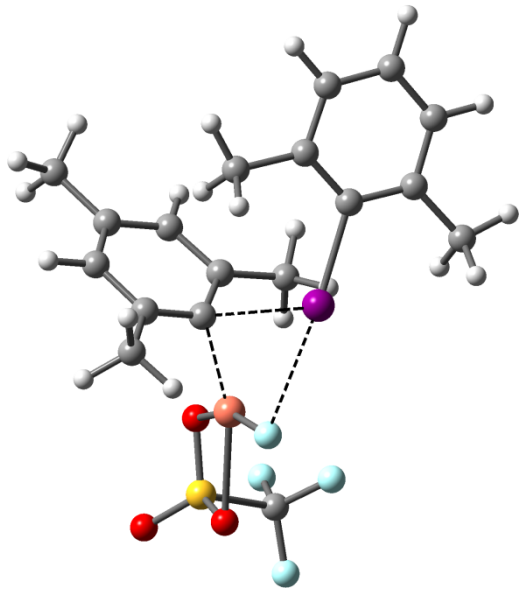
Sum of electronic and zero-point Energies= -1929.160402
Sum of electronic and thermal Energies= -1929.126988
Sum of electronic and thermal Enthalpies= -1929.126044
Sum of electronic and thermal Free Energies= -1929.231553
E(RB-P86) = -1929.49480235 A.U.



C	-3.297991	-0.568983	-0.399190
C	-3.566687	-1.924306	-0.098433
C	-4.159035	0.479374	0.000872
C	-4.739240	-2.205971	0.619059
C	-5.313110	0.130172	0.716189
C	-5.623758	-1.200548	1.035716
H	-4.964047	-3.249622	0.858312
H	-5.988970	0.929141	1.035663
I	-1.545161	-0.096664	-1.494961
C	0.224071	1.301450	0.482582
C	0.032466	2.670706	0.278644
C	0.000041	0.584002	1.660457
C	-0.265995	3.402186	1.449637
C	-0.298821	1.378250	2.786941
C	-0.429162	2.764523	2.680248
H	-0.383681	4.486154	1.362907
H	-0.439335	0.876954	3.748947
Cu	1.730196	0.593558	-0.612358
F	1.072418	0.612064	-2.331026
C	4.510432	-1.815986	0.528275
S	4.259102	0.029680	0.194233
F	3.438006	-2.515984	0.111621
F	5.600889	-2.251889	-0.132194

F	4.684881	-2.025657	1.847342
O	3.925864	0.120993	-1.254581
O	5.477102	0.672684	0.677075
O	2.993538	0.360319	0.972665
C	0.089913	-0.916333	1.786670
H	-0.903110	-1.337460	2.010310
H	0.457600	-1.383030	0.863302
H	0.762033	-1.197785	2.610356
C	0.155151	3.372516	-1.052010
H	0.162664	2.653185	-1.880442
H	-0.678655	4.076960	-1.186504
H	1.088530	3.957551	-1.094718
H	-0.685188	3.352889	3.564330
C	-3.887608	1.929990	-0.309226
H	-2.946459	2.271795	0.150034
H	-3.796969	2.098685	-1.394192
H	-4.701131	2.563326	0.069828
C	-2.670727	-3.059266	-0.528171
H	-2.607388	-3.126660	-1.626233
H	-1.642100	-2.930189	-0.157054
H	-3.054653	-4.016324	-0.149665
C	-6.887535	-1.539692	1.786625
H	-6.801687	-2.506457	2.302910
H	-7.133141	-0.765484	2.528455
H	-7.744286	-1.609813	1.094727

Zero-point correction= 0.334366 (Hartree/Particle)
Thermal correction to Energy= 0.367792
Thermal correction to Enthalpy= 0.368736
Thermal correction to Gibbs Free Energy= 0.263152
Sum of electronic and zero-point Energies= -1929.160176
Sum of electronic and thermal Energies= -1929.126751
Sum of electronic and thermal Enthalpies= -1929.125806
Sum of electronic and thermal Free Energies= -1929.231391
E(RB-P86) = -1929.49454272 A.U.

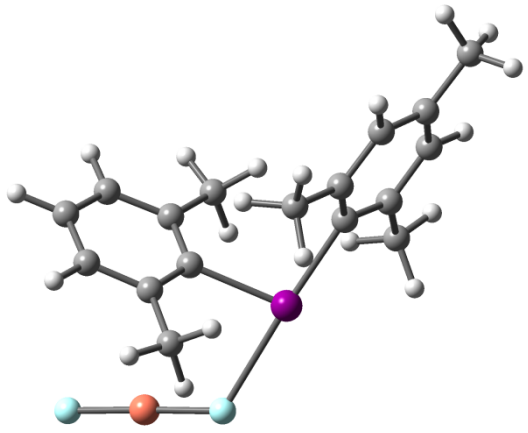


C	-3.555315	-0.908597	0.126404
C	-3.826844	-2.002544	0.980930
C	-4.401630	0.219990	0.034154
C	-4.996007	-1.937601	1.757203
C	-5.555603	0.228017	0.835125
C	-5.851317	-0.835829	1.690007
H	-5.231711	-2.772805	2.421612
H	-6.227074	1.088683	0.780230
H	-6.753028	-0.806567	2.306067
I	-1.814194	-0.993442	-1.093291
C	0.007115	1.153008	-0.135498
C	-0.241328	2.241377	-0.974325
C	-0.128955	1.125060	1.259346
C	-0.454730	3.465607	-0.303920
C	-0.359065	2.379824	1.850117
C	-0.517811	3.552926	1.091714
H	-0.597721	4.361904	-0.916007
H	-0.419648	2.424135	2.942215
Cu	1.496426	0.040529	-0.830136
F	0.736182	-0.870597	-2.242732
C	4.616009	-1.335554	1.021594
S	4.115867	0.095326	-0.111875
F	3.612138	-2.227571	1.122924
F	5.700826	-1.955042	0.516213
F	4.912276	-0.868636	2.250336
O	3.665883	-0.554238	-1.376303
O	5.285181	0.968589	-0.153809
O	2.885175	0.677676	0.560794
C	0.049759	-0.105290	2.110516
H	-0.424754	0.031595	3.091325
H	-0.385215	-0.990841	1.625912
H	1.120142	-0.307961	2.274058

C	-0.768787	4.875124	1.775003
H	-1.435863	4.757310	2.641647
H	0.177413	5.301230	2.149331
H	-1.212974	5.606531	1.085835
C	-0.270386	2.186655	-2.482593
H	-0.016529	1.186013	-2.854154
H	-1.274133	2.453567	-2.849005
H	0.436286	2.916816	-2.906244
C	-4.121235	1.388541	-0.876496
H	-3.175570	1.888174	-0.613075
H	-4.035750	1.068694	-1.927346
H	-4.928156	2.130856	-0.808642
C	-2.944123	-3.222285	1.074691
H	-2.879795	-3.749007	0.109076
H	-1.914398	-2.961403	1.365682
H	-3.340654	-3.925224	1.819896

K, L: adducts

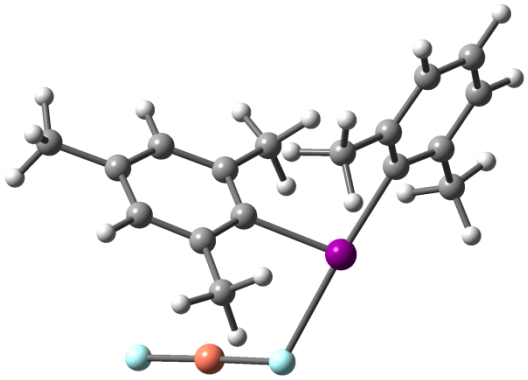
Zero-point correction= 0.311466 (Hartree/Particle)
Thermal correction to Energy= 0.337570
Thermal correction to Enthalpy= 0.338515
Thermal correction to Gibbs Free Energy= 0.251370
Sum of electronic and zero-point Energies= -1067.342413
Sum of electronic and thermal Energies= -1067.316309
Sum of electronic and thermal Enthalpies= -1067.315364
Sum of electronic and thermal Free Energies= -1067.402509
E(RB-P86) = -1067.65387889 A.U.



C	-2.225649	-0.328251	-0.222393
C	-2.934370	-1.260670	0.563654
C	-2.826558	0.813543	-0.789732
C	-4.293878	-0.993247	0.796715
C	-4.185548	1.024243	-0.509223
C	-4.935250	0.139209	0.278611
H	-4.863334	-1.701204	1.405914
H	-4.669914	1.910112	-0.930552
I	-0.158412	-0.791701	-0.639579

C	0.795469	0.959407	0.178742
C	1.525248	1.763195	-0.718426
C	0.675292	1.201415	1.559193
C	2.145685	2.897943	-0.164958
C	1.313765	2.358335	2.042292
C	2.035659	3.197240	1.193329
H	2.725113	3.547220	-0.825617
H	1.242650	2.584476	3.108866
H	2.525436	4.086804	1.595503
Cu	3.662010	-1.076069	0.044970
F	5.052052	-0.664125	1.132924
F	2.275528	-1.521802	-1.078478
C	-2.093014	1.790168	-1.672473
H	-1.281507	2.301123	-1.131346
H	-1.645886	1.282463	-2.542285
H	-2.780428	2.558379	-2.050550
C	-2.325439	-2.519235	1.136715
H	-2.003352	-3.214150	0.344454
H	-1.445428	-2.306534	1.763205
H	-3.061341	-3.045707	1.758862
C	-6.402430	0.385589	0.532518
H	-7.007525	0.043417	-0.323913
H	-6.752437	-0.155870	1.422670
H	-6.610327	1.457055	0.669230
C	1.694780	1.459724	-2.184807
H	0.730991	1.467764	-2.718238
H	2.344892	2.209952	-2.653847
H	2.146803	0.465699	-2.324723
C	-0.061905	0.302472	2.516900
H	-1.135722	0.245116	2.279870
H	0.343564	-0.721798	2.492585
H	0.035965	0.678674	3.543526

Zero-point correction= 0.311739 (Hartree/Particle)
Thermal correction to Energy= 0.337701
Thermal correction to Enthalpy= 0.338645
Thermal correction to Gibbs Free Energy= 0.252537
Sum of electronic and zero-point Energies= -1067.342217
Sum of electronic and thermal Energies= -1067.316255
Sum of electronic and thermal Enthalpies= -1067.315311
Sum of electronic and thermal Free Energies= -1067.401419
E(RB-P86) = -1067.65395649 A.U.

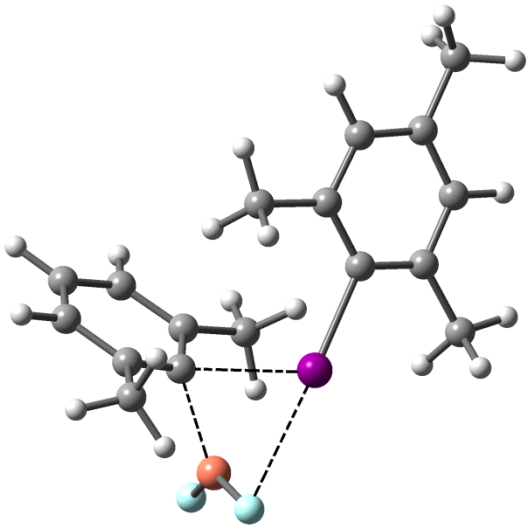


C	-2.603522	-0.137987	-0.068608
C	-3.358111	-0.841556	0.894424
C	-3.086391	0.982809	-0.773137
C	-4.647045	-0.351048	1.169881
C	-4.379234	1.429017	-0.446644
C	-5.149496	0.774142	0.515301
H	-5.257667	-0.871311	1.911865
H	-4.779662	2.300534	-0.970517
I	-0.647534	-0.944993	-0.532755
C	0.582111	0.750476	-0.046435
C	1.344550	1.311468	-1.089915
C	0.600637	1.208150	1.282293
C	2.143361	2.414097	-0.748696
C	1.417887	2.321552	1.544222
C	2.189960	2.937496	0.551494
H	2.749012	2.872236	-1.535972
H	1.449908	2.705949	2.567606
Cu	3.043336	-1.698658	0.092640
F	4.461062	-1.345494	1.165620
F	1.618865	-2.088241	-1.005271
C	-2.303431	1.696005	-1.845057
H	-1.375405	2.136327	-1.449025
H	-2.024998	1.006191	-2.658163
H	-2.901845	2.506377	-2.281467
C	-2.871772	-2.079950	1.608959
H	-2.729206	-2.922554	0.913335
H	-1.912040	-1.912520	2.121150
H	-3.605843	-2.394544	2.362597
C	1.368430	0.779815	-2.500118
H	0.374947	0.829346	-2.973515
H	2.063955	1.366130	-3.114861
H	1.691282	-0.272867	-2.510301
C	-0.173548	0.573101	2.407832
H	-1.260938	0.648555	2.251210
H	0.078144	-0.494989	2.508367
H	0.063915	1.066020	3.359495
H	-6.152278	1.138081	0.750196
C	3.077964	4.114083	0.874905

H	2.786172	4.589694	1.821514
H	4.128214	3.792096	0.971779
H	3.043465	4.870554	0.076799

K, L: TS's

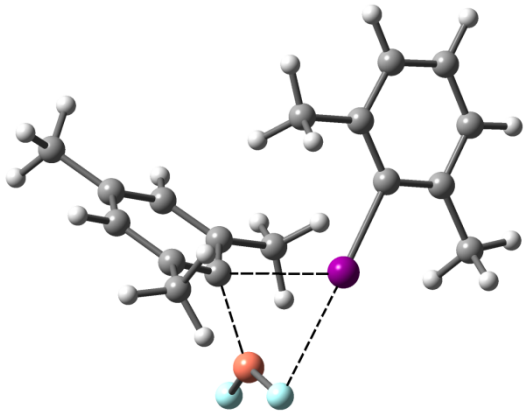
Zero-point correction= 0.309709 (Hartree/Particle)
Thermal correction to Energy= 0.335468
Thermal correction to Enthalpy= 0.336412
Thermal correction to Gibbs Free Energy= 0.251002
Sum of electronic and zero-point Energies= -1067.330952
Sum of electronic and thermal Energies= -1067.305193
Sum of electronic and thermal Enthalpies= -1067.304249
Sum of electronic and thermal Free Energies= -1067.389659
E(RB-P86) = -1067.64066104 A.U.



C	-2.016666	-0.346483	-0.329302
C	-2.806538	-1.147602	0.526928
C	-2.475144	0.873587	-0.873257
C	-4.097892	-0.686188	0.821526
C	-3.773896	1.279105	-0.533015
C	-4.598676	0.521020	0.311272
H	-4.731040	-1.297165	1.471689
H	-4.149171	2.219787	-0.946617
I	-0.073992	-1.044341	-0.839894
C	1.598495	0.807634	0.227648
C	2.147394	1.571940	-0.814377
C	1.058787	1.310396	1.424590
C	2.332695	2.940261	-0.517331
C	1.263822	2.686312	1.640725
C	1.895181	3.489289	0.686769
H	2.810106	3.567975	-1.274755
H	0.914790	3.115656	2.583650
Cu	2.591407	-0.923103	0.486671
F	3.250300	-0.868308	2.222044

F	2.593241	-1.900764	-1.126575
C	2.526582	1.042064	-2.173824
H	3.370195	1.613821	-2.585388
H	2.787152	-0.024792	-2.136858
H	1.678382	1.157680	-2.870131
C	0.370932	0.467689	2.465406
H	0.146955	1.068113	3.357228
H	-0.579672	0.062398	2.084814
H	1.015390	-0.375182	2.759125
C	-1.640945	1.733029	-1.789344
H	-0.713712	2.066349	-1.296675
H	-1.347919	1.184251	-2.698908
H	-2.202191	2.625789	-2.096050
C	-2.336930	-2.459598	1.105972
H	-2.132265	-3.200799	0.317003
H	-1.407394	-2.340981	1.685258
H	-3.102555	-2.878151	1.772802
C	-5.979155	1.003325	0.681693
H	-6.408939	1.636498	-0.107831
H	-6.661647	0.161755	0.868858
H	-5.943819	1.607549	1.604250
H	2.027964	4.556476	0.877781

Zero-point correction= 0.309909 (Hartree/Particle)
Thermal correction to Energy= 0.335591
Thermal correction to Enthalpy= 0.336536
Thermal correction to Gibbs Free Energy= 0.251583
Sum of electronic and zero-point Energies= -1067.330579
Sum of electronic and thermal Energies= -1067.304896
Sum of electronic and thermal Enthalpies= -1067.303952
Sum of electronic and thermal Free Energies= -1067.388904
E(RB-P86) = -1067.64048750 A.U.



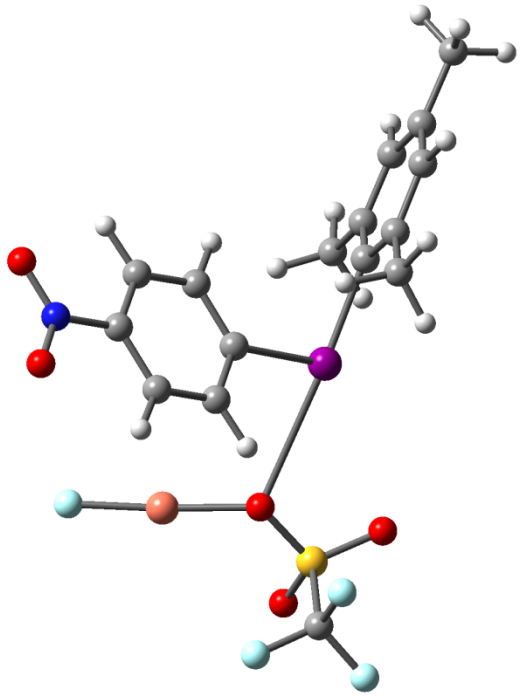
C	-2.383911	0.193776	-0.182991
C	-3.279178	-0.298988	0.794187
C	-2.528600	1.454350	-0.803642
C	-4.359500	0.529158	1.142069
C	-3.627419	2.236658	-0.410614

C	-4.532115	1.782558	0.551223
H	-5.072398	0.174598	1.890618
H	-3.766153	3.217082	-0.873053
H	-5.377795	2.409741	0.842421
I	-0.762286	-1.060819	-0.766328
C	1.490410	0.258586	0.115293
C	2.161727	0.771562	-1.003739
C	1.183582	0.973919	1.284997
C	2.758136	2.036165	-0.811110
C	1.800128	2.232543	1.390844
C	2.592884	2.774745	0.366029
H	3.349308	2.447074	-1.635374
H	1.644649	2.797685	2.315046
Cu	1.870283	-1.678086	0.437533
F	2.545484	-1.784769	2.165989
F	1.541967	-2.680389	-1.127313
C	2.277721	0.082228	-2.338972
H	3.190154	0.404359	-2.859554
H	2.275092	-1.011565	-2.231570
H	1.418431	0.353972	-2.975750
C	0.323980	0.447382	2.403103
H	0.377530	1.113789	3.274368
H	-0.731062	0.384516	2.092931
H	0.660959	-0.556470	2.702854
C	3.241090	4.127592	0.531795
H	3.510011	4.566744	-0.439037
H	2.578194	4.827059	1.062256
H	4.166361	4.042715	1.126505
C	-1.577328	1.976223	-1.850553
H	-0.547150	2.040962	-1.466975
H	-1.554654	1.320502	-2.735954
H	-1.881058	2.979466	-2.178160
C	-3.135869	-1.648749	1.453031
H	-3.190895	-2.466904	0.717494
H	-2.170972	-1.749082	1.975370
H	-3.937095	-1.800175	2.188711

Reactions of [*p*-$NO_2C_6H_4$(Ph)I]BF_4

G-I: adducts

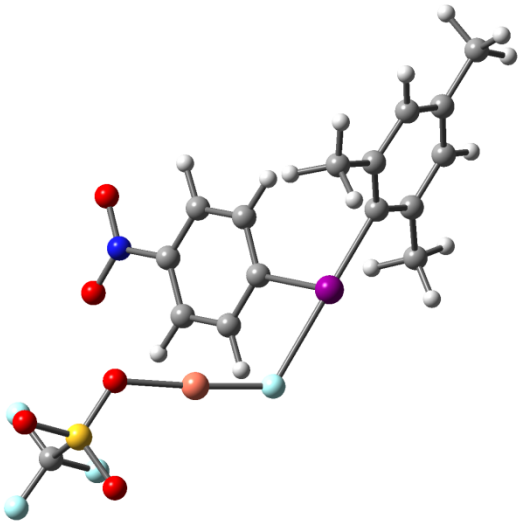
Zero-point correction= 0.284672 (Hartree/Particle)
Thermal correction to Energy= 0.317946
Thermal correction to Enthalpy= 0.318890
Thermal correction to Gibbs Free Energy= 0.209194
Sum of electronic and zero-point Energies= -2055.166109
Sum of electronic and thermal Energies= -2055.132835
Sum of electronic and thermal Enthalpies= -2055.131891
Sum of electronic and thermal Free Energies= -2055.241587
E(RB-P86) = -2055.45078090 A.U.



O	2.139236	-0.680827	0.302324
C	-2.947524	-1.129865	-0.001053
C	-3.580022	-1.547117	1.188645
C	-3.619607	-0.875434	-1.212910
C	-4.974099	-1.688476	1.128388
C	-5.014421	-1.030635	-1.191529
C	-5.706582	-1.435508	-0.041602
H	-5.499046	-2.007804	2.032954
H	-5.570434	-0.829724	-2.111346
I	-0.821793	-0.962779	0.027593
C	-0.662214	1.167098	-0.154081
C	0.389177	1.663687	-0.927735
C	-1.586949	1.981468	0.499148
C	0.518019	3.049125	-1.050505
H	1.088976	1.002408	-1.437295
C	-1.451989	3.365239	0.368621
H	-2.403271	1.570479	1.092981
C	-0.402101	3.872559	-0.399898
H	1.318664	3.484201	-1.647689
H	-2.148905	4.042485	0.861238
Cu	2.700522	0.672826	1.492764
C	3.959484	-1.694316	-1.356558
F	3.146134	2.027559	2.604489
F	4.654658	-2.808662	-1.666475
F	3.209165	-1.342931	-2.421022
F	4.830791	-0.699251	-1.093592
S	2.859928	-2.029855	0.147666
O	1.915577	-3.060410	-0.297197
O	3.786756	-2.335206	1.239694

C	-2.929803	-0.447130	-2.482478
H	-2.449934	0.538636	-2.372419
H	-2.147986	-1.163448	-2.780944
H	-3.654056	-0.375029	-3.303977
C	-2.851845	-1.856853	2.474056
H	-2.168681	-2.713062	2.356694
H	-2.253657	-1.003080	2.827873
H	-3.571857	-2.112677	3.262120
C	-7.202726	-1.621187	-0.064109
H	-7.457149	-2.691656	-0.139752
H	-7.665354	-1.243544	0.859738
H	-7.658758	-1.107970	-0.921785
N	-0.263520	5.340005	-0.534038
O	-1.077223	6.054871	0.069536
O	0.658103	5.771119	-1.242403

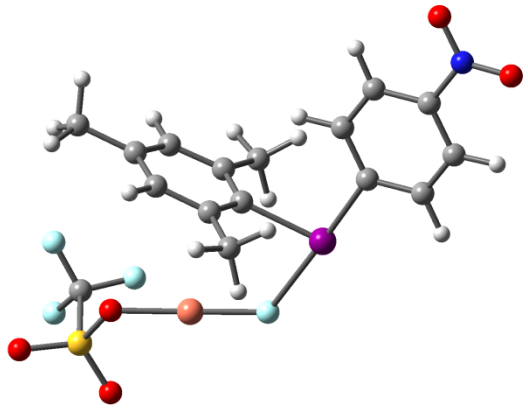
Zero-point correction= 0.284809 (Hartree/Particle)
Thermal correction to Energy= 0.317858
Thermal correction to Enthalpy= 0.318802
Thermal correction to Gibbs Free Energy= 0.208790
Sum of electronic and zero-point Energies= -2055.174593
Sum of electronic and thermal Energies= -2055.141544
Sum of electronic and thermal Enthalpies= -2055.140600
Sum of electronic and thermal Free Energies= -2055.250613
E(RB-P86) = -2055.45940240 A.U.



C	3.798975	-0.773585	-0.044097
C	4.624435	-0.105467	-0.972239
C	4.254432	-1.240504	1.208759
C	5.957041	0.113735	-0.589447
C	5.598084	-0.990965	1.522865
C	6.461097	-0.315524	0.645986
H	6.618458	0.634099	-1.287823
H	5.978591	-1.340479	2.486960

I	1.780362	-1.204103	-0.600160
C	1.026611	0.781766	-0.284431
C	1.677992	1.606812	0.631726
C	-0.092929	1.181834	-1.016044
C	1.182787	2.897717	0.827520
H	2.556250	1.270800	1.184429
C	-0.581275	2.475051	-0.816362
H	-0.574060	0.506086	-1.723001
C	0.062156	3.307765	0.101752
H	1.655665	3.575402	1.537540
H	-1.448423	2.834933	-1.369029
Cu	-2.052305	-1.448030	-0.134573
F	-0.638278	-1.736326	-1.273452
C	-5.370177	0.258562	-0.163982
S	-4.890980	-1.338553	0.732490
F	-5.195124	1.329398	0.639120
F	-6.669136	0.204864	-0.531472
F	-4.618181	0.427888	-1.274485
O	-5.083797	-2.396685	-0.267428
O	-5.729474	-1.349872	1.934872
O	-3.428217	-1.076116	1.091158
C	7.894445	-0.052055	1.034780
H	7.947065	0.715185	1.824856
H	8.370317	-0.959817	1.435997
H	8.484946	0.303361	0.179365
C	3.386633	-1.987107	2.194393
H	2.488969	-1.413566	2.473311
H	3.045417	-2.952043	1.786984
H	3.950805	-2.194423	3.113132
C	4.145319	0.375331	-2.319418
H	3.759095	-0.454313	-2.932576
H	3.336398	1.117297	-2.224471
H	4.968352	0.848205	-2.870983
N	-0.460005	4.674364	0.311997
O	0.122897	5.397685	1.134456
O	-1.452877	5.022901	-0.344977

Zero-point correction= 0.284859 (Hartree/Particle)
Thermal correction to Energy= 0.317861
Thermal correction to Enthalpy= 0.318805
Thermal correction to Gibbs Free Energy= 0.211248
Sum of electronic and zero-point Energies= -2055.177177
Sum of electronic and thermal Energies= -2055.144175
Sum of electronic and thermal Enthalpies= -2055.143231
Sum of electronic and thermal Free Energies= -2055.250787
E(RB-P86) = -2055.46203590 A.U.

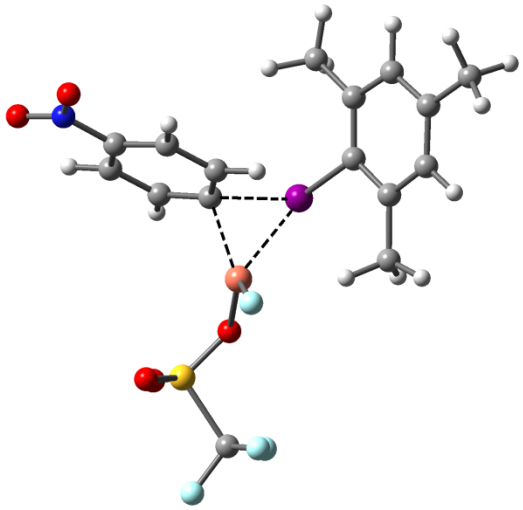


C	-3.545987	-0.626628	0.115951
C	-3.823994	0.731892	0.281928
C	-4.560556	-1.585195	0.007137
C	-5.156086	1.146344	0.340904
H	-3.024196	1.469305	0.364954
C	-5.891582	-1.171690	0.069248
H	-4.335008	-2.644683	-0.129279
C	-6.167057	0.188467	0.233833
I	-1.522349	-1.367279	0.027696
C	-0.586579	0.538445	-0.150754
C	-0.533180	1.124839	-1.428830
C	-0.032182	1.105860	1.014120
C	0.112101	2.369990	-1.509191
C	0.600566	2.347154	0.851837
C	0.679239	2.994968	-0.390544
H	0.171998	2.857192	-2.486194
H	1.044962	2.818098	1.733059
Cu	2.265537	-1.055047	-0.494163
F	0.833334	-2.151543	-0.116592
C	5.339600	0.239344	1.170400
S	5.136235	-0.305668	-0.631127
F	5.134684	1.567935	1.293594
F	6.589663	-0.043442	1.598192
F	4.458502	-0.405823	1.967272
O	5.364530	-1.756242	-0.608106
O	6.074248	0.538305	-1.377712
O	3.690866	0.095795	-0.923159
C	-1.118534	0.499555	-2.669611
H	-0.673201	-0.486309	-2.876012
H	-2.207474	0.358291	-2.579572
H	-0.935426	1.142331	-3.540238
C	-0.083090	0.459089	2.375873
H	-1.119449	0.305262	2.715641
H	0.415013	-0.523089	2.375576
H	0.422191	1.094314	3.114865
C	1.350951	4.339931	-0.510782
H	0.698509	5.134656	-0.112241
H	2.286558	4.369585	0.067135

H	1.576958	4.585031	-1.557548
H	-5.410488	2.198038	0.469374
H	-6.706995	-1.889587	-0.013304
N	-7.574546	0.628301	0.295856
O	-8.458992	-0.236128	0.189272
O	-7.798824	1.839268	0.451246

G-I: TS's

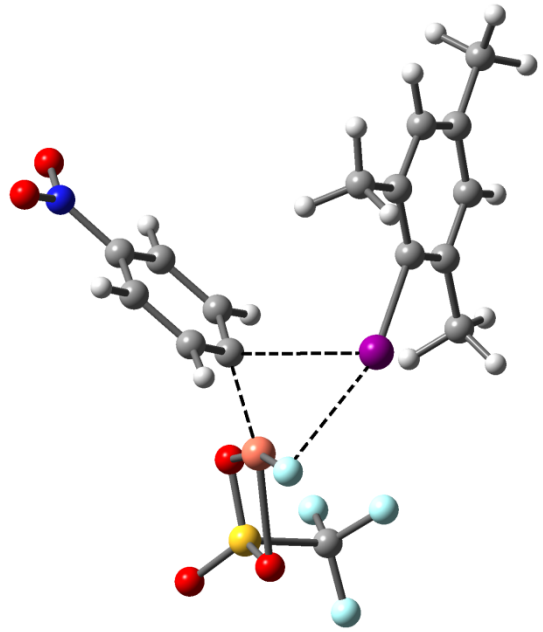
Zero-point correction= 0.282803 (Hartree/Particle)
Thermal correction to Energy= 0.315657
Thermal correction to Enthalpy= 0.316601
Thermal correction to Gibbs Free Energy= 0.209023
Sum of electronic and zero-point Energies= -2055.157548
Sum of electronic and thermal Energies= -2055.124695
Sum of electronic and thermal Enthalpies= -2055.123751
Sum of electronic and thermal Free Energies= -2055.231328
E(RB-P86) = -2055.44035161 A.U.



O	-2.569210	-0.565189	-0.592383
C	2.550565	-1.522101	-0.365837
C	3.778944	-1.023710	-0.855934
C	2.423575	-2.434128	0.704747
C	4.930183	-1.477557	-0.200537
C	3.624426	-2.838801	1.306936
C	4.877283	-2.379812	0.874550
H	5.899958	-1.110388	-0.547072
H	3.568745	-3.537929	2.145540
I	0.793846	-0.916806	-1.380561
C	0.488067	1.200576	-0.196940
C	1.493137	1.498780	0.730778
C	-0.173140	2.174528	-0.961374
C	1.759575	2.840973	0.993231
H	2.025463	0.714889	1.270617
C	0.096155	3.515581	-0.679292
H	-0.890300	1.914649	-1.740364

C	1.054028	3.825115	0.289701
H	2.503079	3.125522	1.737314
H	-0.414307	4.310497	-1.222406
Cu	-0.900773	-0.068016	0.465804
C	-4.843298	-1.438329	0.445125
F	-0.652254	-0.230798	2.326931
F	-6.100361	-1.079316	0.789057
F	-4.917643	-2.427781	-0.472091
F	-4.220268	-1.918649	1.543080
S	-3.915264	0.053393	-0.254467
O	-4.678709	0.429889	-1.450595
O	-3.855906	1.013974	0.857289
C	3.899980	-0.062275	-2.010756
H	3.500134	-0.493807	-2.942091
H	3.357786	0.877354	-1.820530
H	4.954090	0.189463	-2.183854
C	1.109965	-2.955789	1.224387
H	0.489963	-2.141860	1.642061
H	0.527433	-3.451987	0.432552
H	1.285767	-3.688503	2.022653
C	6.144581	-2.862261	1.530533
H	5.958266	-3.220896	2.552160
H	6.576058	-3.700286	0.957179
H	6.904043	-2.067840	1.565050
N	1.353081	5.242787	0.563583
O	0.724562	6.102563	-0.074243
O	2.217467	5.498095	1.417467

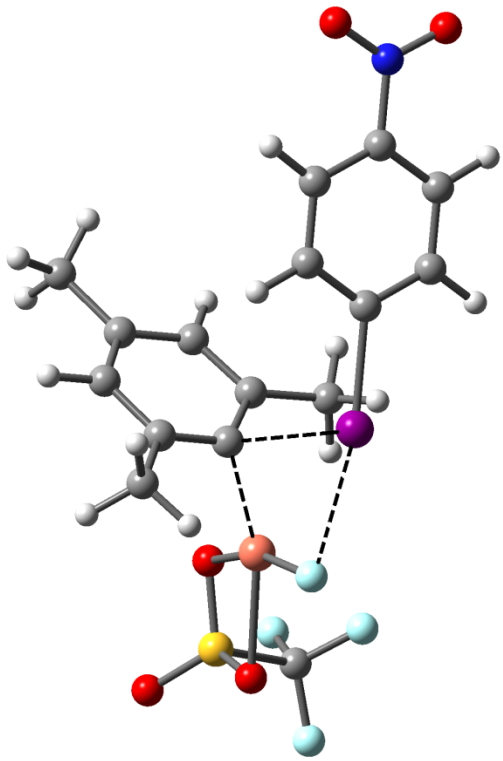
Zero-point correction= 0.283622 (Hartree/Particle)
Thermal correction to Energy= 0.315893
Thermal correction to Enthalpy= 0.316837
Thermal correction to Gibbs Free Energy= 0.214155
Sum of electronic and zero-point Energies= -2055.159553
Sum of electronic and thermal Energies= -2055.127282
Sum of electronic and thermal Enthalpies= -2055.126338
Sum of electronic and thermal Free Energies= -2055.229020
E(RB-P86) = -2055.44317483 A.U.



C	-2.128222	-1.828093	-0.339944
C	-1.723251	-2.819012	0.584842
C	-3.470560	-1.397964	-0.467641
C	-2.722170	-3.386683	1.387547
C	-4.416394	-2.006834	0.367479
C	-4.067234	-2.995697	1.300933
H	-2.435488	-4.162748	2.103007
H	-5.461617	-1.696102	0.282054
I	-0.674572	-0.966493	-1.610030
C	-0.209473	1.462718	-0.377287
C	-0.665811	2.496652	-1.202453
C	-0.570910	1.336817	0.967925
C	-1.430692	3.509842	-0.621782
H	-0.404076	2.525488	-2.259661
C	-1.338938	2.353847	1.537938
H	-0.244633	0.495421	1.579157
C	-1.752800	3.424460	0.737524
H	-1.782392	4.352241	-1.217295
H	-1.620358	2.314101	2.590164
Cu	1.592427	0.841273	-0.862775
F	1.277527	0.846101	-2.703410
C	4.066553	-1.349010	1.124380
S	3.814595	0.443237	0.568675
F	3.181386	-2.154733	0.510461
F	5.313601	-1.745797	0.810250
F	3.897311	-1.440637	2.456347
O	3.795709	0.393983	-0.925437
O	4.868493	1.200925	1.231556
O	2.390223	0.763601	1.007026
C	-0.298853	-3.292622	0.721837
H	0.059885	-3.761877	-0.208255

H	0.385544	-2.461417	0.948671
H	-0.217720	-4.032693	1.528948
C	-3.913877	-0.344598	-1.451680
H	-3.403193	0.615202	-1.276788
H	-3.695227	-0.643947	-2.489194
H	-4.995319	-0.173834	-1.367439
C	-5.108299	-3.603219	2.205904
H	-4.828819	-4.620770	2.514082
H	-5.219958	-3.000920	3.123848
H	-6.093150	-3.638618	1.718128
N	-2.575336	4.483692	1.340609
O	-2.867501	4.381867	2.544670
O	-2.936995	5.426128	0.615136

Zero-point correction= 0.282721 (Hartree/Particle)
Thermal correction to Energy= 0.315528
Thermal correction to Enthalpy= 0.316473
Thermal correction to Gibbs Free Energy= 0.210456
Sum of electronic and zero-point Energies= -2055.159384
Sum of electronic and thermal Energies= -2055.126576
Sum of electronic and thermal Enthalpies= -2055.125632
Sum of electronic and thermal Free Energies= -2055.231649
E(RB-P86) = -2055.44210466 A.U.



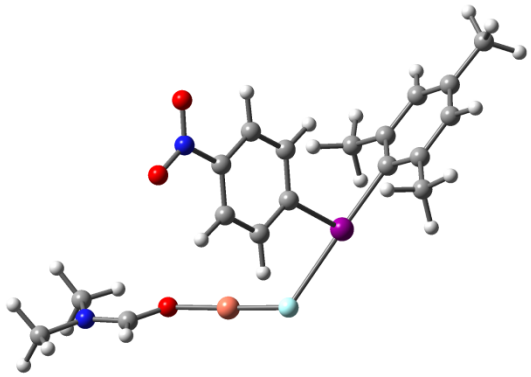
C	-3.139081	-1.020506	-0.100032
C	-3.607178	-1.396034	1.169297
C	-3.900281	-0.187914	-0.935866

C	-4.851165	-0.941516	1.605279
H	-3.011853	-2.041741	1.815855
C	-5.142855	0.271202	-0.500465
H	-3.533735	0.099155	-1.922102
C	-5.599756	-0.113008	0.763803
H	-5.240053	-1.220411	2.584225
H	-5.755114	0.917337	-1.128890
I	-1.261928	-1.726466	-0.761272
C	0.332142	0.728864	-0.541778
C	0.090946	1.388271	-1.748281
C	0.069686	1.208717	0.748640
C	-0.267131	2.746320	-1.611433
C	-0.294618	2.565236	0.798379
C	-0.465994	3.343649	-0.360771
H	-0.410522	3.329570	-2.526647
H	-0.453137	3.012816	1.784575
Cu	1.971406	-0.379969	-0.651469
F	1.356672	-1.932142	-1.435991
C	5.086745	-0.355463	1.652024
S	4.505352	0.306640	-0.022879
F	4.158453	-1.175552	2.180018
F	6.235830	-1.040141	1.493093
F	5.300592	0.668754	2.500263
O	4.159563	-0.910426	-0.819292
O	5.594702	1.155868	-0.493644
O	3.199945	1.011486	0.294905
C	0.248976	0.403682	2.009552
H	-0.181844	0.934164	2.868789
H	-0.230642	-0.583072	1.927321
H	1.318468	0.236014	2.214646
C	-0.868434	4.793804	-0.252852
H	-1.560568	4.956671	0.586020
H	0.017473	5.425776	-0.071110
H	-1.344833	5.148890	-1.177172
C	0.219728	0.760788	-3.115249
H	0.573028	-0.276388	-3.051013
H	-0.756286	0.765051	-3.625350
H	0.919025	1.337761	-3.739448
N	-6.912295	0.372811	1.224832
O	-7.301496	0.021070	2.350986
O	-7.561697	1.109438	0.463873

J: adduct

Zero-point correction=	0.359880 (Hartree/Particle)
Thermal correction to Energy=	0.391321
Thermal correction to Enthalpy=	0.392265
Thermal correction to Gibbs Free Energy=	0.288669
Sum of electronic and zero-point Energies=	-1341.794483
Sum of electronic and thermal Energies=	-1341.763042
Sum of electronic and thermal Enthalpies=	-1341.762098
Sum of electronic and thermal Free Energies=	-1341.865693

E(RB-P86) = -1342.15436276 A.U

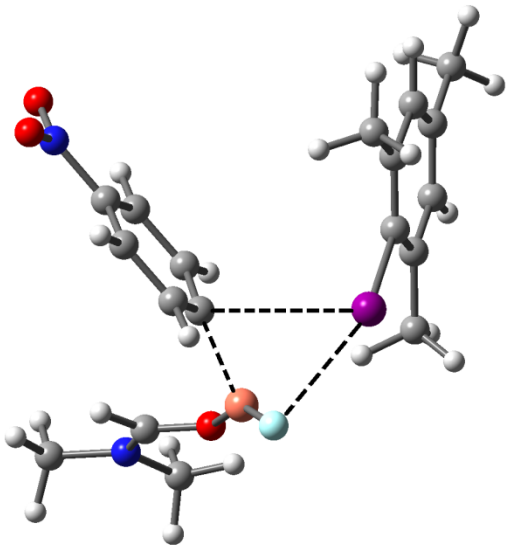


C	-3.087660	-0.875987	0.058078
C	-3.329947	-1.475045	1.312711
C	-4.078712	-0.205456	-0.691305
C	-4.632790	-1.361323	1.821924
C	-5.356813	-0.128273	-0.119488
C	-5.654489	-0.697328	1.127913
H	-4.849723	-1.808285	2.796221
H	-6.141944	0.395237	-0.672362
I	-1.139158	-1.084601	-0.791140
C	-0.483211	0.923651	-0.392578
C	0.586601	1.416708	-1.141282
C	-1.143645	1.667969	0.584150
C	1.017031	2.721434	-0.891609
H	1.075255	0.797269	-1.893813
C	-0.707981	2.972440	0.826716
H	-1.982995	1.260882	1.149146
C	0.365076	3.474762	0.087350
H	1.845600	3.151844	-1.453191
H	-1.190790	3.590668	1.582816
Cu	2.693224	-1.474910	-0.779840
F	1.202076	-1.398547	-1.846974
C	5.234307	-0.899423	0.199420
H	5.365132	-0.196169	-0.635956
O	4.171081	-1.581214	0.343408
N	6.262488	-0.981915	1.037931
C	6.241292	-1.869641	2.202417
H	6.364808	-1.273983	3.118809
H	5.286204	-2.403351	2.231316
H	7.069832	-2.589236	2.129436
C	7.470489	-0.182075	0.827031
H	7.636933	0.475382	1.692817
H	8.338889	-0.846602	0.709357
H	7.357827	0.429930	-0.076129
C	-3.821784	0.423355	-2.038429
H	-3.067414	1.224452	-1.979217
H	-3.457982	-0.316497	-2.769048
H	-4.745335	0.864371	-2.435501

C	-2.282963	-2.219173	2.107575
H	-1.927881	-3.114105	1.572281
H	-1.402693	-1.593173	2.321675
H	-2.701223	-2.549658	3.067373
C	-7.049199	-0.619218	1.696582
H	-7.660140	-1.463602	1.335003
H	-7.038319	-0.667678	2.794630
H	-7.556477	0.306218	1.388367
N	0.826521	4.853655	0.350403
O	0.225235	5.511877	1.213276
O	1.791051	5.277191	-0.305045

J: TS

Zero-point correction= 0.358502 (Hartree/Particle)
Thermal correction to Energy= 0.389397
Thermal correction to Enthalpy= 0.390341
Thermal correction to Gibbs Free Energy= 0.289744
Sum of electronic and zero-point Energies= -1341.775628
Sum of electronic and thermal Energies= -1341.744733
Sum of electronic and thermal Enthalpies= -1341.743789
Sum of electronic and thermal Free Energies= -1341.844385
E(RB-P86) = -1342.13412971 A.U

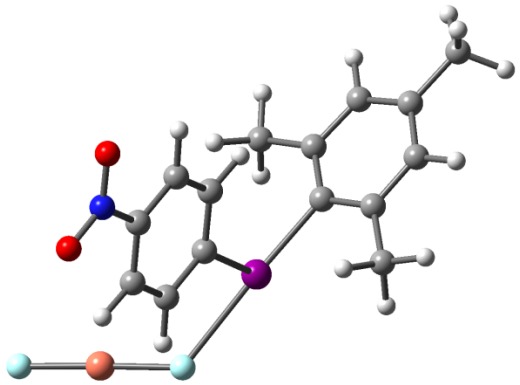


C	-2.657299	-0.196033	-0.095559
C	-2.944199	-1.321106	0.715120
C	-3.227224	1.079922	0.128604
C	-3.846846	-1.131707	1.768548
C	-4.122266	1.197089	1.200075
C	-4.444779	0.112309	2.031139
H	-4.092240	-1.988184	2.403013
H	-4.582349	2.171076	1.388890
I	-1.338510	-0.430625	-1.725734
C	1.394153	0.610117	-0.611120

C	1.918313	1.591074	-1.446949
C	1.095071	0.793489	0.734933
C	2.243686	2.821702	-0.864239
H	2.087011	1.409422	-2.507142
C	1.424376	2.028861	1.303632
H	0.633279	0.018917	1.346828
C	1.996761	3.016012	0.496893
H	2.676933	3.620529	-1.466238
H	1.229584	2.221273	2.358687
Cu	1.503430	-1.189608	-1.322978
F	1.401423	-0.799797	-3.113059
C	2.970072	-2.054747	0.936751
H	3.631664	-1.188919	0.794156
O	1.931855	-2.222836	0.208648
N	3.309508	-2.890099	1.901616
C	2.522676	-4.090529	2.203439
H	2.293960	-4.104556	3.277846
H	1.596325	-4.074975	1.621204
H	3.108834	-4.985239	1.948473
C	4.520844	-2.663286	2.697732
H	4.247024	-2.569288	3.758039
H	5.204903	-3.514807	2.575008
H	5.017755	-1.744734	2.364739
C	-2.919498	2.284261	-0.723671
H	-1.842781	2.515572	-0.718626
H	-3.210315	2.121187	-1.773820
H	-3.460771	3.164719	-0.352777
C	-2.338186	-2.681521	0.484372
H	-2.610803	-3.081613	-0.505332
H	-1.238111	-2.644827	0.525552
H	-2.686464	-3.390233	1.247373
C	-5.388598	0.281193	3.193150
H	-6.043924	1.152820	3.057066
H	-6.012529	-0.613416	3.335628
H	-4.824250	0.433863	4.129282
N	2.333818	4.319297	1.101589
O	2.820272	5.191968	0.365380
O	2.112925	4.471411	2.313525

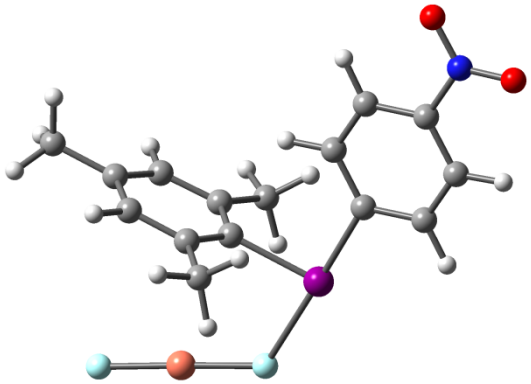
K, L: adducts

Zero-point correction= 0.259892 (Hartree/Particle)
Thermal correction to Energy= 0.285340
Thermal correction to Enthalpy= 0.286285
Thermal correction to Gibbs Free Energy= 0.198119
Sum of electronic and zero-point Energies= -1193.340283
Sum of electronic and thermal Energies= -1193.314835
Sum of electronic and thermal Enthalpies= -1193.313890
Sum of electronic and thermal Free Energies= -1193.402056
E(RB-P86) = -1193.60017490 A.U.



C	-2.385249	-0.515336	-0.069864
C	-2.956584	-0.777047	1.192760
C	-3.083036	0.121223	-1.121467
C	-4.281169	-0.351369	1.387953
C	-4.398838	0.521534	-0.855582
C	-5.014456	0.298218	0.386566
H	-4.747721	-0.538996	2.358935
H	-4.959622	1.022517	-1.649910
I	-0.402541	-1.219620	-0.451508
C	0.568504	0.682738	-0.194752
C	1.853504	0.833498	-0.717657
C	-0.111093	1.700990	0.473203
C	2.486598	2.068079	-0.559675
H	2.348664	0.006451	-1.227598
C	0.529111	2.932264	0.627936
H	-1.118285	1.557882	0.867019
C	1.815957	3.094394	0.109598
H	3.488681	2.234379	-0.953883
H	0.037962	3.754812	1.146795
Cu	3.298928	-2.411089	0.178787
F	4.675498	-2.728000	1.309865
F	1.922039	-2.098862	-1.005198
C	-2.482487	0.386928	-2.480299
H	-1.595803	1.037724	-2.417014
H	-2.170170	-0.545653	-2.976281
H	-3.215282	0.884562	-3.129005
C	-2.232737	-1.482794	2.315182
H	-1.982384	-2.521717	2.047685
H	-1.291850	-0.977984	2.583555
H	-2.864861	-1.512680	3.212484
C	-6.431597	0.754016	0.628936
H	-7.113234	0.345612	-0.133652
H	-6.792347	0.442064	1.618510
H	-6.503949	1.852049	0.568440
N	2.490098	4.398224	0.274423
O	1.878810	5.295867	0.875044
O	3.631049	4.525459	-0.196419

Zero-point correction= 0.260049 (Hartree/Particle)
Thermal correction to Energy= 0.285418
Thermal correction to Enthalpy= 0.286362
Thermal correction to Gibbs Free Energy= 0.198898
Sum of electronic and zero-point Energies= -1193.342088
Sum of electronic and thermal Energies= -1193.316719
Sum of electronic and thermal Enthalpies= -1193.315775
Sum of electronic and thermal Free Energies= -1193.403239
E(RB-P86) = -1193.60213675 A.U.

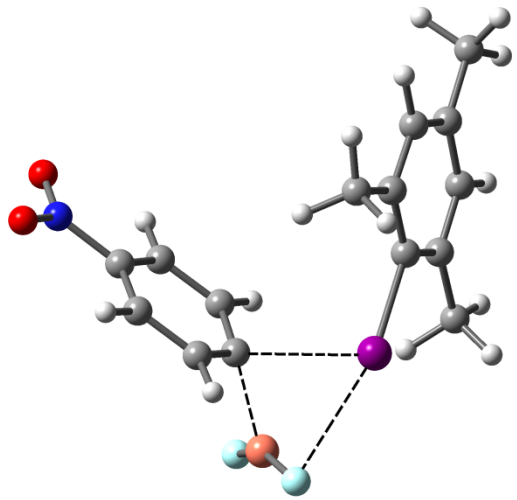


C	-2.029061	-0.620603	0.030370
C	-2.313796	0.744478	0.111290
C	-3.040547	-1.583807	-0.069727
C	-3.646827	1.159737	0.091629
H	-1.517485	1.486204	0.190262
C	-4.372528	-1.170119	-0.087874
H	-2.810814	-2.649239	-0.136156
C	-4.653779	0.196736	-0.007577
H	-3.905378	2.216495	0.152977
H	-5.184224	-1.892821	-0.165058
I	-0.005692	-1.373739	0.056076
C	0.938091	0.535642	0.044924
C	1.140376	1.160465	-1.201222
C	1.341596	1.072363	1.282076
C	1.778130	2.409900	-1.167788
C	1.974307	2.325041	1.233510
C	2.196851	3.007993	0.029904
H	1.955308	2.923956	-2.116572
H	2.305906	2.771783	2.174773
Cu	3.815570	-1.112288	-0.106579
F	5.301033	-0.088664	-0.270324
F	2.324547	-2.190345	0.062049
C	1.148053	0.379985	2.607871
H	1.548779	0.999690	3.420522
H	0.084122	0.191593	2.821089
H	1.669245	-0.590042	2.632915
C	0.720422	0.564979	-2.521472
H	-0.365730	0.385991	-2.562435

H	0.978707	1.245235	-3.343362
H	1.222114	-0.397766	-2.708005
C	2.861657	4.361884	0.020174
H	3.506068	4.483434	-0.862561
H	2.104749	5.163496	-0.015390
H	3.467844	4.518378	0.923256
N	-6.061531	0.637741	-0.028497
O	-6.942326	-0.231966	-0.124198
O	-6.290954	1.855338	0.050444

K, L: TS's

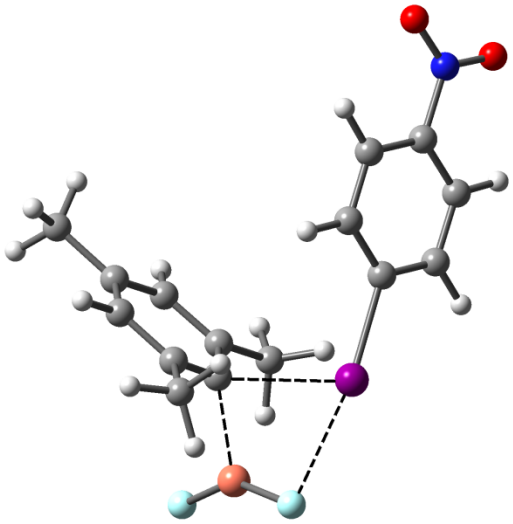
Zero-point correction= 0.258659 (Hartree/Particle)
Thermal correction to Energy= 0.283442
Thermal correction to Enthalpy= 0.284386
Thermal correction to Gibbs Free Energy= 0.199906
Sum of electronic and zero-point Energies= -1193.329670
Sum of electronic and thermal Energies= -1193.304888
Sum of electronic and thermal Enthalpies= -1193.303943
Sum of electronic and thermal Free Energies= -1193.388423
E(RB-P86) = -1193.58832954 A.U.



C	-2.190119	0.104178	-0.300926
C	-3.025213	-0.166376	0.807077
C	-2.252114	1.310073	-1.039525
C	-3.949920	0.827626	1.161377
C	-3.197293	2.257700	-0.629036
C	-4.050302	2.041067	0.466175
H	-4.612643	0.641338	2.011165
H	-3.268449	3.196466	-1.186012
I	-0.790881	-1.368752	-0.887403
C	1.446887	-0.386182	0.100933
C	2.357541	-0.116675	-0.930686
C	1.150182	0.528938	1.118832
C	3.075117	1.077803	-0.877290
H	2.522323	-0.834258	-1.733528

C	1.872083	1.721181	1.158237
H	0.405842	0.315100	1.884766
C	2.825953	1.978744	0.165247
H	3.812482	1.316613	-1.643563
H	1.696039	2.449031	1.950233
Cu	1.574258	-2.294883	0.649343
F	1.669386	-2.228686	2.471201
F	1.565319	-2.994673	-1.073773
C	-2.981902	-1.454530	1.590981
H	-3.236484	-2.319523	0.957884
H	-1.982672	-1.645183	2.011609
H	-3.699814	-1.418928	2.420986
C	-1.368625	1.599996	-2.226806
H	-0.301808	1.584547	-1.954227
H	-1.510686	0.855302	-3.026222
H	-1.597928	2.591073	-2.640103
C	-5.038939	3.098860	0.885857
H	-5.633062	3.449367	0.027555
H	-5.726655	2.725663	1.656938
H	-4.515909	3.979711	1.293759
N	3.566535	3.243041	0.202709
O	4.400159	3.460437	-0.695640
O	3.324158	4.037522	1.129599

Zero-point correction= 0.258135 (Hartree/Particle)
Thermal correction to Energy= 0.283234
Thermal correction to Enthalpy= 0.284178
Thermal correction to Gibbs Free Energy= 0.198494
Sum of electronic and zero-point Energies= -1193.328419
Sum of electronic and thermal Energies= -1193.303321
Sum of electronic and thermal Enthalpies= -1193.302376
Sum of electronic and thermal Free Energies= -1193.388060
E(RB-P86) = -1193.58655415 A.U.

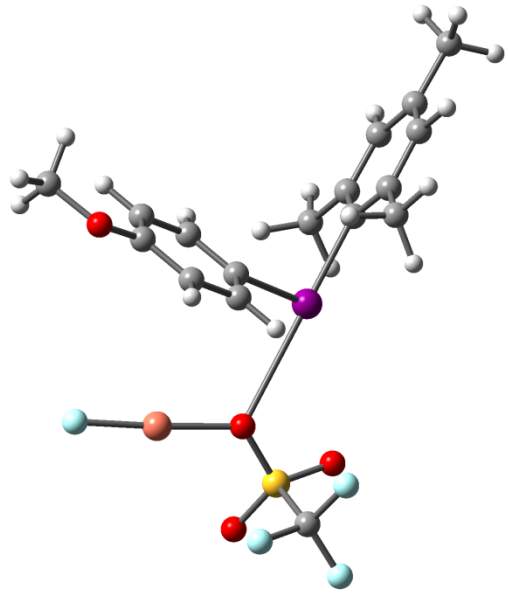


C	-1.708652	-0.938568	-0.206288
C	-2.497592	-1.405948	0.856186
C	-2.208747	-0.009370	-1.131097
C	-3.808737	-0.949013	0.987755
H	-2.102485	-2.126553	1.573525
C	-3.516436	0.455806	-0.995821
H	-1.589990	0.348239	-1.954782
C	-4.296600	-0.024050	0.060215
H	-4.447793	-1.299881	1.797516
H	-3.933177	1.176126	-1.699137
I	0.265071	-1.669846	-0.433680
C	1.670721	0.643481	0.018378
C	1.898311	1.239686	-1.226556
C	1.131308	1.265992	1.153143
C	1.717955	2.638742	-1.252419
C	0.965783	2.657535	1.038102
C	1.251318	3.357934	-0.145487
H	1.939327	3.159175	-2.189272
H	0.602863	3.198251	1.917794
Cu	3.133470	-0.666077	0.502511
F	4.073182	0.217892	1.815758
F	2.884906	-2.127737	-0.625374
C	2.318049	0.502223	-2.472402
H	2.770655	1.195380	-3.193998
H	3.029788	-0.304911	-2.248949
H	1.441747	0.036144	-2.953321
C	0.840856	0.560140	2.451320
H	0.438871	1.265272	3.190580
H	0.110099	-0.252119	2.318060
H	1.764927	0.116872	2.855984
C	1.053061	4.852655	-0.217830
H	1.017287	5.203540	-1.258453
H	0.124110	5.157245	0.286828
H	1.882287	5.378875	0.284290
N	-5.682708	0.461274	0.199562
O	-6.361758	0.020585	1.141238
O	-6.097657	1.284742	-0.632243

Reactions of [*p*-MeOC$_6$H$_4$(Ph)I]BF$_4$

G-I: adducts

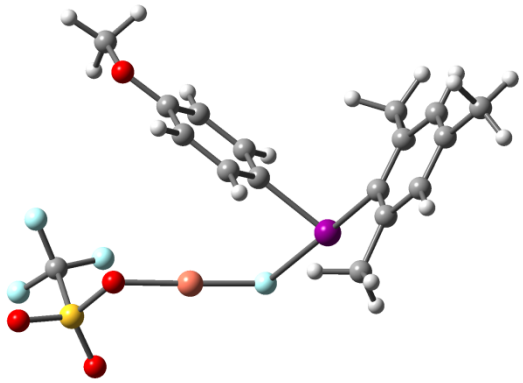
Zero-point correction= 0.313963 (Hartree/Particle)
Thermal correction to Energy= 0.347438
Thermal correction to Enthalpy= 0.348382
Thermal correction to Gibbs Free Energy= 0.238504
Sum of electronic and zero-point Energies= -1965.107646
Sum of electronic and thermal Energies= -1965.074172
Sum of electronic and thermal Enthalpies= -1965.073227
Sum of electronic and thermal Free Energies= -1965.183105
E(RB-P86) = -1965.42160904 A.U.



O	-2.106256	-0.608169	-0.367148
C	3.014654	-0.914719	-0.052531
C	3.719664	-1.211590	-1.236006
C	3.622603	-0.740406	1.205466
C	5.114332	-1.317944	-1.118720
C	5.021340	-0.854923	1.243936
C	5.781859	-1.143562	0.102337
H	5.691981	-1.545022	-2.019284
H	5.524668	-0.713834	2.204604
I	0.878419	-0.787748	-0.186313
C	0.578035	1.283927	0.165427
C	-0.128250	1.658851	1.316161
C	1.045643	2.218084	-0.758211
C	-0.361863	3.011279	1.541198
H	-0.493766	0.917401	2.027354
C	0.818312	3.576924	-0.518999
H	1.583699	1.914857	-1.656859
C	0.111473	3.978024	0.630667
H	-0.911513	3.337745	2.425940
H	1.187213	4.306168	-1.239550
Cu	-2.899335	1.012830	-0.912033
C	-3.652490	-2.113300	1.195812
F	-3.581151	2.607327	-1.429393
F	-4.305262	-3.292143	1.277831
F	-2.745464	-2.052354	2.192977
F	-4.543879	-1.113849	1.361254
S	-2.796525	-1.973005	-0.486790
O	-1.798892	-3.048473	-0.488752
O	-3.881330	-2.008252	-1.471162
C	2.861593	-0.434439	2.470010
H	2.361338	0.545280	2.414164
H	2.085614	-1.190576	2.669749

H	3.543625	-0.413886	3.329999
C	3.067639	-1.434791	-2.579600
H	2.421468	-2.327234	-2.574371
H	2.443871	-0.580487	-2.883209
H	3.834219	-1.584627	-3.351075
C	7.280575	-1.292189	0.188276
H	7.556325	-2.352833	0.313893
H	7.771561	-0.934655	-0.728435
H	7.690629	-0.740567	1.045887
O	-0.167470	5.268875	0.948552
C	0.279613	6.300628	0.044152
H	-0.180054	6.176440	-0.948260
H	-0.054066	7.242918	0.491833
H	1.377090	6.297764	-0.042375

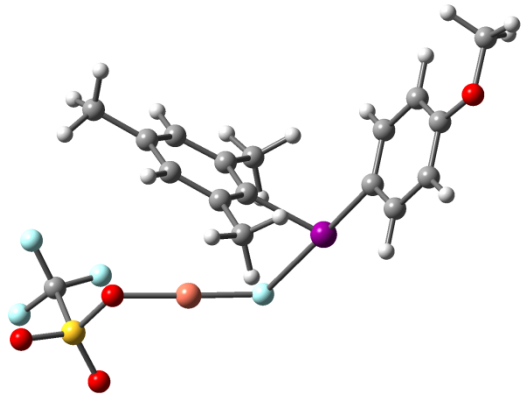
Zero-point correction= 0.314065 (Hartree/Particle)
Thermal correction to Energy= 0.347268
Thermal correction to Enthalpy= 0.348212
Thermal correction to Gibbs Free Energy= 0.239851
Sum of electronic and zero-point Energies= -1965.114203
Sum of electronic and thermal Energies= -1965.081000
Sum of electronic and thermal Enthalpies= -1965.080055
Sum of electronic and thermal Free Energies= -1965.188417
E(RB-P86) = -1965.42826773 A.U.



C	3.885260	-0.490036	-0.103374
C	4.547971	0.453053	-0.914315
C	4.481379	-1.097722	1.021487
C	5.854630	0.805805	-0.540880
C	5.792797	-0.705852	1.332476
C	6.491611	0.244941	0.574608
H	6.388958	1.538727	-1.152447
H	6.280400	-1.165819	2.196914
I	1.894605	-1.105884	-0.632892
C	0.890643	0.689733	-0.106951
C	0.909328	1.127254	1.222399
C	0.216720	1.388665	-1.107852
C	0.238577	2.302749	1.545479

H	1.432368	0.571486	2.001330
C	-0.465409	2.564101	-0.775267
H	0.208218	1.034296	-2.139167
C	-0.452930	3.027234	0.552987
Cu	-1.883816	-1.218628	-0.173267
F	-0.520388	-1.819641	-1.244661
C	-5.368585	0.118008	-0.438317
S	-4.666020	-1.037302	0.886595
F	-5.244900	1.408738	-0.061816
F	-6.679217	-0.148285	-0.632242
F	-4.720123	-0.049584	-1.612614
O	-4.826657	-2.385094	0.325850
O	-5.409725	-0.693730	2.102857
O	-3.216524	-0.566652	0.984076
C	7.888543	0.664725	0.961122
H	7.856829	1.454606	1.730546
H	8.458029	-0.176640	1.382306
H	8.439991	1.065983	0.099070
C	3.799853	-2.141090	1.876423
H	2.849719	-1.776332	2.296456
H	3.573600	-3.054697	1.303870
H	4.449156	-2.426839	2.714668
C	3.926762	1.085543	-2.134855
H	3.571821	0.326085	-2.849475
H	3.062569	1.715573	-1.870421
H	4.658604	1.721117	-2.650800
H	-0.991219	3.107192	-1.559861
H	0.233105	2.671025	2.573134
O	-1.075925	4.159007	0.978717
C	-1.795168	4.940410	0.002681
H	-2.215240	5.785218	0.559174
H	-1.115606	5.311607	-0.780151
H	-2.608007	4.351880	-0.449733

Zero-point correction= 0.314164 (Hartree/Particle)
Thermal correction to Energy= 0.347323
Thermal correction to Enthalpy= 0.348267
Thermal correction to Gibbs Free Energy= 0.240388
Sum of electronic and zero-point Energies= -1965.116015
Sum of electronic and thermal Energies= -1965.082856
Sum of electronic and thermal Enthalpies= -1965.081911
Sum of electronic and thermal Free Energies= -1965.189791
E(RB-P86) = -1965.43017889 A.U.

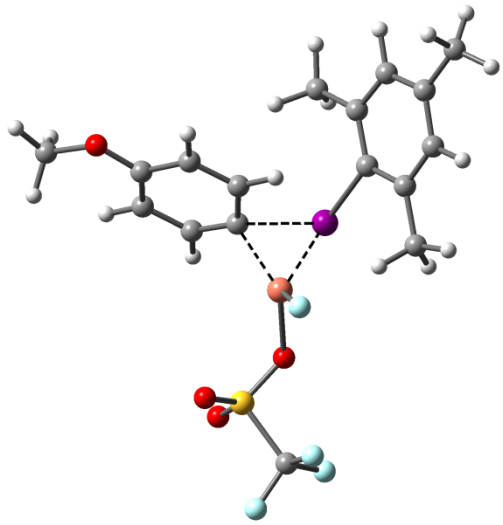


C	3.743304	-0.654553	-0.043352
C	4.337370	0.132129	-1.033258
C	4.466634	-1.060611	1.088612
C	5.667134	0.540062	-0.888711
H	3.783568	0.437328	-1.922430
C	5.794046	-0.665721	1.226554
H	4.007088	-1.681545	1.859982
C	6.401276	0.141516	0.244026
I	1.735482	-1.335683	-0.269423
C	0.752414	0.561010	-0.056974
C	0.722472	1.160068	1.215920
C	0.163717	1.115821	-1.208539
C	0.078215	2.404833	1.301408
C	-0.469907	2.358755	-1.043103
C	-0.516060	3.021003	0.191108
H	0.036353	2.896974	2.277364
H	-0.945326	2.814508	-1.916289
Cu	-2.040399	-1.065031	0.174549
F	-0.703912	-2.119640	-0.519650
C	-5.426626	0.286227	-0.775561
S	-4.839484	-0.362056	0.903340
F	-5.255422	1.622947	-0.857959
F	-6.739404	0.011082	-0.940886
F	-4.737456	-0.296317	-1.781995
O	-5.058478	-1.812992	0.838270
O	-5.603973	0.416302	1.883202
O	-3.369015	0.050409	0.904998
C	1.328859	0.545845	2.451377
H	0.964872	-0.480391	2.616005
H	2.427166	0.499351	2.380425
H	1.075362	1.143213	3.336854
C	0.154602	0.445931	-2.560351
H	1.170486	0.348131	-2.975029
H	-0.278624	-0.564123	-2.497314
H	-0.442260	1.034120	-3.269794
C	-1.178989	4.370062	0.322728
H	-0.426589	5.175991	0.290785
H	-1.891827	4.548832	-0.494294

H	-1.712294	4.461735	1.280296
H	6.376565	-0.970168	2.098339
H	6.117491	1.157875	-1.665212
O	7.698369	0.480802	0.478115
C	8.365112	1.308685	-0.496647
H	9.376224	1.462783	-0.104367
H	8.418309	0.801429	-1.472484
H	7.855253	2.278746	-0.602458

G-I: TS's

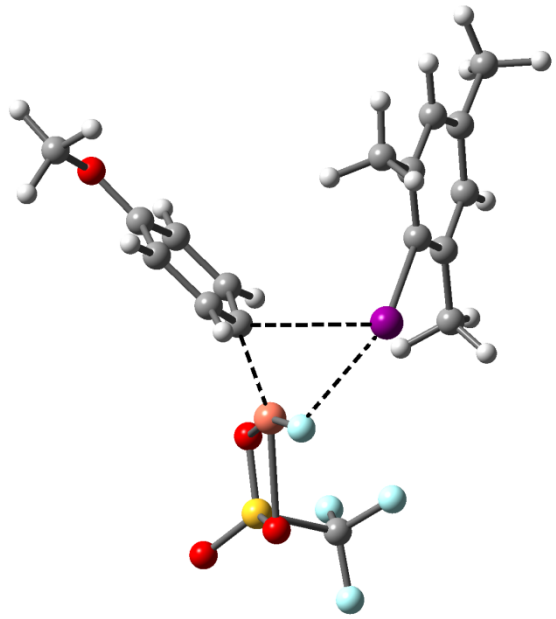
Zero-point correction= 0.312775 (Hartree/Particle)
Thermal correction to Energy= 0.345442
Thermal correction to Enthalpy= 0.346386
Thermal correction to Gibbs Free Energy= 0.241781
Sum of electronic and zero-point Energies= -1965.099029
Sum of electronic and thermal Energies= -1965.066362
Sum of electronic and thermal Enthalpies= -1965.065418
Sum of electronic and thermal Free Energies= -1965.170023
E(RB-P86) = -1965.41180459 A.U.



O	-2.516325	-0.644011	-0.525888
C	2.638555	-1.304457	-0.408632
C	3.840127	-0.689912	-0.825991
C	2.559342	-2.318431	0.570042
C	5.011245	-1.131530	-0.197148
C	3.776401	-2.703779	1.154129
C	5.002192	-2.127400	0.793139
H	5.960804	-0.679364	-0.496378
H	3.755775	-3.486879	1.916831
I	0.852960	-0.707512	-1.383573
C	0.447966	1.369250	0.056827
C	1.482691	1.613416	0.970349
C	-0.147017	2.386515	-0.698544
C	1.780033	2.935618	1.276886

H	2.005311	0.802085	1.479579
C	0.151242	3.714244	-0.375320
H	-0.862402	2.173802	-1.494086
C	1.112572	3.992379	0.615671
H	2.528619	3.171620	2.035695
H	-0.359059	4.512446	-0.913647
Cu	-0.784193	-0.076753	0.507609
C	-4.896933	-1.413843	0.332158
F	-0.792333	-0.632504	2.328420
F	-6.154140	-0.993214	0.602881
F	-4.965894	-2.373907	-0.617945
F	-4.381458	-1.962294	1.454448
S	-3.839502	0.037710	-0.258859
O	-4.512312	0.494614	-1.483912
O	-3.808537	0.965475	0.883736
C	3.912705	0.379745	-1.885853
H	3.546414	0.013609	-2.858012
H	3.308529	1.260367	-1.615714
H	4.950496	0.711182	-2.020060
C	1.276255	-2.970636	1.012380
H	0.596393	-2.242232	1.491586
H	0.738104	-3.423623	0.165050
H	1.489086	-3.764320	1.740627
C	6.282850	-2.550559	1.465689
H	7.116419	-2.591648	0.749224
H	6.563301	-1.824549	2.247512
H	6.179894	-3.533361	1.945940
O	1.488764	5.239101	0.989904
C	0.879329	6.364353	0.319618
H	-0.210439	6.365673	0.474058
H	1.321536	7.251672	0.784625
H	1.112359	6.350135	-0.755734

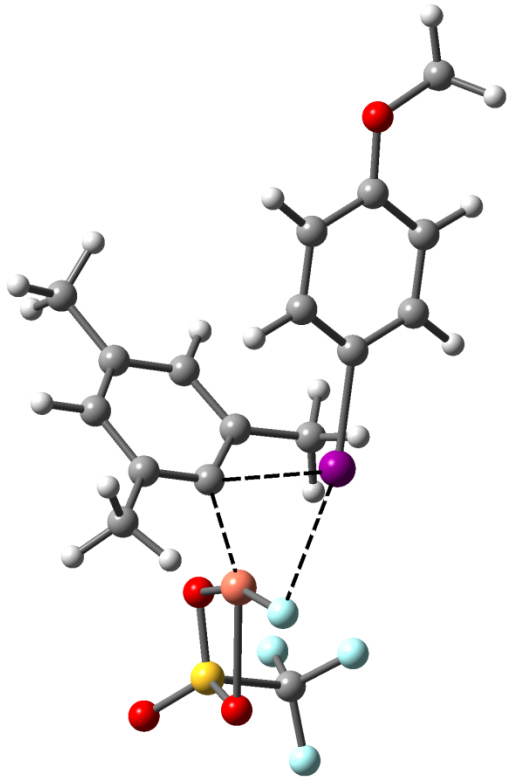
Zero-point correction= 0.312780 (Hartree/Particle)
Thermal correction to Energy= 0.345335
Thermal correction to Enthalpy= 0.346280
Thermal correction to Gibbs Free Energy= 0.242196
Sum of electronic and zero-point Energies= -1965.098125
Sum of electronic and thermal Energies= -1965.065570
Sum of electronic and thermal Enthalpies= -1965.064626
Sum of electronic and thermal Free Energies= -1965.168709
E(RB-P86) = -1965.41090517 A.U.



C	2.160503	-1.695739	0.377768
C	1.727263	-2.730257	-0.483263
C	3.512242	-1.295475	0.472264
C	2.706805	-3.377724	-1.248409
C	4.440970	-1.986156	-0.320987
C	4.064494	-3.027152	-1.181881
H	2.393520	-4.182947	-1.919540
H	5.493501	-1.694187	-0.261664
I	0.730790	-0.702214	1.585853
C	0.225692	1.723958	0.093346
C	0.738918	2.791497	0.827806
C	0.637619	1.435368	-1.211624
C	1.536721	3.732460	0.163909
H	0.482572	2.923216	1.879057
C	1.437703	2.370869	-1.863285
H	0.302520	0.542921	-1.740702
C	1.884191	3.525496	-1.185124
Cu	-1.490574	1.043875	0.684218
F	-1.214914	1.264012	2.537653
C	-4.057135	-1.505586	-0.795746
S	-3.730588	0.352963	-0.648662
F	-3.182321	-2.198120	-0.043152
F	-5.307430	-1.778316	-0.373941
F	-3.934387	-1.893063	-2.080224
O	-3.682485	0.618003	0.823448
O	-4.792368	0.981959	-1.428237
O	-2.319818	0.528927	-1.173969
C	0.286622	-3.158632	-0.598781
H	-0.092762	-3.554816	0.356887
H	-0.364580	-2.316592	-0.878793
H	0.179656	-3.943779	-1.359247

C	3.985911	-0.183698	1.374916
H	3.474544	0.765629	1.151177
H	3.789739	-0.413920	2.434605
H	5.066321	-0.026884	1.255008
C	5.090525	-3.765815	-2.004473
H	5.318435	-4.745901	-1.552200
H	4.722085	-3.959692	-3.023128
H	6.032542	-3.204058	-2.073349
H	1.724537	2.219680	-2.906135
H	1.879533	4.610790	0.710992
O	2.665010	4.365585	-1.915822
C	3.207043	5.529617	-1.258129
H	3.860792	5.237785	-0.422079
H	3.792941	6.049265	-2.023893
H	2.400496	6.186441	-0.897174

Zero-point correction= 0.312292 (Hartree/Particle)
Thermal correction to Energy= 0.345118
Thermal correction to Enthalpy= 0.346062
Thermal correction to Gibbs Free Energy= 0.240680
Sum of electronic and zero-point Energies= -1965.096926
Sum of electronic and thermal Energies= -1965.064100
Sum of electronic and thermal Enthalpies= -1965.063156
Sum of electronic and thermal Free Energies= -1965.168538
E(RB-P86) = -1965.40921803 A.U

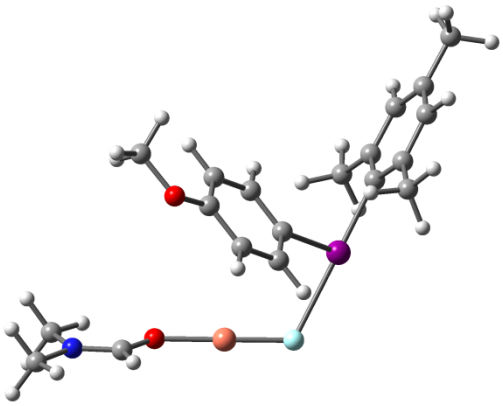


C	-3.366437	-0.953949	-0.181018
C	-3.785303	-1.332303	1.101708
C	-4.198034	-0.157105	-0.989740
C	-5.036981	-0.932925	1.578994
H	-3.144428	-1.946306	1.736827
C	-5.442233	0.243814	-0.517569
H	-3.876134	0.145922	-1.987607
C	-5.871783	-0.139782	0.769868
I	-1.488612	-1.562871	-0.906899
C	0.313299	0.921580	-0.491166
C	0.015768	1.678148	-1.622268
C	0.032831	1.261823	0.837879
C	-0.443570	2.987742	-1.356481
C	-0.425410	2.577524	1.022996
C	-0.666058	3.449438	-0.054723
H	-0.646551	3.640300	-2.211792
H	-0.608190	2.914525	2.048453
Cu	1.883647	-0.257697	-0.728689
F	1.208067	-1.634453	-1.735038
C	4.904526	-0.672476	1.645458
S	4.443283	0.193280	0.026834
F	3.917652	-1.505459	2.027677
F	6.034446	-1.384605	1.470228
F	5.107969	0.240281	2.614638
O	4.090474	-0.908490	-0.913844
O	5.586550	1.044005	-0.286932
O	3.153075	0.925592	0.363510
C	0.248237	0.339170	2.009930
H	-0.060891	0.823916	2.945437
H	-0.331039	-0.589450	1.888699
H	1.308769	0.057717	2.102948
C	-1.175987	4.848144	0.196565
H	-1.964458	4.854059	0.964095
H	-0.362999	5.497263	0.562994
H	-1.577357	5.300387	-0.720799
C	0.182829	1.200207	-3.044851
H	0.401800	0.125366	-3.078946
H	-0.734728	1.394994	-3.620315
H	1.002936	1.743165	-3.542002
H	-5.347697	-1.243900	2.576344
H	-6.101030	0.858518	-1.134475
O	-7.104477	0.307255	1.137707
C	-7.588219	-0.048389	2.448593
H	-6.927006	0.351905	3.232690
H	-8.578665	0.412779	2.528418
H	-7.677229	-1.140998	2.551179

J: adduct

Zero-point correction=	0.389350 (Hartree/Particle)
Thermal correction to Energy=	0.420820
Thermal correction to Enthalpy=	0.421764

Thermal correction to Gibbs Free Energy= 0.319587
Sum of electronic and zero-point Energies= -1251.733783
Sum of electronic and thermal Energies= -1251.702314
Sum of electronic and thermal Enthalpies= -1251.701369
Sum of electronic and thermal Free Energies= -1251.803546
E(RB-P86) = -1252.12313312 A.U

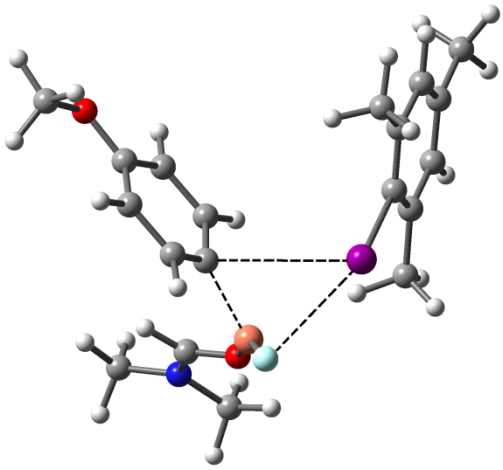


C	-3.189478	-0.423210	0.119169
C	-3.640506	-0.880354	1.373720
C	-3.919270	0.476042	-0.686629
C	-4.875128	-0.381184	1.821827
C	-5.140350	0.938902	-0.175048
C	-5.635908	0.524058	1.070325
H	-5.247535	-0.716185	2.794255
H	-5.720277	1.644773	-0.776969
I	-1.328526	-1.202506	-0.615164
C	-0.212225	0.606708	-0.527389
C	0.442527	1.036673	-1.687625
C	-0.150301	1.319521	0.667556
C	1.183040	2.213513	-1.636312
H	0.383767	0.467493	-2.615499
C	0.589462	2.507075	0.710907
H	-0.665657	0.978565	1.566340
C	1.261769	2.955817	-0.440451
H	1.704525	2.577443	-2.523697
H	0.635196	3.063400	1.646740
Cu	2.419904	-1.682064	-0.525974
F	0.938160	-2.109800	-1.514485
C	4.890974	-0.599550	0.193677
H	4.959936	-0.141971	-0.804313
O	3.898246	-1.313009	0.539514
N	5.916902	-0.352430	1.003126
C	5.972863	-0.889740	2.364175
H	6.038214	-0.059650	3.082715
H	5.070267	-1.478176	2.556417
H	6.863518	-1.526125	2.471018
C	7.043650	0.471025	0.561008
H	7.140486	1.349968	1.215091

H	7.973141	-0.115047	0.608590
H	6.877748	0.803874	-0.470752
C	-3.445151	0.954362	-2.035919
H	-2.520237	1.547374	-1.953070
H	-3.233675	0.111638	-2.713380
H	-4.208408	1.586381	-2.508698
C	-2.887468	-1.868824	2.233665
H	-2.804144	-2.852855	1.745122
H	-1.864884	-1.528555	2.458264
H	-3.410764	-2.015863	3.187746
C	-6.967293	1.025585	1.573441
H	-7.795994	0.516664	1.053305
H	-7.085468	0.841070	2.650258
H	-7.083481	2.103892	1.387890
O	2.009889	4.091087	-0.501159
C	2.117186	4.891617	0.693646
H	2.596469	4.322866	1.505555
H	2.747309	5.743918	0.417154
H	1.127384	5.250154	1.016038

J: TS

Zero-point correction= 0.387743 (Hartree/Particle)
Thermal correction to Energy= 0.418685
Thermal correction to Enthalpy= 0.419629
Thermal correction to Gibbs Free Energy= 0.320229
Sum of electronic and zero-point Energies= -1251.715257
Sum of electronic and thermal Energies= -1251.684315
Sum of electronic and thermal Enthalpies= -1251.683371
Sum of electronic and thermal Free Energies= -1251.782771
E(RB-P86) = -1252.10300008 A.U



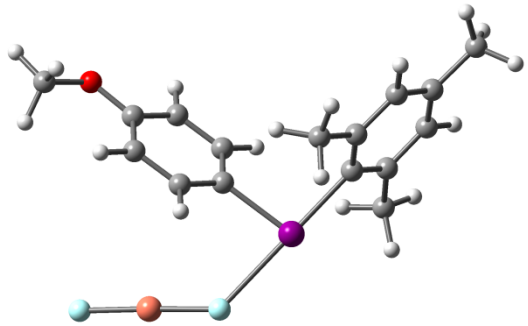
C	-2.643079	-0.102996	-0.153520
C	-2.825633	-1.336479	0.510406
C	-3.348075	1.069904	0.200759
C	-3.760473	-1.366864	1.556598
C	-4.267124	0.968648	1.254549

C	-4.488122	-0.232973	1.946155
H	-3.923975	-2.313972	2.079023
H	-4.829214	1.862616	1.540566
I	-1.261390	-0.002900	-1.756989
C	1.641468	0.840691	-0.342287
C	2.259793	1.931448	-0.930776
C	1.143436	0.825448	0.956854
C	2.564591	3.024834	-0.102200
H	2.542710	1.938476	-1.982554
C	1.444694	1.923040	1.765332
H	0.568659	-0.007291	1.362322
C	2.162033	3.019928	1.245345
H	3.115510	3.861840	-0.531531
H	1.122997	1.935500	2.808876
Cu	1.627629	-0.780781	-1.386152
F	1.599131	-0.060029	-3.063279
C	2.790236	-2.128041	0.827514
H	3.339460	-1.206319	1.067824
O	1.904134	-2.143029	-0.092337
N	3.094652	-3.192468	1.548136
C	2.449165	-4.491104	1.329515
H	1.968658	-4.816310	2.263022
H	1.702031	-4.398077	0.535573
H	3.211236	-5.229393	1.041560
C	4.113827	-3.121785	2.600267
H	3.660154	-3.386341	3.565867
H	4.922667	-3.831009	2.374816
H	4.522610	-2.106158	2.654268
C	-3.159507	2.391029	-0.500989
H	-2.112774	2.729842	-0.448815
H	-3.422052	2.321748	-1.568930
H	-3.793334	3.162518	-0.043455
C	-2.080082	-2.593087	0.140083
H	-2.283874	-2.890308	-0.901217
H	-0.990291	-2.457073	0.227386
H	-2.375674	-3.422472	0.796583
C	-5.465713	-0.293432	3.093121
H	-6.344482	0.340863	2.904268
H	-5.807238	-1.321971	3.276716
H	-4.997173	0.071157	4.023259
O	2.398182	4.032364	2.123045
C	3.076774	5.206699	1.631511
H	2.496205	5.688572	0.829942
H	3.151817	5.880304	2.491913
H	4.085268	4.952987	1.269006

K, L: adducts

Zero-point correction= 0.289429 (Hartree/Particle)
Thermal correction to Energy= 0.314970
Thermal correction to Enthalpy= 0.315915
Thermal correction to Gibbs Free Energy= 0.227907

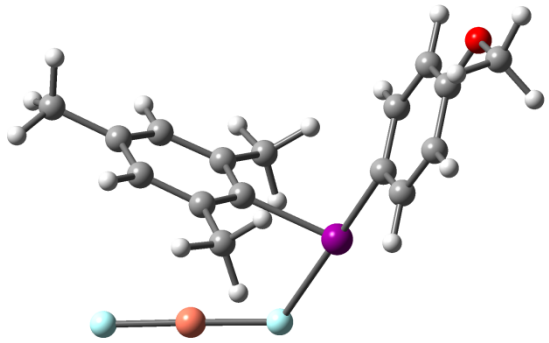
Sum of electronic and zero-point Energies= -1103.278719
Sum of electronic and thermal Energies= -1103.253177
Sum of electronic and thermal Enthalpies= -1103.252233
Sum of electronic and thermal Free Energies= -1103.340241
E(RB-P86) = -1103.56814770 A.U.



C	2.459861	-0.334257	0.106780
C	3.223513	-0.610335	-1.046835
C	2.917490	0.487169	1.156850
C	4.488501	-0.007441	-1.129751
C	4.189536	1.062529	1.007153
C	4.988019	0.829119	-0.120783
H	5.098860	-0.200317	-2.016962
H	4.562810	1.712595	1.803905
I	0.533365	-1.270634	0.286722
C	-0.619669	0.488054	-0.030150
C	-1.582720	0.836186	0.915092
C	-0.396739	1.248668	-1.181999
C	-2.350083	1.988967	0.707884
H	-1.743693	0.233263	1.809173
C	-1.159209	2.395685	-1.381227
H	0.357561	0.965095	-1.917012
C	-2.139928	2.772161	-0.440882
H	-3.100939	2.260770	1.449229
H	-1.010992	3.010710	-2.270920
Cu	-3.397850	-1.787005	-0.043295
F	-5.038149	-1.246239	-0.595701
F	-1.753693	-2.382402	0.528856
C	2.112429	0.772436	2.400615
H	1.175743	1.303039	2.166540
H	1.839233	-0.155649	2.927612
H	2.688860	1.398709	3.094233
C	2.758742	-1.511762	-2.167453
H	2.599886	-2.545163	-1.820536
H	1.810717	-1.167989	-2.609748
H	3.510602	-1.540361	-2.967263
C	6.363110	1.440314	-0.236455
H	7.136140	0.719255	0.078662
H	6.588870	1.724694	-1.274764
H	6.461860	2.330562	0.400639

O	-2.829613	3.908540	-0.735115
C	-3.853500	4.332414	0.187471
H	-3.422971	4.557959	1.175562
H	-4.277939	5.243897	-0.247363
H	-4.637915	3.565690	0.282993

Zero-point correction= 0.289649 (Hartree/Particle)
Thermal correction to Energy= 0.314986
Thermal correction to Enthalpy= 0.315930
Thermal correction to Gibbs Free Energy= 0.230176
Sum of electronic and zero-point Energies= -1103.280280
Sum of electronic and thermal Energies= -1103.254943
Sum of electronic and thermal Enthalpies= -1103.253999
Sum of electronic and thermal Free Energies= -1103.339753
E(RB-P86) = -1103.56992868 A.U.

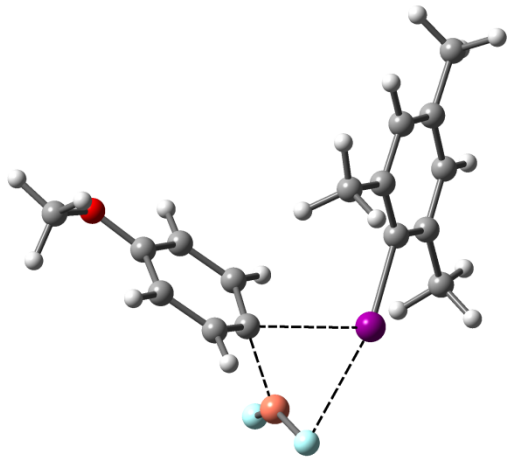


C	-2.222330	-0.554226	0.186575
C	-2.716927	0.080075	1.336492
C	-3.035399	-0.745435	-0.933607
C	-4.029044	0.540612	1.348563
H	-2.093010	0.217509	2.220845
C	-4.359476	-0.291592	-0.919410
H	-2.654536	-1.249838	-1.823857
C	-4.858444	0.360246	0.222168
H	-4.434522	1.041099	2.230235
H	-4.982647	-0.447880	-1.799668
I	-0.234543	-1.329121	0.140663
C	0.797190	0.550782	0.091029
C	0.812956	1.270183	-1.117833
C	1.434139	0.974052	1.272555
C	1.496921	2.496849	-1.102404
C	2.100255	2.208896	1.210743
C	2.139046	2.984615	0.043844
H	1.531118	3.079045	-2.027709
H	2.612877	2.563495	2.109398
Cu	3.610631	-1.154757	-0.313888
F	5.077404	-0.131592	-0.617574
F	2.142514	-2.226162	-0.004132
C	1.465320	0.174534	2.551898
H	2.061516	0.698369	3.310650

H	0.456728	0.018504	2.965274
H	1.914432	-0.817947	2.389774
C	0.153639	0.802117	-2.390521
H	-0.943664	0.783083	-2.294091
H	0.403866	1.478888	-3.218146
H	0.478828	-0.212122	-2.669929
C	2.845291	4.318012	0.023792
H	3.270518	4.530647	-0.967677
H	2.140878	5.133359	0.260234
H	3.653484	4.355183	0.767948
O	-6.123618	0.849056	0.339849
C	-7.012202	0.694651	-0.785205
H	-7.955435	1.158756	-0.477013
H	-6.615578	1.212329	-1.672333
H	-7.178311	-0.369999	-1.011841

K, L: TS's

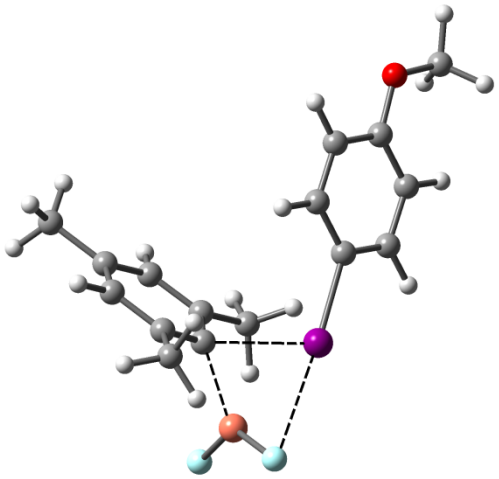
Zero-point correction= 0.287814 (Hartree/Particle)
Thermal correction to Energy= 0.312947
Thermal correction to Enthalpy= 0.313891
Thermal correction to Gibbs Free Energy= 0.228583
Sum of electronic and zero-point Energies= -1103.266239
Sum of electronic and thermal Energies= -1103.241106
Sum of electronic and thermal Enthalpies= -1103.240162
Sum of electronic and thermal Free Energies= -1103.325470
E(RB-P86) = -1103.55405274 A.U.



C	-2.105654	-0.044534	-0.303232
C	-2.936831	-0.499750	0.744478
C	-2.298791	1.196522	-0.952033
C	-4.001647	0.333048	1.120944
C	-3.380781	1.978740	-0.525816
C	-4.244112	1.567609	0.501944
H	-4.660401	0.000026	1.928130
H	-3.548934	2.943066	-1.014329
I	-0.505762	-1.283630	-0.936041

C	1.572707	-0.059508	0.180607
C	2.415277	0.443733	-0.812553
C	1.121402	0.722174	1.250885
C	2.979133	1.713205	-0.629848
H	2.675874	-0.156035	-1.684681
C	1.680817	1.986875	1.418410
H	0.397473	0.346303	1.974264
C	2.614553	2.487890	0.487002
H	3.687650	2.081554	-1.371953
H	1.400589	2.601610	2.276523
Cu	1.896379	-1.973168	0.552631
F	1.992583	-2.239388	2.385284
F	2.008970	-2.599752	-1.231108
C	-2.739060	-1.817267	1.452945
H	-2.819241	-2.667333	0.756914
H	-1.746810	-1.880038	1.926517
H	-3.498069	-1.947249	2.236006
C	-1.407723	1.696273	-2.061855
H	-0.359382	1.778455	-1.734439
H	-1.424288	1.016752	-2.929149
H	-1.736790	2.687789	-2.400543
C	-5.412925	2.426665	0.915247
H	-6.258262	2.292037	0.219170
H	-5.768191	2.165473	1.921976
H	-5.149528	3.494675	0.900821
O	3.090326	3.737710	0.746410
C	4.006154	4.318689	-0.203546
H	3.533369	4.421807	-1.192547
H	4.250289	5.309254	0.195427
H	4.923359	3.714506	-0.284587

Zero-point correction= 0.287623 (Hartree/Particle)
Thermal correction to Energy= 0.312824
Thermal correction to Enthalpy= 0.313768
Thermal correction to Gibbs Free Energy= 0.228523
Sum of electronic and zero-point Energies= -1103.267297
Sum of electronic and thermal Energies= -1103.242095
Sum of electronic and thermal Enthalpies= -1103.241151
Sum of electronic and thermal Free Energies= -1103.326396
E(RB-P86) = -1103.55491923 A.U.



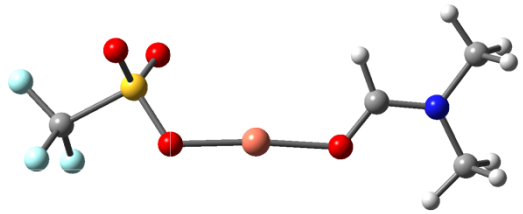
C	-1.804762	-0.770773	-0.351616
C	-2.624433	-1.168655	0.712765
C	-2.274590	0.134463	-1.319613
C	-3.927749	-0.675737	0.811248
H	-2.261587	-1.871209	1.465469
C	-3.567820	0.631934	-1.217984
H	-1.638192	0.446790	-2.149213
C	-4.404187	0.231686	-0.153774
H	-4.556258	-1.001894	1.639451
H	-3.954370	1.333950	-1.959525
I	0.137401	-1.574940	-0.515301
C	1.500490	0.668593	0.073632
C	1.945491	1.217556	-1.138770
C	0.880881	1.388921	1.110341
C	1.906777	2.624125	-1.217893
C	0.864784	2.783797	0.950646
C	1.370090	3.418020	-0.197231
H	2.294594	3.094865	-2.126798
H	0.444498	3.386340	1.762008
Cu	2.588618	-0.875119	0.673492
F	3.433480	-0.296246	2.238261
F	2.762259	-2.367682	-0.535762
C	2.450121	0.413059	-2.312692
H	3.238866	0.963794	-2.844715
H	2.841948	-0.567365	-2.005651
H	1.630086	0.235061	-3.028699
C	0.350351	0.754144	2.369842
H	0.000146	1.524103	3.070304
H	-0.494190	0.079849	2.159830
H	1.143131	0.165311	2.857303
C	1.336030	4.921864	-0.320887
H	1.395027	5.240111	-1.371232
H	0.420066	5.340236	0.121814
H	2.190094	5.373795	0.211591
O	-5.649132	0.776482	-0.148411
C	-6.545447	0.407324	0.920660

H	-6.133055	0.704581	1.897038
H	-7.471714	0.958543	0.726055
H	-6.746036	-0.674974	0.907420

f. Other copper species

Cu(OTf)(DMF)

Zero-point correction= 0.127424 (Hartree/Particle)
Thermal correction to Energy= 0.144755
Thermal correction to Enthalpy= 0.145699
Thermal correction to Gibbs Free Energy= 0.076122
Sum of electronic and zero-point Energies= -1406.689427
Sum of electronic and thermal Energies= -1406.672096
Sum of electronic and thermal Enthalpies= -1406.671152
Sum of electronic and thermal Free Energies= -1406.740728
E(RB-P86) = -1406.81685098 A.U



Cu	-0.756642	-0.524627	-0.332784
O	-2.600810	-0.651555	-0.100857
C	-3.392365	0.340741	-0.034600
H	-3.036442	1.376271	-0.138054
N	-4.699682	0.206508	0.163546
C	-5.575095	1.378407	0.227031
H	-6.333255	1.318599	-0.567426
H	-6.080349	1.411867	1.203268
H	-4.982477	2.291657	0.094360
C	-5.325515	-1.107793	0.325319
H	-6.077150	-1.255364	-0.463855
H	-5.821047	-1.158267	1.305912
H	-4.556920	-1.883996	0.256959
C	3.558570	-0.266092	0.250254
F	3.388551	-1.201694	1.207735
F	4.026045	-0.868129	-0.863481
F	4.481575	0.623224	0.677141
S	1.936051	0.634451	-0.102807
O	1.497401	1.166189	1.194654
O	2.261184	1.594012	-1.164307
O	1.103736	-0.550588	-0.597102

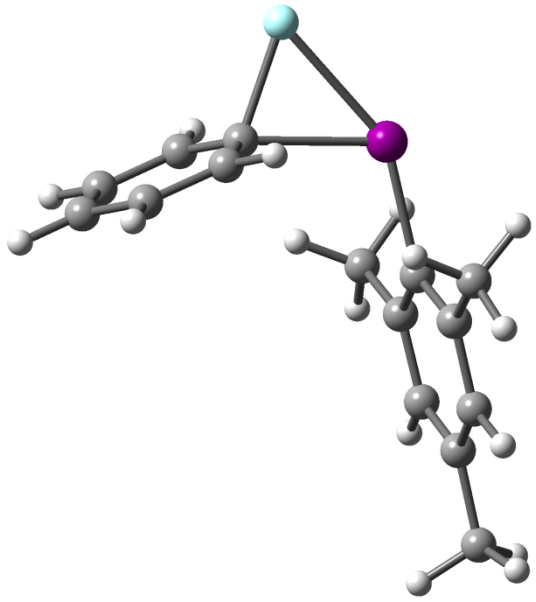
g. Isomerization and reductive elimination reactions of Mes(Ar)IF (Figure 7 and Table 4)

Ar = Ph

TS_ArF

Zero-point correction= 0.254225 (Hartree/Particle)

Thermal correction to Energy= 0.272601
Thermal correction to Enthalpy= 0.273545
Thermal correction to Gibbs Free Energy= 0.205502
Sum of electronic and zero-point Energies= -692.355756
Sum of electronic and thermal Energies= -692.337380
Sum of electronic and thermal Enthalpies= -692.336436
Sum of electronic and thermal Free Energies= -692.404479
E(RB-P86) = -692.609980655 A.U

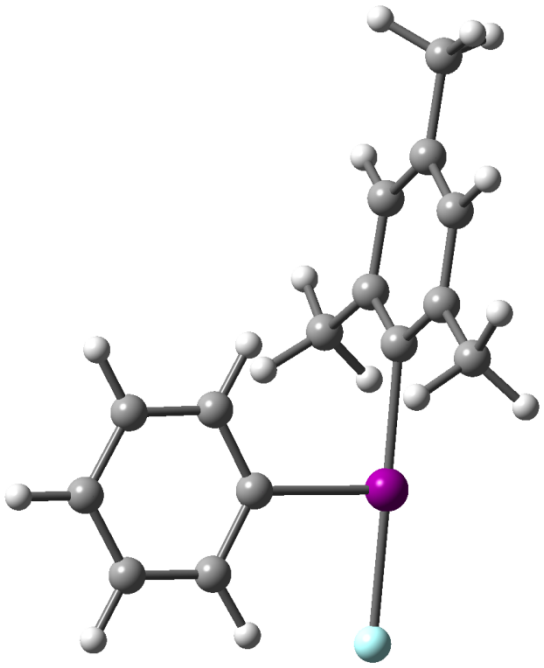


C	2.888979	2.349544	-1.002780
C	2.439769	1.026182	-1.124950
C	2.195124	0.311217	0.046368
C	2.366976	0.855720	1.317698
C	2.817062	2.181826	1.407112
C	3.077692	2.933507	0.255500
H	3.088933	2.919386	-1.913941
H	2.958767	2.619088	2.398847
I	0.577405	-1.402624	-0.117485
C	-1.304357	-0.390192	-0.043420
C	-1.939363	-0.236233	1.206629
C	-1.868917	0.087078	-1.247242
C	-3.178045	0.427103	1.222121
C	-3.106670	0.741270	-1.162615
C	-3.774654	0.926879	0.057559
H	-3.688537	0.552308	2.181602
H	-3.561321	1.115146	-2.084952
F	3.128671	-1.375569	-0.057236
C	-1.364782	-0.753711	2.503928
H	-1.195000	-1.841342	2.467864
H	-0.397606	-0.282371	2.736916
H	-2.050969	-0.543674	3.335560
C	-1.214135	-0.083383	-2.597465

H	-0.241219	0.429748	-2.644448
H	-1.033908	-1.144884	-2.829776
H	-1.853343	0.334011	-3.387267
C	-5.095827	1.655150	0.108872
H	-5.568081	1.561920	1.096824
H	-4.959387	2.729247	-0.099786
H	-5.794604	1.267204	-0.648369
H	2.174039	0.273072	2.218444
H	3.423263	3.965799	0.337438
H	2.305354	0.572818	-2.107005

***anti*-isom**

Zero-point correction= 0.255377 (Hartree/Particle)
Thermal correction to Energy= 0.274263
Thermal correction to Enthalpy= 0.275208
Thermal correction to Gibbs Free Energy= 0.206049
Sum of electronic and zero-point Energies= -692.386143
Sum of electronic and thermal Energies= -692.367257
Sum of electronic and thermal Enthalpies= -692.366313
Sum of electronic and thermal Free Energies= -692.435471
E(RB-P86) = -692.641520354 A.U

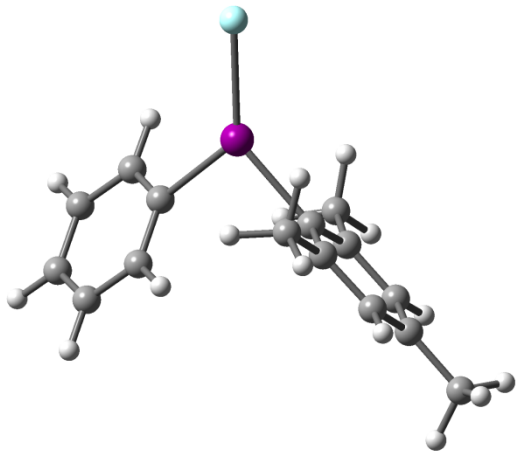


C	3.175547	0.405279	-1.202515
C	1.866121	-0.096230	-1.234812
C	1.224938	-0.346087	0.000303
C	1.866949	-0.110722	1.234766
C	3.179126	0.391864	1.204882
C	3.850142	0.653402	0.003220
H	3.681500	0.609660	-2.151313
H	3.687536	0.585215	2.154414

I	-0.742117	-1.270815	-0.002999
C	-1.790278	0.623955	0.002340
C	-3.182859	0.590309	-0.002503
C	-1.061392	1.811071	0.010363
C	-3.869828	1.812616	0.000604
C	-1.770434	3.021033	0.013301
C	-3.169333	3.024125	0.008405
H	-4.962391	1.807377	-0.003123
H	-1.214515	3.961370	0.019596
F	-2.830481	-2.236426	-0.006845
C	1.199095	-0.334053	-2.570879
H	0.967404	-1.399726	-2.726772
H	0.250692	0.219365	-2.658208
H	1.855443	-0.009420	-3.389899
C	1.205092	-0.362267	2.570920
H	0.256735	0.189605	2.667554
H	0.974834	-1.429599	2.717279
H	1.864315	-0.045339	3.390662
C	5.263346	1.184952	-0.002069
H	5.955104	0.459491	-0.460447
H	5.336331	2.113108	-0.590759
H	5.617432	1.394793	1.016816
H	0.029708	1.811357	0.014282
H	-3.713150	3.971261	0.010737
H	-3.697840	-0.372976	-0.008226

TS_isom

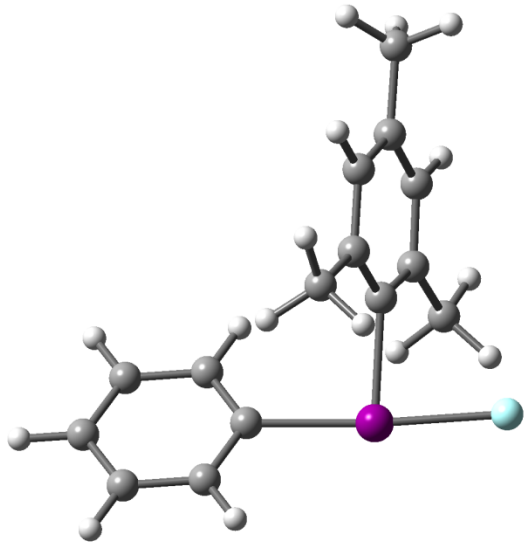
Zero-point correction= 0.254634 (Hartree/Particle)
Thermal correction to Energy= 0.273179
Thermal correction to Enthalpy= 0.274124
Thermal correction to Gibbs Free Energy= 0.204872
Sum of electronic and zero-point Energies= -692.372825
Sum of electronic and thermal Energies= -692.354279
Sum of electronic and thermal Enthalpies= -692.353335
Sum of electronic and thermal Free Energies= -692.422586
E(RB-P86) = -692.627458560 A.U



C	-3.303736	-0.161466	-0.962947
C	-2.047435	0.468458	-0.987947
C	-1.193416	0.225609	0.105152
C	-1.556557	-0.570852	1.209974
C	-2.823398	-1.174065	1.168493
C	-3.706631	-0.987811	0.094757
H	-3.986201	0.009637	-1.800722
H	-3.126700	-1.803575	2.010488
I	0.729943	1.234673	0.125249
C	1.861881	-0.592658	-0.190624
C	2.940093	-0.838142	0.661994
C	1.545094	-1.436365	-1.256807
C	3.723648	-1.978766	0.435638
C	2.331059	-2.577665	-1.459522
C	3.418495	-2.846206	-0.618624
H	4.569301	-2.186599	1.094971
H	2.091088	-3.252960	-2.283917
F	1.495007	3.523696	0.381074
C	-1.694258	1.367111	-2.150884
H	-1.558530	2.412097	-1.829109
H	-0.760721	1.056642	-2.644473
H	-2.496524	1.349259	-2.900645
C	-0.660071	-0.798344	2.401368
H	0.276309	-1.301581	2.112764
H	-0.382784	0.150979	2.886632
H	-1.165352	-1.426965	3.146702
C	-5.051648	-1.672697	0.074804
H	-5.763245	-1.142152	-0.573694
H	-4.957508	-2.702455	-0.309524
H	-5.481227	-1.741207	1.085068
H	0.702072	-1.226115	-1.917022
H	4.029629	-3.735519	-0.786519
H	3.169635	-0.167262	1.492207

***syn*-isom**

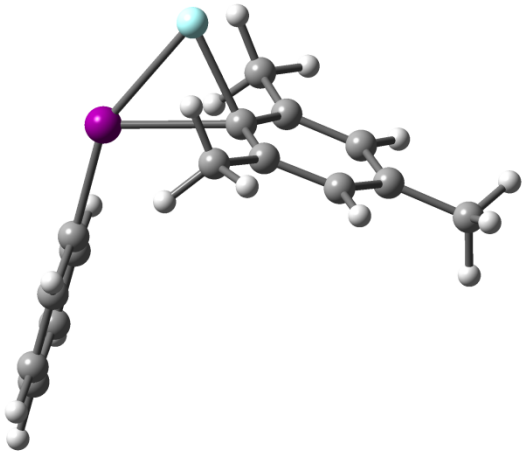
Zero-point correction= 0.255501 (Hartree/Particle)
Thermal correction to Energy= 0.274405
Thermal correction to Enthalpy= 0.275350
Thermal correction to Gibbs Free Energy= 0.205996
Sum of electronic and zero-point Energies= -692.386496
Sum of electronic and thermal Energies= -692.367592
Sum of electronic and thermal Enthalpies= -692.366648
Sum of electronic and thermal Free Energies= -692.436002
E(RB-P86) = -692.641997680 A.U



C	4.131284	-1.356982	0.284560
C	3.217363	-0.311039	0.473988
C	1.972864	-0.358906	-0.165149
C	1.631248	-1.437610	-0.987377
C	2.546807	-2.483629	-1.163620
C	3.795986	-2.443447	-0.531318
H	5.102202	-1.322574	0.784626
H	3.482367	0.528222	1.123290
H	0.659658	-1.476675	-1.485621
H	2.281590	-3.329769	-1.802300
H	4.506905	-3.260461	-0.673728
I	0.663127	1.375001	0.099276
C	-1.091377	0.160817	0.092475
C	-1.935029	0.232313	-1.030660
C	-1.347439	-0.651915	1.212287
C	-3.082520	-0.578231	-1.007878
C	-2.509828	-1.439464	1.165294
C	-3.387500	-1.417323	0.072449
H	-3.755373	-0.545704	-1.869881
H	-2.730405	-2.085706	2.020043
F	-0.811120	3.071291	0.394154
C	-0.454448	-0.710535	2.426315
H	0.551134	-1.082106	2.172625
H	-0.329554	0.284653	2.881818
H	-0.882356	-1.380494	3.184003
C	-1.672851	1.127974	-2.215890
H	-1.574745	2.176933	-1.896219
H	-0.741429	0.852229	-2.736354
H	-2.496416	1.057489	-2.939126
C	-4.644535	-2.253964	0.073098
H	-4.493387	-3.205083	0.604063
H	-5.465646	-1.722035	0.582670
H	-4.980356	-2.473963	-0.950371

TS_MesF

Zero-point correction= 0.254043 (Hartree/Particle)
Thermal correction to Energy= 0.272603
Thermal correction to Enthalpy= 0.273547
Thermal correction to Gibbs Free Energy= 0.204886
Sum of electronic and zero-point Energies= -692.355605
Sum of electronic and thermal Energies= -692.337046
Sum of electronic and thermal Enthalpies= -692.336101
Sum of electronic and thermal Free Energies= -692.404763
E(RB-P86) = -692.609648146 A.U

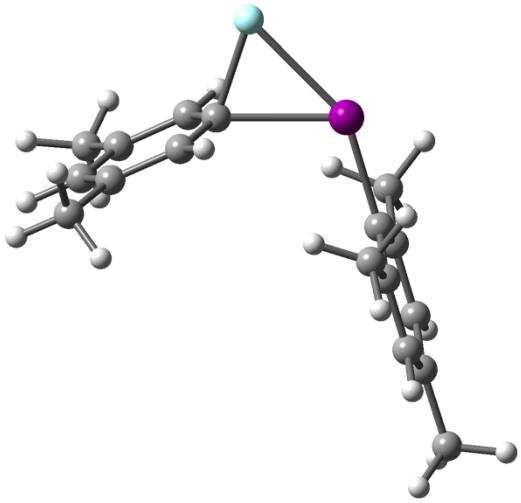


C	-2.860834	1.063092	1.200372
C	-1.895986	0.035314	1.242716
C	-1.445688	-0.405388	0.000833
C	-1.897516	0.034037	-1.241968
C	-2.861877	1.061019	-1.200427
C	-3.350025	1.595085	0.000242
H	-3.239226	1.439598	2.156261
H	-3.241232	1.435985	-2.156620
I	0.795464	-1.360028	0.000298
C	2.182667	0.262266	-0.000267
C	2.632718	0.783196	-1.220814
C	2.632237	0.784641	1.219838
C	3.553375	1.838108	-1.213824
C	3.552872	1.839568	1.211957
C	4.012789	2.366029	-0.001155
H	3.910469	2.245876	-2.162299
H	3.909555	2.248494	2.160089
F	-1.478984	-2.410768	0.000806
C	-1.426327	-0.528509	2.557954
H	-0.365234	-0.291439	2.739627
H	-2.013457	-0.110963	3.387287
H	-1.522242	-1.623742	2.569708
C	-1.428258	-0.532001	-2.556402
H	-0.367359	-0.294790	-2.738982

H	-1.523625	-1.627298	-2.565891
H	-2.016017	-0.116276	-3.386197
C	-4.363922	2.717123	-0.001474
H	-4.936751	2.740544	0.937136
H	-3.872244	3.698749	-0.111220
H	-5.074826	2.615384	-0.835304
H	2.277721	0.374757	2.167521
H	4.729840	3.189884	-0.001502
H	2.278545	0.372175	-2.168133

Ar = 3,5-$Me_2C_6H_4$
TS_ArF

Zero-point correction= 0.306782 (Hartree/Particle)
Thermal correction to Energy= 0.329087
Thermal correction to Enthalpy= 0.330031
Thermal correction to Gibbs Free Energy= 0.252344
Sum of electronic and zero-point Energies= -770.956033
Sum of electronic and thermal Energies= -770.933729
Sum of electronic and thermal Enthalpies= -770.932784
Sum of electronic and thermal Free Energies= -771.010471
E(RB-P86) = -771.262815336 A.U.

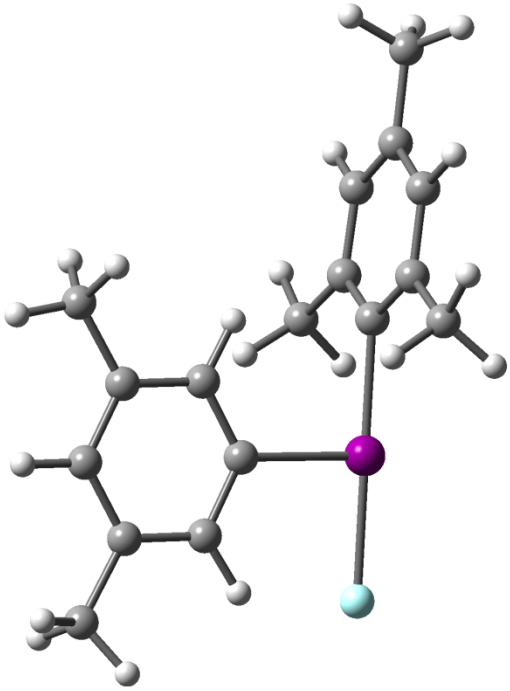


C	2.953537	1.438658	-1.225171
C	2.235112	0.229228	-1.231364
C	1.909814	-0.344540	-0.006089
C	2.251455	0.205551	1.221641
C	2.977247	1.414913	1.226380
C	3.314952	2.015205	0.004990
I	-0.050228	-1.693123	-0.010811
C	-1.685861	-0.315892	0.002751
C	-2.201872	0.115264	1.244592
C	-2.213098	0.123272	-1.230354
C	-3.276865	1.016846	1.218421
C	-3.288676	1.025288	-1.187614
C	-3.834241	1.483771	0.019070

H	-3.688312	1.363309	2.171286
H	-3.709047	1.378325	-2.134038
F	2.443490	-2.219429	-0.030554
C	-1.662661	-0.351849	2.575746
H	-1.722900	-1.447371	2.674863
H	-0.606184	-0.072379	2.707723
H	-2.236051	0.096227	3.398640
C	-1.687516	-0.333773	-2.570421
H	-0.632478	-0.053213	-2.711090
H	-1.748800	-1.428485	-2.677336
H	-2.269258	0.120545	-3.383964
C	-5.008150	2.432651	0.030511
H	-5.952962	1.881335	0.173664
H	-4.929214	3.158783	0.853222
H	-5.088434	2.984562	-0.916800
H	1.989801	-0.285903	2.159549
H	3.876569	2.953855	0.009562
H	1.959641	-0.245861	-2.173509
C	3.381778	2.035214	2.545358
H	3.915332	2.983245	2.388291
H	2.503023	2.237105	3.178252
H	4.042752	1.362332	3.115073
C	3.302039	2.114835	-2.532359
H	2.537918	2.863011	-2.802901
H	4.265072	2.641846	-2.461005
H	3.362239	1.391249	-3.358036

***anti*-isom**

Zero-point correction= 0.308284 (Hartree/Particle)
Thermal correction to Energy= 0.330916
Thermal correction to Enthalpy= 0.331860
Thermal correction to Gibbs Free Energy= 0.253441
Sum of electronic and zero-point Energies= -770.986672
Sum of electronic and thermal Energies= -770.964040
Sum of electronic and thermal Enthalpies= -770.963096
Sum of electronic and thermal Free Energies= -771.041515
E(RB-P86) = -771.294955607 A.U.

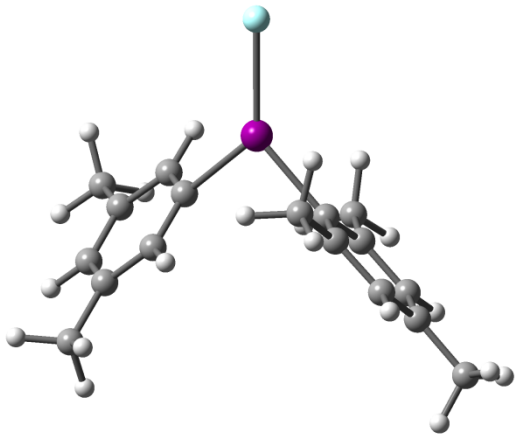


C	-3.408889	0.593038	1.228006
C	-2.172369	-0.072088	1.246472
C	-1.581079	-0.397833	0.005899
C	-2.202201	-0.081967	-1.222440
C	-3.438214	0.583325	-1.179274
C	-4.056437	0.930097	0.030609
H	-3.878312	0.852876	2.181936
H	-3.930591	0.835737	-2.123551
I	0.239598	-1.584932	-0.012142
C	1.549370	0.144984	-0.008060
C	2.919808	-0.096042	0.018402
C	0.993904	1.417972	-0.036547
C	3.790966	1.007362	0.020808
C	1.862374	2.528506	-0.039657
C	3.245307	2.302264	-0.011511
F	2.170573	-2.850446	-0.028754
C	-1.531062	-0.401109	2.575444
H	-1.434374	-1.488444	2.723742
H	-0.519513	0.027381	2.656544
H	-2.134004	-0.001105	3.402149
C	-1.593439	-0.421430	-2.564173
H	-0.579100	-0.004708	-2.668387
H	-1.512254	-1.510171	-2.711734
H	-2.209893	-0.017063	-3.378713
C	-5.371221	1.672152	0.043855
H	-5.961083	1.428426	0.939485
H	-5.202930	2.762543	0.049653
H	-5.973056	1.439124	-0.846522
H	-0.087320	1.569610	-0.060132

H	3.921625	3.162702	-0.017500
H	3.283845	-1.126340	0.032399
C	5.286326	0.797062	0.082179
H	5.643576	0.839662	1.124910
H	5.570833	-0.183886	-0.324089
H	5.822049	1.576988	-0.478828
C	1.294487	3.928613	-0.078588
H	0.694661	4.088549	-0.988743
H	0.631575	4.112473	0.781749
H	2.094656	4.681599	-0.060597

TS_isom

Zero-point correction= 0.307185 (Hartree/Particle)
Thermal correction to Energy= 0.329697
Thermal correction to Enthalpy= 0.330641
Thermal correction to Gibbs Free Energy= 0.251671
Sum of electronic and zero-point Energies= -770.974211
Sum of electronic and thermal Energies= -770.951699
Sum of electronic and thermal Enthalpies= -770.950754
Sum of electronic and thermal Free Energies= -771.029724
E(RB-P86) = -771.281395531 A.U.

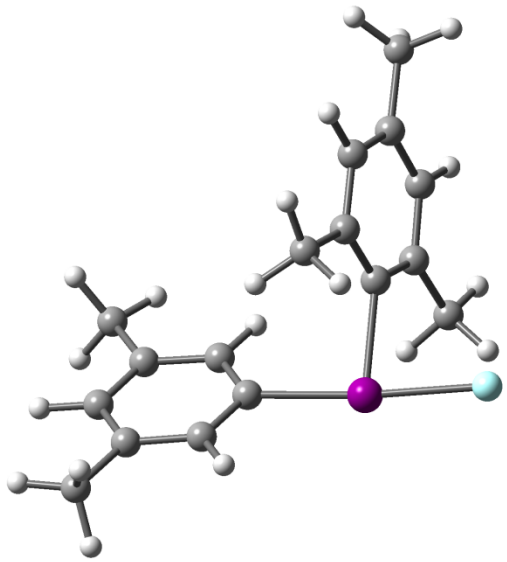


C	-3.564936	-0.892850	-0.748733
C	-2.497330	0.003490	-0.920250
C	-1.583338	0.117312	0.146330
C	-1.721990	-0.583331	1.360494
C	-2.809858	-1.466135	1.463935
C	-3.734824	-1.640393	0.425281
H	-4.288108	-0.999468	-1.562863
H	-2.935097	-2.027807	2.394590
I	0.044828	1.540819	-0.074168
C	1.606520	0.034367	-0.158816
C	2.601323	0.098133	0.813068
C	1.624072	-0.896219	-1.200445
C	3.668980	-0.821312	0.757064
C	2.674105	-1.825855	-1.258555
C	3.681287	-1.766698	-0.276592

F	0.174730	3.973353	-0.181953
C	-2.400968	0.799131	-2.201925
H	-2.507344	1.880103	-2.016924
H	-1.436081	0.651434	-2.710282
H	-3.198470	0.499140	-2.894956
C	-0.771988	-0.435015	2.522502
H	0.233049	-0.810812	2.272410
H	-0.659546	0.618678	2.822836
H	-1.137123	-1.000622	3.390202
C	-4.877784	-2.617045	0.560226
H	-5.773461	-2.262109	0.029706
H	-4.606972	-3.594251	0.125750
H	-5.138660	-2.786522	1.614649
H	0.840229	-0.913751	-1.959878
H	4.506380	-2.484205	-0.324891
H	2.561987	0.841443	1.612839
C	2.723706	-2.869061	-2.349842
H	3.706189	-2.875553	-2.846702
H	2.564179	-3.877560	-1.934536
H	1.952270	-2.691792	-3.111958
C	4.757934	-0.784268	1.803282
H	5.200841	0.220867	1.880992
H	4.357744	-1.039130	2.797972
H	5.560094	-1.497148	1.567371

***syn*-isom**

Zero-point correction= 0.307882 (Hartree/Particle)
Thermal correction to Energy= 0.330810
Thermal correction to Enthalpy= 0.331754
Thermal correction to Gibbs Free Energy= 0.251566
Sum of electronic and zero-point Energies= -770.987392
Sum of electronic and thermal Energies= -770.964464
Sum of electronic and thermal Enthalpies= -770.963520
Sum of electronic and thermal Free Energies= -771.043708
E(RB-P86) = -771.295274049 A.U.

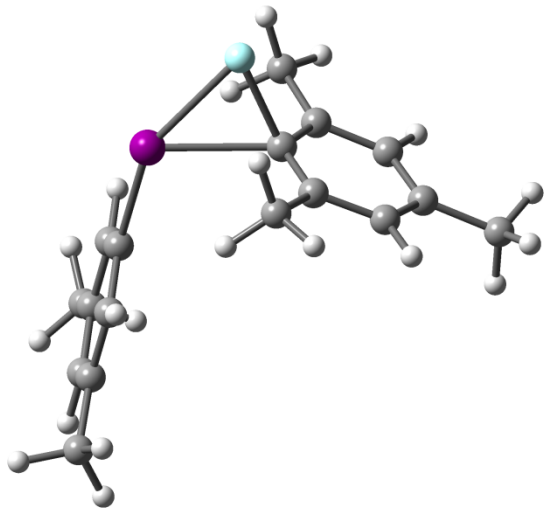


C	-3.912373	0.406340	0.472570
C	-2.814794	-0.478347	0.494186
C	-1.632348	-0.134255	-0.161421
C	-1.506417	1.080310	-0.844639
C	-2.581311	1.982318	-0.865625
C	-3.772264	1.624280	-0.205594
H	-2.899937	-1.427367	1.033018
H	-0.576350	1.340166	-1.357400
H	-4.616506	2.321173	-0.221621
I	-0.037014	-1.629044	-0.168324
C	1.472682	-0.149510	0.127349
C	2.324817	0.144622	-0.952817
C	1.567648	0.467122	1.387985
C	3.306230	1.124899	-0.731201
C	2.570241	1.440597	1.538399
C	3.445732	1.782522	0.499214
H	3.980487	1.377236	-1.555014
H	2.663806	1.940682	2.506891
F	1.727067	-3.063539	-0.125969
C	0.666778	0.137208	2.551618
H	-0.387839	0.358297	2.322358
H	0.726600	-0.930708	2.815506
H	0.953025	0.722872	3.435440
C	2.236753	-0.538777	-2.294850
H	2.333237	-1.629806	-2.182620
H	1.271406	-0.342110	-2.788941
H	3.034879	-0.182105	-2.959715
C	4.530585	2.812147	0.707623
H	4.254397	3.532420	1.491027
H	5.471448	2.328917	1.020943
H	4.741240	3.365749	-0.219013
C	-5.201087	0.041252	1.172412
H	-5.668696	-0.841535	0.706684

H	-5.022683	-0.209561	2.230027
H	-5.924275	0.868029	1.133614
C	-2.466338	3.311472	-1.575723
H	-2.491973	4.145962	-0.855750
H	-1.527605	3.384288	-2.142696
H	-3.303731	3.463385	-2.274739

TS_MesF

Zero-point correction= 0.306393 (Hartree/Particle)
Thermal correction to Energy= 0.328129
Thermal correction to Enthalpy= 0.329073
Thermal correction to Gibbs Free Energy= 0.252470
Sum of electronic and zero-point Energies= -770.956713
Sum of electronic and thermal Energies= -770.934977
Sum of electronic and thermal Enthalpies= -770.934033
Sum of electronic and thermal Free Energies= -771.010636
E(RB-P86) = -771.263105803 A.U.

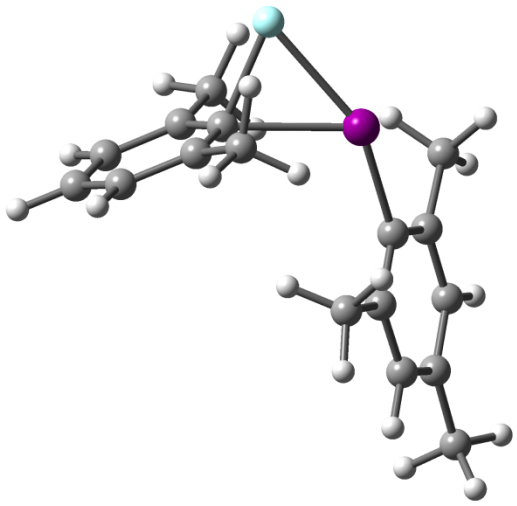


C	2.891114	1.507667	-1.194382
C	2.206547	0.276085	-1.235071
C	1.857957	-0.256103	0.006330
C	2.182347	0.291214	1.247699
C	2.867603	1.522397	1.204948
C	3.221399	2.153037	0.004725
H	3.177047	1.958278	-2.150427
H	3.134571	1.984992	2.160763
I	-0.099154	-1.680075	-0.004010
C	-1.764041	-0.348442	-0.006683
C	-2.307050	0.063889	1.214573
C	-2.278726	0.100067	-1.228250
C	-3.397229	0.951092	1.223757
C	-3.372371	0.981798	-1.236279
C	-3.910081	1.394775	-0.005747
F	2.373614	-2.188923	0.017788
C	1.914592	-0.395939	-2.551468

H	0.830624	-0.466911	-2.738142
H	2.364333	0.169342	-3.379232
H	2.314173	-1.420490	-2.564148
C	1.864702	-0.363530	2.566760
H	0.777252	-0.450347	2.723610
H	2.281223	-1.380657	2.609673
H	2.281134	0.223401	3.396857
C	3.927615	3.490354	0.003765
H	4.563651	3.607120	-0.886217
H	3.204387	4.323777	0.000677
H	4.559543	3.610616	0.896270
H	-1.843858	-0.233636	-2.173046
H	-4.759230	2.085742	-0.005748
H	-1.895278	-0.299101	2.158961
C	-3.983136	1.435724	2.529555
H	-3.561046	2.416289	2.806586
H	-5.073749	1.558911	2.456546
H	-3.765330	0.738058	3.350727
C	-3.969982	1.458532	-2.539617
H	-4.904455	0.917294	-2.763022
H	-4.218228	2.529605	-2.494973
H	-3.281686	1.296288	-3.380984

Ar = 2,6-$Me_2C_6H_4$
TS_ArF

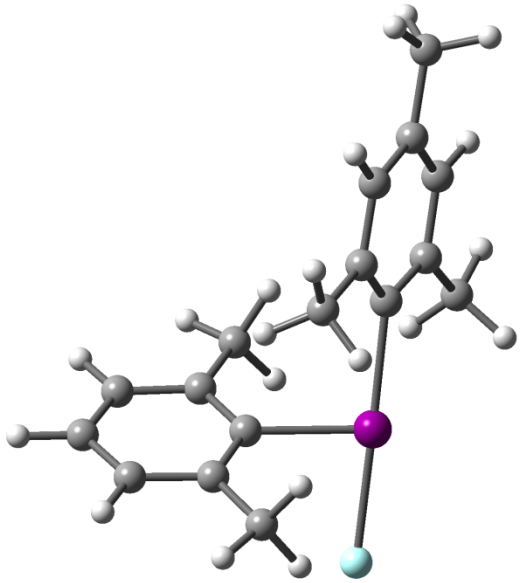
Zero-point correction= 0.307216 (Hartree/Particle)
Thermal correction to Energy= 0.329187
Thermal correction to Enthalpy= 0.330131
Thermal correction to Gibbs Free Energy= 0.254565
Sum of electronic and zero-point Energies= -770.952229
Sum of electronic and thermal Energies= -770.930258
Sum of electronic and thermal Enthalpies= -770.929314
Sum of electronic and thermal Free Energies= -771.004880
E(RB-P86) = -771.259444751 A.U.



C	-2.652146	1.245947	2.295910
C	-2.044479	0.127456	1.686888
C	-2.080893	0.114756	0.292840
C	-2.699817	1.061535	-0.526948
C	-3.278172	2.154853	0.149364
C	-3.252989	2.255284	1.542503
H	-2.641212	1.300954	3.388238
H	-3.770298	2.924397	-0.452337
I	-0.294528	-1.162821	-0.724114
C	1.572336	-0.187641	-0.297373
C	1.822747	1.108088	-0.795946
C	2.516952	-0.893732	0.478753
C	3.056021	1.698015	-0.477995
C	3.734598	-0.250133	0.757026
C	4.021026	1.043125	0.300769
H	3.265528	2.702421	-0.858453
H	4.481058	-0.786659	1.350591
F	-2.755852	-1.662309	-0.381192
C	-1.414320	-0.954262	2.524380
H	-0.313753	-0.915391	2.463537
H	-1.693470	-0.833518	3.580111
H	-1.731010	-1.951085	2.186522
C	-2.820186	0.932698	-2.022252
H	-1.839810	0.780176	-2.499447
H	-3.442068	0.063210	-2.282253
H	-3.276033	1.835539	-2.451062
C	2.295853	-2.298240	0.988881
H	1.381755	-2.377069	1.598247
H	2.191904	-3.017672	0.160704
H	3.145372	-2.617646	1.607736
C	0.840292	1.864046	-1.655727
H	0.605815	1.306123	-2.576754
H	-0.109506	2.043479	-1.128188
H	1.252858	2.839671	-1.946576
C	5.322632	1.722019	0.653518
H	6.111825	0.988911	0.873919
H	5.668828	2.374537	-0.161571
H	5.201626	2.355398	1.548752
H	-3.713465	3.111641	2.039540

***anti*-isom**

Zero-point correction= 0.309303 (Hartree/Particle)
Thermal correction to Energy= 0.331195
Thermal correction to Enthalpy= 0.332139
Thermal correction to Gibbs Free Energy= 0.258202
Sum of electronic and zero-point Energies= -770.979343
Sum of electronic and thermal Energies= -770.957451
Sum of electronic and thermal Enthalpies= -770.956507
Sum of electronic and thermal Free Energies= -771.030444
E(RB-P86) = -771.288646131 A.U

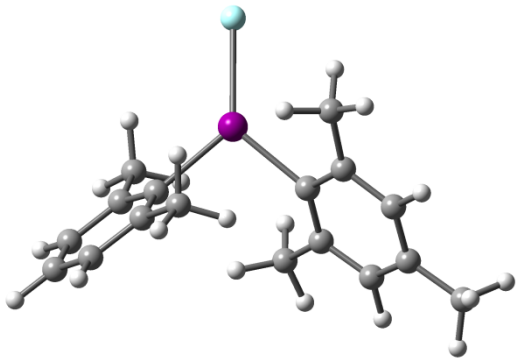


C	-3.685522	-0.158716	0.604927
C	-2.426567	-0.779886	0.607028
C	-1.425269	-0.249047	-0.238861
C	-1.683082	0.840233	-1.095567
C	-2.961021	1.425930	-1.049145
C	-3.971846	0.949440	-0.205568
H	-4.465512	-0.559327	1.260257
H	-3.166567	2.279541	-1.702710
I	0.507300	-1.294943	-0.259664
C	1.691213	0.414499	0.289027
C	2.663099	0.846794	-0.635362
C	1.478993	1.008188	1.547344
C	3.432327	1.963097	-0.260166
C	2.279583	2.123606	1.858430
C	3.239963	2.600024	0.966510
H	4.195740	2.325500	-0.953238
H	2.140867	2.609334	2.827563
F	2.534138	-2.388713	-0.177315
C	0.479738	0.514400	2.561377
H	-0.555287	0.641276	2.207360
H	0.627444	-0.554653	2.781462
H	0.586094	1.071210	3.501841
C	2.927481	0.170797	-1.956065
H	3.159954	-0.893824	-1.797389
H	2.051357	0.223768	-2.622148
H	3.770217	0.652959	-2.469411
C	-0.664856	1.390701	-2.064172
H	0.199215	1.833263	-1.544532
H	-0.279795	0.599394	-2.727539
H	-1.114316	2.169685	-2.694882
C	-2.216008	-1.991283	1.489009
H	-2.039210	-2.902906	0.895008

H	-1.352515	-1.871227	2.160841
H	-3.104912	-2.169662	2.109569
C	-5.339402	1.590136	-0.182475
H	-6.096787	0.919199	-0.620480
H	-5.660354	1.807226	0.848288
H	-5.352467	2.529837	-0.752533
H	3.849763	3.466310	1.233047

TS_isom

Zero-point correction= 0.308300 (Hartree/Particle)
Thermal correction to Energy= 0.329969
Thermal correction to Enthalpy= 0.330913
Thermal correction to Gibbs Free Energy= 0.256446
Sum of electronic and zero-point Energies= -770.968430
Sum of electronic and thermal Energies= -770.946761
Sum of electronic and thermal Enthalpies= -770.945817
Sum of electronic and thermal Free Energies= -771.020283
E(RB-P86) = -771.276729416 A.U.

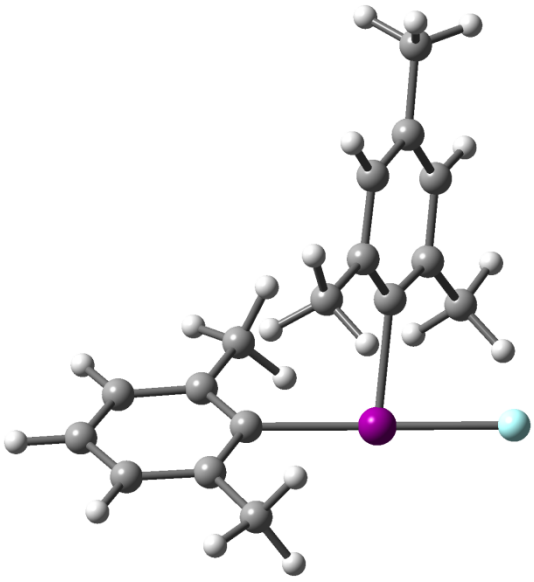


C	3.642266	-0.140331	0.659786
C	2.402664	0.512441	0.760478
C	1.409865	0.144071	-0.169802
C	1.624858	-0.797041	-1.194576
C	2.884559	-1.418977	-1.231905
C	3.902385	-1.108377	-0.320182
H	4.425933	0.124118	1.376106
H	3.069543	-2.165862	-2.009713
I	-0.473554	1.237711	-0.067002
C	-1.814511	-0.461795	0.246582
C	-2.846171	-0.622593	-0.700367
C	-1.676623	-1.260034	1.398295
C	-3.750333	-1.677075	-0.477481
C	-2.606306	-2.303581	1.560072
C	-3.628532	-2.513037	0.633227
H	-4.560552	-1.833133	-1.194060
H	-2.519758	-2.948817	2.438096
F	-0.968246	3.630798	-0.239557
C	2.206919	1.562943	1.828836
H	1.989578	2.551427	1.393587

H	1.373182	1.313361	2.503629
H	3.116234	1.659408	2.437026
C	0.591728	-1.153424	-2.232908
H	-0.311548	-1.588426	-1.777835
H	0.279265	-0.264179	-2.804202
H	0.997844	-1.884433	-2.944784
C	5.255895	-1.770622	-0.411739
H	5.949399	-1.156353	-1.010602
H	5.708326	-1.896600	0.582721
H	5.189296	-2.756394	-0.893726
H	-4.340808	-3.327658	0.782719
C	-0.612340	-1.042956	2.442920
H	0.398689	-1.125094	2.015464
H	-0.700068	-0.041899	2.895729
H	-0.705158	-1.786099	3.245912
C	-3.033588	0.271679	-1.902458
H	-3.254493	1.309901	-1.607051
H	-2.136216	0.298237	-2.539668
H	-3.872540	-0.085133	-2.514896

***syn*-isom**

Zero-point correction= 0.308919 (Hartree/Particle)
Thermal correction to Energy= 0.331040
Thermal correction to Enthalpy= 0.331984
Thermal correction to Gibbs Free Energy= 0.257067
Sum of electronic and zero-point Energies= -770.979801
Sum of electronic and thermal Energies= -770.957681
Sum of electronic and thermal Enthalpies= -770.956736
Sum of electronic and thermal Free Energies= -771.031653
E(RB-P86) = -771.288720468 A.U.

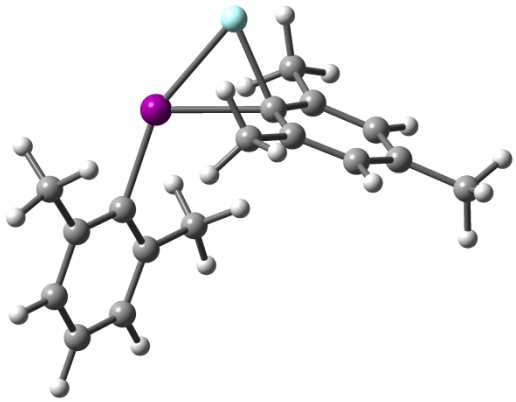


C	3.903786	1.356776	-0.538504
C	2.948453	0.332344	-0.666690

C	1.866882	0.321342	0.243505
C	1.749983	1.271825	1.280338
C	2.729092	2.278805	1.360455
C	3.792610	2.327245	0.458285
H	4.745738	1.381601	-1.235634
H	2.651373	3.027011	2.153912
H	4.543461	3.116898	0.539133
I	0.451225	-1.359263	0.062478
C	-1.305950	-0.148133	-0.162806
C	-2.309129	-0.262842	0.819606
C	-1.414905	0.678841	-1.295058
C	-3.450638	0.537444	0.647324
C	-2.583399	1.454332	-1.399383
C	-3.603149	1.408076	-0.440840
H	-4.246576	0.467164	1.394582
H	-2.693533	2.105976	-2.271180
F	-1.019711	-3.107112	-0.218949
C	-0.378889	0.755384	-2.387476
H	0.582220	1.137600	-2.010202
H	-0.190141	-0.236579	-2.828517
H	-0.718975	1.423504	-3.189734
C	-2.228845	-1.203040	1.994707
H	-2.056157	-2.232545	1.644441
H	-1.400962	-0.938479	2.672037
H	-3.160786	-1.170057	2.574965
C	-4.829344	2.279688	-0.569344
H	-4.707098	3.210977	0.009186
H	-5.012178	2.563805	-1.615559
H	-5.725079	1.771832	-0.182654
C	0.643288	1.249221	2.305327
H	-0.333166	1.497766	1.860404
H	0.549575	0.254560	2.769035
H	0.842422	1.975991	3.104850
C	3.138355	-0.705949	-1.751408
H	3.290815	-1.714209	-1.333303
H	2.270458	-0.762363	-2.426878
H	4.021865	-0.463677	-2.357916

TS_MesF

Zero-point correction= 0.307500 (Hartree/Particle)
Thermal correction to Energy= 0.329314
Thermal correction to Enthalpy= 0.330258
Thermal correction to Gibbs Free Energy= 0.255482
Sum of electronic and zero-point Energies= -770.950508
Sum of electronic and thermal Energies= -770.928695
Sum of electronic and thermal Enthalpies= -770.927751
Sum of electronic and thermal Free Energies= -771.002527
E(RB-P86) = -771.258008763 A.U.

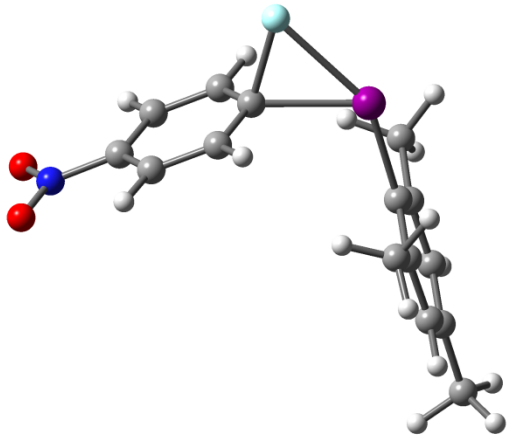


C	-2.834641	0.753696	1.697836
C	-1.813801	-0.180906	1.422510
C	-1.622916	-0.470508	0.074680
C	-2.378122	0.024140	-0.988535
C	-3.371979	0.957386	-0.632526
C	-3.613171	1.342553	0.694299
H	-3.011127	1.013673	2.746589
H	-3.984631	1.372863	-1.439282
I	0.616369	-1.250812	-0.458977
C	2.020645	0.349716	-0.137569
C	1.915121	1.538028	-0.890515
C	3.029019	0.142631	0.830053
C	2.860273	2.548134	-0.641349
C	3.950949	1.185283	1.031700
C	3.867434	2.377098	0.310283
H	2.797636	3.478604	-1.211546
H	4.744845	1.047951	1.770490
F	-1.578143	-2.478529	-0.216384
C	-1.012332	-0.794498	2.540299
H	0.016760	-0.398031	2.553553
H	-1.470685	-0.566866	3.512490
H	-0.944999	-1.885794	2.426690
C	-2.220417	-0.421433	-2.418259
H	-1.179726	-0.321374	-2.763140
H	-2.491963	-1.482559	-2.521761
H	-2.862752	0.174817	-3.080599
C	-4.675106	2.366540	1.026899
H	-5.560944	2.249904	0.384403
H	-4.997511	2.282055	2.074907
H	-4.299158	3.393200	0.879130
H	4.591989	3.175096	0.488545
C	3.174457	-1.132543	1.626100
H	2.266507	-1.361587	2.206443
H	3.367240	-1.999422	0.973941
H	4.013580	-1.048620	2.330157
C	0.857377	1.754854	-1.943837
H	0.948325	1.014795	-2.755616

H -0.157854 1.664675 -1.527545
H 0.953437 2.755406 -2.387010

Ar = *p*-$NO_2C_6H_4$
TS_ArF

Zero-point correction= 0.256090 (Hartree/Particle)
Thermal correction to Energy= 0.277179
Thermal correction to Enthalpy= 0.278123
Thermal correction to Gibbs Free Energy= 0.202708
Sum of electronic and zero-point Energies= -896.959856
Sum of electronic and thermal Energies= -896.938766
Sum of electronic and thermal Enthalpies= -896.937822
Sum of electronic and thermal Free Energies= -897.013238
E(RB-P86) = -897.215945588 A.U

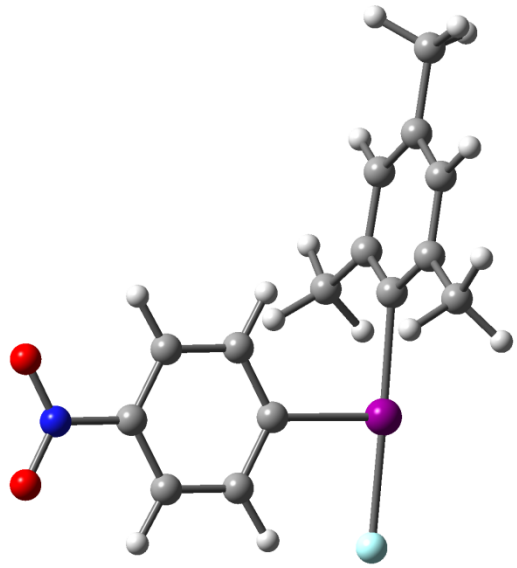


C -2.915651 0.410972 1.221998
C -1.893105 -0.528686 1.228930
C -1.399095 -1.006801 -0.000203
C -1.892600 -0.528201 -1.229346
C -2.915148 0.411461 -1.222458
C -3.421708 0.882202 -0.000241
H -3.323284 0.789463 2.159376
H -3.322388 0.790334 -2.159853
I 0.723472 -1.783096 0.000083
C 1.940175 -0.025532 0.000399
C 2.345956 0.512554 -1.240221
C 2.344753 0.512702 1.240867
C 3.183748 1.637387 -1.203366
C 3.182775 1.637967 1.204360
C 3.609001 2.216786 0.000784
H 3.515175 2.069006 -2.152223
H 3.513284 2.069855 2.153385
F -1.564719 -2.886614 -0.000545
C 1.936489 -0.058151 -2.576773
H 2.244589 -1.109803 -2.684483
H 0.845398 -0.020081 -2.717059
H 2.398433 0.514731 -3.391850

C	1.934448	-0.057330	2.577445
H	0.843332	-0.018535	2.717305
H	2.241874	-1.109128	2.685604
H	2.396410	0.515525	3.392529
C	4.484724	3.445186	-0.000400
H	5.160732	3.455184	-0.867701
H	3.868626	4.358692	-0.055616
H	5.087229	3.510302	0.916791
H	-1.499313	-0.903710	-2.173629
H	-1.500213	-0.904585	2.173220
N	-4.475001	1.876340	-0.000254
O	-4.909919	2.285197	1.098578
O	-4.909456	2.285664	-1.099096

***anti*-isom**

Zero-point correction= 0.257218 (Hartree/Particle)
Thermal correction to Energy= 0.278681
Thermal correction to Enthalpy= 0.279625
Thermal correction to Gibbs Free Energy= 0.203850
Sum of electronic and zero-point Energies= -896.982589
Sum of electronic and thermal Energies= -896.961126
Sum of electronic and thermal Enthalpies= -896.960182
Sum of electronic and thermal Free Energies= -897.035957
E(RB-P86) = -897.239807025 A.U

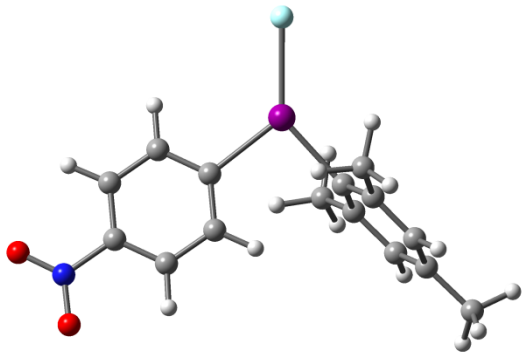


C	3.345618	1.481942	-1.203464
C	2.379319	0.466230	-1.235593
C	1.907010	-0.030913	0.001193
C	2.381567	0.460416	1.236333
C	3.349940	1.478321	1.204793
C	3.845293	1.999155	0.002208
H	3.717607	1.880372	-2.152465
H	3.724883	1.873324	2.153789

I	0.558126	-1.734486	-0.000290
C	-1.213383	-0.510855	0.000595
C	-2.450388	-1.157853	-0.005778
C	-1.087668	0.879329	0.007422
C	-3.608349	-0.378240	-0.005557
C	-2.248427	1.654881	0.007652
C	-3.490534	1.014595	0.001066
H	-4.593941	-0.843114	-0.010536
H	-2.192466	2.742989	0.012930
F	-0.899368	-3.500636	-0.002615
C	1.880861	-0.038407	-2.570749
H	2.116873	-1.104003	-2.719342
H	0.788389	0.068165	-2.666121
H	2.345637	0.525730	-3.390759
C	1.888346	-0.047041	2.572368
H	0.796091	0.058043	2.671669
H	2.126319	-1.112522	2.718566
H	2.355166	0.516311	3.391754
C	4.889292	3.089453	-0.004980
H	5.809283	2.751070	-0.508448
H	4.531850	3.975772	-0.553171
H	5.153115	3.400551	1.015291
H	-0.109690	1.362853	0.012693
H	-2.482869	-2.249705	-0.010278
N	-4.714532	1.835767	0.001202
O	-5.809759	1.249875	-0.003489
O	-4.587973	3.071525	0.005973

TS_isom

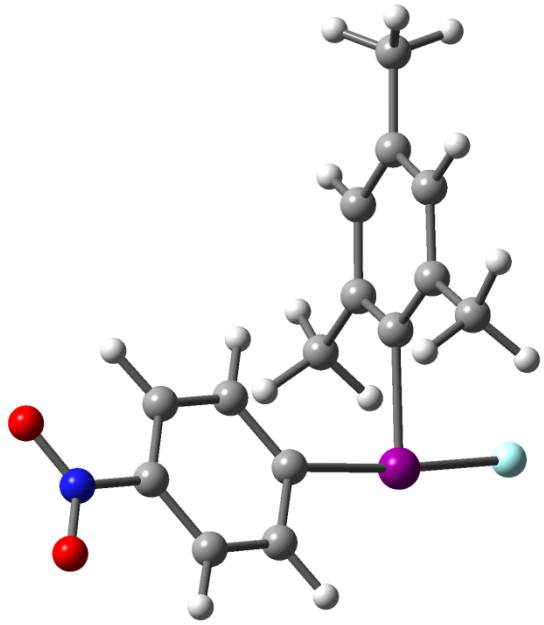
Zero-point correction= 0.256658 (Hartree/Particle)
Thermal correction to Energy= 0.277701
Thermal correction to Enthalpy= 0.278646
Thermal correction to Gibbs Free Energy= 0.203136
Sum of electronic and zero-point Energies= -896.968124
Sum of electronic and thermal Energies= -896.947080
Sum of electronic and thermal Enthalpies= -896.946136
Sum of electronic and thermal Free Energies= -897.021646
E(RB-P86) = -897.224781882 A.U.



C	-3.411204	-1.555776	-1.094121
C	-2.543840	-0.452473	-1.149280
C	-1.875279	-0.110981	0.044035
C	-2.061059	-0.796645	1.262556
C	-2.938339	-1.891891	1.244950
C	-3.623249	-2.283836	0.085204
H	-3.934864	-1.850720	-2.008143
H	-3.088989	-2.451662	2.172647
I	-0.606852	1.642064	0.030812
C	1.247821	0.505353	-0.022982
C	2.404398	1.210233	0.328286
C	1.281609	-0.833166	-0.419352
C	3.634702	0.553590	0.282070
C	2.512558	-1.491279	-0.459176
C	3.668308	-0.787813	-0.109257
H	4.556330	1.068867	0.551009
H	2.579064	-2.536456	-0.760404
F	-0.877949	4.020709	0.050850
C	-2.373226	0.293763	-2.451726
H	-2.716695	1.337109	-2.369982
H	-1.321172	0.320986	-2.774991
H	-2.958060	-0.189814	-3.245444
C	-1.361617	-0.421003	2.546078
H	-0.265677	-0.463136	2.441610
H	-1.620149	0.601314	2.864465
H	-1.648678	-1.108820	3.352461
C	-4.586598	-3.444952	0.113856
H	-5.595361	-3.103268	0.401353
H	-4.670514	-3.921474	-0.873314
H	-4.277692	-4.204321	0.846541
H	0.370211	-1.368553	-0.689425
H	2.363668	2.255509	0.640602
N	4.966988	-1.485031	-0.154564
O	5.983665	-0.843197	0.155858
O	4.975641	-2.677408	-0.501429

***syn*-isom**

Zero-point correction= 0.257499 (Hartree/Particle)
Thermal correction to Energy= 0.278923
Thermal correction to Enthalpy= 0.279867
Thermal correction to Gibbs Free Energy= 0.204202
Sum of electronic and zero-point Energies= -896.984324
Sum of electronic and thermal Energies= -896.962901
Sum of electronic and thermal Enthalpies= -896.961957
Sum of electronic and thermal Free Energies= -897.037621
E(RB-P86) = -897.241823379 A.U

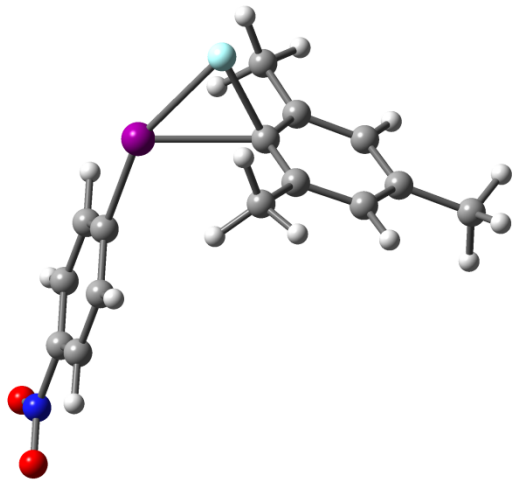


C	-3.649702	-0.768022	0.289801
C	-2.387033	-1.359339	0.335982
C	-1.250648	-0.616318	-0.017432
C	-1.368510	0.720796	-0.416632
C	-2.626965	1.323447	-0.461598
C	-3.750033	0.568920	-0.108637
H	-4.545696	-1.325422	0.561931
H	-2.301425	-2.401600	0.654622
H	-0.487235	1.302978	-0.692744
H	-2.744145	2.362373	-0.769278
I	0.654195	-1.705664	0.021360
C	1.785499	0.100255	0.052319
C	2.411113	0.503641	-1.142015
C	1.887779	0.800572	1.267979
C	3.163830	1.687633	-1.086262
C	2.655658	1.977393	1.249526
C	3.299511	2.435458	0.092366
H	3.657843	2.029586	-2.000341
H	2.750259	2.547044	2.178458
F	2.662057	-2.671753	0.049282
C	1.228754	0.359120	2.551228
H	0.131132	0.335924	2.459483
H	1.554711	-0.650740	2.846106
H	1.482787	1.049190	3.366722
C	2.314594	-0.266256	-2.435473
H	2.682428	-1.296134	-2.308473
H	1.275068	-0.328484	-2.795137
H	2.913190	0.221029	-3.216538
C	4.142051	3.687809	0.118284
H	3.832114	4.363941	0.927704
H	5.203525	3.437931	0.284348

H	4.080943	4.231033	-0.836011
N	-5.078239	1.200805	-0.158604
O	-6.065210	0.514194	0.157168
O	-5.147800	2.389681	-0.515030

TS_MesF

Zero-point correction= 0.255828 (Hartree/Particle)
Thermal correction to Energy= 0.277047
Thermal correction to Enthalpy= 0.277991
Thermal correction to Gibbs Free Energy= 0.202175
Sum of electronic and zero-point Energies= -896.951875
Sum of electronic and thermal Energies= -896.930656
Sum of electronic and thermal Enthalpies= -896.929712
Sum of electronic and thermal Free Energies= -897.005528
E(RB-P86) = -897.207702828 A.U.

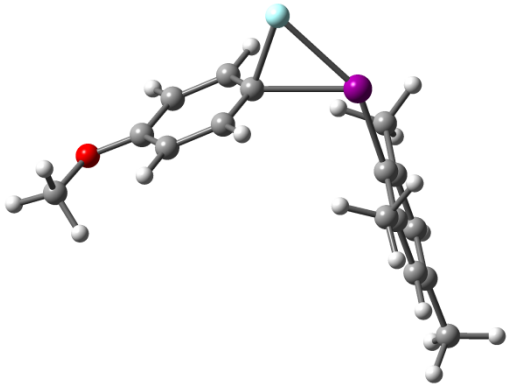


C	3.048061	1.867411	-1.134718
C	2.499821	0.570598	-1.218778
C	2.215127	-0.021858	0.007553
C	2.479940	0.502002	1.269083
C	3.029743	1.800741	1.265820
C	3.310834	2.502634	0.086236
H	3.283478	2.376285	-2.074931
H	3.249162	2.256716	2.236493
I	0.475508	-1.729021	-0.051414
C	-1.416723	-0.737387	-0.028650
C	-2.099695	-0.582223	1.187525
C	-1.957110	-0.249345	-1.228038
C	-3.338348	0.059420	1.205158
C	-3.193959	0.395663	-1.215365
C	-3.864858	0.540252	0.002596
H	-3.892637	0.189595	2.134205
H	-3.637873	0.782093	-2.132397
F	2.923061	-1.923066	-0.042290
C	2.279808	-0.087698	-2.555044

H	1.208397	-0.258024	-2.748707
H	2.673238	0.544860	-3.362170
H	2.779007	-1.066672	-2.596289
C	2.233151	-0.227333	2.563076
H	1.157072	-0.397392	2.728545
H	2.724483	-1.211165	2.558191
H	2.617961	0.355937	3.410536
C	3.873764	3.905263	0.130431
H	4.483559	4.063894	1.032038
H	4.498969	4.114571	-0.750003
H	3.066388	4.657046	0.144901
H	-1.426371	-0.372824	-2.172865
H	-1.676984	-0.961807	2.118853
N	-5.171664	1.222665	0.019509
O	-5.627264	1.637029	-1.059399
O	-5.749363	1.348611	1.112059

Ar = *p*-MeOC$_6$H$_4$
TS_ArF

Zero-point correction= 0.284996 (Hartree/Particle)
Thermal correction to Energy= 0.306312
Thermal correction to Enthalpy= 0.307256
Thermal correction to Gibbs Free Energy= 0.231824
Sum of electronic and zero-point Energies= -806.885056
Sum of electronic and thermal Energies= -806.863740
Sum of electronic and thermal Enthalpies= -806.862796
Sum of electronic and thermal Free Energies= -806.938228
E(RB-P86) = -807.170051643 A.U.

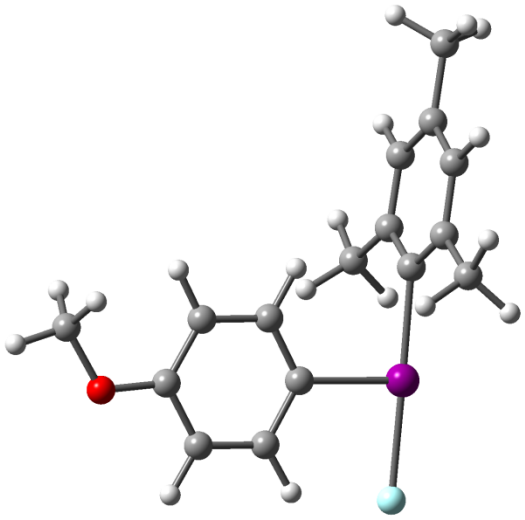


C	-3.076759	0.603383	1.434054
C	-2.145939	-0.433110	1.325299
C	-1.721205	-0.807087	0.051131
C	-2.193094	-0.198311	-1.103195
C	-3.129909	0.843858	-0.979659
C	-3.572997	1.249516	0.287879
H	-3.425660	0.919132	2.420062
H	-3.492964	1.322678	-1.889500
I	0.462646	-1.754507	-0.091826

C	1.820210	-0.104157	-0.022566
C	2.275676	0.451159	-1.238027
C	2.243033	0.376218	1.235900
C	3.188764	1.514891	-1.158850
C	3.156092	1.442271	1.245986
C	3.642989	2.022918	0.066253
H	3.552711	1.958072	-2.090684
H	3.493770	1.828789	2.212311
F	-1.887011	-2.733320	-0.102533
C	1.837946	-0.044679	-2.595814
H	2.096609	-1.105146	-2.743621
H	0.748897	0.044403	-2.730053
H	2.325335	0.537279	-3.389823
C	1.767389	-0.200226	2.548166
H	0.675411	-0.112880	2.657927
H	2.018167	-1.269297	2.636509
H	2.234696	0.328953	3.389773
C	4.647224	3.148826	0.115301
H	4.565044	3.799734	-0.767161
H	4.516636	3.763257	1.017892
H	5.676398	2.751652	0.135597
H	-1.861856	-0.514433	-2.092369
H	-1.779957	-0.937753	2.219425
O	-4.477809	2.261746	0.513929
C	-5.006244	2.937189	-0.637912
H	-5.553483	2.239452	-1.293078
H	-5.698134	3.692430	-0.247259
H	-4.205360	3.432515	-1.211455

***anti*-isom**

Zero-point correction= 0.286453 (Hartree/Particle)
Thermal correction to Energy= 0.308135
Thermal correction to Enthalpy= 0.309079
Thermal correction to Gibbs Free Energy= 0.231354
Sum of electronic and zero-point Energies= -806.918525
Sum of electronic and thermal Energies= -806.896843
Sum of electronic and thermal Enthalpies= -806.895899
Sum of electronic and thermal Free Energies= -806.973624
E(RB-P86) = -807.204977491 A.U.

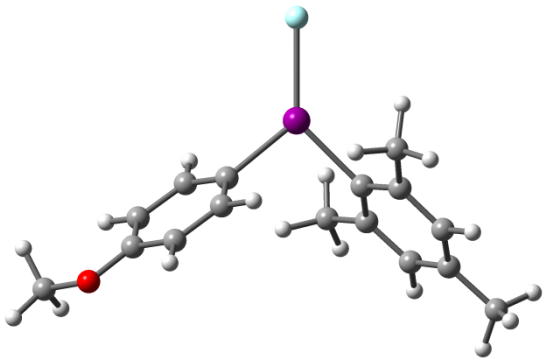


C	-3.172689	1.395767	1.219166
C	-2.177018	0.408059	1.241446
C	-1.714404	-0.090341	0.002067
C	-2.227944	0.374869	-1.226915
C	-3.224850	1.365300	-1.187412
C	-3.711462	1.885260	0.018925
H	-3.535580	1.794957	2.171519
H	-3.628641	1.739760	-2.133066
I	-0.290790	-1.734232	-0.004760
C	1.425686	-0.427141	-0.004722
C	2.693764	-1.008791	0.065841
C	1.249415	0.950402	-0.073672
C	3.811005	-0.175352	0.069096
C	2.377067	1.784397	-0.070705
C	3.662698	1.223282	0.001543
H	4.815620	-0.600626	0.123859
H	2.230718	2.863056	-0.124646
F	1.238523	-3.457076	0.001403
C	-1.636984	-0.066927	2.571331
H	-1.844808	-1.135848	2.737487
H	-0.545124	0.064291	2.637944
H	-2.095496	0.497190	3.395097
C	-1.746901	-0.132777	-2.567581
H	-0.656713	-0.020244	-2.679105
H	-1.977750	-1.200953	-2.706166
H	-2.228653	0.423527	-3.383375
C	-4.789345	2.942525	0.035621
H	-5.706913	2.562276	0.513569
H	-4.470536	3.825608	0.611790
H	-5.047117	3.270063	-0.981178
H	0.254508	1.395539	-0.129280
H	2.783322	-2.096322	0.111074
O	4.822981	1.946175	0.011650
C	4.715556	3.380083	-0.059122

H	5.745755	3.752786	-0.037427
H	4.227721	3.693873	-0.995676
H	4.159426	3.777927	0.804601

TS_isom

Zero-point correction= 0.285990 (Hartree/Particle)
Thermal correction to Energy= 0.307152
Thermal correction to Enthalpy= 0.308096
Thermal correction to Gibbs Free Energy= 0.233344
Sum of electronic and zero-point Energies= -806.906123
Sum of electronic and thermal Energies= -806.884961
Sum of electronic and thermal Enthalpies= -806.884017
Sum of electronic and thermal Free Energies= -806.958770
E(RB-P86) = -807.192113176 A.U.

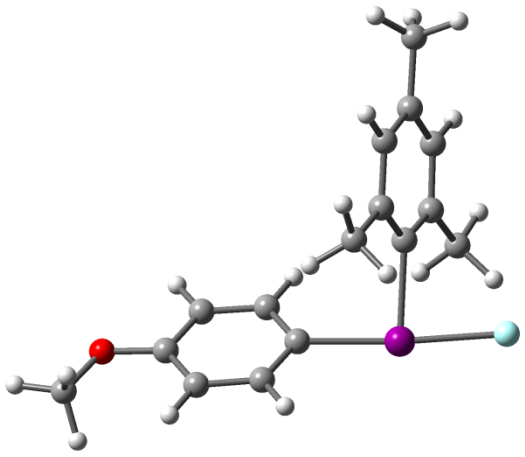


C	3.482572	-1.288814	1.043276
C	2.558692	-0.229810	1.045622
C	1.735936	-0.100494	-0.090204
C	1.825275	-0.950736	-1.210004
C	2.766196	-1.991284	-1.145268
C	3.600802	-2.177664	-0.033891
H	4.129097	-1.415898	1.916778
H	2.844734	-2.674125	-1.996683
I	0.335691	1.567544	-0.134487
C	-1.436049	0.372527	0.129090
C	-2.367605	0.327153	-0.909182
C	-1.682030	-0.265034	1.353284
C	-3.564065	-0.381216	-0.737369
C	-2.864846	-0.978125	1.520744
C	-3.813034	-1.040878	0.478758
H	-4.283432	-0.412600	-1.555479
H	-3.076543	-1.490123	2.461772
F	0.570022	3.985798	-0.386916
C	2.504292	0.699120	2.237010
H	2.743784	1.736977	1.956106
H	1.507878	0.711628	2.704803
H	3.230238	0.382082	2.997715
C	0.965625	-0.800105	-2.440724
H	-0.100093	-0.957334	-2.211064

H	1.059091	0.205627	-2.879947
H	1.257507	-1.533767	-3.204092
C	4.622229	-3.289177	-0.012871
H	4.877243	-3.580683	1.016064
H	4.258396	-4.177887	-0.549050
H	5.555548	-2.969350	-0.506400
H	-0.963971	-0.214100	2.173131
H	-2.179802	0.835400	-1.857025
O	-4.937395	-1.761062	0.750311
C	-5.943903	-1.848695	-0.277859
H	-5.544441	-2.341309	-1.178119
H	-6.746767	-2.458051	0.151417
H	-6.331636	-0.850625	-0.534854

***syn*-isom**

Zero-point correction= 0.286673 (Hartree/Particle)
Thermal correction to Energy= 0.308277
Thermal correction to Enthalpy= 0.309221
Thermal correction to Gibbs Free Energy= 0.233760
Sum of electronic and zero-point Energies= -806.919177
Sum of electronic and thermal Energies= -806.897573
Sum of electronic and thermal Enthalpies= -806.896628
Sum of electronic and thermal Free Energies= -806.972090
E(RB-P86) = -807.205849795 A.U.

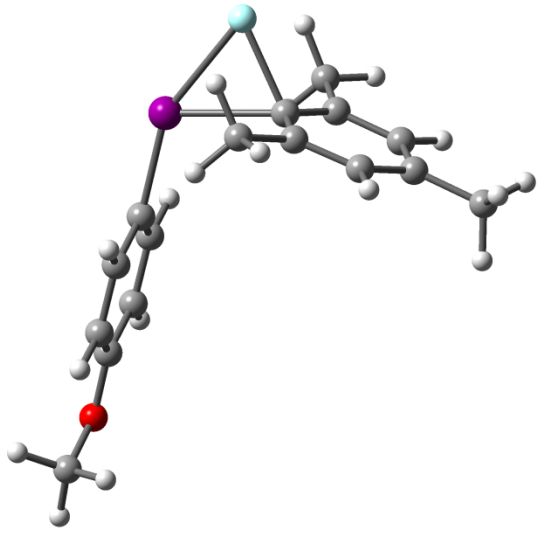


C	-3.723390	-0.084752	0.587506
C	-2.499079	-0.752750	0.737345
C	-1.430680	-0.477465	-0.119736
C	-1.579357	0.476140	-1.138336
C	-2.787239	1.153558	-1.287395
C	-3.868420	0.875010	-0.427470
H	-4.542589	-0.315088	1.268702
H	-2.396728	-1.489661	1.538744
H	-0.755438	0.702469	-1.819321
H	-2.915337	1.900898	-2.073818
I	0.385990	-1.657212	0.087936

C	1.630272	0.080918	0.099468
C	2.446629	0.307320	-1.023480
C	1.595991	0.926398	1.223253
C	3.245707	1.462381	-0.999127
C	2.417591	2.065908	1.178001
C	3.244816	2.352484	0.083770
H	3.888936	1.663564	-1.860987
H	2.407647	2.743971	2.036608
F	2.369088	-2.755566	0.315219
C	0.745283	0.670103	2.441789
H	-0.329187	0.720696	2.203928
H	0.938827	-0.328029	2.865564
H	0.955878	1.417441	3.218520
C	2.510077	-0.623995	-2.208611
H	2.762721	-1.644939	-1.883053
H	1.544730	-0.675425	-2.737694
H	3.269355	-0.282127	-2.924744
C	4.138512	3.569808	0.085873
H	3.697611	4.390953	0.669398
H	5.116542	3.334067	0.538446
H	4.328814	3.929489	-0.935670
O	-5.010337	1.589889	-0.661321
C	-6.144336	1.331886	0.187372
H	-5.912400	1.564139	1.238958
H	-6.936442	1.998738	-0.171350
H	-6.473773	0.284344	0.099392

TS_MesF

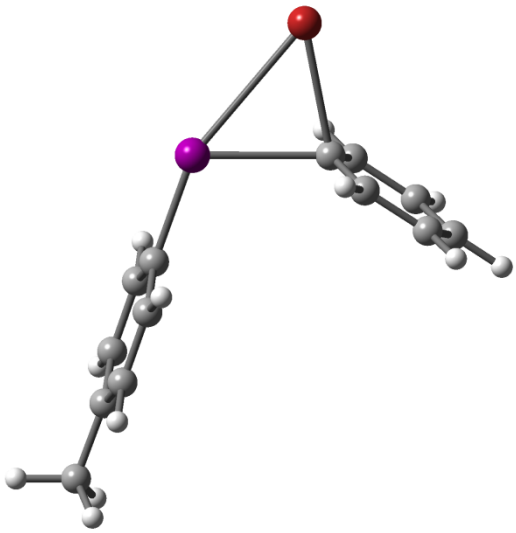
Zero-point correction= 0.285346 (Hartree/Particle)
Thermal correction to Energy= 0.306583
Thermal correction to Enthalpy= 0.307528
Thermal correction to Gibbs Free Energy= 0.232950
Sum of electronic and zero-point Energies= -806.888922
Sum of electronic and thermal Energies= -806.867685
Sum of electronic and thermal Enthalpies= -806.866741
Sum of electronic and thermal Free Energies= -806.941319
E(RB-P86) = -807.174268177 A.U.



C	2.818701	1.885528	-1.114589
C	2.246416	0.604740	-1.248549
C	2.036768	-0.083008	-0.053841
C	2.389885	0.362220	1.218793
C	2.957318	1.652071	1.270390
C	3.171880	2.432532	0.126822
H	2.997842	2.457554	-2.030980
H	3.246201	2.038156	2.253441
I	0.223718	-1.709416	-0.115173
C	-1.602062	-0.643557	0.077987
C	-2.183175	-0.468763	1.345816
C	-2.224499	-0.116977	-1.059412
C	-3.385513	0.221509	1.465379
C	-3.432632	0.579828	-0.943616
C	-4.018270	0.751643	0.323141
H	-3.852896	0.360798	2.442540
H	-3.903158	0.978342	-1.842341
F	2.726630	-1.941764	-0.278791
C	1.913451	0.048057	-2.608519
H	0.823352	-0.022325	-2.758260
H	2.320533	0.694335	-3.398346
H	2.324819	-0.964254	-2.729893
C	2.210206	-0.450505	2.474594
H	1.143176	-0.584479	2.716925
H	2.647043	-1.452831	2.358760
H	2.689486	0.049055	3.327779
C	3.755454	3.824110	0.228593
H	4.395534	4.056055	-0.635957
H	2.960697	4.588937	0.259461
H	4.356949	3.940183	1.142157
H	-1.781708	-0.247708	-2.048747
H	-1.706020	-0.874786	2.239803
O	-5.190450	1.411270	0.549627
C	-5.877189	1.969925	-0.587426

H -6.163957 1.181518 -1.300969
H -6.776907 2.444748 -0.180720
H -5.254543 2.725371 -1.091763

***p*-Tol(Ph)IBr system**
TS_PhBr
Zero-point correction= 0.199441 (Hartree/Particle)
Thermal correction to Energy= 0.215278
Thermal correction to Enthalpy= 0.216222
Thermal correction to Gibbs Free Energy= 0.150955
Sum of electronic and zero-point Energies= -527.320439
Sum of electronic and thermal Energies= -527.304602
Sum of electronic and thermal Enthalpies= -527.303658
Sum of electronic and thermal Free Energies= -527.368925
E(RB-P86) = -527.519879636 A.U

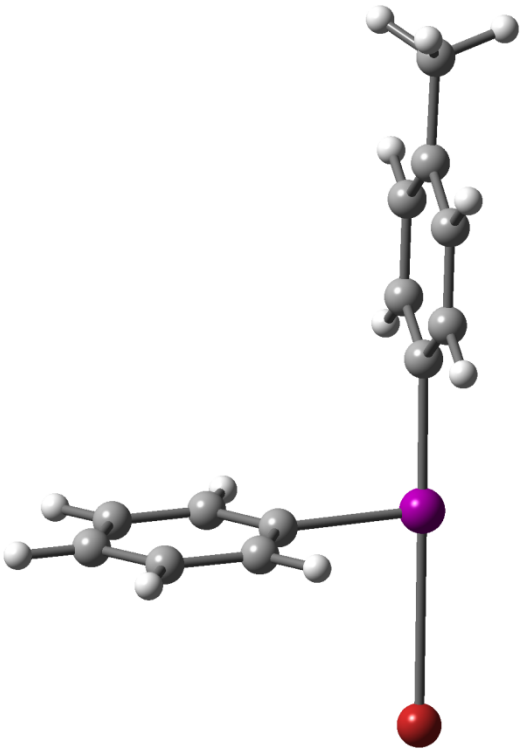


C -1.621681 2.949417 1.216690
C -1.571091 1.544691 1.232746
C -1.561177 0.905614 0.002523
C -1.574664 1.549594 -1.225142
C -1.625237 2.954202 -1.203470
C -1.649554 3.653847 0.008045
H -1.638331 3.479660 2.172326
H -1.644790 3.488163 -2.156981
I -0.094997 -1.176096 -0.004270
C 1.934204 -0.554767 -0.001408
C 2.587962 -0.324863 -1.219754
C 2.594843 -0.359468 1.218306
C 3.921254 0.092394 -1.205956
C 3.929362 0.057340 1.208076
C 4.615629 0.287067 0.002434
H 4.430978 0.271599 -2.156683
H 4.445526 0.208134 2.160137
H 2.082057 -0.530502 2.166612

H	2.069103	-0.469524	-2.169128
H	-1.560037	1.004893	-2.168735
H	-1.553516	0.996333	2.174168
Br	-3.300449	-0.973629	-0.000060
H	-1.686018	4.744902	0.010250
C	6.063801	0.709228	0.001011
H	6.276135	1.410610	-0.819232
H	6.345072	1.184553	0.951281
H	6.722482	-0.164481	-0.140176

***anti*-isom**

Zero-point correction= 0.201222 (Hartree/Particle)
Thermal correction to Energy= 0.217487
Thermal correction to Enthalpy= 0.218431
Thermal correction to Gibbs Free Energy= 0.151433
Sum of electronic and zero-point Energies= -527.353596
Sum of electronic and thermal Energies= -527.337331
Sum of electronic and thermal Enthalpies= -527.336387
Sum of electronic and thermal Free Energies= -527.403385
E(RB-P86) = -527.554818079 A.U

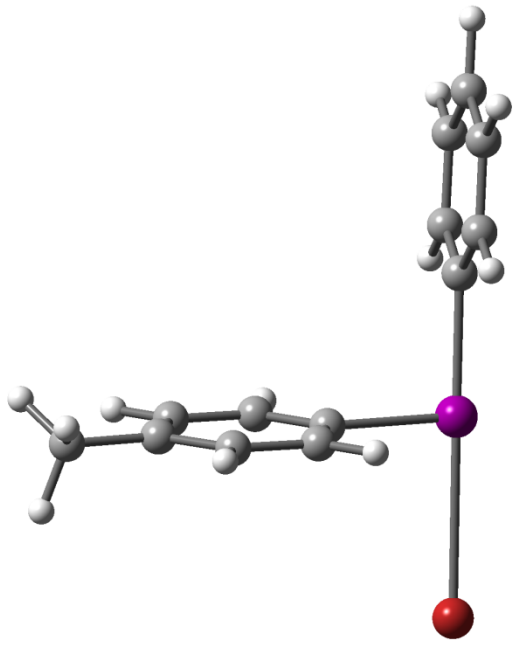


C	-3.873121	-0.356713	1.188728
C	-2.485595	-0.533594	1.200160
C	-1.796176	-0.540676	-0.016256
C	-2.465788	-0.387695	-1.232979
C	-3.854427	-0.211804	-1.221596
C	-4.579179	-0.194917	-0.017089

H	-4.414875	-0.343823	2.138587
H	-1.959129	-0.659139	2.148563
H	-1.925102	-0.399393	-2.181676
H	-4.381640	-0.085261	-2.171150
I	0.348653	-0.866013	-0.010458
C	0.818449	1.213664	0.008205
C	1.071972	1.849848	-1.207411
C	0.844510	1.877232	1.235116
C	1.362123	3.220126	-1.182832
C	1.135717	3.247530	1.234353
C	1.393485	3.915101	0.031619
H	1.564177	3.739039	-2.122214
H	1.162233	3.787411	2.183208
H	0.647610	1.352989	2.171005
H	1.050753	1.304178	-2.151422
Br	3.389271	-1.319214	0.014568
C	-6.079388	-0.032708	-0.015684
H	-6.576176	-1.014176	0.065641
H	-6.415260	0.572727	0.839036
H	-6.433222	0.441434	-0.941963
H	1.622033	4.982804	0.040792

***syn*-isom**

Zero-point correction= 0.201229 (Hartree/Particle)
Thermal correction to Energy= 0.217486
Thermal correction to Enthalpy= 0.218430
Thermal correction to Gibbs Free Energy= 0.151636
Sum of electronic and zero-point Energies= -527.353714
Sum of electronic and thermal Energies= -527.337457
Sum of electronic and thermal Enthalpies= -527.336513
Sum of electronic and thermal Free Energies= -527.403308
E(RB-P86) = -527.554943298 A.U

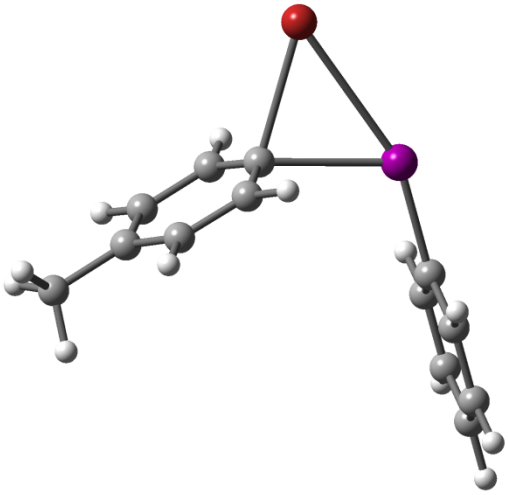


C	-4.327213	0.147991	1.154182
C	-3.004843	-0.316064	1.163080
C	-2.280645	-0.301773	-0.032322
C	-2.839672	0.149446	-1.231461
C	-4.160923	0.614412	-1.222960
C	-4.901546	0.613182	-0.034333
H	-4.904799	0.143896	2.081314
H	-2.555952	-0.678623	2.090044
H	-2.265454	0.144953	-2.160153
H	-4.610606	0.973351	-2.151538
H	-5.932558	0.973486	-0.035862
I	-0.247986	-1.082554	-0.023736
C	0.651954	0.844548	0.017080
C	1.084188	1.405019	-1.184641
C	0.774218	1.505894	1.239584
C	1.657048	2.681001	-1.148936
C	1.350350	2.780542	1.244318
C	1.801831	3.386444	0.058276
H	1.994777	3.133271	-2.085031
H	1.448394	3.310584	2.195389
C	2.447209	4.749732	0.086094
H	2.007842	5.384749	0.868876
H	3.525345	4.662777	0.302082
H	2.345109	5.262048	-0.880965
H	0.433160	1.051563	2.170803
H	0.983333	0.872065	-2.130865
Br	2.604655	-2.212029	0.009890

TS_*p*-TolBr

Zero-point correction= 0.199423 (Hartree/Particle)

Thermal correction to Energy= 0.215326
Thermal correction to Enthalpy= 0.216271
Thermal correction to Gibbs Free Energy= 0.150368
Sum of electronic and zero-point Energies= -527.318970
Sum of electronic and thermal Energies= -527.303067
Sum of electronic and thermal Enthalpies= -527.302123
Sum of electronic and thermal Free Energies= -527.368026
E(RB-P86) = -527.518393261 A.U



C	-1.959115	2.330153	1.224864
C	-1.527565	0.991209	1.239663
C	-1.351862	0.381591	0.011204
C	-1.551597	1.000454	-1.212073
C	-1.982184	2.335981	-1.181712
C	-2.192460	3.022582	0.027081
H	-2.112457	2.830144	2.185738
H	-2.154951	2.841040	-2.136841
I	0.612283	-1.250800	-0.019135
C	2.431406	-0.145641	-0.007929
C	2.970671	0.298115	-1.222746
C	3.057221	0.129536	1.215323
C	4.168217	1.022623	-1.206212
C	4.255649	0.852842	1.213481
C	4.810019	1.298902	0.007374
H	4.598560	1.369737	-2.148279
H	4.754335	1.067336	2.161369
C	-2.642627	4.465677	0.029088
H	-2.874160	4.809733	1.046853
H	-1.861420	5.126965	-0.380311
H	-3.541446	4.605161	-0.591731
H	2.624744	-0.217132	2.155501
H	5.744469	1.864122	0.013339
H	2.471703	0.080145	-2.168577
H	-1.400594	0.484452	-2.159833
H	-1.358750	0.471076	2.182127

Br -2.521590 -1.912702 0.000868

h. Other non-copper containing species

2,6-$Me_2C_6H_3F$

Zero-point correction= 0.142263 (Hartree/Particle)
Thermal correction to Energy= 0.151265
Thermal correction to Enthalpy= 0.152209
Thermal correction to Gibbs Free Energy= 0.108168
Sum of electronic and zero-point Energies= -410.094343
Sum of electronic and thermal Energies= -410.085341
Sum of electronic and thermal Enthalpies= -410.084397
Sum of electronic and thermal Free Energies= -410.128438
E(RB-P86) = -410.236606028 A.U.

C	0.000000	-0.633205	0.000272
C	1.240525	0.012799	0.000042
C	-1.240525	0.012799	0.000070
C	1.212371	1.417661	-0.000129
C	-1.212371	1.417661	-0.000084
C	0.000000	2.115411	0.000042
H	2.159999	1.963113	-0.000312
H	-2.159999	1.963113	-0.000215
F	0.000000	-2.010112	-0.000230
C	2.530014	-0.769732	0.000073
H	2.606212	-1.420879	0.885298
H	2.605315	-1.422527	-0.883993
H	3.392300	-0.089076	-0.000974
C	-2.530014	-0.769732	0.000056
H	-2.605877	-1.421522	-0.884713
H	-2.605650	-1.421885	0.884579
H	-3.392300	-0.089076	0.000282
H	0.000000	3.207775	0.000072

2,6-$Me_2C_6H_3I$

Zero-point correction= 0.140299 (Hartree/Particle)
Thermal correction to Energy= 0.149656
Thermal correction to Enthalpy= 0.150600
Thermal correction to Gibbs Free Energy= 0.104704
Sum of electronic and zero-point Energies= -321.643633
Sum of electronic and thermal Energies= -321.634276
Sum of electronic and thermal Enthalpies= -321.633332
Sum of electronic and thermal Free Energies= -321.679228
E(RB-P86) = -321.783932415 A.U.

C	-2.589516	-1.208104	-0.000124
C	-1.183062	-1.239699	0.000239
C	-0.511223	0.000000	0.000417
C	-1.183062	1.239699	0.000239
C	-2.589516	1.208104	-0.000124
C	-3.288696	0.000000	-0.000224

H	-3.134143	-2.156055	-0.000384
H	-3.134143	2.156055	-0.000384
I	1.622148	0.000000	-0.000080
C	-0.466751	-2.566590	0.000171
H	0.181382	-2.675161	-0.884479
H	0.181824	-2.674945	0.884511
H	-1.189653	-3.394060	0.000422
C	-0.466751	2.566590	0.000171
H	0.181825	2.674945	0.884511
H	0.181382	2.675161	-0.884479
H	-1.189653	3.394060	0.000422
H	-4.381209	0.000000	-0.000475

3,5-$Me_2C_6H_3F$

Zero-point correction= 0.141749 (Hartree/Particle)
Thermal correction to Energy= 0.150955
Thermal correction to Enthalpy= 0.151899
Thermal correction to Gibbs Free Energy= 0.105544
Sum of electronic and zero-point Energies= -410.094411
Sum of electronic and thermal Energies= -410.085205
Sum of electronic and thermal Enthalpies= -410.084261
Sum of electronic and thermal Free Energies= -410.130617
E(RB-P86) = -410.236160433 A.U.

C	-0.000050	1.404456	0.001088
C	1.223938	0.745796	-0.000948
C	-1.223976	0.745732	-0.000655
C	1.229933	-0.659778	-0.004068
C	-1.229875	-0.659868	-0.003842
C	0.000039	-1.339324	-0.006841
F	-0.000072	2.778949	0.001084
H	0.000080	-2.433367	-0.013241
H	-2.152725	1.320621	-0.002283
H	2.152637	1.320766	-0.002798
C	2.538756	-1.415253	0.003791
H	3.208027	-1.063978	-0.797129
H	3.073287	-1.270480	0.957023
H	2.377106	-2.493835	-0.131570
C	-2.538681	-1.415376	0.003654
H	-3.076302	-1.265956	0.954403
H	-3.205399	-1.068048	-0.801146
H	-2.376565	-2.494575	-0.126085

3,5-$Me_2C_6H_3I$

Zero-point correction= 0.139629 (Hartree/Particle)
Thermal correction to Energy= 0.149577
Thermal correction to Enthalpy= 0.150521
Thermal correction to Gibbs Free Energy= 0.101278
Sum of electronic and zero-point Energies= -321.645548
Sum of electronic and thermal Energies= -321.635600
Sum of electronic and thermal Enthalpies= -321.634656

Sum of electronic and thermal Free Energies= -321.683899
E(RB-P86) = -321.785176728 A.U.

C	-0.056887	0.000010	0.002161
C	-0.736596	-1.220699	-0.002389
C	-0.736590	1.220695	-0.002390
C	-2.142810	-1.227762	-0.010220
C	-2.142830	1.227749	-0.010223
C	-2.823528	0.000002	-0.018504
H	-3.917948	-0.000003	-0.036655
H	-0.187527	2.164701	-0.006819
H	-0.187520	-2.164697	-0.006813
C	-2.899768	-2.535824	0.010505
H	-2.322700	-3.342396	-0.464497
H	-3.111498	-2.848850	1.046843
H	-3.865551	-2.446099	-0.508046
C	-2.899728	2.535845	0.010505
H	-3.109195	2.850182	1.046907
H	-2.323646	3.341826	-0.466710
H	-3.866603	2.445509	-0.505883
I	2.066502	-0.000005	0.000472

DMF

Zero-point correction= 0.098925 (Hartree/Particle)
Thermal correction to Energy= 0.105118
Thermal correction to Enthalpy= 0.106062
Thermal correction to Gibbs Free Energy= 0.069745
Sum of electronic and zero-point Energies= -248.502470
Sum of electronic and thermal Energies= -248.496277
Sum of electronic and thermal Enthalpies= -248.495333
Sum of electronic and thermal Free Energies= -248.531650
E(RB-P86) = -248.601394741 A.U.

C	0.858477	-0.647912	0.000027
H	0.751812	-1.754554	-0.000051
O	1.968314	-0.094041	-0.000035
N	-0.342335	-0.018728	0.000129
C	-1.592678	-0.769878	-0.000030
H	-2.188100	-0.527279	-0.894785
H	-1.374038	-1.846150	-0.000058
H	-2.188342	-0.527454	0.894624
C	-0.431370	1.437344	-0.000032
H	-0.970847	1.786489	0.894807
H	0.584674	1.849020	-0.000585
H	-0.971899	1.786028	-0.894369

Fluoride

Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.014159

Sum of electronic and zero-point Energies= -100.021874
Sum of electronic and thermal Energies= -100.020458
Sum of electronic and thermal Enthalpies= -100.019514
Sum of electronic and thermal Free Energies= -100.036033

MesF

Zero-point correction= 0.168677 (Hartree/Particle)
Thermal correction to Energy= 0.179491
Thermal correction to Enthalpy= 0.180436
Thermal correction to Gibbs Free Energy= 0.132252
Sum of electronic and zero-point Energies= -449.393578
Sum of electronic and thermal Energies= -449.382764
Sum of electronic and thermal Enthalpies= -449.381819
Sum of electronic and thermal Free Energies= -449.430003
E(RB-P86) = -449.562255035 A.U

C	-1.057352	0.000000	0.005267
C	-0.405723	1.236338	-0.000909
C	-0.405723	-1.236338	-0.000947
C	0.998249	1.205007	-0.009903
C	0.998249	-1.205007	-0.009966
C	1.718465	0.000000	-0.010640
H	1.540055	2.156148	-0.018896
H	1.540054	-2.156147	-0.019033
F	-2.435292	0.000000	0.010852
C	-1.182212	2.530050	-0.002650
H	-1.837691	2.605682	-0.885230
H	-1.830288	2.612098	0.884793
H	-0.497328	3.389550	-0.008531
C	-1.182214	-2.530049	-0.002626
H	-1.829076	-2.612760	0.885653
H	-1.838899	-2.605021	-0.884352
H	-0.497338	-3.389544	-0.010019
C	3.230983	-0.000001	0.012531
H	3.640042	0.891912	-0.485678
H	3.611730	-0.000037	1.048430
H	3.640041	-0.891880	-0.485740

MesI

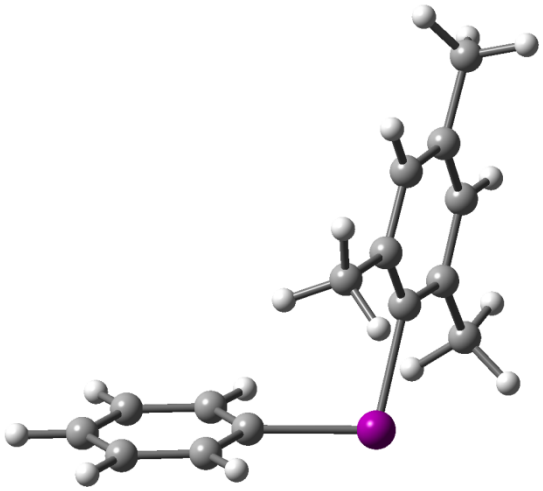
Zero-point correction= 0.166572 (Hartree/Particle)
Thermal correction to Energy= 0.177911
Thermal correction to Enthalpy= 0.178856
Thermal correction to Gibbs Free Energy= 0.127710
Sum of electronic and zero-point Energies= -360.943669
Sum of electronic and thermal Energies= -360.932330
Sum of electronic and thermal Enthalpies= -360.931385
Sum of electronic and thermal Free Energies= -360.982531
E(RB-P86) = -361.110241023 A.U.

C	-2.248256	1.200978	-0.009564
C	-0.843022	1.235594	-0.004246

C	-0.166045	0.000000	-0.000107
C	-0.843023	-1.235594	-0.004246
C	-2.248256	-1.200978	-0.009564
C	-2.970070	0.000001	-0.009047
H	-2.789486	2.152306	-0.016766
H	-2.789487	-2.152305	-0.016765
I	1.966840	0.000000	0.003411
C	-0.131626	2.565517	-0.007116
H	0.514146	2.679271	0.878717
H	0.519049	2.673431	-0.890103
H	-0.856999	3.390890	-0.011710
C	-0.131626	-2.565517	-0.007116
H	0.519049	-2.673431	-0.890103
H	0.514145	-2.679271	0.878717
H	-0.857000	-3.390890	-0.011710
C	-4.480936	0.000000	0.017590
H	-4.891249	-0.892234	-0.477892
H	-4.856246	-0.000044	1.055139
H	-4.891248	0.892275	-0.477819

[Mes(Ph)I]$^{+}$

Zero-point correction= 0.254628 (Hartree/Particle)
Thermal correction to Energy= 0.271691
Thermal correction to Enthalpy= 0.272635
Thermal correction to Gibbs Free Energy= 0.207761
Sum of electronic and zero-point Energies= -592.332083
Sum of electronic and thermal Energies= -592.315020
Sum of electronic and thermal Enthalpies= -592.314076
Sum of electronic and thermal Free Energies= -592.378950
E(RB-P86) = -592.586711059 A.U

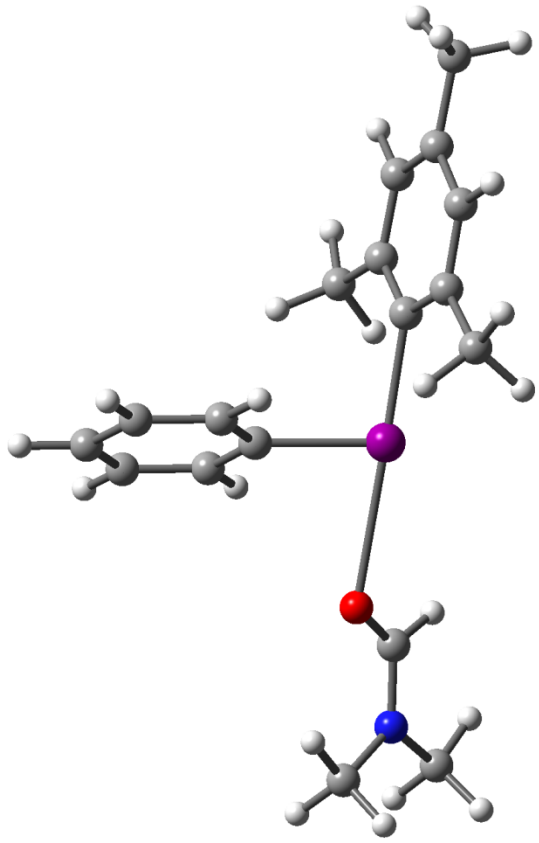


C	-3.264238	-0.063671	1.015150
C	-2.061758	-0.759393	0.811644
C	-1.216421	-0.243107	-0.188809

C	-1.505928	0.883942	-0.981004
C	-2.723635	1.527781	-0.712019
C	-3.611972	1.074274	0.273524
H	-3.947502	-0.434160	1.784197
H	-2.977739	2.413538	-1.300871
I	0.617548	-1.285717	-0.551847
C	2.072667	0.100350	0.180160
C	2.112720	0.388068	1.544845
C	2.966470	0.637807	-0.747428
C	3.098874	1.275762	1.991911
H	1.408901	-0.055035	2.249219
C	3.951153	1.512848	-0.270425
H	2.908394	0.392788	-1.808540
C	4.013551	1.832325	1.089963
H	3.149871	1.521603	3.054419
H	4.663553	1.946430	-0.974982
H	4.781535	2.519089	1.451171
C	-0.596178	1.417494	-2.057001
H	0.345169	1.804928	-1.636115
H	-0.335813	0.639672	-2.792166
H	-1.084436	2.240904	-2.593946
C	-4.925194	1.777134	0.509605
H	-4.846636	2.853681	0.301624
H	-5.704112	1.369952	-0.156930
H	-5.272943	1.641065	1.543266
C	-1.765800	-1.989373	1.634348
H	-1.687683	-2.890065	1.005217
H	-0.824198	-1.895206	2.196270
H	-2.572270	-2.159603	2.359274

***anti*-[Mes(Ph)I(DMF)]$^{+}$**

Zero-point correction= 0.354593 (Hartree/Particle)
Thermal correction to Energy= 0.379965
Thermal correction to Enthalpy= 0.380909
Thermal correction to Gibbs Free Energy= 0.294241
Sum of electronic and zero-point Energies= -840.840830
Sum of electronic and thermal Energies= -840.815458
Sum of electronic and thermal Enthalpies= -840.814514
Sum of electronic and thermal Free Energies= -840.901182
E(RB-P86) = -841.195423031 A.U

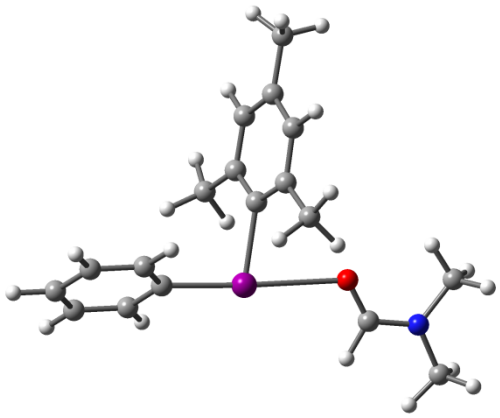


C	3.967698	-0.271166	-1.335125
C	2.566618	-0.197791	-1.267090
C	1.969040	-0.604501	-0.058189
C	2.698246	-1.093730	1.045995
C	4.093225	-1.144904	0.905860
C	4.745878	-0.737557	-0.267448
H	4.458566	0.047727	-2.259061
H	4.684709	-1.517481	1.747216
I	-0.174316	-0.560241	0.106257
C	-0.428425	1.561418	0.179201
C	-1.166053	2.164113	-0.839813
C	0.134874	2.272780	1.238082
C	-1.342137	3.552863	-0.787680
H	-1.597399	1.580852	-1.653803
C	-0.047945	3.661687	1.263144
H	0.698901	1.778235	2.029165
C	-0.783539	4.297666	0.256790
H	-1.914930	4.046693	-1.575294
H	0.384113	4.239907	2.082428
H	-0.922910	5.380131	0.287642
C	-3.603272	-1.202217	-0.316694
O	-2.899087	-0.442874	0.387363
H	-3.162956	-1.835573	-1.112041
N	-4.934133	-1.342645	-0.203202

C	-5.696410	-0.591584	0.792499
H	-6.206402	-1.286886	1.476846
H	-5.007706	0.045239	1.358285
H	-6.452999	0.031885	0.292165
C	-5.675150	-2.255840	-1.070751
H	-4.981212	-2.749434	-1.763058
H	-6.185827	-3.021501	-0.466990
H	-6.428227	-1.701289	-1.651421
C	1.788938	0.308135	-2.455699
H	1.003343	-0.401384	-2.759881
H	1.296715	1.269540	-2.238595
H	2.457433	0.461773	-3.313000
C	2.065600	-1.570894	2.332415
H	1.438518	-0.796093	2.799408
H	1.427016	-2.453828	2.168996
H	2.843465	-1.853143	3.054108
C	6.248028	-0.824803	-0.380362
H	6.737950	-0.473066	0.539996
H	6.566005	-1.869153	-0.536701
H	6.622936	-0.230922	-1.225357

***syn*-[Mes(Ph)I(DMF)]$^{+}$**

Zero-point correction= 0.354587 (Hartree/Particle)
Thermal correction to Energy= 0.379935
Thermal correction to Enthalpy= 0.380879
Thermal correction to Gibbs Free Energy= 0.293996
Sum of electronic and zero-point Energies= -840.841659
Sum of electronic and thermal Energies= -840.816311
Sum of electronic and thermal Enthalpies= -840.815367
Sum of electronic and thermal Free Energies= -840.902250
E(RB-P86) = -841.196245508 A.U.

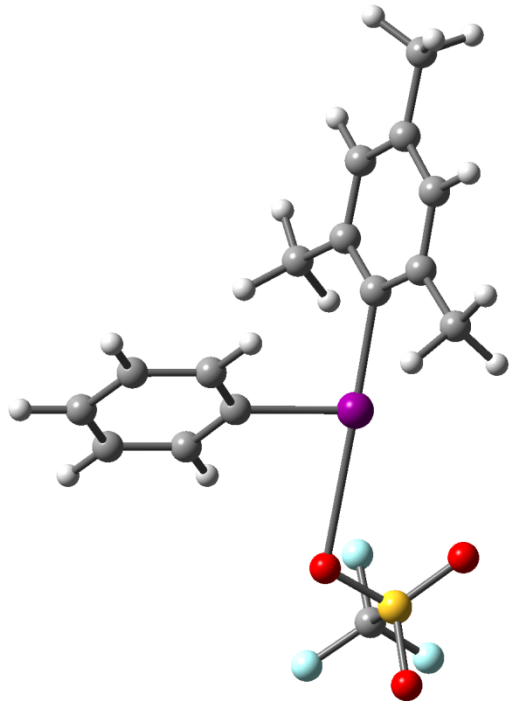


C	-4.474779	-1.004170	1.106617
C	-3.099353	-0.743985	1.135818
C	-2.298123	-1.292958	0.131134
C	-2.821751	-2.098384	-0.884305
C	-4.198678	-2.358189	-0.888504

C	-5.022014	-1.809884	0.100483
H	-5.115500	-0.578423	1.881763
H	-2.678470	-0.125739	1.929919
H	-2.181407	-2.517500	-1.662740
H	-4.622403	-2.985694	-1.675396
H	-6.095162	-2.011282	0.088829
I	-0.170931	-0.986504	0.150757
C	-0.179960	1.147857	-0.013564
C	0.197819	1.886442	1.122949
C	-0.543098	1.714440	-1.247922
C	0.180672	3.283401	0.984285
C	-0.540754	3.118312	-1.307905
C	-0.184756	3.916303	-0.212708
H	0.466518	3.890170	1.848260
H	-0.825508	3.593598	-2.250754
C	3.260743	-1.484524	-0.052150
O	2.499608	-0.497551	0.081417
H	2.871324	-2.520954	-0.090063
N	4.596066	-1.414987	-0.162373
C	5.297135	-0.132463	-0.131731
H	5.855431	0.010611	-1.069399
H	4.561938	0.670723	-0.012691
H	6.006658	-0.114947	0.709536
C	5.407694	-2.620767	-0.318228
H	4.758081	-3.505275	-0.320844
H	5.965332	-2.581431	-1.266401
H	6.125218	-2.703948	0.512256
C	0.626170	1.268902	2.430816
H	-0.166353	0.643855	2.871114
H	1.513880	0.631514	2.295331
H	0.876463	2.053728	3.156557
C	-0.925300	0.914380	-2.466815
H	-0.145624	0.183610	-2.732788
H	-1.861738	0.356203	-2.308783
H	-1.074446	1.579913	-3.327048
C	-0.164772	5.420923	-0.324830
H	-0.494343	5.895978	0.610749
H	0.857823	5.779986	-0.529719
H	-0.809064	5.771516	-1.143173

***anti*-Mes(Ph)I(OTf)**

Zero-point correction= 0.279876 (Hartree/Particle)
Thermal correction to Energy= 0.306874
Thermal correction to Enthalpy= 0.307818
Thermal correction to Gibbs Free Energy= 0.214773
Sum of electronic and zero-point Energies= -1554.224585
Sum of electronic and thermal Energies= -1554.197587
Sum of electronic and thermal Enthalpies= -1554.196643
Sum of electronic and thermal Free Energies= -1554.289687
E(RB-P86) = -1554.50446068 A.U.

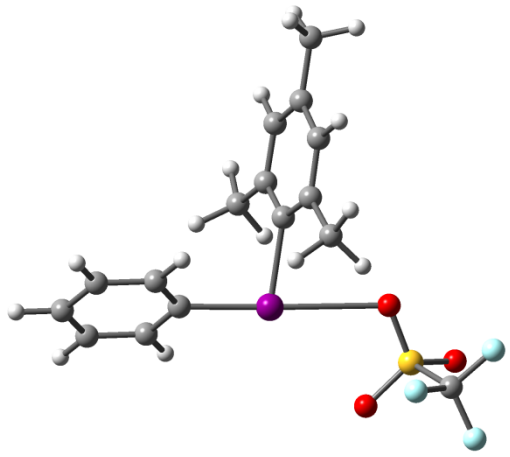


C	-4.208840	-0.722041	1.519934
C	-2.854375	-0.403970	1.339814
C	-2.301771	-0.685392	0.073645
C	-3.023497	-1.282137	-0.979700
C	-4.371808	-1.580901	-0.725267
C	-4.981727	-1.308957	0.507186
H	-4.667697	-0.502798	2.488287
H	-4.959821	-2.040156	-1.524888
I	-0.234088	-0.241541	-0.266230
C	-0.418236	1.894743	-0.269617
C	0.491872	2.625337	0.493135
C	-1.426360	2.484363	-1.030860
C	0.378215	4.021964	0.485195
H	1.271507	2.133275	1.074604
C	-1.525167	3.881748	-1.014384
H	-2.126380	1.889435	-1.618866
C	-0.626267	4.646539	-0.262085
H	1.079055	4.615714	1.075706
H	-2.308446	4.366174	-1.601050
H	-0.709835	5.735180	-0.258031
C	4.184994	-0.735937	0.933092
S	3.311473	-0.835371	-0.741670
F	3.285562	-0.718148	1.946972
F	4.938921	0.385755	1.022170
F	4.998265	-1.804325	1.113395
O	4.420396	-0.840224	-1.712095
O	2.519281	-2.081061	-0.644245
O	2.482377	0.408260	-0.755159
C	-2.073108	0.214846	2.471081

H	-1.188521	-0.388870	2.729678
H	-1.716536	1.225226	2.214654
H	-2.700484	0.298216	3.368163
C	-2.430329	-1.618219	-2.327494
H	-1.995282	-0.734912	-2.820062
H	-1.631573	-2.372278	-2.243153
H	-3.204738	-2.026309	-2.990367
C	-6.427938	-1.664379	0.749234
H	-6.997671	-1.689331	-0.190429
H	-6.508248	-2.662857	1.211232
H	-6.907320	-0.949094	1.433137

***syn*-Mes(Ph)I(OTf)**

Zero-point correction= 0.280119 (Hartree/Particle)
Thermal correction to Energy= 0.307033
Thermal correction to Enthalpy= 0.307977
Thermal correction to Gibbs Free Energy= 0.215248
Sum of electronic and zero-point Energies= -1554.224818
Sum of electronic and thermal Energies= -1554.197903
Sum of electronic and thermal Enthalpies= -1554.196959
Sum of electronic and thermal Free Energies= -1554.289688
E(RB-P86) = -1554.50493660 A.U



C	4.215562	-2.186899	-1.519992
C	3.027928	-1.472810	-1.321657
C	2.237317	-1.797168	-0.217111
C	2.582098	-2.809854	0.681660
C	3.767481	-3.522888	0.456387
C	4.581995	-3.210010	-0.636971
H	4.848929	-1.942821	-2.375471
H	4.052128	-4.318309	1.148278
I	0.377945	-0.776588	0.104802
C	1.148269	1.219746	0.079432
C	0.842303	2.021181	-1.037524
C	1.903469	1.648616	1.184634
C	1.363178	3.323781	-1.022866

C	2.396070	2.963754	1.124221
C	2.141618	3.810989	0.038483
H	1.146365	3.975303	-1.874254
H	2.993789	3.329311	1.963905
C	-4.239057	-0.243332	-0.676994
S	-3.150788	-0.324626	0.868411
F	-3.558053	-0.656090	-1.773284
F	-4.669532	1.021087	-0.901851
F	-5.326595	-1.038787	-0.535709
O	-4.044676	0.142245	1.943186
O	-2.737173	-1.743204	0.928484
O	-2.036084	0.616370	0.539146
C	-0.007389	1.564389	-2.196907
H	0.425125	0.686895	-2.702389
H	-1.018057	1.286297	-1.860534
H	-0.101123	2.368307	-2.938557
C	2.201703	0.791568	2.388111
H	1.278179	0.412564	2.853412
H	2.819701	-0.080895	2.122415
H	2.748469	1.372275	3.142333
C	2.681290	5.219785	0.007955
H	3.305045	5.383280	-0.885087
H	1.860843	5.953896	-0.034535
H	3.289144	5.436633	0.896861
H	2.741524	-0.684031	-2.018668
H	5.507336	-3.765565	-0.802576
H	1.952224	-3.044208	1.541675

***p*-MeOC$_6$H$_4$F**

Zero-point correction= 0.120196 (Hartree/Particle)
Thermal correction to Energy= 0.128196
Thermal correction to Enthalpy= 0.129140
Thermal correction to Gibbs Free Energy= 0.087529
Sum of electronic and zero-point Energies= -446.024367
Sum of electronic and thermal Energies= -446.016367
Sum of electronic and thermal Enthalpies= -446.015423
Sum of electronic and thermal Free Energies= -446.057034
E(RB-P86) = -446.144563009 A.U.

C	-1.830002	-0.119944	-0.000003
C	-1.343837	1.186719	0.000009
C	-0.986201	-1.221914	-0.000084
C	0.036129	1.387638	-0.000021
H	-2.036105	2.030496	0.000040
C	0.401871	-1.017711	-0.000130
H	-1.401224	-2.231376	-0.000113
C	0.916354	0.289143	-0.000091
H	0.448949	2.398506	-0.000025
H	1.062277	-1.884448	-0.000250
F	-3.189436	-0.320387	0.000129
O	2.254050	0.598846	-0.000119

C	3.186092	-0.495268	0.000194
H	3.067940	-1.118608	-0.901063
H	4.180943	-0.035270	0.000519
H	3.067297	-1.118555	0.901424

***p*-MeOC$_6$H$_4$I**

Zero-point correction= 0.118300 (Hartree/Particle)
Thermal correction to Energy= 0.127023
Thermal correction to Enthalpy= 0.127968
Thermal correction to Gibbs Free Energy= 0.082862
Sum of electronic and zero-point Energies= -357.576932
Sum of electronic and thermal Energies= -357.568208
Sum of electronic and thermal Enthalpies= -357.567264
Sum of electronic and thermal Free Energies= -357.612369
E(RB-P86) = -357.695231496 A.U.

C	-0.205176	0.082013	-0.000011
C	0.400324	1.347186	0.000028
C	0.575492	-1.075020	-0.000020
C	1.791182	1.443912	0.000060
H	-0.203256	2.256670	0.000035
C	1.973991	-0.979534	0.000011
H	0.109899	-2.061666	-0.000053
C	2.587727	0.283450	0.000052
H	2.277440	2.421961	0.000092
H	2.563813	-1.896164	-0.000003
O	3.941531	0.487653	0.000076
C	4.787117	-0.676900	0.000176
H	4.619304	-1.287802	-0.901206
H	5.814203	-0.294882	0.000268
H	4.619128	-1.287773	0.901543
I	-2.316919	-0.081174	-0.000058

***p*-NO$_2$C$_6$H$_4$F**

Zero-point correction= 0.091056 (Hartree/Particle)
Thermal correction to Energy= 0.098959
Thermal correction to Enthalpy= 0.099903
Thermal correction to Gibbs Free Energy= 0.057512
Sum of electronic and zero-point Energies= -536.092506
Sum of electronic and thermal Energies= -536.084602
Sum of electronic and thermal Enthalpies= -536.083658
Sum of electronic and thermal Free Energies= -536.126049
E(RB-P86) = -536.183561626 A.U.

C	2.060948	0.000003	-0.000038
C	1.395902	-1.227083	-0.000051
C	1.395873	1.227073	0.000045
C	0.003161	-1.225041	-0.000108
H	1.963394	-2.158245	-0.000132
C	0.003132	1.225029	0.000154
H	1.963375	2.158231	0.000126

C	-0.674696	-0.000011	0.000024
H	-0.559734	-2.157705	-0.000166
H	-0.559768	2.157688	0.000220
F	3.417227	0.000028	-0.000002
N	-2.142980	-0.000060	0.000042
O	-2.729220	1.096752	-0.000259
O	-2.729201	-1.096705	0.000199

_p_-$NO_2C_6H_4I$

Zero-point correction= 0.088775 (Hartree/Particle)
Thermal correction to Energy= 0.097469
Thermal correction to Enthalpy= 0.098413
Thermal correction to Gibbs Free Energy= 0.052354
Sum of electronic and zero-point Energies= -447.642914
Sum of electronic and thermal Energies= -447.634219
Sum of electronic and thermal Enthalpies= -447.633275
Sum of electronic and thermal Free Energies= -447.679335
E(RB-P86) = -447.731688450 A.U.

C	0.436148	-0.000001	0.000007
C	-0.253077	-1.222237	-0.000069
C	-0.253077	1.222235	0.000079
C	-1.647253	-1.222646	-0.000072
H	0.288370	-2.168744	-0.000130
C	-1.647253	1.222647	0.000067
H	0.288370	2.168743	0.000142
C	-2.326157	0.000001	-0.000009
H	-2.207351	-2.157362	-0.000129
H	-2.207351	2.157362	0.000119
N	-3.796022	-0.000004	-0.000014
O	-4.381380	1.097085	-0.000061
O	-4.381380	-1.097082	0.000072
I	2.540683	0.000000	0.000000

PhF

Zero-point correction= 0.089091 (Hartree/Particle)
Thermal correction to Energy= 0.094425
Thermal correction to Enthalpy= 0.095369
Thermal correction to Gibbs Free Energy= 0.060144
Sum of electronic and zero-point Energies= -331.493963
Sum of electronic and thermal Energies= -331.488629
Sum of electronic and thermal Enthalpies= -331.487685
Sum of electronic and thermal Free Energies= -331.522910
E(RB-P86) = -331.583054196

C	0.926059	0.000001	0.000018
C	0.260861	1.222812	0.000004
C	0.260861	-1.222812	0.000001
C	-1.139787	1.212557	-0.000001
H	0.828515	2.154997	-0.000003
C	-1.139786	-1.212557	-0.000003

H	0.828518	-2.154995	-0.000007
C	-1.840875	0.000000	0.000010
H	-1.681721	2.160880	-0.000003
H	-1.681721	-2.160880	-0.000008
H	-2.932737	-0.000001	0.000012
F	2.297238	0.000000	-0.000018

PhI

Zero-point correction= 0.087011 (Hartree/Particle)
Thermal correction to Energy= 0.093070
Thermal correction to Enthalpy= 0.094015
Thermal correction to Gibbs Free Energy= 0.055129
Sum of electronic and zero-point Energies= -243.044927
Sum of electronic and thermal Energies= -243.038868
Sum of electronic and thermal Enthalpies= -243.037924
Sum of electronic and thermal Free Energies= -243.076810
E(RB-P86) = -243.131938219

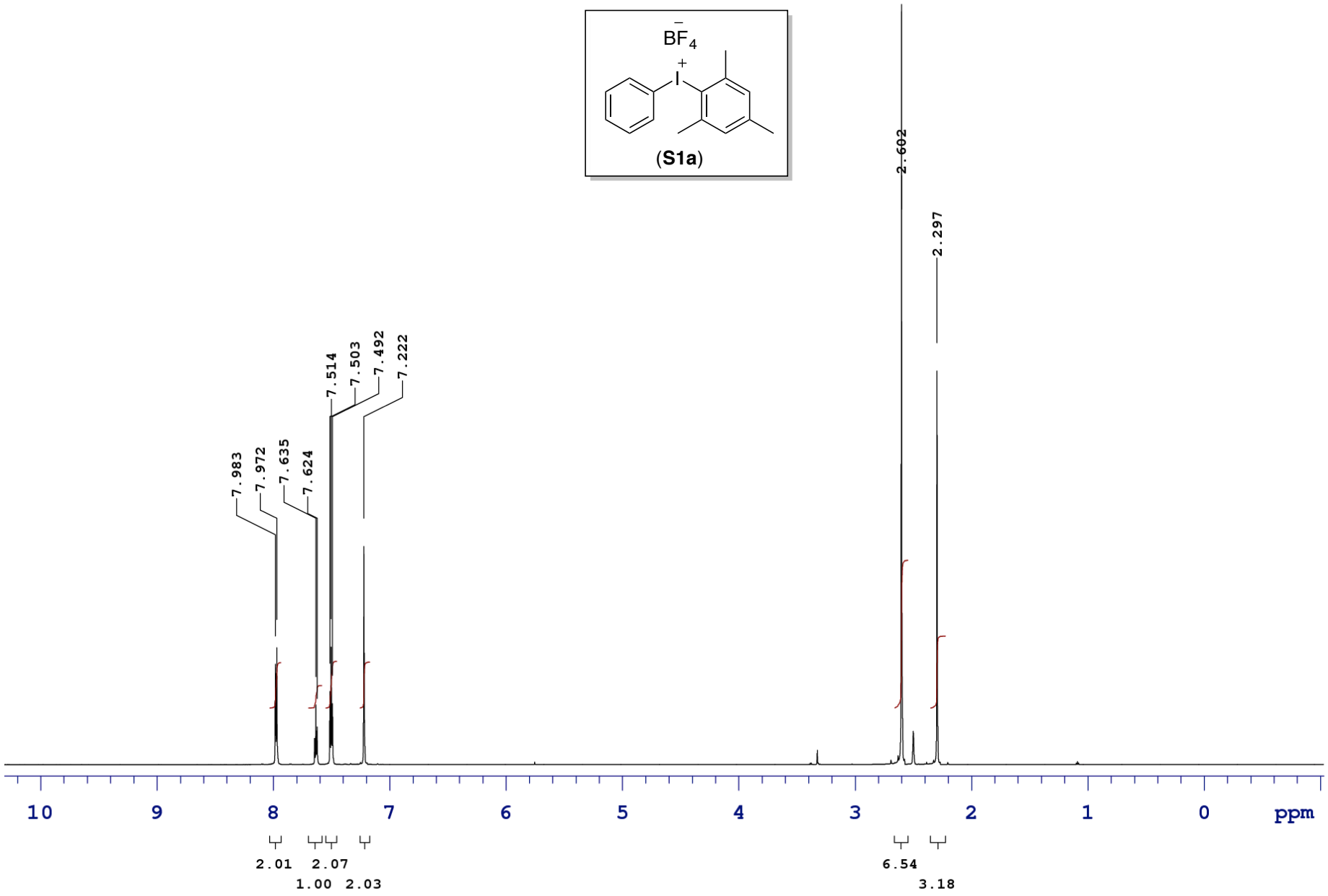
C	-2.650496	-1.210673	0.000003
C	-1.249408	-1.219590	0.000001
C	-0.562925	0.000000	0.000001
C	-1.249408	1.219590	0.000002
C	-2.650496	1.210673	0.000003
C	-3.352634	0.000000	0.000004
H	-3.189971	-2.160779	0.000003
H	-0.706401	-2.166121	0.000001
H	-0.706401	2.166121	0.000001
H	-3.189971	2.160779	0.000004
H	-4.444737	0.000000	0.000005
I	1.557164	0.000000	-0.000002

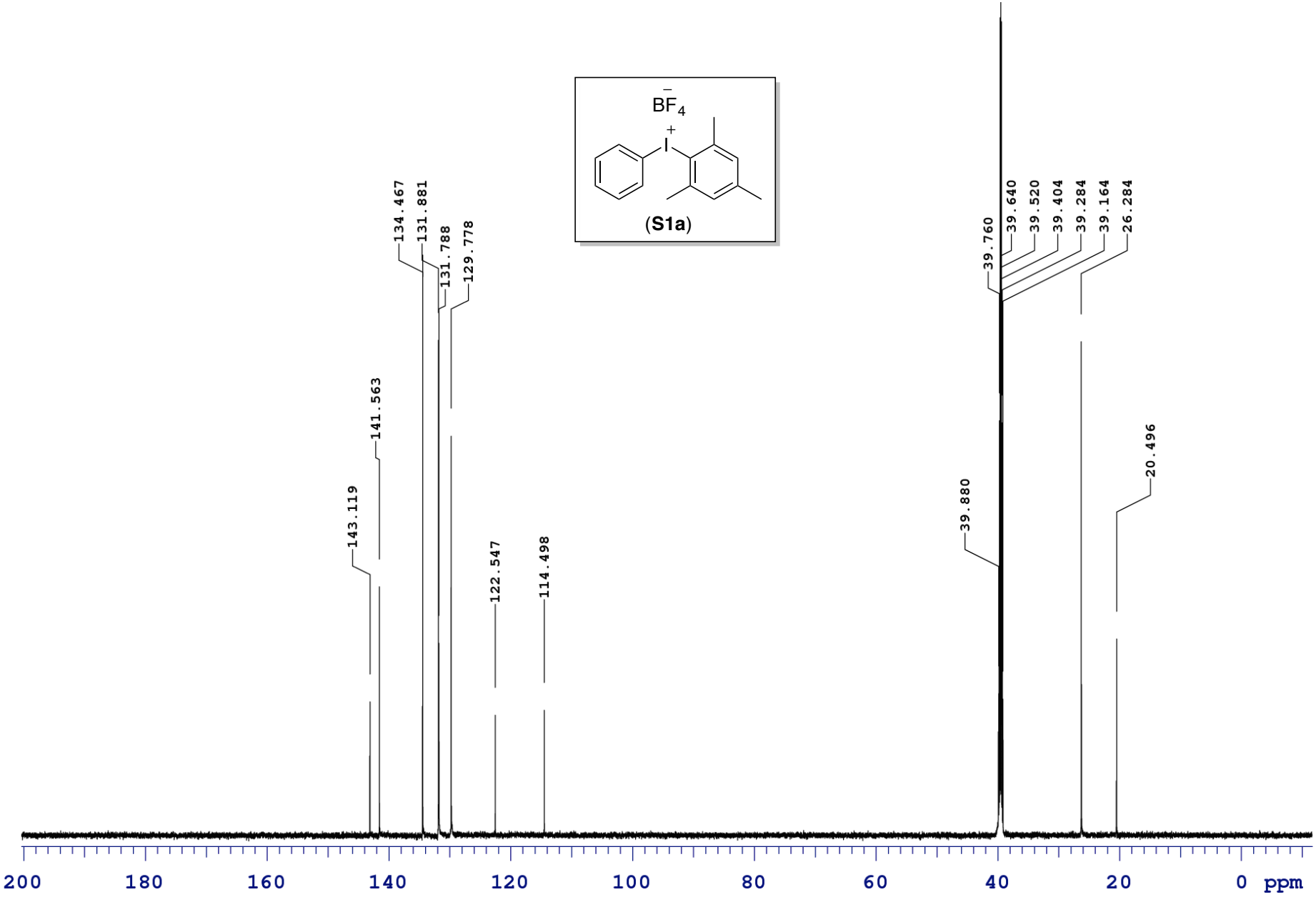
Triflate

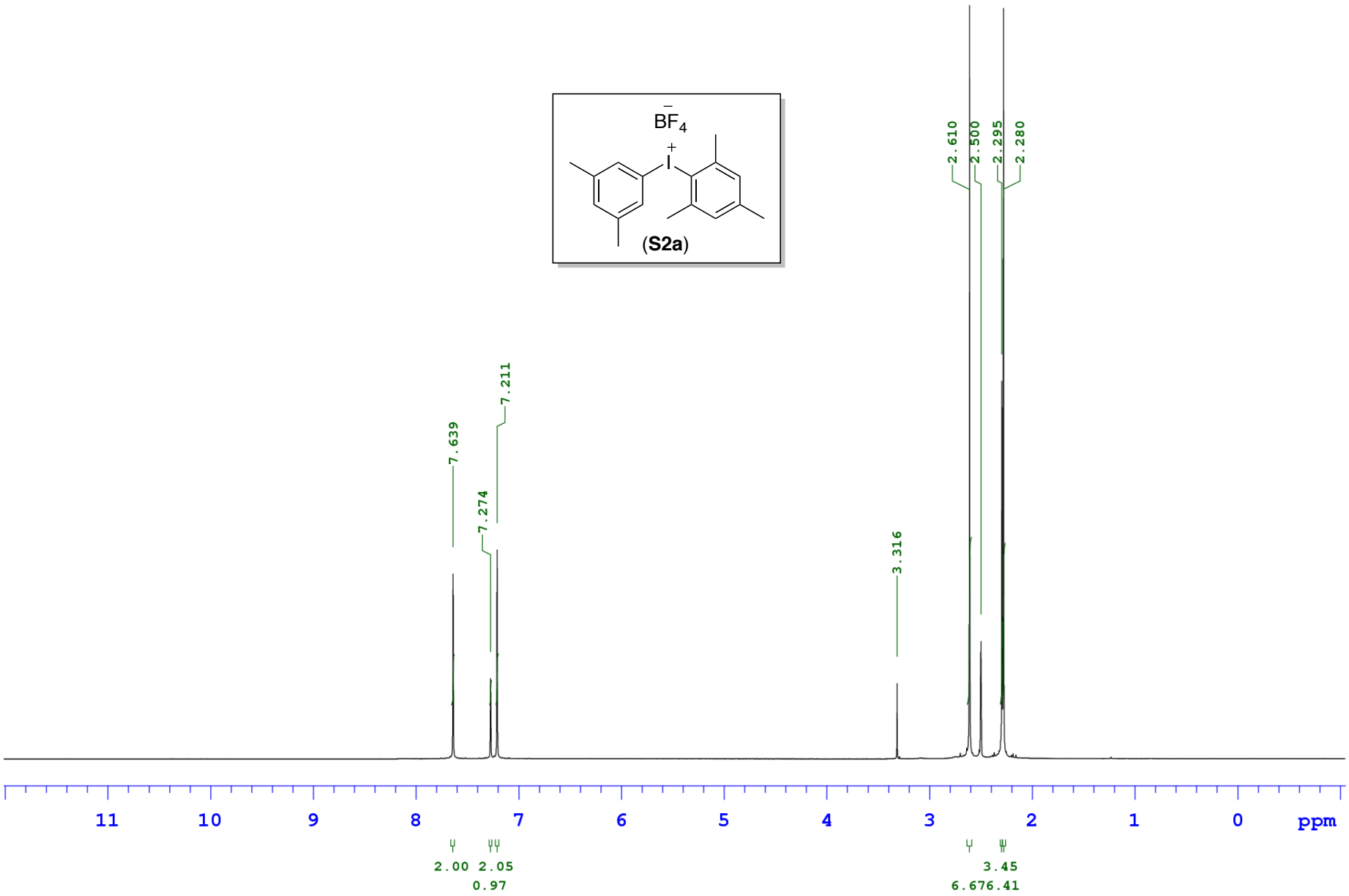
Zero-point correction= 0.025069 (Hartree/Particle)
Thermal correction to Energy= 0.032555
Thermal correction to Enthalpy= 0.033499
Thermal correction to Gibbs Free Energy= -0.007757
Sum of electronic and zero-point Energies= -961.884545
Sum of electronic and thermal Energies= -961.877059
Sum of electronic and thermal Enthalpies= -961.876115
Sum of electronic and thermal Free Energies= -961.917371
E(RB-P86) = -961.909614744

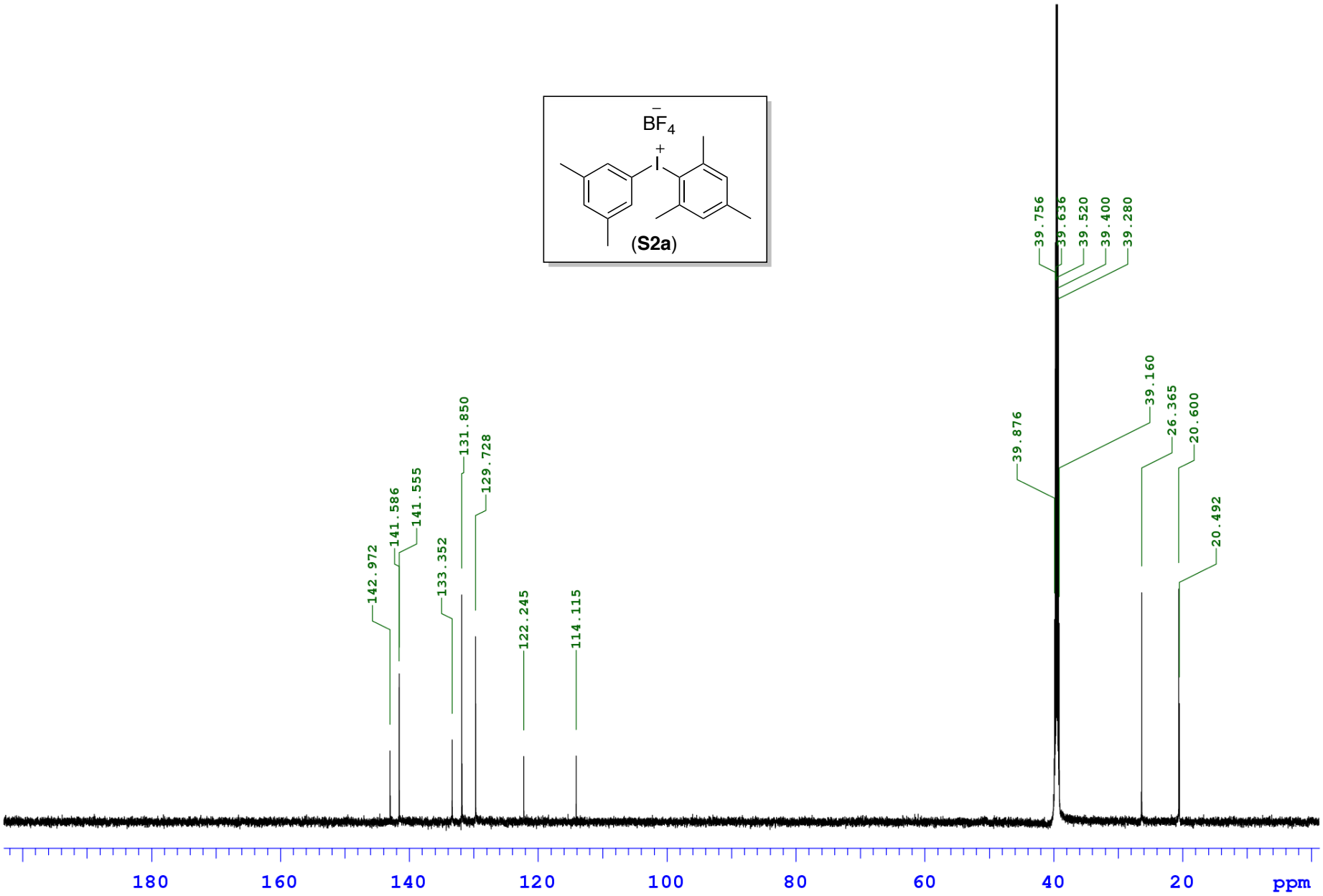
C	-0.963869	0.000049	-0.000001
S	0.928228	-0.000025	-0.000004
F	-1.455632	-0.643848	1.089799
F	-1.455569	-0.621948	-1.102516
F	-1.455539	1.265870	0.012661
O	1.259763	0.734515	-1.242160
O	1.259684	0.708522	1.257177
O	1.259583	-1.443107	-0.014946

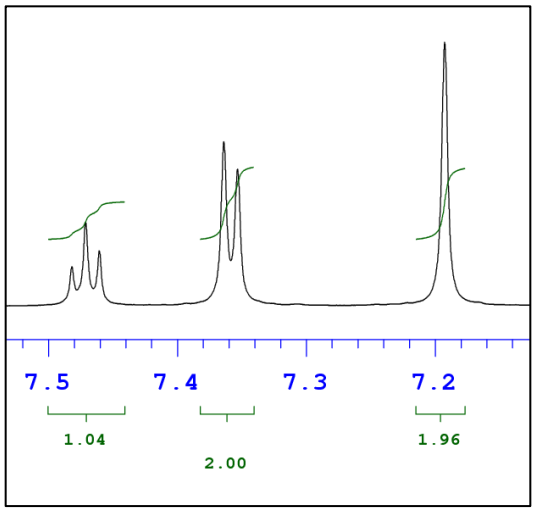
V. ^{1}H, ^{13}C, and ^{19}F NMR Spectra of Diaryliodonium Salts

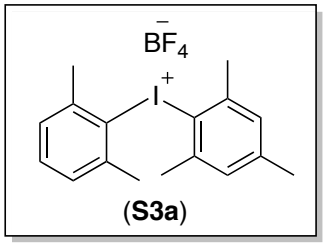

BF4
(S1a)
7.983
7.972
7.635
7.624
7.514
7.503
7.492
7.222
2.602
2.297
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.07
1.00
2.03
6.54
3.18


BF4
(S1a)
143.119
141.563
134.467
131.881
131.788
129.778
122.547
114.498
39.880
39.760
39.640
39.520
39.404
39.284
39.164
26.284
20.496
200
180
160
140
120
100
80
60
40
20
0
ppm


BF4
(S2a)
7.639
7.274
7.211
3.316
2.610
2.500
2.295
2.280
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00 2.05
0.97
3.45
6.676.41

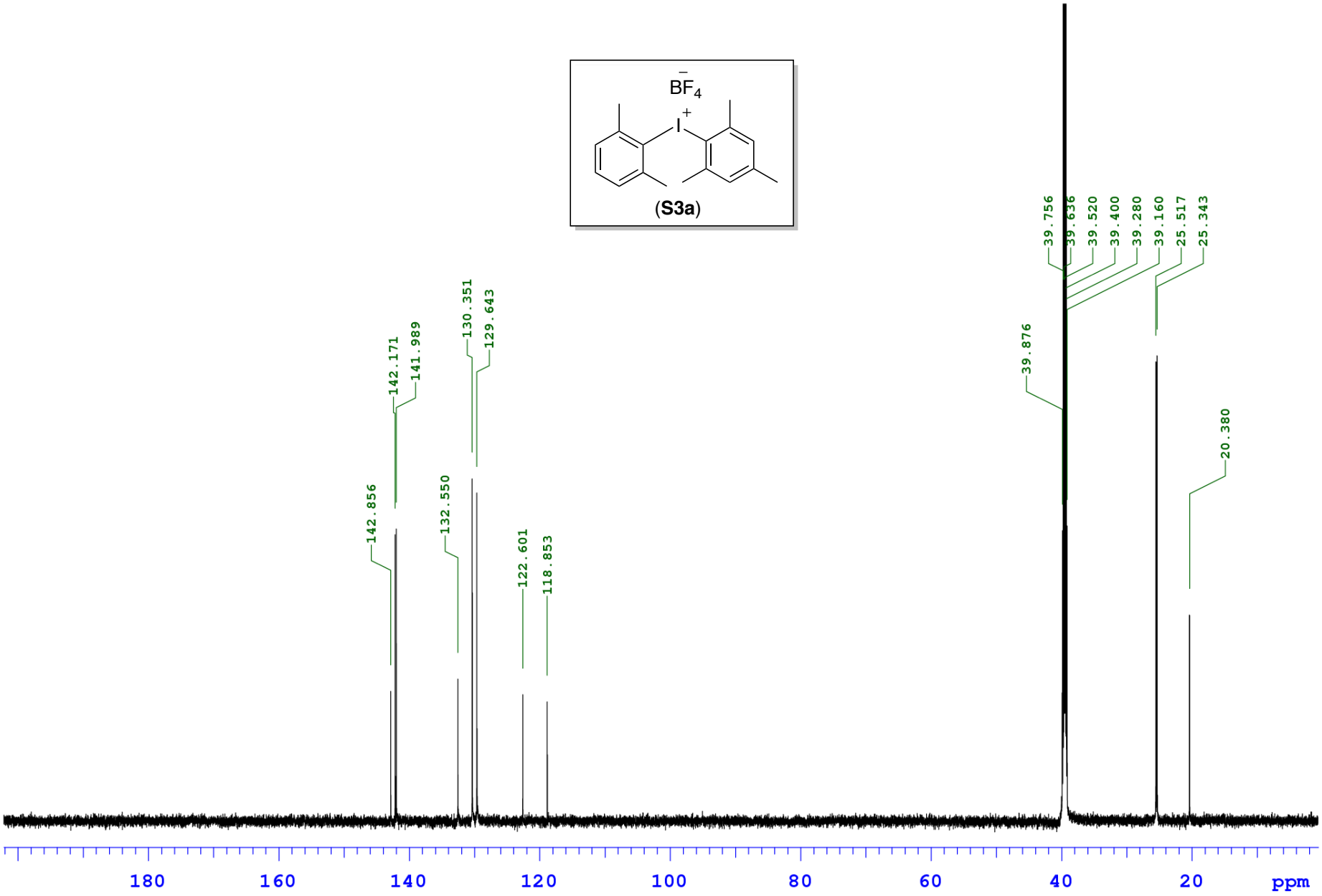

BF4
(S2a)
142.972
141.586
141.555
133.352
131.850
129.728
122.245
114.115
39.876
39.756
39.636
39.520
39.400
39.280
39.160
26.365
20.600
20.492
180
160
140
120
100
80
60
40
20
ppm

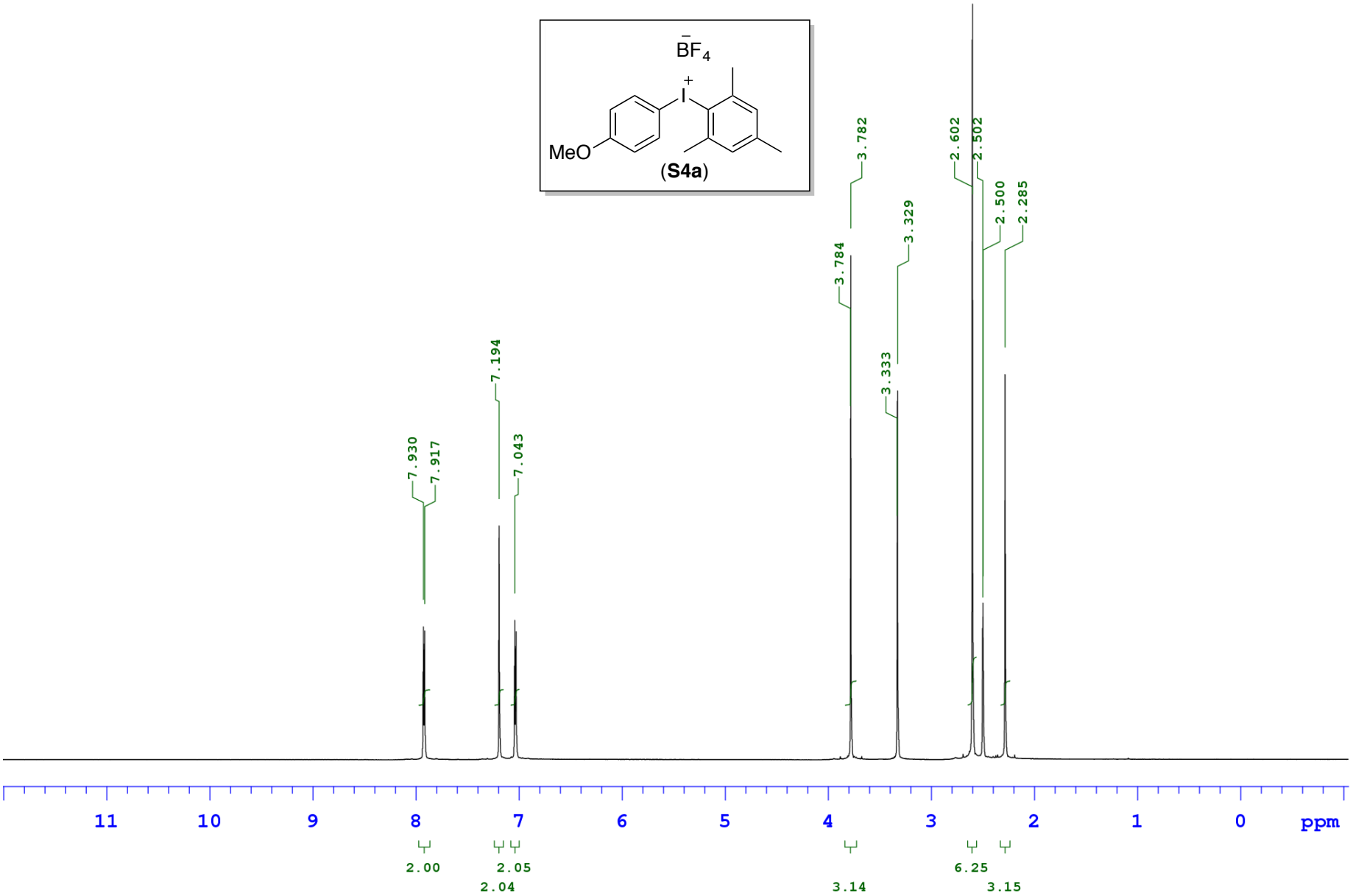

7.5
7.4
7.3
7.2
1.04
2.00
1.96

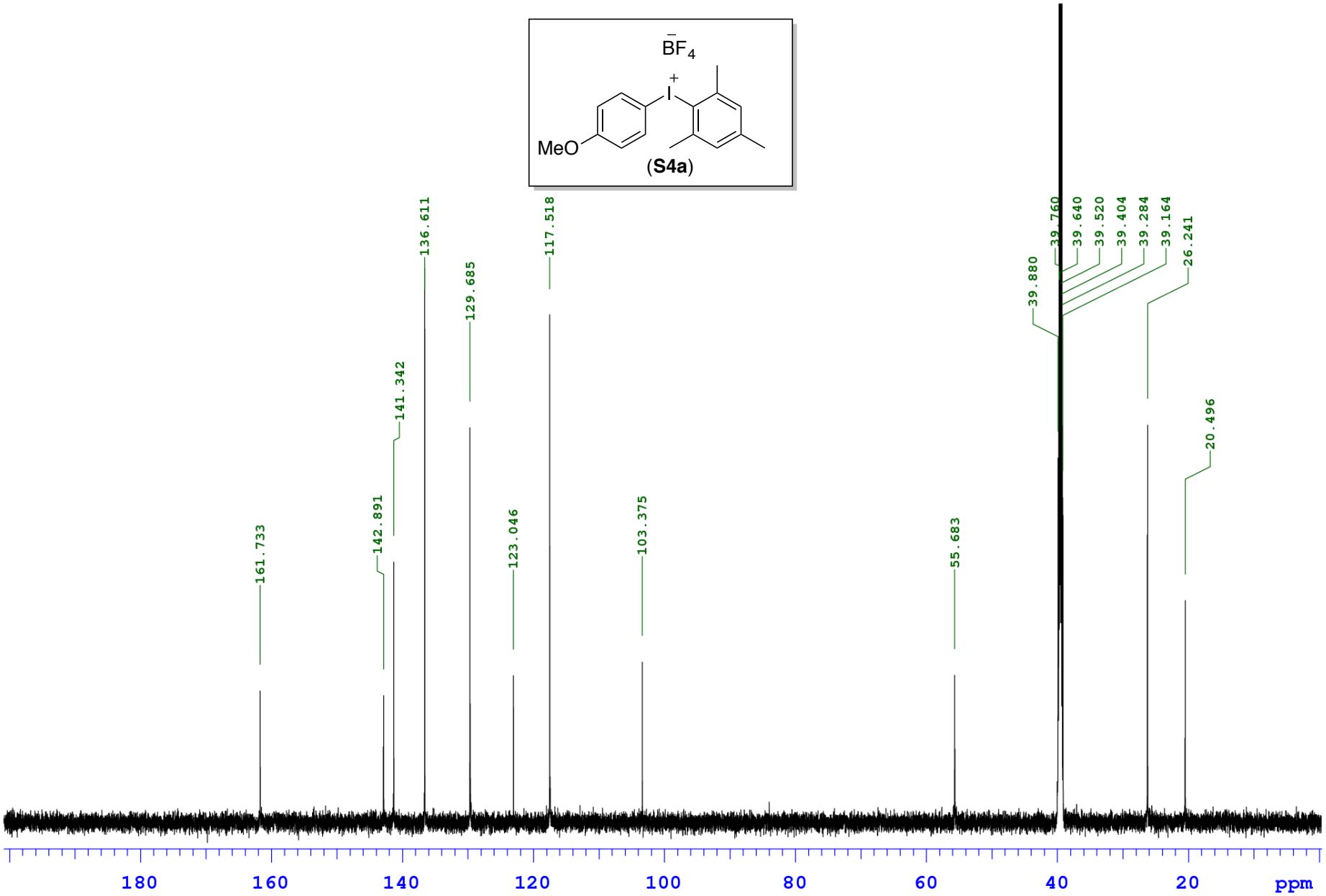

BF4
I+

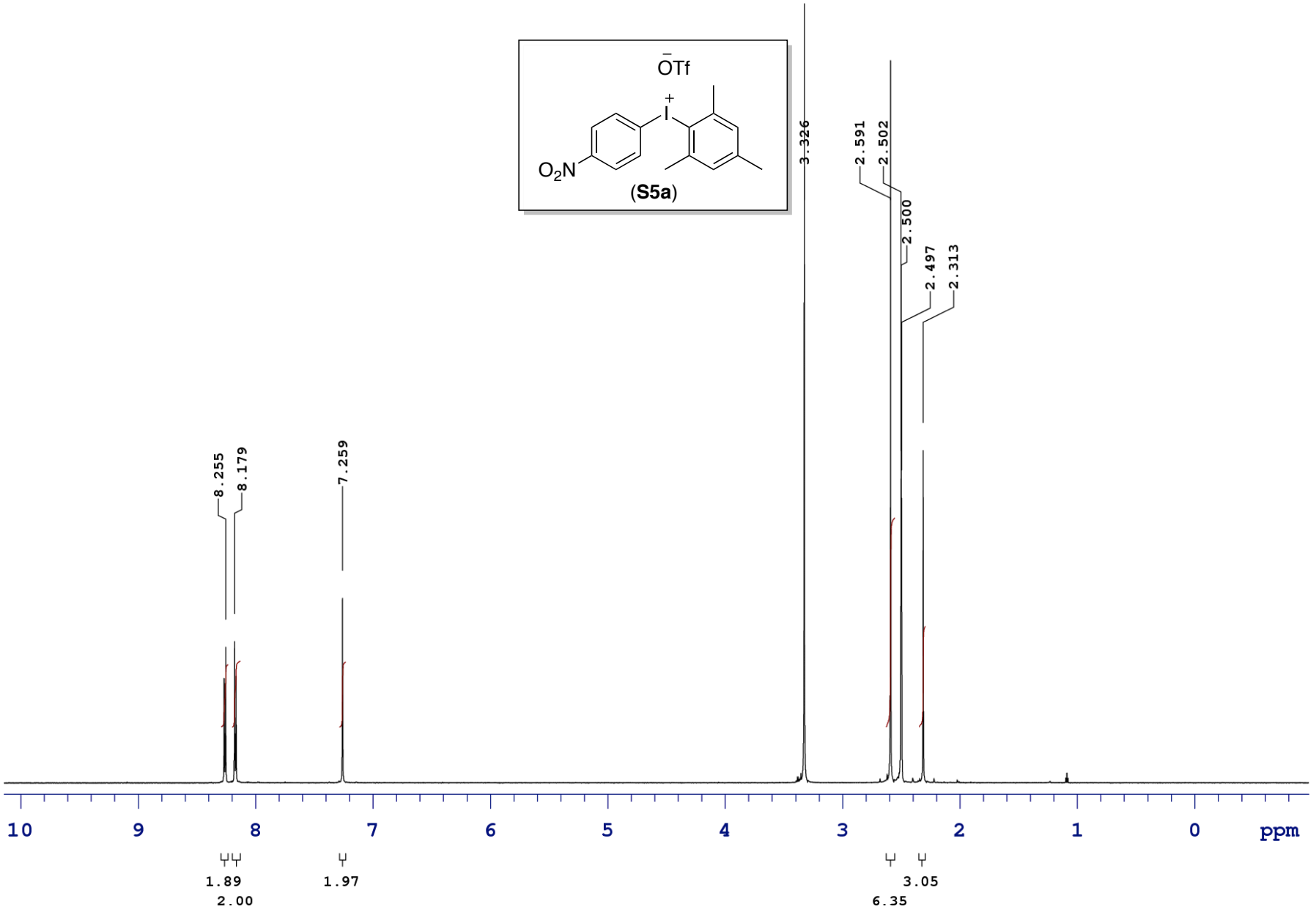
(**S3a**)

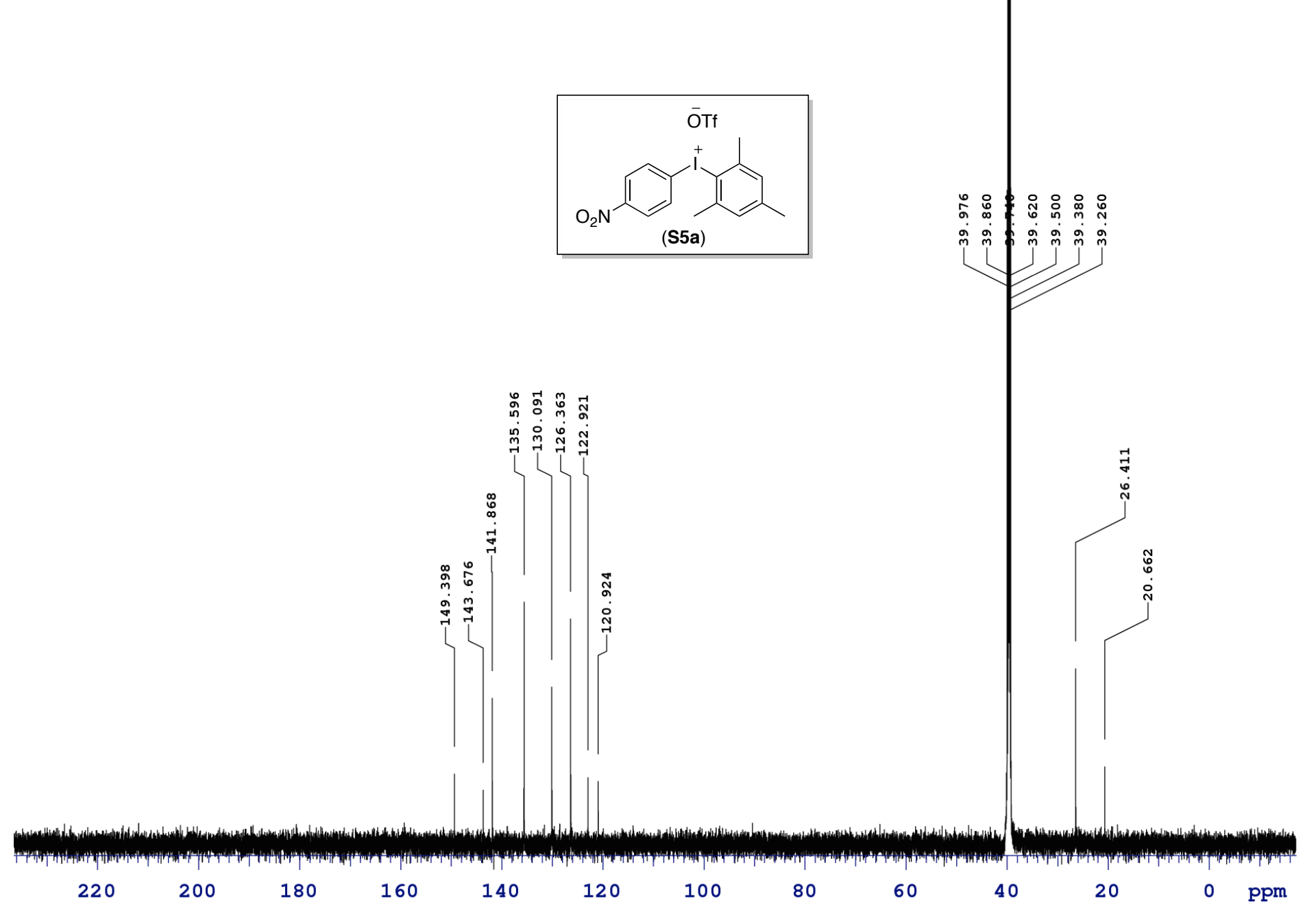
2.500
2.456
2.280
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.04
4.96
2.00
3.11
6.68


BF4
I+
(S3a)
142.856
142.171
141.989
132.550
130.351
129.643
122.601
118.853
39.876
39.756
39.636
39.520
39.400
39.280
39.160
25.517
25.343
20.380
180
160
140
120
100
80
60
40
20
ppm


BF4
MeO
(S4a)
7.930
7.917
7.194
7.043
3.784
3.782
3.333
3.329
2.602
2.502
2.500
2.285
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.05
2.04
3.14
6.25
3.15


BF4
MeO
(S4a)
161.733
142.891
141.342
136.611
129.685
123.046
117.518
103.375
55.683
39.880
39.760
39.640
39.520
39.404
39.284
39.164
26.241
20.496
180
160
140
120
100
80
60
40
20
ppm


OTf
I
O2N
(S5a)
8.255
8.179
7.259
3.326
2.591
2.502
2.500
2.497
2.313
10
9
8
7
6
5
4
3
2
1
0
ppm
1.89
2.00
1.97
6.35
3.05


OTf
I
O2N
(S5a)
149.398
143.676
141.868
135.596
130.091
126.363
122.921
120.924
39.976
39.860
39.620
39.500
39.380
39.260
26.411
20.662
220
200
180
160
140
120
100
80
60
40
20
0
ppm