Anexo V

Coordenadas cartesianas de cálculos teóricos

ILUROS DE AZOMETINO TRIFLUOROMETILADOS EN REACCIONES DE CICLOADICIÓN 1,3-DIPOLAR CATALÍTICA ASIMÉTRICA

1. Theoretical calculations

Geometries were initially fully optimized at the DFT (B3LYP)[1] level. LANL2DZ + f (1.611) basis set[2] with effective core potential (ECP) was used for Ag and the standard 6-31G(d)[3] basis for all other atoms. Single point energies were calculated at the M06[4] / LANL2TZ(f)[5]-6-311+G(2df,2p)[6] level which is generally considered to be more accurate for energetics. The reported free energies include zero-point energies and thermal corrections calculated at 298 K with B3LYP/LANL2DZ(f)-6-31G(d). Solvation energy corrections were also calculated by M06 / LANL2TZ(f)–6-311+G(2df,2p) single point calculations with the SMD solvation model[7] in THF for all structures. All calculations were performed with Gaussian 09.[8]

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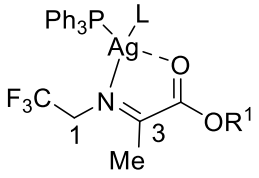
[5] (a) P. J. Hay, W. R. Wadt, *J. Chem. Phys*. **1985**, *82*, 270.(b) P. J. Hay, W. R. Wadt, *J. Chem. Phys*. **1985**, *82*, 284. (c) P. J. Hay, W. R. Wadt, *J. Chem. Phys*. **1985**, *82*, 299.

[6] (a) A. D. McLean and G. S. Chandler, *J. Chem. Phys*. **1980**, *72,* 5639-48. (b) K. Raghavachari, J. S. Binkley, R. Seeger, and J. A. Pople, *J. Chem. Phys.*, **1980**, *72,* 650-54. (c) T. Clark, J. Chandrasekhar, G.W. Spitznagel, P.V.R. Schleyer, *J. Comp. Chem*. **1983**, *4*, 294.

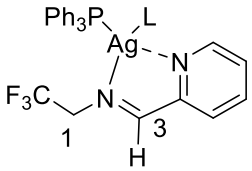
[7] A. V, Marenich, C. J. Cramer, D. G. Truhlar. *J. Phys. Chem. B* **2009**, *113*, 6378.

[8] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Table S1. Natural charges (q_i) from the NBO analysis of complexes **IA**, **IB**, **IIA** and **IIB**.



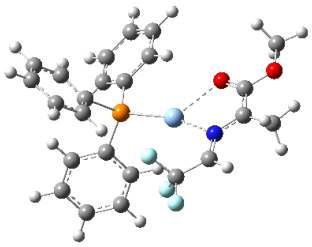
IA, without L
IB, L=OAc



IIA, without L
IIB, L=OAc

	IA	**IB**	**IIA**	**IIB**
q_1	-0.18	-0.20	-0.18	-0.20
q_3	-0.04	-0.06	-0.13	-0.14

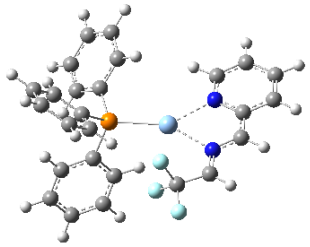
Cartesian coordinates (Å) and energies (hartrees) of all the optimized structures.



IA

E(RB3LYP) = -1919.66577184
H(correction)= 0.442559
G(correction)= 0.338760
E(RM06) = -1919.25775737
E(SMD$_{THF}$RM06) = -1919.28376002
Number of imaginary frequencies: 0

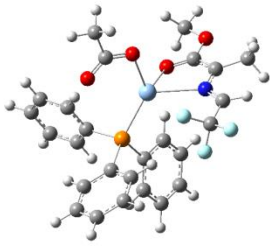
47	0	1.00666	0.09401	-0.05971
15	0	-1.42253	0.17428	-0.00351
7	0	3.17667	-0.63765	-0.05017
6	0	-2.27905	-0.75018	-1.34413
6	0	-2.05008	1.89835	-0.14144
6	0	-2.12111	-0.4983	1.56081
6	0	3.45309	-1.92043	-0.07659
6	0	4.10346	0.34007	-0.0288
6	0	-1.68058	-0.77964	-2.61383
6	0	-3.49844	-1.41549	-1.14707
6	0	-3.34436	2.19602	-0.59871
6	0	-1.19161	2.94935	0.22048
6	0	-3.20051	0.09365	2.23336
6	0	-1.53036	-1.65696	2.09417
1	0	4.46202	-2.32309	-0.07072
6	0	2.35178	-2.90598	-0.06517
6	0	3.6047	1.6798	0.00757
6	0	5.5689	0.00991	-0.03521
1	0	-0.72409	-0.28732	-2.77282
6	0	-2.29968	-1.44534	-3.6712
6	0	-4.11244	-2.08669	-2.20653
1	0	-3.96324	-1.41926	-0.16576
1	0	-4.00908	1.39493	-0.90872
6	0	-3.77767	3.52019	-0.67314
6	0	-1.63202	4.27227	0.14854
1	0	-0.17325	2.73861	0.53816
6	0	-3.68769	-0.47023	3.41451
1	0	-3.6565	0.99815	1.84313
6	0	-2.02694	-2.21994	3.26978
1	0	-0.67826	-2.11469	1.59848
9	0	2.82754	-4.16242	-0.17378
9	0	1.58896	-2.87347	1.08374
9	0	1.43732	-2.73162	-1.07076
8	0	2.40328	2.03459	0.01219
8	0	4.582	2.63067	0.03985
1	0	5.84638	-0.60559	0.83538
1	0	5.84524	-0.57165	-0.92906
1	0	6.17678	0.91456	-0.018
1	0	-1.82543	-1.46253	-4.64845
6	0	-3.5169	-2.10017	-3.46894
1	0	-5.05433	-2.60315	-2.04221
1	0	-4.77982	3.73999	-1.03135
6	0	-2.92378	4.55943	-0.2954
1	0	-0.95864	5.07745	0.42875
6	0	-3.105	-1.62807	3.93224
1	0	-4.52093	-0.00054	3.93034
1	0	-1.56244	-3.11554	3.67279
6	0	4.13408	3.98481	0.07314
1	0	-3.99431	-2.62725	-4.29046
1	0	-3.26173	5.59035	-0.35795
1	0	-3.48379	-2.06337	4.85302
1	0	3.53217	4.18029	0.96614
1	0	5.04143	4.5918	0.09143
1	0	3.53679	4.22559	-0.81181



IIA

E(RB3LYP) = -1899.56318525
H(correction)= 0.438888
G(correction)= 0.338544
E(RM06) = -1899.10885037
E(SMD$_{THF}$RM06) = -1899.13857089
Number of imaginary frequencies: 0

47	0	1.11162	0.05742	-0.08476
15	0	-1.3142	-0.31826	-0.01505
6	0	-2.0642	0.19921	1.58364
6	0	-1.71569	-2.11247	-0.16266
6	0	-2.33239	0.49406	-1.31503
6	0	-1.28621	0.08366	2.74716
6	0	-3.3694	0.70402	1.68317
6	0	-2.73483	-2.73277	0.57495
6	0	-0.95464	-2.88486	-1.05593
6	0	-3.45644	-0.12152	-1.88832
6	0	-1.96115	1.78057	-1.73925
1	0	-0.26493	-0.28473	2.68199
6	0	-1.80898	0.44882	3.98731
6	0	-3.8873	1.07611	2.92548
1	0	-3.97879	0.81643	0.79171
1	0	-3.32571	-2.15389	1.27818
6	0	-2.98891	-4.0974	0.41728
6	0	-1.21705	-4.24503	-1.21908
1	0	-0.15002	-2.42033	-1.62151
6	0	-4.20112	0.54368	-2.86394
1	0	-3.74727	-1.12143	-1.58118
6	0	-2.7138	2.44231	-2.71024
1	0	-1.08435	2.26489	-1.32168
1	0	-1.19513	0.35616	4.87886
6	0	-3.1107	0.94689	4.07823
1	0	-4.8975	1.47135	2.98979
1	0	-3.77719	-4.56772	0.99896
6	0	-2.23411	-4.85445	-0.48016
1	0	-0.62196	-4.82917	-1.91567
6	0	-3.83267	1.82632	-3.27469
1	0	-5.06696	0.05653	-3.30449
1	0	-2.41613	3.4367	-3.03087
1	0	-3.51462	1.24173	5.04288
1	0	-2.43258	-5.9161	-0.59904
1	0	-4.41166	2.34073	-4.03698
7	0	2.96558	1.51392	-0.00919
6	0	2.86779	2.82306	0.04441
6	0	4.11776	0.84086	0.01351
1	0	3.73527	3.48203	0.08754
6	0	1.54883	3.46825	-0.05124
1	0	5.06222	1.38663	0.06436
6	0	4.16469	-0.58058	-0.02361
9	0	1.63003	4.78884	0.21377
9	0	0.95597	3.36336	-1.29598
9	0	0.60571	2.94017	0.79619
6	0	5.41319	-1.26781	-0.01093
7	0	3.00373	-1.30606	-0.06984
6	0	5.44868	-2.6453	-0.04241
1	0	6.32977	-0.68533	0.02363
6	0	3.06194	-2.64713	-0.09931
6	0	4.24351	-3.37283	-0.08732
1	0	6.40366	-3.16542	-0.03233
1	0	2.10075	-3.15699	-0.13285
1	0	4.22833	-4.45718	-0.11057

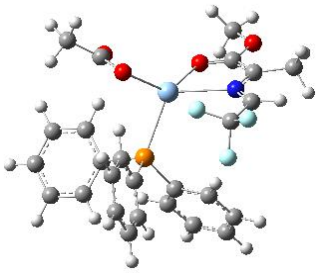


IB

E(RB3LYP) = -2148.21988027
H(correction)= 0.497879
G(correction)= 0.378359
E(RM06) = -2147.78709107
E(SMD$_{THF}$RM06) = -2147.86276057
Number of imaginary frequencies: 0

47	0	-0.84486	-0.24215	-0.87904
15	0	1.389	0.19087	0.24795
7	0	-2.90784	-0.40584	0.61472
6	0	1.27969	1.02008	1.89781
6	0	2.44053	1.34506	-0.74266
6	0	2.51042	-1.24571	0.56668
6	0	-3.27742	-1.54204	1.14815
6	0	-3.70819	0.6755	0.55594
6	0	0.20987	1.91061	2.09583
6	0	2.18548	0.79973	2.9467
6	0	3.20924	2.37319	-0.17491
6	0	2.4406	1.17299	-2.13885
6	0	3.90282	-1.18775	0.40325
6	0	1.92568	-2.45393	0.98171
1	0	-4.24287	-1.71768	1.62146
6	0	-2.31729	-2.6585	1.24978
6	0	-3.1473	1.85444	-0.02294
6	0	-5.11726	0.62587	1.08361
1	0	-0.51397	2.06993	1.29854
6	0	0.06731	2.57682	3.31421
6	0	2.03232	1.46179	4.16712
1	0	3.00935	0.10484	2.81331
1	0	3.20558	2.52432	0.90058
6	0	3.97512	3.21368	-0.98621
6	0	3.21691	2.01316	-2.94016
1	0	1.83048	0.39017	-2.59465
6	0	4.69517	-2.30918	0.65914
1	0	4.36835	-0.26618	0.06744
6	0	2.72125	-3.5698	1.2447
1	0	0.84858	-2.52521	1.09581
9	0	-2.94702	-3.79708	1.64704
9	0	-1.65505	-2.95352	0.0952
9	0	-1.30711	-2.45831	2.17081
8	0	-1.99464	2.02032	-0.46417
8	0	-4.03111	2.92082	-0.05651
1	0	-5.70445	-0.16069	0.58107
1	0	-5.14132	0.38492	2.1601
1	0	-5.62966	1.57764	0.93862
1	0	-0.76632	3.26043	3.45516
6	0	0.97483	2.35418	4.35256
1	0	2.7389	1.27635	4.97318
1	0	4.56245	4.01035	-0.53453

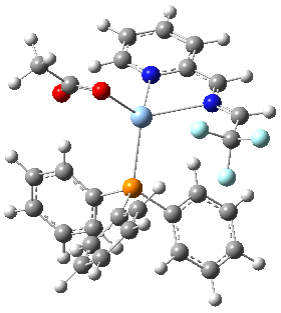
6	0	3.98272	3.03322	-2.37077
1	0	3.21034	1.87126	-4.01814
6	0	4.10688	-3.50189	1.08326
1	0	5.77259	-2.24981	0.52203
1	0	2.25266	-4.49728	1.56408
6	0	-3.51852	4.10457	-0.65196
1	0	0.85339	2.86626	5.30452
1	0	4.57756	3.6896	-3.00257
1	0	4.7237	-4.37627	1.27807
1	0	-3.20188	3.92909	-1.68546
1	0	-4.33938	4.82743	-0.62779
1	0	-2.6595	4.49752	-0.09611
8	0	-1.4884	-0.89589	-2.94473
6	0	-0.50726	-1.2021	-3.70147
8	0	0.71056	-1.13689	-3.42806
6	0	-0.91783	-1.70391	-5.09962
1	0	-1.50871	-0.93436	-5.6109
1	0	-0.04081	-1.95346	-5.70366
1	0	-1.5598	-2.58739	-5.00253



IB'

E(RB3LYP) = -2148.21773327
H(correction)= 0.498022
G(correction)= 0.380049
E(SMD$_{THF}$RM06) = -2147.86033983
Number of imaginary frequencies: 0

47	0	-0.88368	0.85898	-0.62816
15	0	1.28411	-0.12701	0.49303
7	0	-2.94741	-0.59936	-0.2803
8	0	0.02099	1.45143	-2.74353
6	0	1.07966	-1.0571	2.07764
6	0	2.64005	1.08534	0.84436
6	0	2.12884	-1.34231	-0.61783
6	0	-3.12255	-1.78034	-0.81875
6	0	-3.86887	-0.01128	0.50568
6	0	0.31959	2.67776	-2.56258
6	0	0.23249	-2.18214	2.06656
6	0	1.61573	-0.63526	3.30386
6	0	2.38893	2.44287	0.59268
6	0	3.91022	0.69891	1.30788
6	0	2.85314	-2.45311	-0.15878
6	0	2.03786	-1.10523	-2.00068
1	0	-4.00233	-2.40235	-0.65396
6	0	-2.06759	-2.41749	-1.63002
6	0	-3.53656	1.28108	1.01787
6	0	-5.17611	-0.68983	0.81495
8	0	0.16169	3.32656	-1.50216
6	0	0.94654	3.38964	-3.77461
1	0	-0.22591	-2.50671	1.137
6	0	-0.03775	-2.8784	3.24349
6	0	1.33295	-1.32997	4.48336
1	0	2.25563	0.24012	3.34256
1	0	1.43564	2.75628	0.16938
6	0	3.38913	3.39398	0.82408
6	0	4.90093	1.6514	1.54183
1	0	4.12721	-0.35174	1.48143
6	0	3.48724	-3.30778	-1.06226
1	0	2.90945	-2.66153	0.90596
6	0	2.68196	-1.96008	-2.89779
1	0	1.45726	-0.2607	-2.37229
9	0	-2.60976	-3.3172	-2.50078
9	0	-1.31242	-1.55957	-2.35005
9	0	-1.15718	-3.1641	-0.89511
8	0	-2.49354	1.93136	0.83429
8	0	-4.52932	1.83063	1.8097
1	0	-5.74297	-0.91283	-0.10488
1	0	-5.02195	-1.65836	1.32047
1	0	-5.80195	-0.06912	1.45718
1	0	0.31297	3.25495	-4.65861
1	0	1.08652	4.45641	-3.57916
1	0	1.91862	2.93511	-4.00415
1	0	-0.69166	-3.74649	3.212
6	0	0.51193	-2.45678	4.45772
1	0	1.75805	-0.98463	5.42328
1	0	3.18288	4.44054	0.61491
6	0	4.63906	3.00475	1.3036
1	0	5.87854	1.33855	1.90234
6	0	3.4061	-3.06028	-2.43422
1	0	4.04108	-4.16852	-0.69342
1	0	2.60174	-1.77003	-3.96524
6	0	-4.23203	3.11976	2.33003
1	0	0.29218	-2.9965	5.37596
1	0	5.41361	3.74782	1.48144
1	0	3.89684	-3.72853	-3.13853
1	0	-4.04342	3.84216	1.52897
1	0	-5.11395	3.41684	2.90537
1	0	-3.35076	3.0971	2.98062

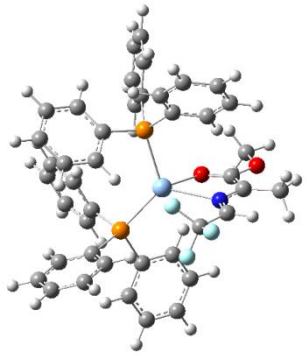


IIB

E(RB3LYP) = -2128.11853386
H(correction)= 0.494061
G(correction)= 0.377927
E(RM06) = -2127.64160165
E(SMD$_{THF}$RM06) = -2127.71883015
Number of imaginary frequencies: 0

47	0	1.07038	-0.07048	-0.82023
15	0	-1.23157	-0.34217	0.34018
7	0	1.99257	2.23167	-0.08178
8	0	1.26767	-1.0715	-2.91256
6	0	-1.68517	0.89604	1.63808
6	0	-1.37503	-1.95769	1.2332
6	0	-2.7097	-0.33623	-0.77613
6	0	1.47809	3.3957	-0.39853
6	0	3.02655	2.07552	0.74428
6	0	1.48546	-2.30595	-2.71008
6	0	-0.63524	1.49069	2.35648
6	0	-3.00516	1.26872	1.93595
6	0	-2.15614	-2.14194	2.38621
6	0	-0.64568	-3.04389	0.71787

6	0	-3.77886	-1.23722	-0.65824
6	0	-2.73276	0.61007	-1.81581
1	0	1.83331	4.34319	0.0179
6	0	0.29343	3.48165	-1.26386
1	0	3.49723	2.95406	1.20183
6	0	3.61366	0.80173	1.00973
8	0	1.51445	-2.89652	-1.59949
6	0	1.73967	-3.16713	-3.96175
1	0	0.39455	1.24861	2.10669
6	0	-0.90356	2.41254	3.36926
6	0	-3.27075	2.19792	2.94395
1	0	-3.82828	0.83817	1.37285
1	0	-2.70738	-1.30637	2.80769
6	0	-2.22279	-3.39148	3.00539
6	0	-0.72343	-4.29265	1.34063
1	0	0.00245	-2.91809	-0.15171
6	0	-4.85382	-1.1858	-1.54929
1	0	-3.76946	-1.98676	0.12712
6	0	-3.81205	0.66385	-2.69804
1	0	-1.90411	1.30034	-1.93809
9	0	0.20672	4.7079	-1.85493
9	0	0.2581	2.54979	-2.2584
9	0	-0.92129	3.32398	-0.61609
6	0	4.76268	0.68672	1.84541
7	0	3.08101	-0.32602	0.45264
1	0	2.72127	-3.64951	-3.88048
1	0	0.99246	-3.96843	-4.01496
1	0	1.7011	-2.57133	-4.87756
1	0	-0.07848	2.86531	3.91328
6	0	-2.22075	2.76759	3.66695
1	0	-4.29898	2.47917	3.16067
1	0	-2.82866	-3.51845	3.90008
6	0	-1.50912	-4.4716	2.48049
1	0	-0.1517	-5.12237	0.93257
6	0	-4.87517	-0.2332	-2.56883
1	0	-5.67216	-1.89512	-1.4467
1	0	-3.81362	1.40182	-3.49628
6	0	5.33504	-0.55088	2.06893
1	0	5.18139	1.58591	2.29228
6	0	3.65373	-1.51513	0.66819
1	0	-2.42796	3.49402	4.44949
1	0	-1.55819	-5.44434	2.96538
1	0	-5.71005	-0.19595	-3.26494
6	0	4.78209	-1.69385	1.46665
1	0	6.21503	-0.63495	2.70533
1	0	3.17208	-2.34756	0.15758
1	0	5.20871	-2.68189	1.6104



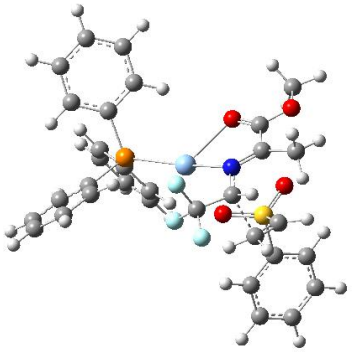
ID

E(RB3LYP) = -2955.96276045
H(correction)= 0.735933
G(correction)= 0.588903
E(RM06) = -2955.23581094

$E(SMD_{THF}RM06)$ = -2955.27443073
Number of imaginary frequencies: 0

47	0	0.01581	-0.63061	0.01059
15	0	-2.15039	0.79783	0.08171
15	0	2.3797	0.34759	0.08417
7	0	-0.5477	-2.88399	-0.74426
6	0	-2.72832	1.19674	1.78696
6	0	-3.63725	0.07387	-0.73116
6	0	-1.93852	2.43697	-0.7424
6	0	3.65765	-0.93252	0.43435
6	0	2.54898	1.56057	1.46691
6	0	3.02553	1.26795	-1.3784
6	0	-0.70853	-3.18468	-2.00839
6	0	-0.84275	-3.73241	0.26356
6	0	-1.78531	1.16398	2.82652
6	0	-4.06257	1.51609	2.08823
6	0	-3.85131	-1.30666	-0.5836
6	0	-4.5516	0.83214	-1.47784
6	0	-2.39902	3.64777	-0.20387
6	0	-1.24197	2.4571	-1.96432
6	0	3.26406	-2.06018	1.17501
6	0	4.98524	-0.83025	-0.00947
6	0	3.54035	1.46595	2.45349
6	0	1.61523	2.60924	1.54017
6	0	3.84373	2.40295	-1.26335
6	0	2.6784	0.80339	-2.65792
1	0	-1.05322	-4.15147	-2.36864
6	0	-0.29658	-2.231	-3.0581
6	0	-0.58361	-3.26407	1.58893
6	0	-1.37742	-5.11044	-0.01882
1	0	-0.75625	0.8893	2.61307
6	0	-2.16349	1.46751	4.13566
6	0	-4.43906	1.81394	3.39862
1	0	-4.80977	1.52233	1.3
1	0	-3.13649	-1.91091	-0.03059
6	0	-4.97243	-1.90938	-1.15429
6	0	-5.66739	0.22234	-2.05532
1	0	-4.39015	1.89725	-1.61459
1	0	-2.93009	3.65376	0.74296
6	0	-2.17537	4.85173	-0.87738
6	0	-1.02886	3.65935	-2.63788
1	0	-0.86615	1.52899	-2.38675
1	0	2.23317	-2.15854	1.50889
6	0	4.19247	-3.05797	1.47707
6	0	5.90608	-1.83612	0.2885
1	0	5.29917	0.029	-0.59453
1	0	4.26708	0.66102	2.41488
6	0	3.59809	2.40153	3.49011
6	0	1.68204	3.5477	2.56929
1	0	0.83567	2.69457	0.78693
6	0	4.3101	3.05624	-2.40592
1	0	4.11254	2.78221	-0.28217
6	0	3.15362	1.45527	-3.7969
1	0	2.04077	-0.06809	-2.76839
9	0	-0.79313	-2.58872	-4.26148
9	0	-0.69774	-0.93653	-2.82829
9	0	1.06637	-2.12857	-3.22702
8	0	-0.11884	-2.15069	1.92564
8	0	-0.88779	-4.17781	2.56252
1	0	-2.31682	-5.06731	-0.59331
1	0	-0.67196	-5.7003	-0.62567
1	0	-1.5694	-5.65794	0.90399
1	0	-1.42209	1.43775	4.92948
6	0	-3.48986	1.79368	4.42356
1	0	-5.47518	2.0569	3.61954
1	0	-5.12711	-2.97811	-1.03359

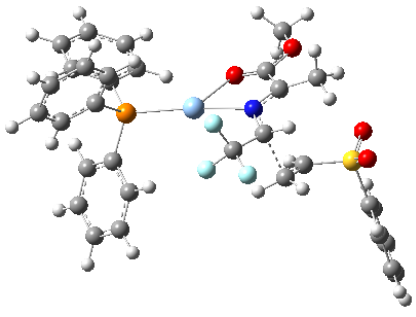
6	0	-5.88165	-1.14732	-1.89151
1	0	-6.3672	0.81903	-2.6347
1	0	-2.53581	5.78275	-0.44742
6	0	-1.49356	4.86021	-2.09496
1	0	-0.48851	3.65793	-3.58053
1	0	3.8782	-3.92703	2.04881
6	0	5.51214	-2.94967	1.03359
1	0	6.9302	-1.75048	-0.06537
1	0	4.37025	2.31338	4.24995
6	0	2.67269	3.44395	3.54981
1	0	0.95441	4.35381	2.60927
6	0	3.96778	2.5833	-3.67413
1	0	4.94078	3.9355	-2.30286
1	0	2.88051	1.08216	-4.78034
6	0	-0.65714	-3.75638	3.90494
1	0	-3.78625	2.02196	5.44403
1	0	-6.74902	-1.62087	-2.34382
1	0	-1.31915	5.79782	-2.61603
1	0	6.22984	-3.73361	1.2609
1	0	2.71965	4.17035	4.35679
1	0	4.33115	3.09354	-4.56234
1	0	-1.24395	-2.86513	4.14824
1	0	-0.96862	-4.59481	4.53169
1	0	0.40104	-3.53338	4.07587



TSIA*endo*

E(RB3LYP) = -2777.86182267
H(correction)= 0.599144
G(correction)= 0.472332
E(RM06) = -2777.34129687
E(SMD_{THF}RM06) = -2777.37475599
Imaginary frequencies: 1 (-272.4091 cm^{-1})

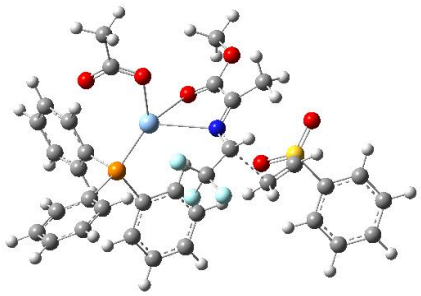
47	0	0.2679	-0.72617	-0.11288
15	0	2.37988	0.50941	-0.09111
7	0	-1.25114	-2.48286	0.26549
6	0	3.16136	0.76129	1.5574
6	0	2.21056	2.19055	-0.82151
6	0	3.67403	-0.31917	-1.10716
6	0	-1.68458	-2.73542	1.52582
6	0	-2.00916	-2.80411	-0.76265
6	0	3.01422	-0.25408	2.51711
6	0	3.89043	1.91367	1.88925
6	0	0.96059	2.825	-0.73075
6	0	3.27021	2.84893	-1.46675
6	0	5.04255	-0.25704	-0.80366
6	0	3.25462	-1.04325	-2.23599
1	0	-2.30027	-3.6157	1.71105
6	0	-0.69779	-2.54805	2.63356
6	0	-3.12128	-1.25947	1.78719
6	0	-1.56587	-2.28673	-2.07978
6	0	-3.12708	-3.82129	-0.70492
1	0	2.42302	-1.13647	2.29035
6	0	3.60543	-0.12717	3.77426
6	0	4.47372	2.03994	3.15168
1	0	3.99518	2.71755	1.16707
1	0	0.11753	2.31418	-0.2722
6	0	0.78578	4.10686	-1.2559
6	0	3.08781	4.12842	-1.99318
1	0	4.23366	2.35815	-1.57056
6	0	5.97561	-0.89651	-1.62275
1	0	5.38041	0.28088	0.07717
6	0	4.19133	-1.67366	-3.05538
1	0	2.19492	-1.12237	-2.46815
9	0	0.37772	-3.38048	2.56851
9	0	-0.17465	-1.28747	2.68489
9	0	-1.29574	-2.77156	3.82625
6	0	-3.71407	-0.89604	0.57873
1	0	-3.7211	-1.828	2.49382
1	0	-2.43934	-0.55331	2.24924
8	0	-0.58104	-1.57638	-2.27543
8	0	-2.36711	-2.67232	-3.08791
1	0	-2.71479	-4.84088	-0.65082
1	0	-3.76444	-3.67969	0.17011
1	0	-3.75176	-3.75971	-1.59539
1	0	3.48222	-0.9193	4.50762
6	0	4.33639	1.01907	4.09392
1	0	5.03203	2.93914	3.39847
1	0	-0.18678	4.58581	-1.1844
6	0	1.8469	4.76062	-1.88447
1	0	3.91319	4.62784	-2.49374
6	0	5.55261	-1.60177	-2.75075
1	0	7.03273	-0.84556	-1.37555
1	0	3.85508	-2.23075	-3.92559
1	0	-4.6222	-1.33684	0.18488
16	0	-3.15366	0.4648	-0.33155
6	0	-2.10868	-2.0511	-4.35585
1	0	4.7883	1.12068	5.07698
1	0	1.7053	5.75505	-2.29949
1	0	6.28014	-2.1012	-3.38497
8	0	-3.40215	0.26651	-1.77584
8	0	-1.77489	0.81167	0.14087
6	0	-4.16403	1.89464	0.13118
1	0	-1.10004	-2.28717	-4.70526
1	0	-2.8555	-2.46188	-5.03637
1	0	-2.22171	-0.9681	-4.26483
6	0	-5.27094	2.22703	-0.65253
6	0	-3.84604	2.62916	1.2769
6	0	-6.07323	3.30638	-0.27802
1	0	-5.4789	1.65535	-1.55072
6	0	-4.65248	3.70737	1.64108
1	0	-2.96929	2.36689	1.85984
6	0	-5.76729	4.0443	0.86773
1	0	-6.93343	3.57438	-0.88566
1	0	-4.40826	4.28771	2.52684
1	0	-6.3931	4.88487	1.1555



TSIA*exo*

E(RB3LYP) = -2777.8480121
H(correction)= 0.599410
G(correction)= 0.469335
E(RM06) = -2777.32571896
E(SMD_{THF}RM06) = -2777.36647476
Imaginary frequencies: 1 (-311.8064 cm^{-1})

47	0	0.89718	0.32702	-0.55907
15	0	3.09506	-0.07088	0.40161
7	0	-1.07517	0.2711	-1.64967
6	0	3.00985	-1.16618	1.87753
6	0	3.90145	1.48243	0.96415
6	0	4.31013	-0.87549	-0.71958
6	0	-1.63947	-0.90634	-2.02646
6	0	-1.78081	1.39375	-1.70971
6	0	2.17327	-2.29367	1.80689
6	0	3.72991	-0.91936	3.05538
6	0	3.08488	2.58395	1.26913
6	0	5.29455	1.60184	1.09741
6	0	5.29408	-1.76152	-0.25443
6	0	4.246	-0.58157	-2.09077
1	0	-2.38218	-0.90948	-2.82212
6	0	-0.72707	-2.08526	-2.15209
6	0	-2.87906	-1.3114	-0.46938
6	0	-1.21459	2.53177	-0.96103
6	0	-2.91019	1.65852	-2.67876
1	0	1.59589	-2.48764	0.90664
6	0	2.07445	-3.16525	2.89072
6	0	3.62017	-1.79119	4.1413
1	0	4.36953	-0.04566	3.13082
1	0	2.00756	2.5205	1.13784
6	0	3.65476	3.77561	1.72101
6	0	5.85849	2.79718	1.54453
1	0	5.93965	0.76654	0.84117
6	0	6.20518	-2.33066	-1.14614
1	0	5.34233	-2.01612	0.80015
6	0	5.16124	-1.14769	-2.97795
1	0	3.47266	0.0843	-2.4663
9	0	0.2578	-1.92825	-3.07838
9	0	-0.07365	-2.3854	-0.98287
9	0	-1.42623	-3.18481	-2.49628
6	0	-3.42249	-0.14284	0.0655
1	0	-3.54254	-1.97698	-1.01602
1	0	-2.12193	-1.81878	0.12225
8	0	-0.23638	2.48875	-0.20336
8	0	-1.88312	3.67876	-1.16734
1	0	-2.50569	2.03692	-3.63065
1	0	-3.50666	0.77094	-2.88517
1	0	-3.59086	2.40766	-2.27583
1	0	1.42521	-4.03371	2.82414
6	0	2.79635	-2.91467	4.0605
1	0	4.17814	-1.58801	5.05134
1	0	3.01424	4.62181	1.95316
6	0	5.03941	3.88379	1.86075
1	0	6.9376	2.8807	1.64087
6	0	6.14233	-2.02287	-2.50654
1	0	6.9607	-3.01888	-0.77701
1	0	5.09957	-0.91462	-4.03716
1	0	-2.97276	0.40453	0.88575
16	0	-5.03631	0.37151	-0.33569
6	0	-1.45037	4.81204	-0.40629
1	0	2.7108	-3.58927	4.9079
1	0	5.48094	4.81488	2.2055
1	0	6.84942	-2.47126	-3.19895
8	0	-5.43811	-0.29267	-1.59807
8	0	-5.13111	1.84084	-0.19298
6	0	-6.12031	-0.30345	0.94922
1	0	-0.41294	5.0649	-0.64342
1	0	-2.11804	5.62486	-0.69309
1	0	-1.5347	4.60959	0.66504
6	0	-6.705	-1.55908	0.76891
6	0	-6.35255	0.43719	2.11048
6	0	-7.52317	-2.08201	1.77102
1	0	-6.53402	-2.10004	-0.15602
6	0	-7.17018	-0.09491	3.10857
1	0	-5.91395	1.42463	2.21081
6	0	-7.75232	-1.35418	2.94185
1	0	-7.9882	-3.05488	1.63462
1	0	-7.35999	0.47775	4.01267
1	0	-8.39121	-1.76423	3.71965

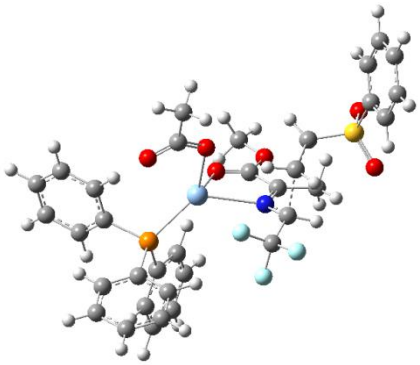


TSIB*endo*

E(RB3LYP) = -3006.41324746
H(correction)= 0.6543175
G(correction)= 0.5090005
E(RM06) = -3005.8663556
E(SMD_{THF}RM06) = -3005.94861909
Imaginary frequencies: 1 (-208.6985cm^{-1})

47	0	-1.55571	1.24113	0.17699
15	0	-2.34213	-1.07228	-0.26274
8	0	-2.2397	3.33407	0.58329
7	0	0.95371	1.67163	0.92292
6	0	-1.03788	-2.3528	-0.51106
6	0	-3.34981	-1.12749	-1.81039
6	0	-3.45813	-1.81701	1.00992
6	0	-3.48029	3.46069	0.29514
6	0	1.34045	1.43194	2.18891
6	0	1.50408	2.56162	0.13364
6	0	0.22549	-1.91358	-0.93866
6	0	-1.24706	-3.7241	-0.28942
6	0	-3.3161	-2.19628	-2.71905
6	0	-4.17336	-0.01852	-2.07739
6	0	-4.56644	-2.61518	0.6879
6	0	-3.18322	-1.55208	2.36192
8	0	-4.239	2.57988	-0.15941
6	0	-4.0505	4.86658	0.55066
1	0	1.85294	2.18741	2.78759
6	0	0.43886	0.5819	3.00665
6	0	3.10853	0.11315	1.95768
6	0	0.99927	2.55032	-1.25139
6	0	2.48649	3.64487	0.52912
1	0	0.41889	-0.8536	-1.08268
6	0	1.25254	-2.83326	-1.16695
6	0	-0.21817	-4.63999	-0.51402
1	0	-2.21119	-4.07508	0.06789
1	0	-2.66735	-3.04697	-2.53302
6	0	-4.10357	-2.16734	-3.87226
6	0	-4.96281	-0.0029	-3.22931
1	0	-4.18673	0.8348	-1.39745
6	0	-5.37316	-3.14975	1.69507

1	0	-4.80684	-2.81061	-0.35289
6	0	-3.98716	-2.09316	3.36571
1	0	-2.34549	-0.9154	2.62857
1	0	-3.51048	5.60055	-0.05939
1	0	-5.11698	4.90888	0.313
1	0	-3.89535	5.14627	1.59915
9	0	0.98954	0.34574	4.23133
9	0	-0.80318	1.11257	3.2588
9	0	0.18425	-0.63618	2.4496
6	0	4.13794	0.69488	1.25387
1	0	3.16666	0.07462	3.04101
1	0	2.52494	-0.67084	1.48757
8	0	0.1453	1.80237	-1.72158
8	0	1.59545	3.50341	-2.0172
1	0	2.84048	3.50864	1.5532
1	0	3.35715	3.6455	-0.13161
1	0	2.01481	4.63558	0.45967
1	0	2.22105	-2.46076	-1.48433
6	0	1.03025	-4.19571	-0.95811
1	0	-0.39102	-5.69934	-0.33678
1	0	-4.06437	-2.9988	-4.57254
6	0	-4.93125	-1.07212	-4.12746
1	0	-5.59491	0.85929	-3.4265
6	0	-5.08357	-2.8932	3.03614
1	0	-6.23145	-3.76244	1.42886
1	0	-3.76155	-1.87736	4.407
1	0	4.84422	1.39543	1.68794
16	0	4.45842	0.36238	-0.41677
6	0	1.17585	3.53665	-3.38093
1	0	1.83148	-4.91146	-1.12933
1	0	-5.54139	-1.0488	-5.02784
1	0	-5.71461	-3.30566	3.81992
8	0	4.98243	1.57404	-1.08643
8	0	3.34697	-0.40899	-1.01617
6	0	5.86901	-0.78706	-0.38732
1	0	0.10002	3.72291	-3.45448
1	0	1.73786	4.35221	-3.84131
1	0	1.40332	2.58997	-3.88025
6	0	7.16044	-0.30149	-0.60029
6	0	5.65193	-2.14623	-0.14031
6	0	8.24405	-1.18204	-0.55514
1	0	7.29689	0.75315	-0.81587
6	0	6.7379	-3.01962	-0.09814
1	0	4.63919	-2.50872	0.00585
6	0	8.0359	-2.5394	-0.30204
1	0	9.25091	-0.8075	-0.72449
1	0	6.57219	-4.07781	0.08945
1	0	8.8804	-3.2236	-0.26917



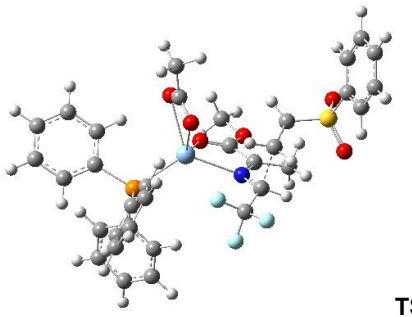
TSIB*exo*

E(RB3LYP) = -3006.41691226
H(correction)= 0.654845

G(correction)= 0.511304
E(RM06) = -3005.86917085
E(SMD_{THF}RM06) = -3005.95083024
Imaginary frequencies: 1 (-293.1855 cm^{-1})

47	0	0.74072	-0.23359	-0.53901
15	0	3.20115	-0.15436	-0.02283
8	0	-0.7274	-1.57395	-1.61993
7	0	-1.01575	1.04384	0.81568
6	0	4.24118	-0.3327	-1.53897
6	0	3.81518	1.41183	0.74636
6	0	3.84386	-1.45909	1.11732
6	0	-0.15015	-2.5879	-2.14694
6	0	-1.72067	0.35365	1.74442
6	0	-1.44056	2.18887	0.32369
6	0	3.77363	-1.20536	-2.53789
6	0	5.44695	0.35939	-1.73502
6	0	3.16744	2.60584	0.38661
6	0	4.8755	1.46344	1.66442
6	0	5.04171	-2.15353	0.89268
6	0	3.08166	-1.76904	2.25641
8	0	1.0758	-2.82153	-2.17158
6	0	-1.10789	-3.59696	-2.80169
1	0	-2.43729	0.86455	2.38807
6	0	-0.96754	-0.67727	2.51665
6	0	-3.07607	-0.70452	0.62922
6	0	-0.66892	2.70523	-0.81644
6	0	-2.5166	3.0854	0.90518
1	0	2.82852	-1.73586	-2.40677
6	0	4.52065	-1.38571	-3.70441
1	0	5.81064	1.04608	-0.97621
6	0	6.18155	0.17809	-2.90871
1	0	2.32485	2.57458	-0.30017
6	0	3.58825	3.8246	0.92124
6	0	5.28725	2.68426	2.20386
1	0	5.37607	0.54766	1.96461
6	0	5.47437	-3.13018	1.79282
1	0	5.63422	-1.93751	0.00905
6	0	3.5218	-2.73856	3.15772
1	0	2.13901	-1.26173	2.43677
1	0	-1.80502	-3.98528	-2.04998
1	0	-1.71156	-3.09503	-3.5667
1	0	-0.55783	-4.42726	-3.25283
9	0	-1.79647	-1.32821	3.37227
9	0	-0.37145	-1.62725	1.74952
9	0	0.04306	-0.16385	3.29527
6	0	-3.82204	0.108	-0.2204
1	0	-2.34174	-1.34089	0.14158
1	0	-3.55621	-1.12026	1.51193
8	0	0.28581	2.17126	-1.38499
8	0	-1.12175	3.92299	-1.22899
1	0	-3.07887	2.59406	1.69913
1	0	-2.06933	4.00451	1.31211
1	0	-3.24273	3.38293	0.14554
6	0	5.72077	-0.69735	-3.89454
1	0	4.15088	-2.063	-4.47011
1	0	7.11141	0.72392	-3.05233
1	0	3.07637	4.74057	0.63663
6	0	4.64703	3.86762	1.83112
1	0	6.10679	2.70846	2.9184
6	0	4.71796	-3.42271	2.92854
1	0	6.40208	-3.66451	1.60159
1	0	2.91926	-2.9677	4.03286
1	0	-3.53918	0.31396	-1.24528
16	0	-5.27993	0.8676	0.29281
6	0	-0.46371	4.46687	-2.37159
1	0	6.29244	-0.83611	-4.80959

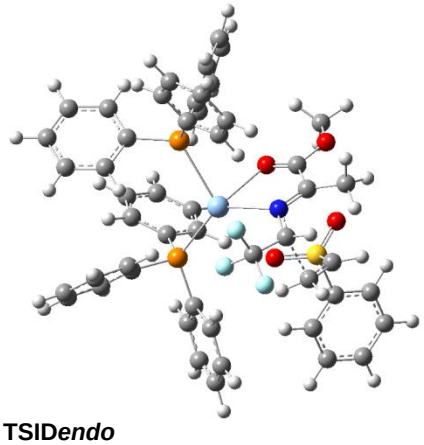
1	0	4.96528	4.81715	2.25498
1	0	5.05319	-4.18606	3.62666
8	0	-5.52635	2.07932	-0.52617
8	0	-5.31135	0.95023	1.77561
6	0	-6.64777	-0.25382	-0.1326
1	0	-0.53619	3.78706	-3.22587
1	0	-0.978	5.40573	-2.58744
1	0	0.59576	4.65372	-2.16673
6	0	-7.22536	-0.18865	-1.40331
6	0	-7.09811	-1.18704	0.80457
6	0	-8.25207	-1.07167	-1.73982
1	0	-6.87773	0.56236	-2.10544
6	0	-8.12581	-2.06701	0.46162
1	0	-6.65251	-1.19949	1.79392
6	0	-8.70182	-2.014	-0.81052
1	0	-8.70553	-1.02123	-2.72707
1	0	-8.48101	-2.79199	1.19039
1	0	-9.50229	-2.70093	-1.07514



TSIB'*exo*

E(RB3LYP) = -3006.41547507
H(correction)= 0.654611
G(correction)= 0.510838
E(SMD_{THF}RM06) = -3005.9499031
Imaginary frequencies: 1 (-273.6571 cm^{-1})

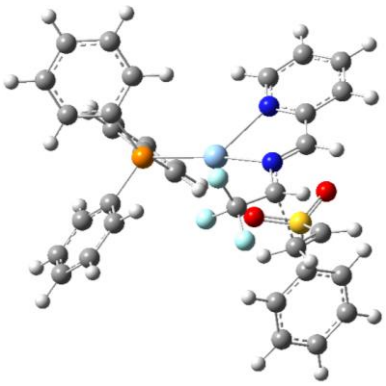
7	0	1.00415	1.49794	-0.70817
6	0	1.58432	0.86073	-1.75324
6	0	1.58061	2.51083	-0.09558
1	0	2.36216	1.35584	-2.33453
6	0	0.6881	0.07753	-2.64896
6	0	2.81133	-0.5487	-0.81762
6	0	0.8783	2.99273	1.10612
6	0	2.75581	3.32216	-0.60067
9	0	1.41902	-0.60323	-3.56995
9	0	-0.09338	-0.82768	-2.01489
9	0	-0.18344	0.85756	-3.37935
6	0	3.62482	0.02256	0.15221
1	0	1.99089	-1.1674	-0.46126
1	0	3.25401	-0.85105	-1.76298
8	0	-0.11568	2.50038	1.63536
8	0	1.45174	4.11718	1.619
1	0	3.29377	2.81801	-1.4031
1	0	2.41815	4.30346	-0.96724
1	0	3.47974	3.50288	0.19699
1	0	3.34673	0.11057	1.19553
16	0	5.17909	0.66598	-0.23108
6	0	0.84688	4.61673	2.81127
8	0	5.55076	1.70067	0.76293
8	0	5.25628	0.96357	-1.68398
6	0	6.38418	-0.67134	0.03025
1	0	0.85785	3.8596	3.60103
1	0	1.44522	5.48234	3.10372
1	0	-0.19097	4.9149	2.63034
6	0	6.92794	-0.87196	1.30171
6	0	6.74349	-1.50075	-1.03487
6	0	7.82726	-1.9186	1.50904
1	0	6.65531	-0.19767	2.10725
6	0	7.64418	-2.54532	-0.82062
1	0	6.32959	-1.30666	-2.01895
6	0	8.18415	-2.75875	0.45047
1	0	8.25395	-2.07594	2.49694
1	0	7.92872	-3.19077	-1.64842
1	0	8.88525	-3.57374	0.61453
1	0	-2.50738	1.11517	-2.44615
6	0	-3.42222	1.56713	-2.07139
6	0	-4.00496	1.09965	-0.87737
6	0	-3.9974	2.62453	-2.77382
15	0	-3.1117	-0.24802	0.01745
6	0	-5.15497	1.74121	-0.39554
1	0	-3.53367	2.96913	-3.69462
6	0	-5.15069	3.24998	-2.2904
47	0	-0.69253	0.26808	0.63461
6	0	-4.18492	-0.67416	1.46269
6	0	-3.32718	-1.7148	-1.08722
6	0	-5.72173	2.80957	-1.09716
1	0	-5.61056	1.41204	0.53251
1	0	-5.59178	4.08122	-2.83522
8	0	0.16689	-2.09904	1.02481
6	0	-3.61178	-0.6199	2.743
6	0	-5.5207	-1.09171	1.32906
6	0	-4.3505	-1.8226	-2.04189
6	0	-2.41489	-2.77336	-0.93333
1	0	-6.61194	3.29607	-0.70495
6	0	0.10309	-1.91877	2.27773
1	0	-2.55991	-0.36592	2.85951
6	0	-4.37516	-0.95167	3.8672
6	0	-6.27885	-1.41605	2.45331
1	0	-5.96688	-1.17221	0.34145
6	0	-4.47208	-2.97451	-2.82118
1	0	-5.04575	-1.0007	-2.18849
6	0	-2.5486	-3.92531	-1.71147
1	0	-1.59112	-2.68832	-0.22477
8	0	-0.28731	-0.85752	2.84102
6	0	0.54584	-3.08928	3.16708
1	0	-3.91659	-0.91245	4.85188
6	0	-5.70696	-1.3408	3.72723
1	0	-7.31197	-1.73517	2.33569
6	0	-3.57351	-4.03034	-2.65395
1	0	-5.26638	-3.04403	-3.56114
1	0	-1.83477	-4.7359	-1.58854
1	0	1.60671	-3.30055	2.98831
1	0	0.3951	-2.86671	4.22665
1	0	-0.01136	-3.99386	2.89653
1	0	-6.29688	-1.59838	4.60402
1	0	-3.6658	-4.92602	-3.26413



TSID*endo*

E(RB3LYP) = -3814.14342516
H(correction)= 0.892560
G(correction)= 0.723191
E(SMD_{THF}RM06) = -3813.35875462
Imaginary frequencies: 1 (-269.2564 cm^{-1})

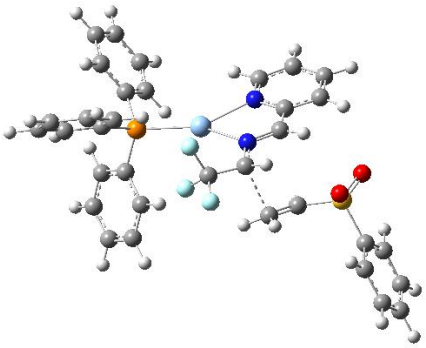
47	0	-0.34959	-0.22228	-0.35013
15	0	0.48385	2.17733	0.11733
15	0	-3.01259	-0.57029	0.17426
7	0	0.57019	-2.11118	-1.63374
6	0	2.21111	2.78208	-0.16306
6	0	0.2197	2.32481	1.9344
6	0	-0.45335	3.55766	-0.68186
6	0	-3.22502	-1.57922	1.7051
6	0	-3.91203	-1.50861	-1.13766
6	0	-4.12773	0.87461	0.4837
6	0	1.1344	-1.92696	-2.8498
6	0	0.84183	-3.20169	-0.941
6	0	2.78198	2.54856	-1.42435
6	0	2.93121	3.52584	0.78131
6	0	1.06846	1.57418	2.77152
6	0	-0.86575	3.00868	2.50289
6	0	-0.45869	4.87207	-0.18606
6	0	-1.08915	3.29453	-1.90447
6	0	-2.49245	-1.19626	2.84139
6	0	-4.06381	-2.69957	1.78428
6	0	-3.1552	-2.28028	-2.03361
6	0	-5.30912	-1.47278	-1.28191
6	0	-5.03454	0.9405	1.55289
6	0	-4.04498	1.96449	-0.39754
1	0	1.35664	-2.78618	-3.48355
6	0	0.62001	-0.80841	-3.69039
6	0	3.10776	-1.4703	-2.30629
6	0	0.42286	-3.18004	0.47818
6	0	1.31361	-4.51833	-1.5233
1	0	2.24099	1.96663	-2.16427
6	0	4.04071	3.06204	-1.73795
6	0	4.19625	4.02941	0.46876
1	0	2.51229	3.70994	1.76543
1	0	1.88231	0.99587	2.34083
6	0	0.85158	1.54736	4.14904
6	0	-1.08157	2.96922	3.88329
1	0	-1.55179	3.56677	1.87428
6	0	-1.11393	5.88886	-0.87988
1	0	0.05528	5.10407	0.74219
6	0	-1.73224	4.31719	-2.60775
1	0	-1.06217	2.29019	-2.31915
1	0	-1.8128	-0.35005	2.7917
6	0	-2.61795	-1.90369	4.03586
6	0	-4.17538	-3.41731	2.97835
1	0	-4.63051	-3.01625	0.91457
1	0	-2.07218	-2.29829	-1.95141
6	0	-3.78448	-3.01434	-3.04116
6	0	-5.93437	-2.20453	-2.2922
1	0	-5.90838	-0.86714	-0.60829
1	0	-5.11197	0.11316	2.25086
6	0	-5.83891	2.06914	1.73078
6	0	-4.85041	3.08913	-0.22152
1	0	-3.33936	1.93964	-1.22194
9	0	-0.65562	-0.99151	-4.13793
9	0	0.60177	0.40187	-3.05031
9	0	1.3947	-0.65284	-4.78928
6	0	3.50767	-2.25397	-1.23033
1	0	3.50546	-1.70306	-3.29101
1	0	2.93301	-0.41452	-2.12542
8	0	-0.02552	-2.20515	1.07855
8	0	0.58909	-4.36879	1.08432
1	0	0.45422	-5.14644	-1.80533
1	0	1.93168	-4.38393	-2.41206
1	0	1.89549	-5.07365	-0.78711
1	0	4.46774	2.87572	-2.71979
6	0	4.75211	3.80451	-0.79165
1	0	4.74413	4.60215	1.21261
1	0	1.51874	0.969	4.78257
6	0	-0.22081	2.24701	4.71021
1	0	-1.92611	3.5056	4.308
6	0	-1.75369	5.61347	-2.09203
1	0	-1.11535	6.89966	-0.48042
1	0	-2.21198	4.09795	-3.55798
1	0	-2.04687	-1.5917	4.90612
6	0	-3.4583	-3.01867	4.10717
1	0	-4.82617	-4.28675	3.02365
1	0	-3.18507	-3.60276	-3.73046
6	0	-5.17345	-2.97855	-3.17197
1	0	-7.0159	-2.16686	-2.39435
1	0	-6.53566	2.10504	2.56439
6	0	-5.75028	3.14456	0.84565
1	0	-4.76202	3.92465	-0.91055
1	0	3.96307	-3.23209	-1.33859
16	0	3.56163	-1.65892	0.40205
6	0	0.42802	-4.36648	2.51042
1	0	5.73313	4.20371	-1.03571
1	0	-0.38832	2.22148	5.78379
1	0	-2.2554	6.4094	-2.63606
1	0	-3.54867	-3.57573	5.03613
1	0	-5.6619	-3.54417	-3.96112
1	0	-6.37455	4.02264	0.98891
8	0	3.31773	-2.76493	1.35616
8	0	2.76028	-0.4105	0.49304
6	0	5.2787	-1.16232	0.70288
1	0	-0.57026	-4.02166	2.79052
1	0	0.57893	-5.40209	2.81923
1	0	1.18482	-3.71788	2.95882
6	0	6.17794	-2.09086	1.23261
6	0	5.68695	0.13544	0.38673
6	0	7.50669	-1.71552	1.43717
1	0	5.82716	-3.08298	1.49704
6	0	7.01629	0.50204	0.59957
1	0	4.96794	0.84753	-0.00322
6	0	7.92729	-0.42155	1.11933
1	0	8.21138	-2.43121	1.85258
1	0	7.33784	1.51306	0.36344
1	0	8.96197	-0.13143	1.28285



TSIIA*endo*

E(RB3LYP) = -2757.76573158
H(correction)= 0.595144
G(correction)= 0.470077
E(RM06) = -2757.19644414
E(SMD$_{THF}$RM06) = -2757.23410912
Imaginary frequencies: 1 (-186.3326 cm^{-1})

47	0	0.29432	-0.9106	0.18407
15	0	2.25339	0.53389	-0.19171
7	0	-1.20783	-2.33129	1.32977
6	0	2.11409	1.34277	-1.84235
6	0	3.84623	-0.3917	-0.24558
6	0	2.56576	1.91916	0.98189
6	0	-1.61347	-2.12411	2.59443
6	0	-1.98032	-2.98718	0.49294
6	0	0.8349	1.7484	-2.26224
6	0	3.21453	1.5596	-2.686
6	0	3.81222	-1.74272	-0.62685
6	0	5.08056	0.19333	0.07761
6	0	3.02132	3.17922	0.56468
6	0	2.33864	1.69121	2.349
1	0	-2.33513	-2.80872	3.04527
6	0	-0.6322	-1.59156	3.57219
6	0	-3.10815	-0.47701	2.31084
1	0	-2.85573	-3.52646	0.86265
6	0	-1.64753	-3.17109	-0.90873
1	0	-0.03278	1.56756	-1.63137
6	0	0.66953	2.37533	-3.49823
6	0	3.0407	2.1807	-3.9246
1	0	4.20592	1.2376	-2.38163
1	0	2.85891	-2.21442	-0.85414
6	0	4.9894	-2.48762	-0.7027
6	0	6.25639	-0.55631	0.0077
1	0	5.12333	1.23136	0.39347
6	0	3.25692	4.18841	1.50067
1	0	3.18465	3.37626	-0.4904
6	0	2.5826	2.70032	3.28094
1	0	1.95512	0.73264	2.68404
9	0	0.39754	-2.43283	3.87164
9	0	-0.03492	-0.43398	3.14748
9	0	-1.24698	-1.30611	4.74566
6	0	-3.73778	-0.63834	1.10027
1	0	-3.62624	-0.76361	3.22066
1	0	-2.34382	0.28308	2.42374
6	0	-2.41754	-4.03638	-1.71292
7	0	-0.58886	-2.50558	-1.42862
1	0	-0.32382	2.68318	-3.81281
6	0	1.76966	2.59169	-4.33106
1	0	3.89921	2.33974	-4.57191
1	0	4.9477	-3.53261	-0.99747
6	0	6.21368	-1.89548	-0.38513
1	0	7.20543	-0.09346	0.26498
6	0	3.04182	3.95014	2.85928
1	0	3.60562	5.16172	1.16551
1	0	2.40166	2.5116	4.33556
1	0	-4.64985	-1.20476	0.94968
16	0	-3.20892	0.21728	-0.32295
6	0	-2.08827	-4.20586	-3.04879
1	0	-3.26408	-4.55737	-1.2752
6	0	-0.28217	-2.67583	-2.71867
1	0	1.63602	3.07204	-5.29675
1	0	7.12972	-2.47797	-0.43438
1	0	3.22299	4.73783	3.58575
8	0	-3.58287	-0.53273	-1.53765
8	0	-1.7947	0.65849	-0.12207
6	0	-4.16297	1.75517	-0.38989
6	0	-0.99224	-3.51355	-3.57489
1	0	-2.67695	-4.86848	-3.67782
1	0	0.5702	-2.10569	-3.08252
6	0	-5.32968	1.795	-1.15607
6	0	-3.73792	2.87158	0.33531
1	0	-0.7015	-3.61068	-4.61578
6	0	-6.08407	2.96916	-1.18935
1	0	-5.62187	0.92145	-1.7293
6	0	-4.49804	4.04046	0.29403
1	0	-2.81612	2.82543	0.90581
6	0	-5.67165	4.08925	-0.46388
1	0	-6.99071	3.01029	-1.78711
1	0	-4.17141	4.91531	0.8498
1	0	-6.26067	5.00206	-0.49325

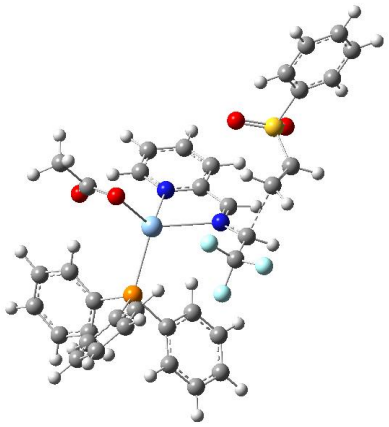


TSIIA*exo*

E(RB3LYP) = -2757.76001912
H(correction)= 0.595832
G(correction)= 0.471065
E(RM06) = -2757.18960197
E(SMD$_{THF}$RM06) = -2757.23119782
Imaginary frequencies: 1 (-241.7820 cm^{-1})

47	0	0.92374	0.52523	-0.52818
15	0	3.1163	-0.13754	0.33035
7	0	-1.13377	0.0163	-1.43327
6	0	3.04088	-0.75876	2.06302
6	0	4.26992	1.29868	0.38883
6	0	3.99791	-1.45777	-0.59541
6	0	-1.64172	-1.21767	-1.6434
6	0	-1.92476	1.06146	-1.57382
6	0	1.94944	-1.56886	2.41736
6	0	4.02957	-0.48376	3.01995
6	0	3.91436	2.40217	1.18573
6	0	5.42744	1.37575	-0.39714
6	0	5.2043	-2.00839	-0.12885
6	0	3.4309	-1.95129	-1.77868
1	0	-2.46318	-1.34015	-2.34943
6	0	-0.69301	-2.35926	-1.64677
6	0	-2.95837	-1.47351	0.0512

1	0	-2.8815	0.96839	-2.08179
6	0	-1.50185	2.39792	-1.19891
1	0	1.17763	-1.78983	1.68468
6	0	1.85657	-2.10167	3.70332
6	0	3.92821	-1.01348	4.30774
1	0	4.87225	0.15234	2.76628
1	0	3.01446	2.36436	1.79519
6	0	4.71026	3.54593	1.20875
6	0	6.21739	2.52909	-0.38001
1	0	5.7156	0.53942	-1.0253
6	0	5.83809	-3.0213	-0.84597
1	0	5.64405	-1.65126	0.79813
6	0	4.06822	-2.96872	-2.49341
1	0	2.48004	-1.56479	-2.13092
9	0	0.21283	-2.34105	-2.67875
9	0	0.07475	-2.42427	-0.51355
9	0	-1.35348	-3.53223	-1.74187
6	0	-3.56069	-0.2612	0.32393
1	0	-3.5185	-2.25088	-0.45826
1	0	-2.18644	-1.82685	0.72871
6	0	-2.39828	3.48307	-1.31292
7	0	-0.23921	2.58752	-0.73696
1	0	1.00862	-2.72822	3.96537
6	0	2.84386	-1.82313	4.65101
1	0	4.6972	-0.79099	5.04268
1	0	4.42741	4.38622	1.83699
6	0	5.86464	3.6131	0.42276
1	0	7.11089	2.57469	-0.99671
6	0	5.27144	-3.50113	-2.03107
1	0	6.77002	-3.44148	-0.47755
1	0	3.61408	-3.3479	-3.4043
1	0	-3.19741	0.45355	1.05263
16	0	-5.04846	0.20317	-0.46122
6	0	-1.9733	4.75548	-0.96721
1	0	-3.41685	3.28897	-1.63175
6	0	0.1586	3.82552	-0.41005
1	0	2.76624	-2.23223	5.6546
1	0	6.48129	4.50749	0.43505
1	0	5.76445	-4.295	-2.58558
8	0	-5.19387	-0.60106	-1.69634
8	0	-5.12096	1.68105	-0.52368
6	0	-6.39809	-0.29966	0.63336
6	0	-0.66099	4.94383	-0.51136
1	0	-2.65556	5.59777	-1.04582
1	0	1.18298	3.91612	-0.05501
6	0	-6.98192	-1.55805	0.47177
6	0	-6.83148	0.57247	1.63473
1	0	-0.28762	5.92485	-0.23605
6	0	-8.007	-1.95005	1.33374
1	0	-6.64703	-2.20307	-0.33387
6	0	-7.85586	0.17076	2.4929
1	0	-6.38287	1.55694	1.7182
6	0	-8.44086	-1.08976	2.34586
1	0	-8.47205	-2.92456	1.21051
1	0	-8.20307	0.84518	3.27125
1	0	-9.24039	-1.39809	3.01437

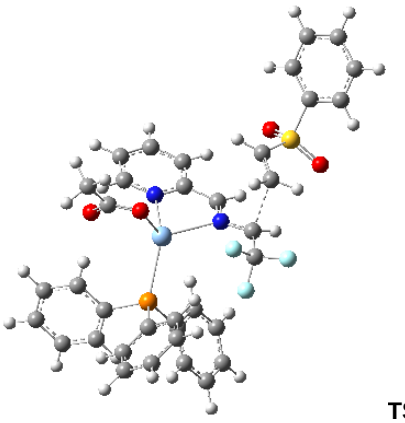


TSIIB*endo*

E(RB3LYP) = -2986.31730983
H(correction)= 0.650457
G(correction)= 0.508938
E(RM06) = -2985.72214286
E(SMD_{THF}RM06) = -2985.80741243
Imaginary frequencies: 1 (-167.8871 cm^{-1})

47	0	-0.67058	0.61492	0.62737
7	0	1.08305	-0.71655	-0.7033
8	0	-0.61519	1.30304	2.83876
15	0	-3.03101	-0.21775	-0.11549
6	0	1.3524	-2.02898	-0.58489
6	0	1.64908	0.01518	-1.63084
6	0	-1.05698	2.49371	2.84984
6	0	-4.16759	1.16073	-0.60005
6	0	-3.12639	-1.35567	-1.57232
6	0	-3.97631	-1.12227	1.19374
1	0	1.72403	-2.6017	-1.4384
6	0	0.50542	-2.82624	0.32862
6	0	3.42098	-2.02662	0.37908
1	0	2.29749	-0.43482	-2.38809
6	0	1.48595	1.45892	-1.67327
8	0	-1.50735	3.13715	1.8659
6	0	-1.02235	3.22196	4.20459
6	0	-3.96071	2.41167	0.00747
6	0	-5.2021	1.01737	-1.53973
6	0	-2.16562	-1.18318	-2.58169
6	0	-4.0855	-2.36899	-1.71923
6	0	-5.35464	-0.96864	1.4082
6	0	-3.25279	-1.98893	2.03075
9	0	1.04567	-4.06401	0.53197
9	0	0.34472	-2.25567	1.55204
9	0	-0.77484	-3.0721	-0.11852
6	0	4.35216	-1.56669	-0.51418
1	0	3.09657	-1.3902	1.19577
1	0	3.29384	-3.09471	0.51855
6	0	2.26271	2.24055	-2.55561
7	0	0.58359	2.042	-0.84962
1	0	-0.30489	4.05011	4.15031
1	0	-2.00448	3.6598	4.41758
1	0	-0.73122	2.55018	5.01629
1	0	-3.13827	2.56023	0.70988
6	0	-4.79526	3.48655	-0.31106
1	0	-5.35879	0.06238	-2.03278
6	0	-6.02721	2.09817	-1.85605
1	0	-1.38958	-0.43223	-2.45945
6	0	-2.18237	-1.98507	-3.72308
6	0	-4.09563	-3.17742	-2.85839
1	0	-4.82207	-2.53391	-0.93818
6	0	-5.99867	-1.67674	2.4257

1	0	-5.92586	-0.28733	0.78489
6	0	-3.90062	-2.70087	3.04063
1	0	-2.18196	-2.10142	1.89495
1	0	4.78587	-2.18333	-1.29624
16	0	4.99549	0.05145	-0.49861
6	0	2.0967	3.61752	-2.56903
1	0	3.01413	1.7562	-3.17106
6	0	0.44282	3.3721	-0.85363
6	0	-5.82764	3.33516	-1.23833
1	0	-4.62197	4.44869	0.16438
1	0	-6.8223	1.97379	-2.58809
1	0	-1.42965	-1.8385	-4.49362
6	0	-3.14794	-2.98423	-3.86509
1	0	-4.84317	-3.96152	-2.95569
6	0	-5.27427	-2.54722	3.2416
1	0	-7.06668	-1.54259	2.58213
1	0	-3.32571	-3.36632	3.67958
8	0	4.27459	0.89067	0.47644
8	0	5.21417	0.5107	-1.89087
6	0	6.66898	-0.15378	0.18156
6	0	1.16899	4.20722	-1.70253
1	0	2.69784	4.23176	-3.23623
1	0	-0.27463	3.75851	-0.13233
1	0	-6.46843	4.17819	-1.48782
1	0	-3.15449	-3.61644	-4.74993
1	0	-5.77513	-3.095	4.0365
6	0	6.86005	-0.08776	1.56445
6	0	7.74666	-0.38469	-0.67645
1	0	1.01855	5.28246	-1.6745
6	0	8.13936	-0.26931	2.09015
1	0	6.01122	0.12195	2.20747
6	0	9.02385	-0.56756	-0.14269
1	0	7.57712	-0.39731	-1.74834
6	0	9.22166	-0.51397	1.23933
1	0	8.29348	-0.21342	3.16506
1	0	9.86661	-0.74392	-0.80713
1	0	10.21775	-0.654	1.65251

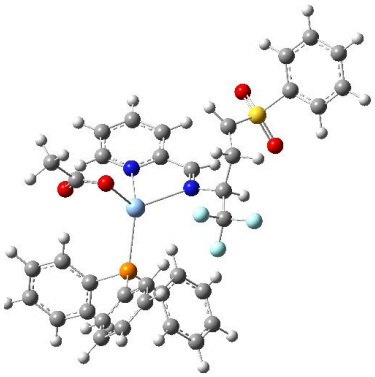


TSIIB*exo*

E(RB3LYP) = -2986.32653256
H(correction)= 0.650820
G(correction)= 0.510127
E(RM06) = -2985.73141165
E(SMD$_{THF}$RM06) = -2985.81462897
Imaginary frequencies: 1 (-154.3177 cm^{-1})

47	0	-0.84417	0.70999	0.62692
7	0	1.11139	-0.46096	-0.50637
8	0	-0.80468	1.48372	2.81919
6	0	1.53321	-1.71768	-0.3035
6	0	1.74806	0.32051	-1.35091
6	0	-1.36649	2.62261	2.79943
1	0	2.13657	-2.23874	-1.04975
6	0	0.69622	-2.61091	0.5276
6	0	3.38987	-1.31112	0.96164
1	0	2.52072	-0.07451	-2.01276
6	0	1.45729	1.73842	-1.4556
6	0	4.06728	-0.25992	0.40011
8	0	-1.88463	3.18791	1.80109
6	0	-1.42126	3.3821	4.13678
9	0	1.37057	-3.75181	0.83726
9	0	0.30915	-2.04503	1.70675
9	0	-0.47593	-3.02911	-0.05882
1	0	2.77439	-1.13106	1.83604
1	0	3.72732	-2.3294	0.80483
6	0	2.2569	2.57129	-2.27198
7	0	0.42697	2.25622	-0.74381
1	0	3.89038	0.78189	0.63918
16	0	5.28135	-0.51976	-0.82165
1	0	-0.95487	4.36744	4.01898
1	0	-2.46764	3.55435	4.41725
1	0	-0.91739	2.83149	4.93536
6	0	1.97532	3.92751	-2.33928
1	0	3.10198	2.13809	-2.79888
6	0	0.17416	3.56839	-0.80051
8	0	5.23675	0.56661	-1.82797
8	0	5.24538	-1.93426	-1.2577
6	0	6.87122	-0.30163	0.02548
6	0	0.91251	4.4496	-1.59045
1	0	2.58651	4.58004	-2.9597
1	0	-0.64343	3.90277	-0.1649
6	0	7.45	0.96785	0.0913
6	0	7.49535	-1.40328	0.61572
1	0	0.6683	5.50771	-1.60811
6	0	8.65948	1.13633	0.76745
1	0	6.95914	1.80151	-0.40031
6	0	8.70556	-1.22716	1.28735
1	0	7.03694	-2.38299	0.52852
6	0	9.28661	0.04163	1.36809
1	0	9.11521	2.12209	0.82031
1	0	9.19816	-2.08171	1.74496
1	0	10.22923	0.17551	1.89329
1	0	-3.45732	2.46235	0.61635
6	0	-4.22019	2.24279	-0.13262
6	0	-4.28869	0.97407	-0.73557
6	0	-5.1151	3.24507	-0.51632
15	0	-3.0774	-0.30221	-0.16272
6	0	-5.24717	0.74148	-1.73596
6	0	-6.07123	3.00489	-1.50478
1	0	-5.0489	4.22186	-0.04375
6	0	-3.02295	-1.50152	-1.56977
6	0	-4.00516	-1.2321	1.14041
1	0	-5.29827	-0.22624	-2.22629
6	0	-6.13269	1.75123	-2.11758
1	0	-6.75911	3.79239	-1.80499
6	0	-1.98583	-1.35488	-2.50424
6	0	-3.94958	-2.54093	-1.74457
6	0	-5.38938	-1.12115	1.34021
6	0	-3.26254	-2.07316	1.98706
1	0	-6.86669	1.55804	-2.89688
1	0	-1.23584	-0.58272	-2.35501
6	0	-1.89499	-2.21013	-3.60312
6	0	-3.85274	-3.40128	-2.84012
1	0	-4.74362	-2.68452	-1.01731
6	0	-6.02031	-1.84467	2.35542
1	0	-5.97587	-0.46263	0.70678
6	0	-3.8973	-2.80092	2.99356
1	0	-2.18717	-2.15292	1.86176

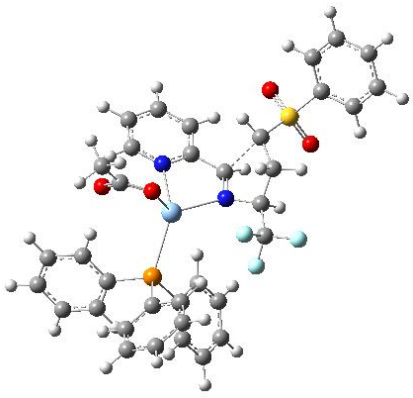
1	0	-1.08307	-2.08554	-4.31495
6	0	-2.82839	-3.23448	-3.77436
1	0	-4.57541	-4.20526	-2.95994
6	0	-5.27705	-2.68857	3.18178
1	0	-7.09349	-1.74369	2.50089
1	0	-3.3082	-3.44642	3.63999
1	0	-2.75029	-3.9079	-4.62461
1	0	-5.76797	-3.2484	3.97442



intB*exo*

E(RB3LYP) = -2986.3414391
H(correction)= 0.6538571
G(correction)= 0.5123781
E(RM06) = -2985.75047013
E(SMD$_{THF}$RM06) = -2985.83476202
Number of imaginary frequencies: 0

47	0	-0.95088	0.76095	0.71184
7	0	1.18634	-0.03774	-0.26594
8	0	-1.11555	1.58451	2.87669
6	0	1.95669	-1.21442	-0.01891
6	0	1.77452	0.7954	-1.06691
6	0	-1.80239	2.64886	2.78678
1	0	2.38929	-1.64929	-0.92981
6	0	1.10716	-2.29164	0.62558
6	0	3.20714	-0.82992	0.91995
1	0	2.57337	0.48457	-1.73809
6	0	1.32571	2.19292	-1.19404
6	0	3.97298	0.34511	0.44062
8	0	-2.32821	3.11515	1.7415
6	0	-2.01088	3.44274	4.08739
9	0	1.84204	-3.40254	0.88357
9	0	0.55974	-1.90217	1.80587
9	0	0.07553	-2.68413	-0.16345
1	0	2.80161	-0.61796	1.91464
1	0	3.79891	-1.75118	0.99486
6	0	2.12399	3.12129	-1.88108
7	0	0.16955	2.54717	-0.60207
1	0	4.01076	1.26469	1.01112
16	0	5.14525	0.2171	-0.76023
1	0	-1.62623	4.46168	3.96012
1	0	-3.08402	3.52907	4.29661
1	0	-1.511	2.96756	4.93518
6	0	1.69627	4.44378	-1.95183
1	0	3.07825	2.80268	-2.29123
6	0	-0.22984	3.82182	-0.65823
8	0	5.47025	1.56423	-1.30425
8	0	4.76114	-0.87454	-1.70381
6	0	6.73737	-0.35858	-0.07428
6	0	0.49743	4.8059	-1.33222
1	0	2.29906	5.18637	-2.46916
1	0	-1.14661	4.04028	-0.11504
6	0	7.6357	0.56529	0.47136
6	0	7.02301	-1.72678	-0.02024
1	0	0.13644	5.83025	-1.35447
6	0	8.81136	0.11953	1.07512
1	0	7.41137	1.62486	0.39679
6	0	8.20011	-2.16809	0.58796
1	0	6.33076	-2.42615	-0.47777
6	0	9.09553	-1.2485	1.13996
1	0	9.51202	0.84069	1.49093
1	0	8.4225	-3.23258	0.62378
1	0	10.01298	-1.59412	1.61102
1	0	-3.7698	2.18289	0.52925
6	0	-4.46567	1.86084	-0.24717
6	0	-4.3357	0.59484	-0.8451
6	0	-5.47372	2.73044	-0.67212
15	0	-2.98704	-0.50679	-0.22128
6	0	-5.21232	0.23143	-1.88084
6	0	-6.34745	2.36017	-1.69601
1	0	-5.56164	3.70737	-0.20347
6	0	-2.6966	-1.65976	-1.638
6	0	-3.83231	-1.57817	1.0277
1	0	-5.10867	-0.73474	-2.36579
6	0	-6.2123	1.10936	-2.30307
1	0	-7.12437	3.04543	-2.02786
6	0	-1.68779	-1.31656	-2.55252
6	0	-3.41503	-2.84845	-1.83958
6	0	-5.22622	-1.68419	1.14694
6	0	-3.01883	-2.29873	1.91925
1	0	-6.88173	0.81679	-3.10896
1	0	-1.09403	-0.4222	-2.38412
6	0	-1.42231	-2.12779	-3.65593
6	0	-3.14245	-3.66427	-2.94002
1	0	-4.18299	-3.1434	-1.1303
6	0	-5.79465	-2.50053	2.12796
1	0	-5.87048	-1.12161	0.47817
6	0	-3.58963	-3.11962	2.89188
1	0	-1.93809	-2.21154	1.85776
1	0	-0.6345	-1.84938	-4.35102
6	0	-2.14946	-3.30377	-3.85276
1	0	-3.70419	-4.58497	-3.07992
6	0	-4.97856	-3.22205	3.00035
1	0	-6.87699	-2.56726	2.21131
1	0	-2.94588	-3.66834	3.57445
1	0	-1.93427	-3.94246	-4.70597
1	0	-5.42174	-3.85335	3.76684

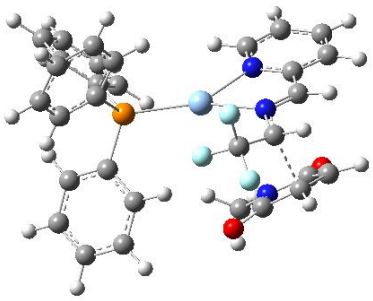


TSintB*exo*

E(RB3LYP) = -2986.34060654
H(correction)= 0.653054
G(correction)= 0.515979
E(RM06) = -2985.74886121

E(SMD$_{THF}$RM06) = -2985.83200874
Imaginary frequencies: 1 (-82.3096 cm^{-1})

47	0	-0.75643	0.64759	0.6281
7	0	1.10935	-0.31945	-0.5843
15	0	-3.01506	-0.36322	-0.159
8	0	-0.78527	1.40214	2.82804
6	0	1.84019	-1.50689	-0.30518
6	0	1.86212	0.50948	-1.28473
6	0	-4.26118	0.8895	-0.70883
6	0	-2.95916	-1.56666	-1.56345
6	0	-3.90306	-1.31883	1.15312
6	0	-1.36614	2.53132	2.82382
1	0	2.26754	-1.9887	-1.20005
6	0	0.99241	-2.56183	0.37756
6	0	3.08792	-1.07224	0.607
1	0	2.50441	0.14516	-2.08961
6	0	1.52685	1.95173	-1.36209
6	0	3.69484	0.18118	0.06692
6	0	-4.21598	2.15086	-0.08789
6	0	-5.21963	0.65217	-1.70802
6	0	-1.89505	-1.45067	-2.47157
6	0	-3.90943	-2.58172	-1.75957
6	0	-5.28111	-1.22033	1.39554
6	0	-3.13135	-2.17119	1.96184
8	0	-1.88241	3.10864	1.83134
6	0	-1.44991	3.26218	4.17582
9	0	1.73663	-3.66026	0.67206
9	0	0.44967	-2.13813	1.54826
9	0	-0.037	-2.98518	-0.39379
1	0	2.70392	-0.89858	1.61664
1	0	3.77913	-1.92047	0.64929
6	0	2.32692	2.82904	-2.11168
7	0	0.46149	2.38894	-0.66763
1	0	3.71703	1.07089	0.68853
16	0	5.07077	0.06382	-0.95127
1	0	-3.45246	2.37562	0.65893
6	0	-5.13428	3.13932	-0.45129
1	0	-5.25305	-0.30835	-2.21344
6	0	-6.12812	1.64875	-2.07009
1	0	-1.12083	-0.70897	-2.29524
6	0	-1.80327	-2.30886	-3.56888
6	0	-3.81199	-3.4438	-2.8533
1	0	-4.72275	-2.70496	-1.04979
6	0	-5.87743	-1.96646	2.41547
1	0	-5.88954	-0.55428	0.79123
6	0	-3.7312	-2.92174	2.97264
1	0	-2.05855	-2.23957	1.80468
1	0	-0.99809	4.25708	4.08436
1	0	-2.5024	3.41186	4.44626
1	0	-0.94713	2.70344	4.96941
6	0	1.99831	4.18061	-2.13429
1	0	3.21261	2.4491	-2.61114
6	0	0.15451	3.69101	-0.67996
8	0	5.3675	1.39796	-1.53289
8	0	4.89322	-1.10214	-1.8565
6	0	6.55008	-0.33675	0.03396
6	0	-6.0905	2.89389	-1.43847
1	0	-5.08634	4.11007	0.03579
1	0	-6.86166	1.45178	-2.84889
1	0	-0.97031	-2.20926	-4.26011
6	0	-2.76206	-3.30459	-3.76407
1	0	-4.55384	-4.22725	-2.99078
6	0	-5.1056	-2.82121	3.20345
1	0	-6.94641	-1.87508	2.59436
1	0	-3.11978	-3.57511	3.58983
6	0	0.89131	4.62694	-1.40738
1	0	2.60798	4.88094	-2.70069
1	0	-0.69572	3.96661	-0.05948
6	0	7.25218	0.68821	0.67626
6	0	6.94261	-1.66888	0.19124
1	0	-6.79661	3.67095	-1.72315
1	0	-2.68401	-3.97895	-4.61363
1	0	-5.5697	-3.39865	3.99954
1	0	0.61015	5.67629	-1.39064
6	0	8.34467	0.37545	1.48505
1	0	6.94704	1.71833	0.5204
6	0	8.03666	-1.97525	1.00329
1	0	6.40048	-2.44417	-0.34047
6	0	8.73666	-0.95633	1.65403
1	0	8.89533	1.17182	1.98061
1	0	8.34637	-3.01098	1.12323
1	0	9.58822	-1.19742	2.28599

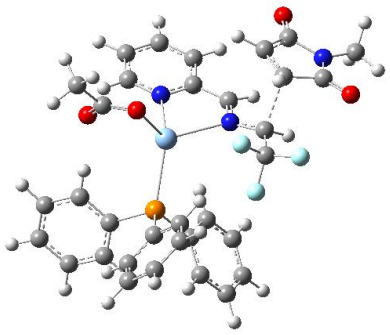


TSIIA*endo'*

E(RB3LYP) = -2298.30298575
H(correction)= 0.545601
G(correction)= 0.428956
E(SMD$_{THF}$RM06) = -2297.79639501
Imaginary frequencies: 1 (-251.8748 cm^{-1})

47	0	-0.35775	0.40014	-0.56178
15	0	2.00553	0.17964	0.03739
7	0	-2.35765	-0.53494	-1.2844
6	0	2.30503	-0.65503	1.64593
6	0	2.85947	1.80684	0.19268
6	0	2.97954	-0.753	-1.21355
6	0	-2.68716	-1.84519	-1.27135
6	0	-3.34481	0.33779	-1.39286
6	0	1.36477	-1.5982	2.09031
6	0	3.42687	-0.37029	2.44263
6	0	2.201	2.82837	0.89856
6	0	4.11837	2.06863	-0.36548
6	0	4.06952	-1.56735	-0.87146
6	0	2.6051	-0.64291	-2.5624
1	0	-3.56813	-2.16162	-1.83658
6	0	-1.58779	-2.85201	-1.40852
6	0	-3.73069	-2.03404	0.56685
1	0	-4.31347	0.03187	-1.78502
6	0	-3.13844	1.76106	-1.18984
1	0	0.48055	-1.8293	1.50539
6	0	1.55029	-2.25361	3.30897
6	0	3.60813	-1.03122	3.65799
1	0	4.15081	0.37275	2.12068
1	0	1.21993	2.64184	1.33008
6	0	2.79578	4.07951	1.05441
6	0	4.70748	3.32744	-0.21712
1	0	4.63862	1.29385	-0.91983
6	0	4.77608	-2.24955	-1.86381
1	0	4.35964	-1.67866	0.16874
6	0	3.31763	-1.31942	-3.55214
1	0	1.74679	-0.03459	-2.83838

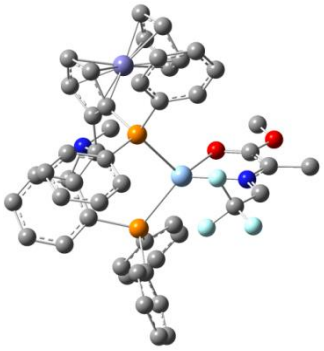
9	0	-1.14846	-2.96098	-2.69626
9	0	-0.4911	-2.56352	-0.66566
9	0	-2.01814	-4.08038	-1.05007
6	0	-4.58387	-0.93109	0.64285
6	0	-2.64333	-1.80711	1.58477
1	0	-4.03074	-3.0548	0.36133
6	0	-4.21042	2.66513	-1.32565
7	0	-1.90199	2.20222	-0.85098
1	0	0.80091	-2.96708	3.63783
6	0	2.67093	-1.97321	4.0921
1	0	4.47778	-0.80459	4.26918
1	0	2.27797	4.8579	1.60827
6	0	4.05064	4.33256	0.49305
1	0	5.6819	3.51924	-0.65826
6	0	4.40424	-2.12469	-3.20368
1	0	5.6143	-2.88326	-1.58722
1	0	3.01504	-1.22842	-4.59154
6	0	-4.02756	0.05528	1.55364
1	0	-5.57722	-0.83009	0.22759
7	0	-2.79373	-0.50348	2.02895
8	0	-1.78663	-2.58964	1.97643
6	0	-3.99553	4.01971	-1.12366
1	0	-5.19614	2.28603	-1.57688
6	0	-1.70441	3.51364	-0.66516
1	0	2.81174	-2.47917	5.0436
1	0	4.51089	5.31026	0.60636
1	0	4.95283	-2.66099	-3.9731
8	0	-4.45253	1.13915	1.93182
6	0	-2.03783	0.07422	3.12112
6	0	-2.71141	4.46547	-0.79144
1	0	-4.81697	4.72419	-1.2207
1	0	-0.69031	3.80766	-0.40373
1	0	-2.09178	-0.56057	4.01313
1	0	-0.98412	0.19614	2.85217
1	0	-2.48178	1.04846	3.33588
1	0	-2.49774	5.51624	-0.62592



TSIIB*exo'*

E(RB3LYP) = -2526.86701594
H(correction)= 0.601136
G(correction)= 0.466771
E(SMD$_{THF}$RM06) = -2526.37332089
Imaginary frequencies: 1 (-249.5448 cm^{-1})

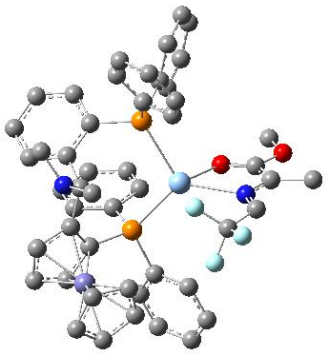
47	0	0.24865	0.83306	-0.67571
7	0	-1.90786	-0.16756	0.17397
8	0	0.60817	1.71051	-2.80042
15	0	2.25445	-0.43171	0.32867
6	0	-2.45657	-1.37355	-0.10194
6	0	-2.61008	0.65711	0.91767
6	0	1.24853	2.79391	-2.633
6	0	3.52137	0.67718	1.09597
6	0	1.90365	-1.65476	1.67107
6	0	3.21957	-1.41778	-0.90349
1	0	-3.01911	-1.9034	0.67271
6	0	-1.61993	-2.30542	-0.91743
1	0	-3.43538	0.30009	1.53798
6	0	-2.23711	2.05858	1.08489
8	0	1.65101	3.26674	-1.53702
6	0	1.56279	3.60713	-3.90056
6	0	3.64103	1.97814	0.57627
6	0	4.34767	0.28552	2.1625
6	0	0.83941	-1.36788	2.54104
6	0	2.62897	-2.84101	1.85968
6	0	4.62108	-1.48336	-0.9215
6	0	2.49544	-2.11195	-1.88823
9	0	-2.32761	-3.38549	-1.31113
9	0	-1.12121	-1.71767	-2.03796
9	0	-0.52734	-2.79239	-0.24564
6	0	-3.0997	2.94634	1.75939
7	0	-1.07467	2.48797	0.5471
1	0	1.12747	4.60952	-3.80952
1	0	2.64784	3.73631	-3.99448
1	0	1.17373	3.12123	-4.79893
1	0	2.98358	2.32008	-0.22512
6	0	4.58999	2.85535	1.10831
1	0	4.2511	-0.70955	2.58686
6	0	5.28859	1.1707	2.69169
1	0	0.24204	-0.4745	2.37941
6	0	0.52664	-2.23214	3.59037
6	0	2.30866	-3.71033	2.90504
1	0	3.4405	-3.09204	1.18287
6	0	5.28407	-2.2363	-1.89381
1	0	5.19765	-0.93856	-0.18012
6	0	3.16067	-2.86947	-2.85236
1	0	1.41152	-2.05597	-1.90433
6	0	-2.73825	4.28271	1.87018
1	0	-4.05325	2.58254	2.13073
6	0	-0.73896	3.77919	0.64469
6	0	5.41431	2.45735	2.16225
1	0	4.67038	3.859	0.69843
1	0	5.91943	0.85554	3.51997
1	0	-0.30221	-1.996	4.25289
6	0	1.26069	-3.40585	3.7755
1	0	2.87666	-4.62867	3.03476
6	0	4.55602	-2.93338	-2.8591
1	0	6.3711	-2.27249	-1.89749
1	0	2.58515	-3.39905	-3.60714
6	0	-1.53325	4.71643	1.30701
1	0	-3.39599	4.98472	2.37795
1	0	0.19168	4.04747	0.14856
1	0	6.14523	3.14793	2.5773
1	0	1.009	-4.08565	4.58596
1	0	5.07286	-3.5154	-3.61852
1	0	-1.22008	5.75475	1.36603
6	0	-4.1376	-0.83022	-1.26032
6	0	-4.4935	0.48157	-0.90868
6	0	-5.16085	-1.73718	-0.62953
1	0	-3.71034	-1.11897	-2.21338
1	0	-4.12034	1.40209	-1.33265
6	0	-5.57345	0.44707	0.05307
7	0	-5.89279	-0.93409	0.2424
8	0	-5.33891	-2.93618	-0.79122
8	0	-6.17206	1.33768	0.65595
6	0	-6.99	-1.40048	1.05388
1	0	-7.01589	-2.48983	0.97419
1	0	-6.85402	-1.10665	2.10076
1	0	-7.94582	-0.98631	0.70915



IC

E(RB3LYP) = -3406.28451319
H(correction)= 0.894395
G(correction)= 0.738077
E(SMD$_{THF}$RM06) = -3405.53284094
Number of imaginary frequencies: 0

47	0	0.34145	0.66324	-0.92148
15	0	-1.35948	0.85567	1.00978
15	0	2.42132	-0.51165	0.17708
7	0	0.32003	2.10966	-2.84974
6	0	-2.11745	-0.74066	1.48188
6	0	-2.78712	1.9902	0.6984
6	0	-0.69821	1.5408	2.59676
6	0	3.80029	0.67841	0.48354
6	0	3.21213	-1.88853	-0.75996
6	0	2.04653	-1.23639	1.85548
6	0	0.59173	3.38806	-2.76114
6	0	0.02371	1.49787	-4.01684
6	0	-1.53074	-2.06831	1.36525
6	0	-3.42713	-0.90182	2.06161
26	0	-3.33578	-1.90025	0.26545
6	0	-3.02004	2.43717	-0.61022
6	0	-3.61474	2.45962	1.73178
6	0	-0.00881	2.76625	2.54334
6	0	-0.85867	0.9062	3.83567
6	0	3.56213	1.78523	1.3185
6	0	5.03175	0.59286	-0.18331
6	0	2.74446	-2.16993	-2.05246
6	0	4.25791	-2.65982	-0.22438
6	0	2.91329	-0.97952	2.93403
6	0	0.87215	-1.9932	2.09661
1	0	0.58733	4.07293	-3.60556
6	0	0.86252	4.00059	-1.44426
6	0	-0.23441	0.09731	-3.95669
6	0	-0.01238	2.27445	-5.30469
6	0	-0.0916	-2.45529	0.99474
6	0	-2.49719	-2.99609	1.85839
1	0	-4.13466	-0.10455	2.23798
6	0	-3.65687	-2.28678	2.28262
6	0	-3.06395	-2.2474	-1.78464
6	0	-3.97155	-3.20349	-1.23337
6	0	-3.61661	-0.95154	-1.57943
6	0	-4.86286	-1.09792	-0.90127
6	0	-5.08408	-2.49278	-0.68885
1	0	-2.35327	2.12987	-1.41083
6	0	-4.08535	3.29678	-0.88837
6	0	-4.67783	3.31917	1.45376
1	0	-3.41777	2.16762	2.75925
1	0	0.12566	3.27529	1.59309
6	0	0.49556	3.34314	3.70904
6	0	-0.34278	1.48355	4.99945
1	0	-1.38366	-0.04113	3.89577
1	0	2.60922	1.88828	1.82929
6	0	4.54127	2.75888	1.50397
6	0	6.00561	1.5794	-0.00622
1	0	5.23667	-0.24103	-0.84566
1	0	1.91601	-1.59956	-2.4664
6	0	3.3233	-3.20181	-2.79835
6	0	4.83352	-3.68575	-0.97286
1	0	4.61923	-2.45935	0.7807
1	0	3.81756	-0.40537	2.76686
6	0	2.63609	-1.4321	4.22187
6	0	0.60183	-2.42246	3.40517
9	0	1.37488	5.24208	-1.58578
9	0	-0.25244	4.13932	-0.64373
9	0	1.7364	3.28705	-0.66995
8	0	-0.22737	-0.63613	-2.93793
8	0	-0.51097	-0.45828	-5.17773
1	0	-0.75138	3.09065	-5.26188
1	0	0.96	2.7472	-5.51589
1	0	-0.26675	1.63212	-6.14749
1	0	0.17682	-1.93961	0.05941
7	0	-0.00031	-3.93149	0.81023
1	0	-2.35215	-4.0667	1.87293
1	0	-4.56975	-2.7275	2.66242
1	0	-2.10363	-2.43547	-2.24281
1	0	-3.83329	-4.27656	-1.20301
1	0	-3.14637	-0.02337	-1.86548
1	0	-5.5043	-0.2915	-0.57122
1	0	-5.92666	-2.93271	-0.17117
1	0	-4.25089	3.63486	-1.90767
6	0	-4.92002	3.73332	0.1412
1	0	-5.31052	3.67371	2.26336
1	0	1.01686	4.29538	3.65363
6	0	0.33185	2.70268	4.94067
1	0	-0.47288	0.97697	5.95232
1	0	4.3396	3.60302	2.15793
6	0	5.7673	2.66072	0.84099
1	0	6.95244	1.49627	-0.53334
1	0	2.95443	-3.41293	-3.79861
6	0	4.36672	-3.95717	-2.26309
1	0	5.6426	-4.2755	-0.5499
1	0	3.32975	-1.21718	5.03032
6	0	1.46666	-2.15199	4.46169
1	0	-0.29966	-3.0013	3.58203
6	0	-0.8045	-1.85141	-5.191
6	0	-0.50834	-4.34627	-0.49482
6	0	1.30402	-4.55921	1.03211
1	0	-5.74504	4.40731	-0.07379
1	0	0.72895	3.1521	5.84708
1	0	6.52622	3.42617	0.97871
1	0	4.81471	-4.75828	-2.84518
1	0	1.231	-2.50649	5.46171
1	0	-1.73144	-2.06798	-4.64963
1	0	-0.92211	-2.1156	-6.24417
1	0	0.00669	-2.43668	-4.74622
1	0	0.12613	-3.99633	-1.33098
1	0	-1.51561	-3.96362	-0.64085
1	0	-0.54549	-5.44123	-0.53329
1	0	1.16208	-5.64445	0.96952
1	0	1.68932	-4.33317	2.02645
1	0	2.06696	-4.27869	0.28836



IC'

E(RB3LYP) = -3406.28484088
H(correction)= 0.894314
G(correction)= 0.736993
E(SMD_{THF}RM06) = -3405.52663197
Number of imaginary frequencies: 0

47	0	0.67312	0.90275	-0.58725
15	0	2.23924	-1.11154	0.05095
15	0	-1.32105	0.92193	1.06359
7	0	1.00112	2.30991	-2.51434
6	0	3.85459	-0.44082	0.64943
6	0	2.72541	-2.36605	-1.20829
6	0	1.60151	-2.08787	1.50393
6	0	-2.41851	-0.52749	1.22849
6	0	-2.45242	2.36914	0.86703
6	0	-0.65681	1.18162	2.77104
6	0	0.5339	1.99663	-3.70287
6	0	1.83853	3.34248	-2.3056
6	0	3.81877	0.67647	1.50248
6	0	5.10076	-0.95744	0.26393
6	0	2.55938	-2.04144	-2.5633
6	0	3.27664	-3.6128	-0.86729
6	0	2.45265	-2.29911	2.60476
6	0	0.25472	-2.5285	1.58806
6	0	-2.08049	-1.89748	0.89218
6	0	-3.73785	-0.53998	1.80655
26	0	-3.83763	-1.28154	-0.11781
6	0	-2.54875	2.97392	-0.39566
6	0	-3.1807	2.91031	1.9386
6	0	0.33539	2.16596	2.93546
6	0	-1.081	0.44922	3.88827
1	0	0.74963	2.5591	-4.60778
6	0	-0.49059	0.94928	-3.8427
6	0	2.23059	3.59026	-0.95124
6	0	2.29505	4.20844	-3.44782
1	0	2.86747	1.11598	1.78363
6	0	5.00128	1.23713	1.98335
6	0	6.28368	-0.38059	0.73366
1	0	5.15502	-1.80947	-0.40506
1	0	2.1081	-1.09351	-2.84027
6	0	2.94773	-2.94227	-3.55826
6	0	3.66286	-4.51077	-1.86339
1	0	3.40305	-3.88188	0.17783
1	0	3.48346	-1.96728	2.55196
6	0	2.00352	-2.90876	3.7739
6	0	-0.18113	-3.1126	2.78772
6	0	-0.73748	-2.44938	0.41627
6	0	-3.19452	-2.71105	1.26032
1	0	-4.29119	0.33379	2.12247
6	0	-4.20599	-1.88329	1.82942
6	0	-4.36889	-2.22795	-1.8989
6	0	-3.6231	-1.04751	-2.19369
6	0	-5.53575	-1.84301	-1.17331
6	0	-4.32974	0.06573	-1.6511
6	0	-5.50962	-0.42323	-1.01914
1	0	-1.97515	2.57951	-1.2293
6	0	-3.37907	4.08076	-0.58812
6	0	-4.00907	4.01655	1.74388
1	0	-3.08689	2.47945	2.93139
1	0	0.69836	2.72386	2.07499
6	0	0.87093	2.41947	4.19856
6	0	-0.533	0.70114	5.14915
1	0	-1.83738	-0.32071	3.7772
9	0	-0.68337	0.6217	-5.13738
9	0	-0.2016	-0.22219	-3.17473
9	0	-1.73344	1.29971	-3.35287
8	0	1.91141	2.93144	0.0616
8	0	3.03791	4.68536	-0.81078
1	0	2.81827	3.61476	-4.21407
1	0	1.44339	4.68945	-3.95525
1	0	2.97091	4.99164	-3.10536
1	0	4.95503	2.09296	2.65166
6	0	6.23781	0.71212	1.59926
1	0	7.24053	-0.79075	0.42139
1	0	2.81081	-2.67954	-4.60359
6	0	3.50058	-4.17562	-3.21042
1	0	4.08787	-5.4724	-1.58783
1	0	2.68886	-3.05698	4.60405
6	0	0.67228	-3.30767	3.87042
1	0	-1.2173	-3.42679	2.86514
1	0	-0.32319	-1.73975	-0.31164
7	0	-0.94812	-3.76021	-0.26445
1	0	-3.25205	-3.77461	1.07761
1	0	-5.18405	-2.20865	2.16042
1	0	-4.08534	-3.24188	-2.14725
1	0	-2.67952	-0.98848	-2.71505
1	0	-6.28521	-2.51354	-0.77317
1	0	-4.00864	1.09621	-1.68867
1	0	-6.23644	0.17192	-0.48173
1	0	-3.44226	4.53984	-1.57102
6	0	-4.11211	4.60206	0.47962
1	0	-4.56618	4.42695	2.5822
1	0	1.63204	3.18706	4.31408
6	0	0.43938	1.68841	5.30872
1	0	-0.87023	0.12357	6.00613
6	0	3.47565	4.97286	0.51432
1	0	7.15871	1.1573	1.96656
1	0	3.79894	-4.8772	-3.98487
1	0	0.29732	-3.76886	4.78027
6	0	-0.99465	-3.62361	-1.7166
6	0	-0.13035	-4.90674	0.11608
1	0	-4.75159	5.46818	0.33099
1	0	0.8627	1.88449	6.29044
1	0	4.03801	4.1332	0.93479
1	0	4.12011	5.85005	0.42555
1	0	2.62963	5.19634	1.17269
1	0	-0.00035	-3.47187	-2.17286
1	0	-1.62731	-2.77868	-1.98685
1	0	-1.43196	-4.52975	-2.15392
1	0	-0.53709	-5.78711	-0.39595
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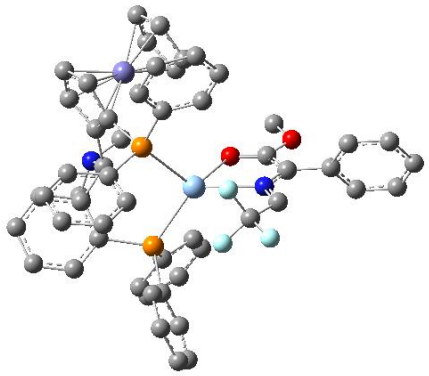

IIIDa

E(RB3LYP) = -3598.0146838
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G(correction)= 0.784609
E(SMD$_{THF}$RM06) = -3597.17620236
Number of imaginary frequencies: 0

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15	0	0.83125	2.4368	-0.28623
7	0	-3.07625	0.30066	0.57031
6	0	2.12392	-2.10829	0.0206
6	0	0.16688	-2.82162	2.06975
6	0	2.05475	-0.73623	2.58177
6	0	0.56711	3.78188	0.95148
6	0	0.6308	3.27881	-1.91476
6	0	2.65685	2.06383	-0.1796
6	0	-3.5775	0.58064	1.74286
6	0	-3.8098	0.0305	-0.53841
6	0	2.61999	-1.49613	-1.20276
6	0	2.73907	-3.40694	0.1296
6	0	-1.19705	-3.05892	1.84663
6	0	0.86284	-3.65566	2.96031
6	0	1.43936	-0.07639	3.66121
6	0	3.44831	-0.8825	2.58083
6	0	0.7937	3.49526	2.30987
6	0	0.03455	5.03374	0.60904
6	0	-0.3947	2.84511	-2.76809
6	0	1.46649	4.33138	-2.3258
6	0	3.49986	2.92112	0.55179
6	0	3.21909	0.90393	-0.77045
1	0	-4.64366	0.61396	1.95627
6	0	-2.67839	0.83297	2.88984
6	0	-3.08484	-0.20947	-1.74424
6	0	-5.3017	-0.00853	-0.50617
6	0	2.44596	-0.05109	-1.69167
6	0	3.50355	-2.43744	-1.81156
1	0	2.5446	-4.12736	0.91127
6	0	3.57851	-3.60532	-0.99997
1	0	-1.76048	-2.38898	1.20315
6	0	-1.84201	-4.13265	2.46442
6	0	0.21775	-4.72736	3.57848
1	0	1.90629	-3.45646	3.18721
1	0	0.3604	0.04791	3.67857
6	0	2.20629	0.41269	4.7188
6	0	4.21334	-0.38174	3.63808
1	0	3.94007	-1.38537	1.75499
1	0	1.18335	2.52511	2.60416
6	0	0.5249	4.44656	3.29154
6	0	-0.24763	5.98001	1.59806
1	0	-0.16485	5.27727	-0.42871
1	0	-1.02737	2.01101	-2.47447
6	0	-0.58555	3.46359	-4.00784
6	0	1.27097	4.94698	-3.56147
1	0	2.2735	4.66666	-1.67992
1	0	3.08594	3.81246	1.00948
6	0	4.85608	2.65072	0.71785
6	0	4.58346	0.63982	-0.57363
9	0	-3.37031	1.29774	3.95047
9	0	-2.00522	-0.28666	3.33037
9	0	-1.68241	1.7352	2.63022
8	0	-1.83984	-0.19608	-1.90055
8	0	-3.89469	-0.47976	-2.81035
6	0	-6.07454	0.94325	-1.19157
6	0	-5.97721	-0.99131	0.23822
1	0	1.3764	0.20602	-1.63991
7	0	2.93217	0.06634	-3.09505
1	0	4.0056	-2.27054	-2.75368
1	0	4.13568	-4.50496	-1.22799
26	0	1.60507	-3.32262	-1.58499
1	0	-2.89967	-4.30213	2.28177
6	0	-1.13479	-4.97206	3.32625
1	0	0.76863	-5.36483	4.26518
1	0	1.71615	0.9112	5.55114
6	0	3.5961	0.2631	4.70956
1	0	5.29367	-0.50026	3.62119
1	0	0.71256	4.20705	4.33478
6	0	0.00147	5.69335	2.93957
1	0	-0.66183	6.94353	1.31292
1	0	-1.38213	3.11973	-4.6623
6	0	0.24208	4.5142	-4.40422
1	0	1.92212	5.76108	-3.86903
1	0	5.4776	3.33718	1.28654
6	0	5.40118	1.49634	0.15763
1	0	5.00708	-0.25097	-1.0273
6	0	-3.25103	-0.75124	-4.05132
6	0	-7.46855	0.90982	-1.14407
1	0	-5.56998	1.70954	-1.77352
6	0	-7.37109	-1.02402	0.29491
1	0	-5.39779	-1.74019	0.77314
6	0	1.94187	-0.42603	-4.04923
6	0	3.4056	1.37906	-3.53865
6	0	-0.09293	-3.07896	-2.79279
1	0	-1.63802	-5.80332	3.8129
1	0	4.19217	0.64825	5.53271
1	0	-0.21755	6.43094	3.70691
1	0	0.09188	4.99353	-5.36803
1	0	6.45581	1.26566	0.2834
1	0	-2.67658	-1.68243	-4.00544
1	0	-4.05664	-0.8513	-4.78159
1	0	-2.5787	0.06238	-4.34213
6	0	-8.12302	-0.07301	-0.39832
1	0	-8.04505	1.6553	-1.68662
1	0	-7.87039	-1.79713	0.87407
1	0	1.04182	0.21528	-4.09986
1	0	1.63388	-1.43257	-3.77681
1	0	2.39139	-0.45948	-5.04859
1	0	3.82684	1.25483	-4.54314
1	0	4.19892	1.75556	-2.89252
1	0	2.61277	2.1415	-3.60097
6	0	0.87052	-3.90483	-3.44956
6	0	-0.45123	-3.71587	-1.57041
1	0	-0.47116	-2.11908	-3.11469
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6	0	0.28761	-4.93127	-1.46381
1	0	-1.1431	-3.32392	-0.84073
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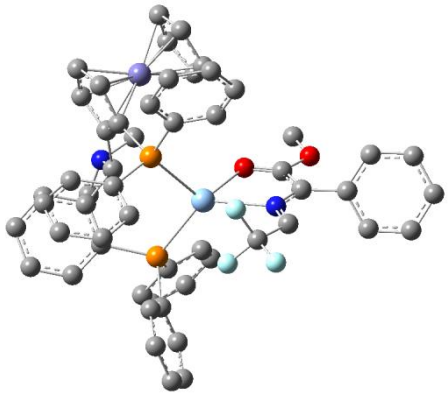

IIIDb

E(RB3LYP) = -3598.01513647
H(correction)= 0.950322
G(correction)= 0.785912
E(SMD$_{THF}$RM06) = -3597.1772752
Number of imaginary frequencies: 0

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15	0	0.77017	2.44224	-0.3672
6	0	-3.5722	0.52258	1.76424
6	0	-3.81043	-0.05237	-0.51194
6	0	2.17293	-2.05939	0.06237
6	0	0.26023	-2.75767	2.15669
6	0	2.09986	-0.61075	2.58233
6	0	0.49625	3.80595	0.84731
6	0	0.52428	3.24576	-2.00857
6	0	2.60478	2.11254	-0.28076
1	0	-4.63444	0.494	1.99711
6	0	-2.6697	0.81593	2.89895
6	0	-3.08298	-0.32282	-1.71084
6	0	-5.30101	-0.10726	-0.47859
6	0	2.63636	-1.47778	-1.18878
6	0	2.81953	-3.33929	0.20508
6	0	-1.10065	-3.03448	1.96198
6	0	0.98965	-3.54786	3.06048
6	0	1.48006	0.05414	3.65616
6	0	3.49732	-0.71154	2.562
6	0	0.74777	3.54868	2.2071
6	0	-0.06407	5.04118	0.48937
6	0	-0.51064	2.77751	-2.8318
6	0	1.33434	4.30244	-2.4583
6	0	3.43962	3.0135	0.40634
6	0	3.18415	0.94791	-0.84486
9	0	-3.36662	1.26427	3.9639
9	0	-1.95053	-0.2732	3.34368
9	0	-1.71243	1.75195	2.61808
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6	0	3.53301	-2.41885	-1.77879
1	0	2.65257	-4.03686	1.01329
6	0	3.64627	-3.55701	-0.93027
1	0	-1.69106	-2.39767	1.30931
6	0	-1.7099	-4.10447	2.62115
6	0	0.38052	-4.61623	3.71941
1	0	2.03104	-3.31673	3.26559
1	0	0.39804	0.1438	3.68815
6	0	2.24679	0.59222	4.6898
6	0	4.2618	-0.16185	3.59512
1	0	3.9927	-1.21669	1.73978
1	0	1.16106	2.59179	2.5124
6	0	0.47472	4.51258	3.17512
6	0	-0.34998	6.00017	1.46508
1	0	-0.28199	5.26164	-0.54987
1	0	-1.1232	1.93988	-2.50767
6	0	-0.73628	3.36597	-4.08018
6	0	1.10484	4.8876	-3.70283
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1	0	4.22058	-4.45095	-1.13705
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1	0	0.68182	4.29598	4.21968
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1	0	-1.54036	2.99593	-4.71067
6	0	0.06672	4.42044	-4.51532
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1	0	5.41951	3.50023	1.09018
6	0	5.36742	1.62227	0.02258
1	0	4.99584	-0.17045	-1.09978
1	0	-2.67505	-1.83254	-3.94057
1	0	-4.04483	-1.00722	-4.74217
1	0	-2.56196	-0.09657	-4.315
6	0	-8.12246	-0.20257	-0.37741
1	0	-8.01122	1.9023	0.08389
1	0	-7.90185	-2.29412	-0.85741
6	0	1.91798	-0.5465	-4.06085
6	0	3.2831	1.35196	-3.62858
6	0	-0.04971	-3.17284	-2.70068
1	0	-1.44463	-5.72878	4.01487
1	0	4.23622	0.91023	5.46622
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1	0	-0.11017	4.87628	-5.48597
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1	0	0.98009	0.03796	-4.11552
1	0	1.675	-1.56228	-3.75892
1	0	2.35664	-0.57873	-5.06498
1	0	3.70435	1.21687	-4.63158
1	0	4.057	1.79592	-3.00213
1	0	2.44649	2.06408	-3.71025
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