

Supporting Information

A DFT Investigation on the Mechanism of Photoinduced Radical Borylation of Alkyl Bromides: Elucidation for Base-Mediated Photoinduced SET and S_N2 Processes

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Table of Contents	Pages
Change in spin density during the B–B homolysis (Figure S1).	2
Two MeO [−] and 4-PhPy promotes the cleavage of B–B bonds in B ₂ cat ₂ (Figure S2).	2
The photoinduced SET process following the S _N 2 of INT-A with counter-cation.(Figure S3).	3
The reaction pathway involving INT-A to R [•] considering the counter-cation (Figure S4).	3
The SET process between 2D and alkyl bromine or nucleophilic substitution (Figure S5).	4
The SET process between INT-AB and alkyl bromine or nucleophilic substitution (Figure S6).	4
B ₂ cat ₂ /B ₂ pin ₂ captures R [•] to produce boride products (Figure S7).	5
The computational details of oxidation potentials .	6
The calculated excitations of intermediate 6A at different computational levels (Table S1).	7
Computed low-lying singlet-to-in 5A , 6A , INT-A, 2D , 2C , INT-AB, INT-B, 1E (Table S2).	7
The computational details of activation barrier of single electron transfer step.	8
Details of estimation of the activation barriers for SET steps (Table S3).	9
Table of calculated energies and energy corrections (Table S4).	10
Cartesian coordinates of all calculated compounds.	13-149

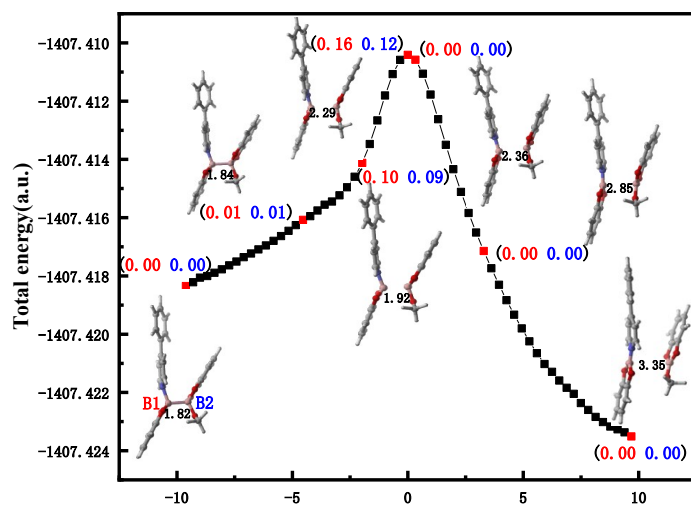


Figure S1. Change in spin density during the B-B hemolysis

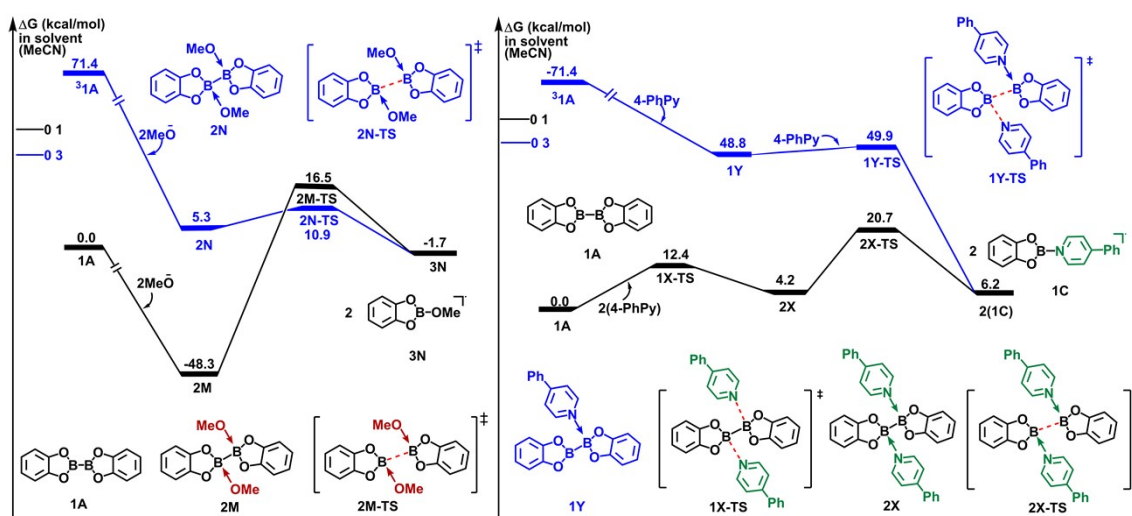


Figure S2. Two MeO^- and two 4-PhPy promote the cleavage of B-B bonds in B_2cat_2 .

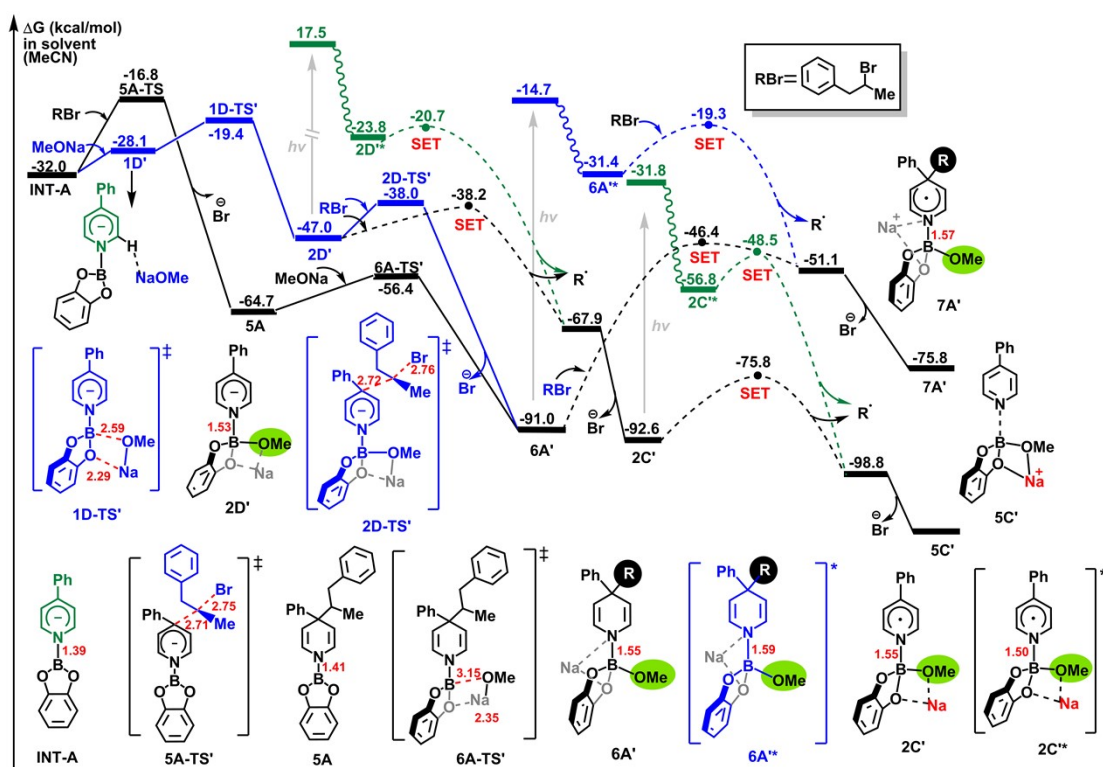


Figure S3. The photoinduced SET process following the S_N2 of INT-A with counter-cation (MeONa).

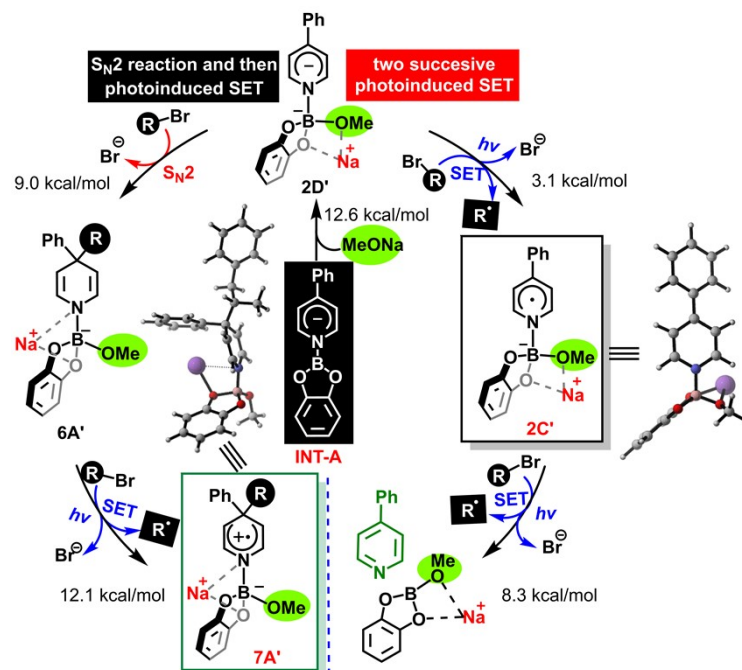


Figure S4. The reaction pathway involving INT-A to R' considering the counter-cation (MeONa).

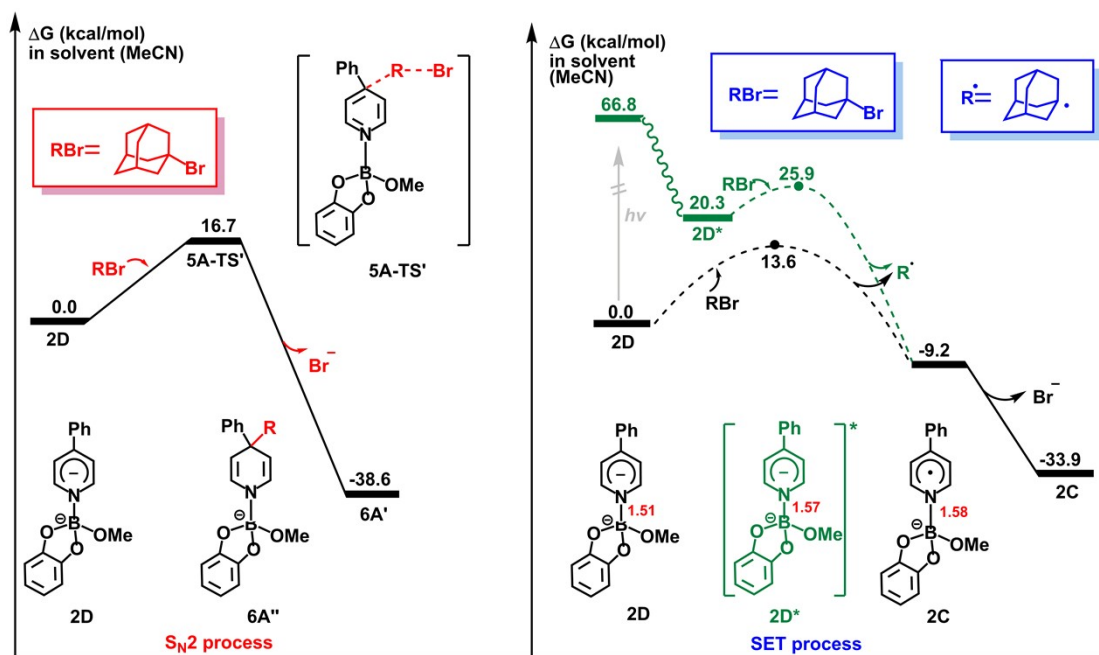


Figure S5. The SET process between 2D and alkyl bromine or nucleophilic substitution.

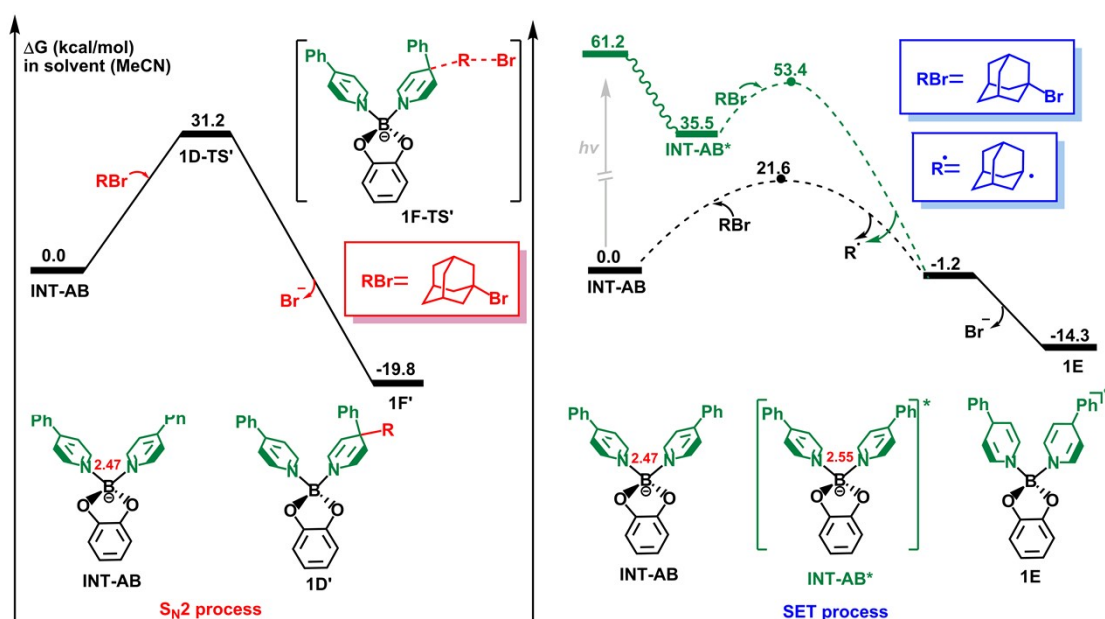


Figure S6. The SET process between INT-AB and alkyl bromine or nucleophilic substitution.

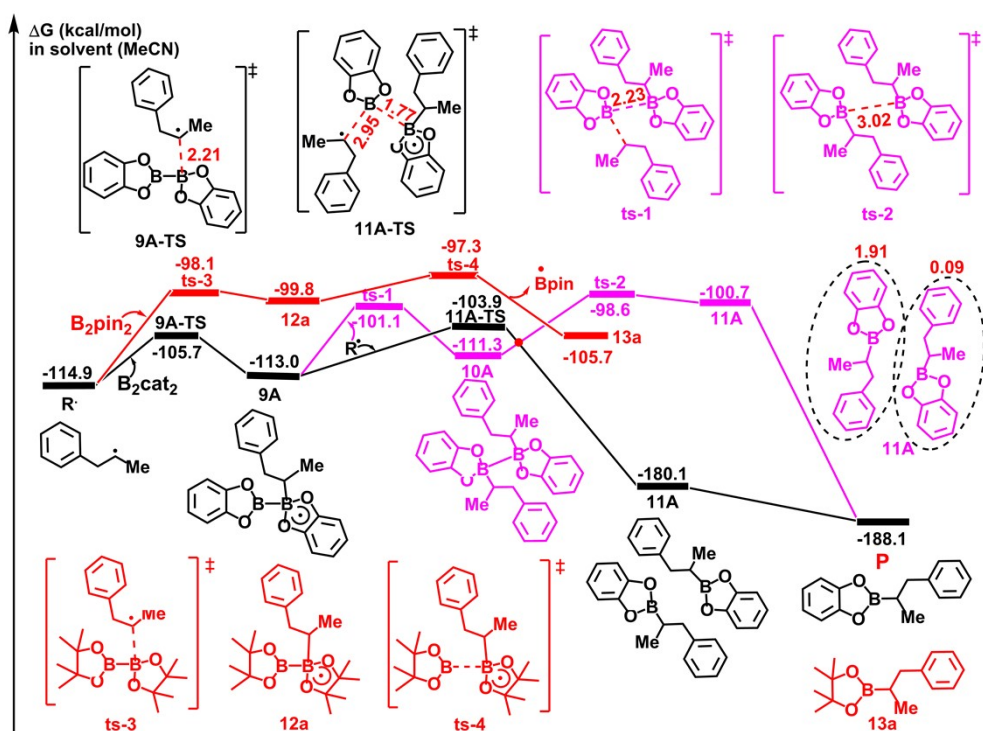
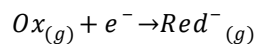


Figure S7. B₂cat₂/B₂pin₂ captures R• to produce boride products.

The computational details of oxidation potentials.

The theoretical prediction of redox potential requires the difference of the free energy (ΔG) associated with the process:



The ΔG of the reduction process in solution can be obtained by frequency calculations. The solvent effects of acetonitrile were included with the SMD model by single point calculations at M06L/6-311++G(d,p) level on the basis of the optimized geometries by B3LYP/6-31G(d). Therefore, the electronic and thermal free energies in solution, G_{sol} , were obtained by taking account the thermodynamic corrections to the energy in solution, as the equation listed in the following:

$$G_{sol} = E_{SMD} + (G - E)_g$$

The ΔG value associated with the reference normal hydrogen electrode (NHE) half-reaction has been calculated to be -4.44 V (in acetonitrile). So the reference standard calomel electrode (SCE) should be -4.20 V. The reduction potentials ($E_{1/2}$) can be calculated according to the Nernst equation $E_0 = -\Delta G_0 / nF$.

The computational levels of excitations.

The excitations of possible SEDs were evaluated using Time-Dependent Density Functional Theory (TD-DFT). Considering potential functional dependence of excitation energies, a benchmarking protocol was implemented: intermediate **6A** was selected as a representative system for comparative analysis across hybrid exchange-correlation functional B3LYP and long-range correction functional CAM-B3LYP. The 6-31+G(d) basis set with diffusion functions was applied. As summarized in the following Table S1, the B3LYP/6-31+G(d)-derived vertical excitation energies align most closely with experimental irradiation conditions.

Table S1 The calculated exactions of intermediate **6A** at different computational levels.

B3LYP/6-31+G(d)				CAM-B3LYP/6-31+G(d)			
states	<i>E</i> (eV)	λ (nm)	<i>f</i>	states	<i>E</i> (eV)	λ (nm)	<i>f</i>
S₁	2.88	430	0.0156	S₁	3.94	315	0.0305
S₂	2.95	421	0.0247	S₂	4.15	299	0.0114
S₃	3.11	399	0.0079	S₃	4.23	293	0.0029
S₄	3.16	392	0.0016	S₄	4.30	288	0.0129
S₅	3.23	383	0.0048	S₅	4.46	278	0.0037
S₆	3.36	369	0.0009	S₆	4.49	276	0.0088
S₇	3.42	362	0.0011	S₇	4.53	274	0.0018
S₈	3.45	359	0.0048	S₈	4.59	270	0.0049
S₉	3.60	344	0.0007	S₉	4.64	267	0.0509
S₁₀	3.62	343	0.0035	S₁₀	4.74	262	0.0503

Table S2. Computed low-lying singlet-to-in **5A**, **6A**, **INT-A**, **2D**, **2C**, **INT-AB**, **INT-B**, **1E**.

intermediate	excitation energy		
	eV	kcal/mol	nm
5A	4.495	103.7	275
6A	2.946	67.9	421
INT-A	3.004	69.3	413
2D	2.895	66.8	428
2C	2.440	56.3	508
INT-AB	2.653	61.2	467
INT-B	2.967	68.4	418
1E	2.522	58.1	492

The computational details of activation barrier of single electron transfer step.

According to the Marcus equation, the reorganization energy λ is normally decomposed into internal energy (λ_i) and external energy (λ_0). The internal reorganization energy λ_i can be estimated according to the equation (S1-S3):

$$\lambda_{i1} = [E^D(Q_P) + E^A(Q_P)] - [E^D(Q_R) + E^A(Q_R)] \quad (S1)$$

$$\lambda_{i2} = [E^{D+}(Q_R) + E^{A-}(Q_R)] - [E^{D+}(Q_P) + E^{A-}(Q_P)] \quad (S2)$$

$$\lambda_i = (\lambda_{i1} + \lambda_{i2})/2 \quad (S3)$$

where λ_{i1} represents the difference between the energy of the reactants (R) in the geometry characteristic of the products and that in their equilibrium geometry, λ_{i2} is the difference between the energy of the products (P) in the characteristic of the reactants and that in their equilibrium geometry. Q_R and Q_P are the equilibrium geometries of the reactants and products, respectively. In addition, the external reorganization energy λ_0 may be calculated from equation (S4-S6):

$$\lambda_0 = (332 \text{ kcal/mol}) \left(\frac{1}{2a_1} + \frac{1}{2a_2} - \frac{1}{R} \right) \left(\frac{1}{\epsilon_{OP}} - \frac{1}{\epsilon} \right) \quad (S4)$$

$$\lambda = \lambda_0 + \lambda_i \quad (S5)$$

$$\Delta G^{0\neq} = \frac{(\Delta G_r + \lambda)^2}{4\lambda} \quad (S6)$$

where α_1 is the radii of the oxidant, α_2 is the radii of the reductant, $R = \alpha_1 + \alpha_2$, ϵ_{OP} is the optical dielectric constant ($\epsilon_{OP} = 1.81$), ϵ is the static dielectric constant for the MeCN solvent ($\epsilon = 35.69$), and ΔG_r is the free energy change of the reaction.

Table S3. Details of estimation of the activation barriers for SET steps.

SET steps	a1 (Å)	a2 (Å)	R (Å)	λ (kcal/mol)	ΔG_r (kcal/mol)	ΔG_{SET} (kcal/mol)
5A	8.35	4.16	12.51	77.25	49.2	51.8
5A*	8.72	4.16	12.88	99.33	-6.2	21.9
6A	8.21	4.16	12.37	77.24	26.9	35.1
6A*	8.12	4.16	12.28	74.58	-22.2	9.2
INT-A	7.62	4.16	11.78	78.35	-3.1	18.1
INT-A*	7.60	4.16	11.76	70.55	-30.8	5.6
2C	6.95	4.16	11.11	84.33	-4.9	18.7
2C*	6.81	4.16	10.97	111.55	-79.3	2.3
2D	7.19	4.16	11.35	79.64	-24.8	9.4
2D*	7.08	4.16	11.24	71.90	-38.5	3.9
INT-AB	7.25	4.16	11.41	78.15	-7.3	16.1
INT-AB*	8.26	4.16	12.42	74.84	-3.9	16.8
INT-B	7.22	4.16	11.38	98.29	-7.7	20.9
INT-B*	8.27	4.16	13.43	74.74	0.4	18.9
1E	7.12	4.16	11.28	21.39	9.6	11.2
1E*	8.53	4.16	12.69	90.48	-39.7	7.1
2D'	7.04	4.16	11.20	70.98	-20.9	8.8
2D'*	6.93	4.16	11.09	74.56	-44.1	3.1
2C'	9.68	4.16	11.14	79.10	-6.2	16.8
2C'*	6.87	4.16	11.03	76.61	-26.3	8.3
6A'	7.92	4.16	12.08	20.39	39.9	44.6
6A'*	8.02	4.16	12.18	82.99	-19.7	12.1

The excited states were obtained by geometry optimization of the triplet state at B3LYP/6-31+G(d) (energy data in Table S4, the structure coordinates are provided later).

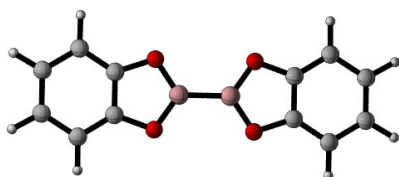
Table S4. The calculated energies and energy corrections.

Stationary point	Sum of electronic and thermal Free Energies-B3LYP 6-31G(d), (a.u.)	Thermal correction to Gibbs Free Energy at 298.15 K (a.u.)	Single-point energy-M06L 6-311++G(d,P), SCRF (Acetonitrile) (a.u.)	Solvation correction energy (Acetonitrile) (a.u.)
1A(B ₂ cat ₂)	-812.734580	0.1462390	-812.99354560	-812.84730660
4-PhPy	-479.2073070	0.1357850	-479.40686910	-479.27108410
MeO ⁻	-115.0585470	0.0135420	-115.21930010	-115.20575810
1A-TS	-1291.930772	0.3004140	-1292.4099005	-1292.1094865
2A	-1291.931232	0.3030520	-1292.4177093	-1292.1146573
2a	-927.8963240	0.1814720	-928.28506050	-928.10358850
2a-TS	-1407.080210	0.3391660	-1407.6996556	-1407.3604896
3A/ ¹ 3a*	-1407.083032	0.3390080	-1407.7055537	-1407.3665457
3A-TS	-1407.071181	0.3392320	-1407.6842549	-1407.3450229
3a-ts	-1407.072375	0.3381900	-1407.6840553	-1407.3458653
4A	-1407.094565	0.3358910	-1407.6982139	-1407.3623229
INT-A	-885.5898980	0.2150910	-886.00147730	-885.78638630
3A/ ³ 3a	-1407.067099	0.3368380	-1407.6715406	-1407.3347026
3a-ts1	-1407.050442	0.3343820	-1407.6519634	-1407.3175814
4a	-1407.052945	0.3337350	-1407.6537408	-1407.3200058
5a	-885.5441210	0.2126130	-885.95089470	-885.73828170
1B-TS	-1771.125924	0.4544890	-1771.8241125	-1771.3696235
1B	-1771.129246	0.4614040	-1771.8442375	-1771.3828335
2B-TS	-1771.275289	0.4660790	-1771.8239703	-1771.3578913
¹ 2B	-1771.308151	0.4696020	-1771.8491706	-1771.3795686
³ 2B	-1771.226443	0.4668100	-1771.7773021	-1771.3104921
2B-TS'	-1771.092436	0.4630510	-1771.8194656	-1771.3564146
1C	-885.5702470	0.2191820	-885.90899630	-885.6898143
¹ 3B	-1886.309117	0.5033430	-1887.1444550	-1886.6411120
3B-TS	-1886.290639	0.5031460	-1887.1259051	-1886.6227591
INT-B	-1364.811985	0.3767160	-1365.4407773	-1365.0640613
³ 3B	-1886.252641	0.4972580	-1887.0847520	-1886.5874940
2b-TS	-1886.252782	0.4970400	-1887.0842753	-1886.5872353
1C+2C	-1886.317822	0.4910540	-1887.1270353	-1886.6359813
1b-TS	-1886.290742	0.4988380	-1887.1201057	-1886.6212677
1b	-1886.3079650	0.4915350	-1887.1287492	-1886.6372142
AB-TS1	-1364.7829110	0.3703680	-1365.4159573	-1365.0455893
INT-AB	-1364.806818	0.373530	-1365.4382268	-1365.0646968
AB-TS2	-1364.782402	0.3759110	-1365.4112975	-1365.0353865
5A-TS	-3806.725577	0.3758610	-3809.6555489	-3809.2796879
5A	-1234.994207	0.3863610	-1235.5480714	-1235.1617104

5A*	-1234.892941	0.3794090	-1235.4413721	-1235.0619631
6A-TS	-1350.069058	0.4166160	-1350.7653506	-1350.3487346
6A	-1350.168360	0.4217360	-1350.8465059	-1350.4247699
6A*	-1350.0744050	0.4147640	-1350.7507181	-1350.3359541
7A	-1350.0720620	0.4207860	-1350.6906370	-1350.2698510
1D	-1000.571904	0.2418100	-1001.2193252	-1000.9775152
1D-TS	-1000.565375	0.2452180	-1001.2143185	-1000.9691005
2D	-1000.640830	0.2497570	-1001.2820770	-1001.0323200
2D*	-1000.602760	0.2451570	-1001.2457280	-1001.0005710
2D-TS	-3921.812857	0.4082120	-3924.9454172	-3924.5372052
INT-A*	-885.5425840	0.2098880	-885.9521545	-885.7422665
1C-TS	-1000.640667	0.2478350	-1001.1271775	-1000.8793425
2C	-1000.752858	0.2544370	-1001.2149305	-1000.9604935
2C*	-1000.685944	0.2483330	-1001.0902199	-1000.8418869
2C-TS	-3806.650609	0.3778330	-3809.5312748	-3809.1534418
3C	-1234.751366	0.3850520	-1235.3581102	-1234.9730582
3C-TS	-1000.714109	0.2494660	-1001.1771002	-1000.9276342
4C	-479.2049490	0.1294550	-479.4845938	-479.3551388
4C-TS	-3921.865974	0.4163680	-3924.8575962	-3924.4412282
7A-TS	-1350.066053	0.4192480	-1350.6780798	-1350.2588318
8A	-828.563859	0.2973240	-828.9772498	-828.6799258
8A-TS	-828.548290	0.2950260	-828.9622249	-828.6671989
R*	-349.391677	0.1355620	-349.5707890	-349.4352270
9A-TS	-1162.102959	0.3055240	-1162.5733583	-1162.2678343
9A	-1162.113623	0.3062010	-1162.5857517	-1162.2795507
11A-TS	-1511.470158	0.4683520	-1512.1686684	-1511.7003164
11A	-1511.619732	0.4659520	-1512.2877358	-1511.8217838
P	-755.815625	0.2248520	-756.1420593	-755.9172073
10a-TS	-1162.088022	0.3043920	-1162.5562319	-1162.2518399
10a	-406.288631	0.0612810	-406.4055130	-406.3442320
ts-1	-1511.474964	0.4675990	-1512.1634483	-1511.6958493
ts-2	-1511.467447	0.4656550	-1512.1575234	-1511.6918684
11A	-1511.470929	0.4621890	-1512.1573428	-1511.6951538
1F-TS	-4285.923944	0.5333860	-4289.0867182	-4288.5533322
1F	-1714.187715	0.5428290	-1714.9707444	-1714.4279154
2F-TS	-1829.251807	0.5723530	-1830.1821327	-1829.6097797
INT-B*	-1364.8812690	0.3717140	-1365.4397886	-1365.0680746
INT-AB*	-1364.8226450	0.3696230	-1365.4396770	-1365.0700540
1E	-1365.1507283	0.3767200	-1365.3410294	-1364.9643094
1E*	-1364.6847030	0.3702580	-1365.2559983	-1364.8857403
1E-TS	-4286.046341	0.5387770	-4288.9688493	-4288.4300723
2E	-1713.979564	0.5424480	-1714.8025270	-1714.2600790
3E	-1829.211041	0.5725280	-1830.0577386	-1829.4852106

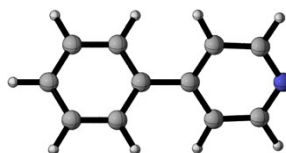
3E-TS	-1829.209147	0.5717750	-1830.0494856	-1829.4777106
4E	-1479.7977190	0.4141030	-1480.4546098	-1480.0405068
4E-TS	-1479.7965200	0.4145690	-1480.4488411	-1480.0342721
5E-TS	-1479.8376980	0.4075450	-1480.5449918	-1480.1374468
1D'	-1163.0295750	0.2453490	-1163.4724510	-1163.2271020
1-TS'	-1162.9996970	0.2477340	-1163.4609794	-1163.2132454
2D'	-1163.0503400	0.2534580	-1163.5108372	-1163.2573792
2D'*	-1163.0692210	0.2527540	-1163.4731610	-1163.2204070
2D-TS'	-4084.1791460	0.4118180	-4087.1723710	-4086.7605530
6A'	-1512.4606570	0.4208270	-1513.0715344	-1512.6507074
6A'*	-1350.0744050	0.4147640	-1350.7507181	-1350.3359541
6A-TS'	-1512.3991570	0.4191380	-1513.0136015	-1512.5944635
7A'	-1512.2326340	0.4207770	-1512.8958515	-1512.4750745
2C'	-1163.0287380	0.2551820	-1163.4339488	-1163.1787668
2C'*	-1162.9298950	0.2508560	-1163.3003169	-1163.0494609
5C'	-1162.8868560	0.2588960	-1163.3355455	-1163.0766495

Cartesian coordinates of all calculated compounds (including imaginary frequencies of transition states).



1A(B₂cat₂)

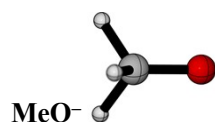
C	2.93711000	0.69741900	-0.00042200
C	2.93747100	-0.69753000	0.00048400
C	4.11118300	-1.43283100	0.00084600
C	5.30591900	-0.70013100	0.00025600
C	5.30560200	0.70097600	-0.00065800
C	4.11056700	1.43317800	-0.00102300
H	4.09867800	-2.51755200	0.00154200
H	6.25253300	-1.23247200	0.00051300
H	6.25198400	1.23373500	-0.00109600
H	4.09766100	2.51789500	-0.00172900
O	1.63311300	1.14485200	-0.00058600
O	1.63358000	-1.14554900	0.00088400
B	0.84312100	-0.00058900	0.00023600
C	-2.93719500	0.69741100	0.00050300
C	-2.93738800	-0.69753800	-0.00041200
C	-4.11112600	-1.43284300	-0.00101500
C	-5.30587500	-0.70017500	-0.00068800
C	-5.30564500	0.70093200	0.00022900
C	-4.11062300	1.43316700	0.00086800
H	-4.09864000	-2.51756500	-0.00171500
H	-6.25246500	-1.23256300	-0.00115700
H	-6.25205100	1.23364300	0.00045300
H	-4.09770000	2.51788300	0.00156800
O	-1.63312700	1.14490300	0.00091700
O	-1.63356800	-1.14549600	-0.00053200
B	-0.84311800	-0.00039100	0.00023300



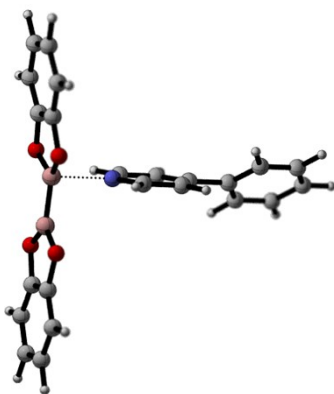
4-PhPy

C	2.87618800	-1.07623900	-0.37029800
C	1.48374400	-1.12841400	-0.38871000
C	0.74556400	-0.00000600	0.00000000
C	1.48374200	1.12841000	0.38871200
C	2.87618100	1.07624500	0.37030200

H	3.45666600	-1.94567500	-0.67580000
H	0.98064800	-2.02941500	-0.72670300
H	0.98063500	2.02940600	0.72670100
H	3.45666000	1.94568200	0.67579300
N	3.58197300	0.00000200	-0.00000200
C	-0.73837100	-0.00000300	0.00000100
C	-1.45813400	-1.14936300	0.36670300
C	-1.45812900	1.14936000	-0.36670400
C	-2.85199500	-1.14883400	0.36843600
H	-0.92047600	-2.04043200	0.67840100
C	-2.85198900	1.14883700	-0.36843800
H	-0.92046600	2.04042500	-0.67840400
C	-3.55457300	0.00000300	0.00000000
H	-3.38985200	-2.04539700	0.66485300
H	-3.38984400	2.04540200	-0.66485500
H	-4.64114700	0.00000700	-0.00000100



C	0.00000000	0.00000000	-0.52089900
H	0.00000000	1.02954000	-1.06079300
H	0.89160800	-0.51477000	-1.06079300
H	-0.89160800	-0.51477000	-1.06079300
O	0.00000000	0.00000000	0.78847100

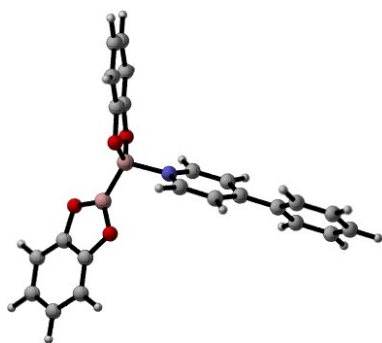


1A-TS

Imaginary frequency: -71.62

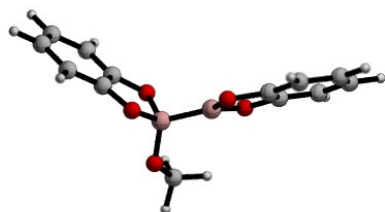
C	1.69029900	3.17582200	-0.65915100
C	1.69954900	3.15798300	0.73970500
C	1.53295800	4.31341600	1.48427500
C	1.34959400	5.50927100	0.77166400
C	1.34031100	5.52713200	-0.62623500
C	1.51405000	4.34995700	-1.37159400
H	1.54660300	4.28839500	2.56928400
H	1.21407000	6.43729800	1.32001200
H	1.19763500	6.46886000	-1.14882600

H	1.51328100	4.35261700	-2.45696900
O	1.89581400	1.90399300	-1.13706300
O	1.91098100	1.87416100	1.18235200
B	1.92097700	1.07636400	0.01215300
C	3.15580600	-2.52057200	0.64268200
C	3.08081500	-2.51812700	-0.75067000
C	3.39380500	-3.63703900	-1.50415600
C	3.79095400	-4.78010900	-0.79510800
C	3.86632000	-4.78247600	0.60294100
C	3.54774700	-3.64194300	1.35441700
H	3.33420000	-3.62267600	-2.58744600
H	4.04645500	-5.68152900	-1.34467300
H	4.17926800	-5.68570700	1.11879000
H	3.60467400	-3.63113100	2.43789300
O	2.79135600	-1.27865100	1.11339300
O	2.66850200	-1.27442800	-1.17496800
B	2.49098400	-0.51320200	-0.01613500
C	-0.84514700	0.26740500	-1.13401900
C	-2.18110200	-0.11403400	-1.18299700
C	-2.89704100	-0.29195700	0.01258400
C	-2.19848400	-0.06770600	1.21066300
C	-0.86129900	0.31038600	1.16626500
H	-0.26031200	0.41442300	-2.03838900
H	-2.65350400	-0.29469900	-2.14309200
H	-2.69945700	-0.15978200	2.16891700
H	-0.29269300	0.50475700	2.07212600
N	-0.19490700	0.47620600	0.01726200
C	-4.32398800	-0.69522500	0.00988300
C	-4.82817900	-1.56143900	0.99430900
C	-5.20281200	-0.21869300	-0.97724300
C	-6.16906800	-1.94127300	0.98980700
H	-4.15904500	-1.96223800	1.75046700
C	-6.54477800	-0.59453300	-0.97779900
H	-4.83887700	0.47334800	-1.73140800
C	-7.03252100	-1.45817700	0.00473600
H	-6.53802300	-2.62064700	1.75327400
H	-7.21143900	-0.20679300	-1.74315400
H	-8.07826900	-1.75277500	0.00280400



C	-1.52529800	3.00818300	0.74205800
C	-1.52542000	3.06334500	-0.66032300
C	-1.55278000	4.27143100	-1.33600900
C	-1.57935700	5.44713800	-0.56413200
C	-1.57960100	5.39298100	0.82977700
C	-1.55347200	4.16130300	1.50868500
H	-1.55855300	4.30133700	-2.42146200
H	-1.60223000	6.41075300	-1.06593600
H	-1.60195600	6.31498900	1.40453300
H	-1.55766300	4.10728800	2.59314300
O	-1.51407600	1.70844300	1.16995600
O	-1.51695600	1.79914900	-1.18871900
B	-1.34352200	0.90300100	-0.04703600
C	-3.79088500	-2.10209800	-0.39004600
C	-2.80760400	-2.66654500	0.42353000
C	-2.89943500	-3.96648600	0.89166600
C	-4.03522600	-4.69436900	0.50688500
C	-5.02142500	-4.12858000	-0.30971300
C	-4.91613600	-2.81042300	-0.77734500
H	-2.12927100	-4.39488800	1.52489500
H	-4.14997400	-5.71810700	0.85152900
H	-5.88848800	-4.72100100	-0.58757500
H	-5.67470700	-2.36072400	-1.40943900
O	-3.43312100	-0.80944400	-0.69728400
O	-1.81663400	-1.73305600	0.63620300
B	-2.21440700	-0.57711400	-0.05620800
C	0.90622100	0.07398500	1.08238200
C	2.23079600	-0.33005400	1.11627000
C	3.00273500	-0.31273600	-0.05844600
C	2.36375600	0.12800300	-1.23007800
C	1.03351500	0.51529700	-1.19140600
H	0.27476100	0.08206700	1.96318700
H	2.65334400	-0.67933600	2.05193800
H	2.90880700	0.20009900	-2.16487300
H	0.49870900	0.88048500	-2.06123800

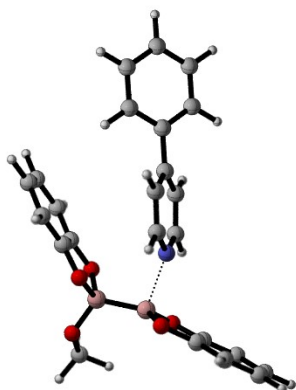
N	0.31848200	0.48623900	-0.05405300
C	4.42158100	-0.73675200	-0.06115800
C	4.96806500	-1.40537300	-1.16974600
C	5.25010500	-0.47871100	1.04412200
C	6.30224900	-1.80682500	-1.17082700
H	4.33689200	-1.63930600	-2.02229200
C	6.58595100	-0.87452400	1.03867900
H	4.85482400	0.06261000	1.89886000
C	7.11591500	-1.54132300	-0.06767300
H	6.70478000	-2.33306100	-2.03174200
H	7.21494000	-0.65609800	1.89705100
H	8.15684100	-1.85214600	-0.07015600



2a

C	-2.66821900	0.08213300	0.69218500
C	-2.68015100	-0.58019900	-0.56104600
C	-3.71934100	-1.43493000	-0.90244800
C	-4.76278600	-1.63095400	0.02741500
C	-4.75169300	-0.98082900	1.25847600
C	-3.69627000	-0.11033700	1.60545400
H	-3.71763000	-1.93741100	-1.86670500
H	-5.58372400	-2.29992600	-0.22593400
H	-5.56376900	-1.14292500	1.96554900
O	-1.56865000	0.84246800	0.82628200
O	-1.59008000	-0.27302200	-1.28363100
B	-0.82891300	0.78235300	-0.51982100
C	2.93105900	0.25432100	0.51880300
C	2.77534400	-0.78460400	-0.40625300
C	3.81777300	-1.64331900	-0.71706700
C	5.04247600	-1.42703300	-0.06369500
C	5.19785300	-0.38895700	0.86040200
C	4.13449700	0.47575700	1.16910500
H	3.68448500	-2.44635700	-1.43562300
H	5.88367000	-2.08069100	-0.28194900
H	6.15804600	-0.24661400	1.35058500
H	4.24229100	1.28494600	1.88514800

O	1.75210800	0.93425500	0.62628600
O	1.49877300	-0.76742400	-0.88692900
B	0.82340400	0.30873100	-0.25316500
O	-0.96961100	2.03714600	-1.25048600
C	-0.49947400	3.20092700	-0.63663200
H	-0.99774400	3.39864000	0.32737000
H	0.58820000	3.17627000	-0.43740400
H	-0.69576700	4.05694000	-1.30073400
H	-3.67723900	0.40247700	2.56425700

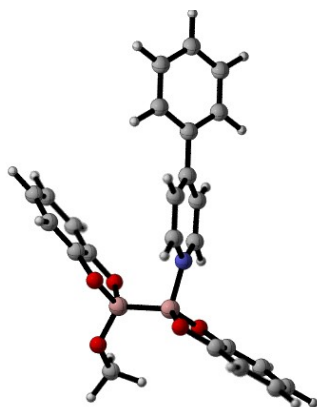


2a-TS

Imaginary frequency: -108.11

C	-3.79926800	-1.18058100	-0.55824300
C	-3.78825900	-1.06905300	0.84356700
C	-4.57148400	-1.89458000	1.63603200
C	-5.37725100	-2.84975400	0.98918100
C	-5.38796300	-2.95942700	-0.40229000
C	-4.59243400	-2.11737500	-1.20168200
H	-4.55767000	-1.79843100	2.71808200
H	-6.00077200	-3.51159300	1.58642400
H	-6.01975700	-3.70544500	-0.87946000
H	-4.59508800	-2.19107600	-2.28573000
O	-2.96566400	-0.25329700	-1.10087500
O	-2.95079700	-0.07135200	1.22182200
B	-2.29651800	0.40272600	0.01383000
C	0.56042700	2.53091600	0.77356500
C	0.69016000	2.40562900	-0.63501100
C	1.91163900	2.64184100	-1.25415600
C	3.01911600	2.99964800	-0.45480100
C	2.89161800	3.11895600	0.92703500
C	1.64900800	2.88603800	1.55882800
H	2.00330900	2.54201300	-2.33317600
H	3.98089900	3.18650500	-0.92972600
H	3.75122800	3.40861200	1.52977300
H	1.53580100	2.97956100	2.63649900
O	-0.68101100	2.22237700	1.17774600

O	-0.46123200	2.01398000	-1.19577700
B	-1.52406900	1.96808200	-0.06662200
C	-0.01420600	-1.13902200	-1.06135600
C	1.32970700	-1.48518900	-1.14056600
C	2.12768000	-1.40932700	0.01042100
C	1.50040000	-1.02439800	1.20336900
C	0.14417100	-0.71872700	1.19605200
H	-0.65812900	-1.12461500	-1.93577000
H	1.76590400	-1.75359600	-2.09813600
H	2.06553500	-0.95688800	2.12754800
H	-0.37589300	-0.38818100	2.08919400
N	-0.59820300	-0.76572500	0.08339900
C	3.58394100	-1.68987900	-0.03567800
C	4.49241300	-0.81875400	0.58897000
C	4.08409600	-2.81644400	-0.70763600
C	5.86204100	-1.07805400	0.54856200
H	4.11988400	0.08624500	1.06146300
C	5.45400600	-3.07553300	-0.74344900
H	3.38902700	-3.50156100	-1.18631700
C	6.34811400	-2.20802800	-0.11281200
H	6.55255200	-0.38670300	1.02526800
H	5.82259700	-3.95826500	-1.26071100
H	7.41655300	-2.40784200	-0.14234000
C	-3.21548100	3.17215200	-1.35047500
H	-2.60064400	3.26965900	-2.26212200
H	-3.86797000	2.29276800	-1.49497000
H	-3.86193700	4.06127500	-1.28479200
O	-2.43982400	3.09295000	-0.19109300

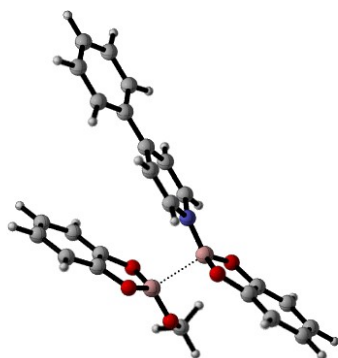


3A/13a

C	-3.64004200	-1.28003200	-0.59525000
C	-3.61433500	-1.26147100	0.81603500
C	-4.45476000	-2.08147800	1.55506100
C	-5.33313200	-2.93391100	0.85700600
C	-5.35832700	-2.95119500	-0.53623700
C	-4.50548600	-2.11551200	-1.28496300

H	-4.42993500	-2.05682800	2.64122500
H	-5.99986500	-3.58567600	1.41802500
H	-6.04445200	-3.61596900	-1.05707200
H	-4.51862200	-2.11724300	-2.37173400
O	-2.75641000	-0.38623900	-1.10138600
O	-2.71421300	-0.35950000	1.26781600
B	-1.99020000	0.15044100	0.06548500
C	0.55435000	2.69239300	0.73872200
C	0.53775700	2.69827700	-0.67955700
C	1.61586400	3.20200600	-1.39621500
C	2.72650900	3.70286700	-0.68366400
C	2.74288400	3.69374300	0.70824200
C	1.64772800	3.18398000	1.43894600
H	1.59471200	3.20321500	-2.48355000
H	3.57804200	4.09962600	-1.23402500
H	3.60602600	4.08546900	1.24402500
H	1.64730600	3.17537700	2.52650000
O	-0.56663400	2.14283200	1.23701100
O	-0.59248400	2.15066800	-1.15444600
B	-1.49807800	1.86233200	0.06716500
C	0.07805600	-0.88388700	-1.12371300
C	1.40674300	-1.26550100	-1.18326900
C	2.15719900	-1.39761200	-0.00245600
C	1.48311500	-1.14717500	1.20545700
C	0.14967700	-0.77967500	1.19709900
H	-0.53334400	-0.73559200	-2.00482100
H	1.86890300	-1.41929500	-2.15298600
H	1.99393800	-1.25802500	2.15643600
H	-0.41062800	-0.56856400	2.09883500
N	-0.54791000	-0.64769700	0.04838500
C	3.58821000	-1.77324400	-0.02713700
C	4.49781200	-1.20074100	0.87962300
C	4.07627800	-2.71037100	-0.95484700
C	5.84496400	-1.55757500	0.86144500
H	4.14843500	-0.44240300	1.57411200
C	5.42328800	-3.06719000	-0.97168400
H	3.38621500	-3.17922400	-1.65111400
C	6.31468500	-2.49359100	-0.06232400
H	6.53223000	-1.09222300	1.56363300
H	5.77623400	-3.80038800	-1.69297500
H	7.36592900	-2.77018200	-0.07659400
C	-3.48940800	2.87853800	-0.92116400
H	-2.98776500	3.07709500	-1.88343100
H	-4.07407300	1.95194600	-1.04360500

H	-4.19637000	3.70119400	-0.73286200
O	-2.58575000	2.81571900	0.14464100

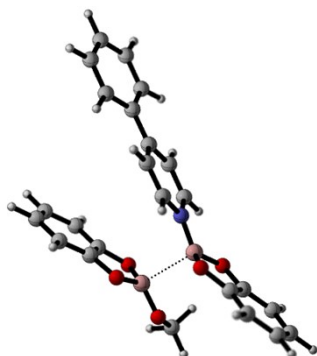


3A-TS

Imaginary frequency: -289.40

C	-3.81507200	-1.33565100	-0.44816200
C	-3.76372000	-1.09693700	0.93852600
C	-4.87718300	-1.28538600	1.74143900
C	-6.06301300	-1.72474300	1.12077700
C	-6.11348200	-1.96031700	-0.25213700
C	-4.97873100	-1.76549800	-1.06460700
H	-4.82680500	-1.09686000	2.80958800
H	-6.95248900	-1.87992100	1.72714500
H	-7.04113500	-2.29846400	-0.70819100
H	-5.00424900	-1.94888500	-2.13489800
O	-2.60544000	-1.08167200	-1.01618900
O	-2.52236600	-0.68880500	1.30348100
B	-1.76337400	-0.60555800	0.07129700
C	0.22687200	2.57236900	0.70828800
C	0.48919700	2.42339600	-0.66426700
C	1.69979400	2.80715100	-1.21504100
C	2.65807500	3.36551600	-0.34964400
C	2.39494600	3.52194100	1.01155600
C	1.16462500	3.12446200	1.56552100
H	1.89522000	2.67424600	-2.27468400
H	3.62212400	3.66854000	-0.75029400
H	3.15460100	3.95219000	1.65989600
H	0.95038100	3.23603300	2.62425000
O	-1.02570500	2.12526800	1.00050600
O	-0.59936000	1.89034100	-1.29203800
B	-1.56990200	1.65878500	-0.24793600
C	0.33102800	-1.22857300	-1.11334400
C	1.68314200	-1.39920500	-1.14472500
C	2.50782000	-1.29501500	0.01542300
C	1.77047800	-1.04470400	1.21292400
C	0.41587700	-0.89430100	1.23562400
H	-0.28878900	-1.29522300	-1.99764700

H	2.12454100	-1.60861600	-2.11479700
H	2.27945000	-1.02557000	2.17240200
H	-0.14409400	-0.73327900	2.14734200
N	-0.36139800	-0.92692500	0.06829900
C	3.94810200	-1.45975200	-0.01003100
C	4.77375200	-1.05518800	1.07564000
C	4.62880900	-2.04128000	-1.11582100
C	6.15212600	-1.23137600	1.05956300
H	4.32162300	-0.56176400	1.93082200
C	6.00812500	-2.20782100	-1.12839500
H	4.05611100	-2.39274300	-1.96950500
C	6.79510700	-1.81008200	-0.04080400
H	6.73738500	-0.89743400	1.91542300
H	6.47746200	-2.66532000	-1.99851800
H	7.87425000	-1.94193300	-0.05306400
C	-3.38408700	1.90479300	-1.82416700
H	-2.91432300	2.71914900	-2.39346700
H	-3.18229100	0.95854600	-2.33887200
H	-4.46716500	2.06611400	-1.79549200
O	-2.92102400	1.87871000	-0.48790600

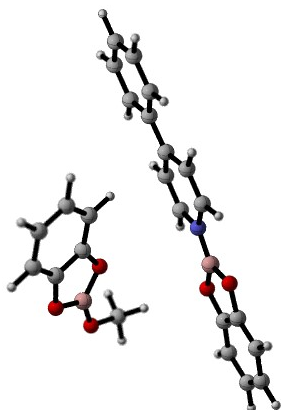


3a-ts

Imaginary frequency: -449.35

C	-3.79571100	-1.36923900	-0.43266000
C	-3.74335100	-1.11448800	0.95080900
C	-4.85440400	-1.29859400	1.75790100
C	-6.03902200	-1.75045200	1.14408700
C	-6.09050000	-2.00208700	-0.22599900
C	-4.95806100	-1.81159800	-1.04256600
H	-4.80322200	-1.09758200	2.82370400
H	-6.92687400	-1.90273800	1.75351000
H	-7.01727600	-2.34984700	-0.67652200
H	-4.98433200	-2.00766100	-2.11056400
O	-2.58729600	-1.11619000	-1.00486400
O	-2.50258700	-0.69599400	1.30831100
B	-1.74730600	-0.62605000	0.07538200
C	0.16679900	2.60925500	0.70194500

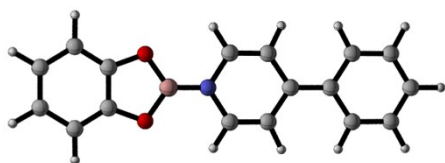
C	0.45855100	2.44499600	-0.66235500
C	1.68235700	2.81734600	-1.19082100
C	2.62353600	3.37992900	-0.30990300
C	2.33113500	3.55177200	1.04360500
C	1.08733200	3.16572000	1.57457300
H	1.90081400	2.67170500	-2.24417300
H	3.59786900	3.67380100	-0.69185100
H	3.07859800	3.98485900	1.70402000
H	0.85038000	3.28876400	2.62711800
O	-1.09512100	2.16991300	0.97000800
O	-0.61977300	1.90946700	-1.30791600
B	-1.60734300	1.69041100	-0.28260400
C	0.35252600	-1.23151000	-1.11064600
C	1.70385600	-1.40028700	-1.14257500
C	2.53253200	-1.28798400	0.01672900
C	1.79386700	-1.02728000	1.21380100
C	0.44020800	-0.87737100	1.23653100
H	-0.26798500	-1.30579700	-1.99400500
H	2.14309300	-1.61558600	-2.11225500
H	2.30270300	-0.99587000	2.17288800
H	-0.11806100	-0.70786100	2.14796200
N	-0.34061200	-0.92576000	0.07084600
C	3.97085100	-1.45126200	-0.00996200
C	4.79715600	-1.07054300	1.08547600
C	4.65541200	-2.00783800	-1.12782300
C	6.17538700	-1.24440000	1.06639500
H	4.34514700	-0.59885900	1.95286900
C	6.03457900	-2.17281300	-1.14215000
H	4.08563300	-2.33976200	-1.99115500
C	6.82105700	-1.79819700	-0.04565000
H	6.75908700	-0.92918500	1.93052500
H	6.50496600	-2.61025200	-2.02209800
H	7.90035000	-1.92859100	-0.05971900
C	-3.39842200	1.84262200	-1.89308500
H	-2.93754100	2.65231300	-2.47579500
H	-3.16702400	0.88762200	-2.37782700
H	-4.48492500	1.98021200	-1.88511200
O	-2.95645900	1.86213500	-0.54869600



4A

C	-3.86632400	-1.50241000	-0.35255500
C	-3.74437400	-1.84991800	1.00226100
C	-4.85788400	-2.03350600	1.80523600
C	-6.12003100	-1.85864200	1.20669000
C	-6.24082100	-1.51439300	-0.13955900
C	-5.10382700	-1.32851900	-0.94899400
H	-4.75167000	-2.30099900	2.85199600
H	-7.01477500	-1.99490100	1.80891600
H	-7.22816400	-1.38530000	-0.57584400
H	-5.18606400	-1.06140000	-1.99813000
O	-2.62519800	-1.37996500	-0.91253400
O	-2.42666200	-1.96202600	1.33649300
B	-1.70491900	-1.67928000	0.13992200
C	-0.07282000	3.68306600	0.62755800
C	0.37951600	2.44962500	0.14970900
C	1.52039700	1.83841800	0.63684900
C	2.21085900	2.53430600	1.64238700
C	1.76516500	3.77006200	2.12252700
C	0.60089200	4.37335200	1.61923400
H	1.86084800	0.87408100	0.26903900
H	3.11372100	2.09084800	2.05223900
H	2.32758000	4.27647500	2.90279500
H	0.24115500	5.33055800	1.98373600
O	-1.23174400	4.04316200	-0.03663800
O	-0.48589900	2.00520800	-0.83537400
B	-1.46042500	2.99185600	-0.92638000
C	0.35662400	-1.47413700	-1.22759800
C	1.70544600	-1.40339400	-1.30922200
C	2.60029400	-1.58212000	-0.18878300
C	1.89188900	-1.95445900	1.01457800
C	0.54521700	-2.03414700	1.11373300
H	-0.29515200	-1.34944200	-2.08318600
H	2.10843900	-1.20998900	-2.30019000

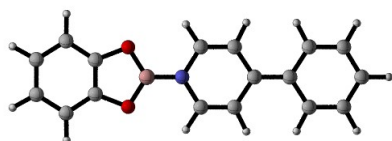
H	2.44700700	-2.21418400	1.91236700
H	0.03424600	-2.33134400	2.02124100
N	-0.32508200	-1.72325100	0.01267400
C	4.02662500	-1.47124000	-0.27539800
C	4.89340100	-1.67122600	0.84970600
C	4.71051400	-1.14619500	-1.49305500
C	6.27402200	-1.56669200	0.75772700
H	4.46283200	-1.90973500	1.81856400
C	6.09183700	-1.04429900	-1.57063800
H	4.13364800	-0.96728600	-2.39666000
C	6.91063700	-1.25294100	-0.45143500
H	6.87132100	-1.73258900	1.65523900
H	6.54409200	-0.79381000	-2.53108100
H	7.99272000	-1.16996000	-0.51748200
C	-2.66927000	1.88188900	-2.67620800
H	-1.87364300	1.88560500	-3.43038500



INT-A

C	-3.95725800	0.70249400	-0.00063500
C	-3.95730300	-0.70247800	-0.00061100
C	-5.13797700	-1.42719100	-0.00149900
C	-6.34255300	-0.69729800	-0.00242100
C	-6.34252500	0.69735800	-0.00244500
C	-5.13793500	1.42722100	-0.00154900
H	-5.12517200	-2.51272700	-0.00147400
H	-7.28761400	-1.23496100	-0.00312900
H	-7.28756900	1.23505500	-0.00317300
H	-5.12512000	2.51275900	-0.00156400
O	-2.67438400	1.16570800	0.00033300
O	-2.67441900	-1.16574900	0.00037600
B	-1.85046300	-0.00007300	0.00101100
C	0.31597600	1.20732600	0.00369100
C	1.66938000	1.19610800	0.00296500
C	2.47646400	0.00000200	0.00166000
C	1.66941700	-1.19611400	0.00303300
C	0.31601300	-1.20737800	0.00376900
H	-0.26910100	2.11883400	0.00528300
H	2.14749700	2.17252100	0.00403100
H	2.14756600	-2.17251400	0.00418400
H	-0.26905600	-2.11889000	0.00541700
N	-0.46335700	-0.00002400	0.00256600

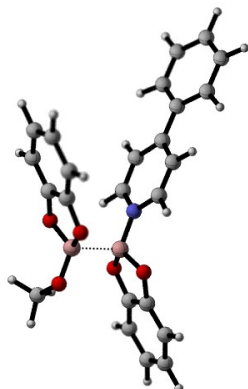
C	3.90709400	0.00001200	-0.00006600
C	4.68850700	1.20396700	-0.00100000
C	4.68850400	-1.20394200	-0.00110900
C	6.07553600	1.19655100	-0.00242900
H	4.18340100	2.16635500	-0.00068400
C	6.07553400	-1.19652900	-0.00253500
H	4.18339300	-2.16632900	-0.00090900
C	6.80767700	0.00001000	-0.00316400
H	6.60278700	2.15179800	-0.00304600
H	6.60278200	-2.15177800	-0.00323900
H	7.89512700	0.00000900	-0.00432300



³INT-A*

C	3.95926900	-0.68728500	-0.03945100
C	3.93086000	0.69688500	0.04993200
C	5.10106800	1.47226200	0.10533700
C	6.31321400	0.74257900	0.06265900
C	6.34267600	-0.64577400	-0.02732600
C	5.14747300	-1.41890400	-0.08158100
H	5.06922800	2.55347000	0.17660700
H	7.25419600	1.28915900	0.10154900
H	7.30265900	-1.15719400	-0.05742500
H	5.15114000	-2.50077400	-0.15025800
O	2.65842400	-1.17247800	-0.07910900
O	2.61211800	1.13155700	0.06843700
B	1.85196600	-0.03509100	-0.01176100
C	-0.31206600	-1.24594400	-0.10103600
C	-1.70649400	-1.24311800	-0.09190900
C	-2.44915500	-0.02533500	-0.01945400
C	-1.66623300	1.17058400	0.05300200
C	-0.29250100	1.14825700	0.05972800
H	0.27853400	-2.14986700	-0.17326600
H	-2.20841600	-2.19443900	-0.22152400
H	-2.14552500	2.13706700	0.16301600
H	0.31756200	2.03808400	0.13868400
N	0.42425900	-0.06103100	-0.02100900
C	-3.90239300	0.00944400	-0.00148300
C	-4.66596400	-1.17894300	0.19397400
C	-4.63545600	1.20640300	-0.18497500
C	-6.06351100	-1.15041800	0.20770100
H	-4.15553000	-2.11618200	0.38803900
C	-6.03041700	1.22972200	-0.17195900

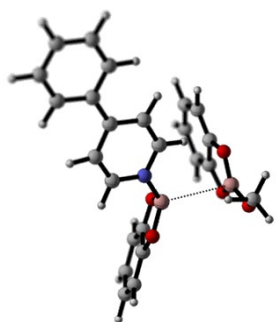
H	-4.10337700	2.13354100	-0.37684600
C	-6.76078500	0.04369400	0.02468400
H	-6.61144300	-2.07857500	0.36759400
H	-6.55156200	2.17359900	-0.32244200
H	-7.84894200	0.05750800	0.03046400



3A/3a

C	-3.33004500	-1.70200100	-0.58699700
C	-3.30431600	-1.62690400	0.81864200
C	-4.27439900	-2.24817300	1.58997700
C	-5.28589400	-2.95865800	0.91845800
C	-5.31153700	-3.03300300	-0.47489400
C	-4.32639600	-2.39833900	-1.25367500
H	-4.24523900	-2.18087000	2.67333200
H	-6.06019600	-3.45551900	1.49841100
H	-6.10484600	-3.58766700	-0.97065300
H	-4.33446200	-2.45068100	-2.33854100
O	-2.28130100	-1.02175300	-1.11560300
O	-2.23742700	-0.90407200	1.23453600
B	-1.59660500	-0.39848200	0.02445400
C	-0.36546600	2.81710100	0.87586000
C	-0.20761500	2.84643600	-0.52384200
C	0.84908300	3.52130300	-1.11581900
C	1.75615200	4.18492300	-0.27046600
C	1.59929400	4.15803500	1.11611100
C	0.53032800	3.46649100	1.71286800
H	0.96384800	3.53051900	-2.19579500
H	2.59637100	4.71950100	-0.70725700
H	2.31805100	4.67340800	1.74898800
H	0.40038400	3.43507200	2.79068000
O	-1.46292000	2.10261400	1.21790500
O	-1.20399400	2.14978500	-1.12582800
B	-2.01996700	1.58438000	-0.03536200
C	0.62263200	-0.60730900	-1.18215300
C	1.96480000	-0.83458000	-1.23654000
C	2.75198900	-1.07456400	-0.05482200

C	1.98629700	-1.01031500	1.16342900
C	0.64453900	-0.77202700	1.16790600
H	0.02871200	-0.43411800	-2.07074900
H	2.42431800	-0.84786800	-2.21878600
H	2.47181100	-1.12170900	2.12682200
H	0.06739400	-0.71665600	2.08229600
N	-0.08377600	-0.58746900	0.00691500
C	4.16717400	-1.34973200	-0.08710600
C	4.89045900	-1.75603400	1.07459000
C	4.93908400	-1.23826800	-1.28263900
C	6.25176500	-2.02173100	1.03925200
H	4.36384200	-1.88502000	2.01498900
C	6.30012700	-1.50565000	-1.30826600
H	4.46002900	-0.91410600	-2.20118500
C	6.98392100	-1.90243700	-0.15030900
H	6.75298800	-2.33384700	1.95446500
H	6.84204100	-1.39806900	-2.24687700
H	8.05037000	-2.11152400	-0.17427200
C	-3.99613700	1.72027700	-1.43525500
H	-3.67480400	2.61410500	-1.98999800
H	-3.73481700	0.83760900	-2.03343700
H	-5.08581300	1.75099500	-1.31514900
O	-3.42007500	1.67470000	-0.14938500

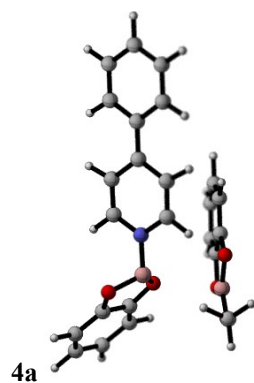


3a-ts1

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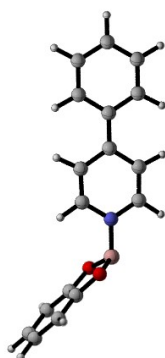
C	1.98308200	-2.89675700	0.16456000
C	2.29678000	-1.85351400	-0.73028500
C	3.27602800	-2.01250300	-1.70050100
C	3.94788200	-3.24970100	-1.76017700
C	3.63697900	-4.28091000	-0.87538400
C	2.64023300	-4.11668400	0.10780200
H	3.51008400	-1.20145100	-2.38400400
H	4.72406200	-3.39702300	-2.50839000
H	4.17100800	-5.22674900	-0.93862200
H	2.38817000	-4.91308800	0.80270600
O	1.00487200	-2.50680800	1.01893400

O	1.53036200	-0.76840000	-0.47520200
B	0.71709500	-1.09433500	0.72335300
C	3.35981300	2.18075200	-0.40111400
C	2.12236100	2.71073400	-0.01705200
C	1.41097000	3.57060100	-0.83307500
C	1.99102300	3.89761400	-2.07051300
C	3.22801400	3.37314000	-2.45307400
C	3.94009700	2.49701100	-1.61623600
H	0.44590300	3.96300900	-0.52941000
H	1.46024500	4.56591400	-2.74337100
H	3.64800100	3.64098900	-3.41914700
H	4.89844100	2.07681000	-1.90404600
O	3.84104700	1.36729700	0.59175400
O	1.79511400	2.24318700	1.23345800
B	2.85299800	1.38335800	1.58483400
C	-1.63466800	-1.78468400	0.00616400
C	-2.96279400	-1.56457800	-0.21431000
C	-3.59641400	-0.31211000	0.10704500
C	-2.68908500	0.64997300	0.67661600
C	-1.36644300	0.37631900	0.87424700
H	-1.16424400	-2.73499200	-0.21728600
H	-3.54039800	-2.38639000	-0.62487100
H	-3.03555800	1.63958700	0.95496800
H	-0.68020800	1.10402200	1.29292500
N	-0.79143400	-0.83551900	0.55570200
C	-4.99723400	-0.05127600	-0.11367300
C	-5.63011700	1.15010600	0.32970200
C	-5.84991400	-0.97746900	-0.78869100
C	-6.97915600	1.39479200	0.11845500
H	-5.04945800	1.89585200	0.86380700
C	-7.19805100	-0.72393700	-0.99496400
H	-5.43655800	-1.90560500	-1.17101600
C	-7.79134700	0.46508900	-0.54681800
H	-7.40974600	2.32701300	0.48205600
H	-7.79994800	-1.46458800	-1.52007900
H	-8.84796200	0.66057800	-0.71109200
C	1.96005500	0.67591400	3.69925500
H	1.53319800	1.65474500	3.95180500
H	1.18858100	0.03941000	3.24560100
H	2.35496200	0.20883900	4.60602200
O	3.04641200	0.80836100	2.78514600



C	-2.75622700	2.66700800	-0.15786100
C	-2.97708900	1.30858600	-0.46170600
C	-4.03354700	0.91279300	-1.26847500
C	-4.87958700	1.91731900	-1.77971900
C	-4.66003400	3.26190900	-1.48462100
C	-3.58597700	3.65816500	-0.66251700
H	-4.19605000	-0.13890300	-1.48384000
H	-5.71906300	1.63350500	-2.41101800
H	-5.32764400	4.02004500	-1.88899400
H	-3.40546800	4.70286500	-0.42425200
O	-1.68133000	2.80452100	0.65425700
O	-2.04481100	0.53598600	0.14769500
B	-1.21157700	1.44793000	0.99292200
C	-1.89410000	-2.85525600	-0.67457700
C	-0.77505800	-2.60517800	0.12844300
C	0.50689500	-2.91317700	-0.28789300
C	0.63613500	-3.50765000	-1.55417300
C	-0.48089800	-3.77020900	-2.35166400
C	-1.77784800	-3.44246300	-1.92160400
H	1.36717800	-2.67771600	0.32941300
H	1.62814900	-3.75607300	-1.92143600
H	-0.34665600	-4.22673300	-3.32898700
H	-2.65250800	-3.62914100	-2.53683500
O	-3.03116500	-2.44014800	-0.02432100
O	-1.18132600	-2.04278800	1.31423900
B	-2.56928600	-1.89445600	1.18325500
C	0.92071400	1.76972000	-0.37079300
C	2.24992900	1.60140300	-0.62634500
C	3.12271400	0.90246100	0.28052200
C	2.44531400	0.41752800	1.45599100
C	1.10936400	0.61436800	1.65797100
H	0.27032500	2.30957600	-1.04945000
H	2.63690100	2.03206000	-1.54411800
H	2.98574400	-0.12838600	2.22187600

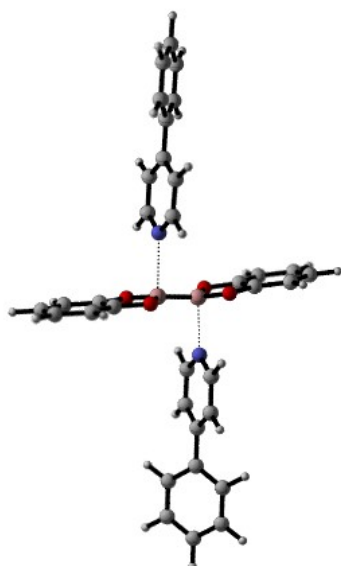
H	0.59345200	0.24543600	2.53748900
N	0.30232800	1.28949700	0.77072600
C	4.53134800	0.70991100	0.03902000
C	5.39241800	0.08912700	0.99490100
C	5.16393700	1.12670800	-1.17189400
C	6.74743100	-0.09300900	0.75921300
H	4.98678000	-0.24541700	1.94462000
C	6.51978700	0.94063500	-1.39828700
H	4.57198700	1.59487400	-1.95208200
C	7.33986400	0.32795400	-0.43976900
H	7.35679800	-0.57046000	1.52559200
H	6.94797100	1.27589100	-2.34209700
H	8.40183900	0.18322900	-0.62109700
C	-2.89541000	-0.81009600	3.29939100
H	-2.27432600	-1.49600800	3.89025800
H	-2.30027800	0.06833500	3.00803600
H	-3.75484300	-0.49814800	3.90023900
O	-3.41170900	-1.46557500	2.13930200



5a

C	-3.76146400	0.15217400	-0.70202900
C	-3.76552200	0.05665600	0.70750600
C	-4.78324500	-0.60860300	1.37732700
C	-5.81618000	-1.18443100	0.60785100
C	-5.81217100	-1.09033900	-0.78197500
C	-4.77514000	-0.41652200	-1.46102900
H	-4.77519000	-0.67837300	2.46185300
H	-6.62722900	-1.70640700	1.11212000
H	-6.62006700	-1.53948000	-1.35654100
H	-4.76083200	-0.33985700	-2.54501200
O	-2.68566800	0.84994700	-1.12280200
O	-2.69202000	0.69096000	1.22451100
B	-1.97143000	1.32961900	0.09095800
C	-0.05980900	-0.36555500	0.00685700
C	1.25293600	-0.73717200	-0.01585900
C	2.32201700	0.22707200	0.02049200
C	1.85448800	1.58807200	0.08533800

C	0.52455900	1.89735300	0.11005200
H	-0.86175500	-1.09474900	-0.02734200
H	1.46879600	-1.79886200	-0.07959100
H	2.55684100	2.41331400	0.13374500
H	0.16143600	2.91873600	0.16540000
N	-0.47257500	0.95200200	0.07132400
C	3.71759700	-0.13296700	-0.00577100
C	4.75810800	0.84383300	-0.07977500
C	4.15930700	-1.49119200	0.04051600
C	6.10001900	0.49322600	-0.10462800
H	4.50093200	1.89719200	-0.13341900
C	5.50363800	-1.83169700	0.01531300
H	3.42780200	-2.29015500	0.11157600
C	6.50234000	-0.84943000	-0.05762900
H	6.85007400	1.28102100	-0.16561600
H	5.78207400	-2.88411900	0.05696600
H	7.55491300	-1.12048700	-0.07721600



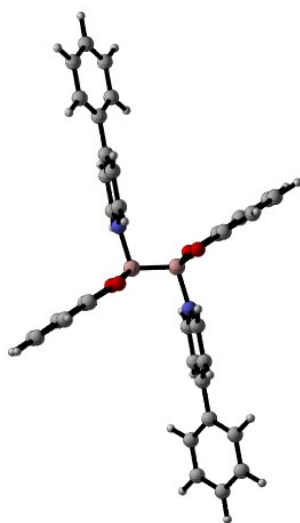
1B-TS

Imaginary frequency: -47.86

C	0.01757500	-3.01335500	0.71016100
C	0.01345400	-3.01478900	-0.68810100
C	0.00467300	-4.19258500	-1.41610100
C	-0.00230600	-5.39169800	-0.68572400
C	0.00194500	-5.39028400	0.71255500
C	0.01324700	-4.18973700	1.44050100
H	0.00260600	-4.18185200	-2.50148500
H	-0.01136800	-6.33765500	-1.22008100
H	-0.00367500	-6.33517400	1.24884200
H	0.01799900	-4.17681300	2.52583900
O	0.04020100	-1.71750900	1.16444200

O	0.03348700	-1.71973100	-1.14517500
B	-0.02717800	-0.91029500	0.00917200
C	-0.00971000	2.85557600	-0.69072700
C	-0.00958300	2.85507000	0.70886900
C	-0.08810400	4.03035200	1.43680500
C	-0.16573400	5.22897700	0.70873500
C	-0.16566600	5.22949400	-0.68891000
C	-0.08810400	4.03137800	-1.41783700
H	-0.08940600	4.01811600	2.52227100
H	-0.22723500	6.17193100	1.24504700
H	-0.22689600	6.17286000	-1.22453500
H	-0.08902400	4.01995100	-2.50332200
O	0.06146900	1.56454300	-1.15111100
O	0.06188400	1.56375000	1.16827400
B	0.20826100	0.75934300	0.00830800
C	-3.12320500	-0.52002600	1.15294100
C	-4.49712600	-0.30200700	1.19581300
C	-5.22114800	-0.21028000	-0.00372500
C	-4.49215900	-0.34724000	-1.19593600
C	-3.11825900	-0.56164400	-1.13937500
H	-2.53491900	-0.58805700	2.06505200
H	-4.99389200	-0.17761300	2.15293200
H	-4.99332800	-0.31170100	-2.15817000
H	-2.52775400	-0.67548300	-2.04546400
N	-2.43979400	-0.65045500	0.01024200
C	-6.68632000	0.02271300	-0.01136500
C	-7.28151500	0.82549800	-0.99876300
C	-7.51169400	-0.55320200	0.96872600
C	-8.65763000	1.04657700	-1.00464200
H	-6.65745900	1.30196400	-1.74958300
C	-8.88834000	-0.33533500	0.96015900
H	-7.07414900	-1.19765400	1.72604400
C	-9.46658900	0.46618600	-0.02595800
H	-9.09728800	1.67929800	-1.77094600
H	-9.51076400	-0.79800700	1.72133900
H	-10.53954800	0.63744600	-0.03146700
C	3.11582200	0.55829400	-1.14617900
C	4.49625100	0.39785000	-1.19878500
C	5.22951200	0.30124200	-0.00474800
C	4.50276700	0.37753200	1.19468700
C	3.12220700	0.54078500	1.15216100
H	2.51717600	0.64279100	-2.04961700
H	4.99887700	0.37329000	-2.16037400
H	5.00439000	0.28374600	2.15255400

H	2.52735000	0.59870600	2.06018900
N	2.43849400	0.63069200	0.00550100
C	6.70207700	0.12377400	-0.01038000
C	7.50458800	0.73900600	0.96481800
C	7.32661400	-0.66518800	-0.99082300
C	8.88830800	0.57241700	0.95807900
H	7.04336100	1.37404300	1.71596500
C	8.70987700	-0.83527500	-0.99429600
H	6.72118000	-1.17153500	-1.73726100
C	9.49601900	-0.21622400	-0.02072500
H	9.49294800	1.06479500	1.71484100
H	9.17315100	-1.45823100	-1.75456100
H	10.57455400	-0.34759800	-0.02453500

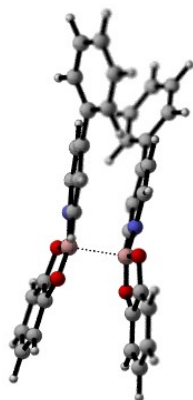


1B

C	-0.58014000	2.85187500	0.70703400
C	-0.58220100	2.84859400	-0.69890300
C	-0.95027900	3.97263700	-1.42000300
C	-1.32279500	5.12170200	-0.69730900
C	-1.32106700	5.12482600	0.69690100
C	-0.94653800	3.97915200	1.42388800
H	-0.94847900	3.95911600	-2.50611600
H	-1.61421000	6.01816300	-1.23845600
H	-1.61152700	6.02355700	1.23475000
H	-0.94276000	3.97040600	2.51001200
O	-0.20701400	1.62998500	1.18970100
O	-0.21101700	1.62432600	-1.17688900
B	0.21100000	0.84236000	0.00797700
C	0.58219500	-2.84848300	-0.69894100
C	0.58011300	-2.85178800	0.70699800
C	0.94643000	-3.97909900	1.42384000
C	1.32089100	-5.12478300	0.69683700
C	1.32264300	-5.12163500	-0.69737500

C	0.95021100	-3.97253800	-1.42005700
H	0.94263900	-3.97037300	2.50996400
H	1.61128500	-6.02354500	1.23467000
H	1.61400800	-6.01811000	-1.23852600
H	0.94843000	-3.95899700	-2.50616900
O	0.21110200	-1.62418100	-1.17690200
O	0.20706400	-1.62987700	1.18966900
B	-0.21094100	-0.84224800	0.00795700
C	2.56000400	0.81057200	1.16454200
C	3.93787200	0.67228000	1.19791200
C	4.66693800	0.58598800	-0.00018000
C	3.93087800	0.64813300	-1.19567300
C	2.55336300	0.78663900	-1.15750500
H	1.95162000	0.87493200	2.05861700
H	4.43906600	0.60521800	2.15731300
H	4.43207700	0.61553600	-2.15685500
H	1.94133700	0.84706500	-2.04934400
N	1.88098100	0.87140200	0.00472000
C	6.14024600	0.43417300	-0.00344100
C	6.77810500	-0.35267400	-0.97734600
C	6.93050100	1.07358300	0.96663600
C	8.16402300	-0.49715300	-0.97886200
H	6.18234300	-0.87967700	-1.71704400
C	8.31680200	0.93329900	0.96016400
H	6.45839300	1.70766000	1.71175300
C	8.93824500	0.14652400	-0.01164500
H	8.63873100	-1.11952000	-1.73230700
H	8.91254200	1.44414900	1.71154100
H	10.01896900	0.03522200	-0.01461500
C	-2.55331100	-0.78643700	-1.15754100
C	-3.93083500	-0.64799300	-1.19570600
C	-4.66690200	-0.58603200	-0.00020900
C	-3.93784800	-0.67245100	1.19788200
C	-2.55997300	-0.81068000	1.16450000
H	-1.94127800	-0.84671000	-2.04938500
H	-4.43203700	-0.61529900	-2.15688300
H	-4.43906200	-0.60553900	2.15728200
H	-1.95159300	-0.87513300	2.05857200
N	-1.88094400	-0.87132800	0.00467700
C	-6.14022000	-0.43427600	-0.00346000
C	-6.93045500	-1.07388900	0.96650200
C	-6.77809800	0.35272400	-0.97722200
C	-8.31676100	-0.93365100	0.96004600
H	-6.45832900	-1.70808400	1.71150600

C	-8.16402400	0.49715800	-0.97872000
H	-6.18235300	0.87988100	-1.71682400
C	-8.93822600	-0.14671900	-0.01162500
H	-8.91248700	-1.44465800	1.71132800
H	-8.63874300	1.11964700	-1.73205800
H	-10.01895400	-0.03545700	-0.01456800

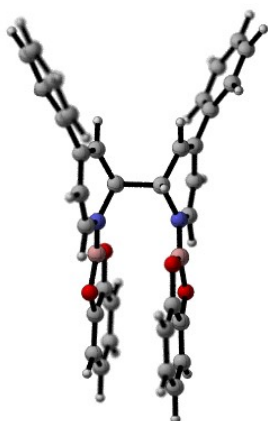


2B-TS

Imaginary frequency: -326.17

B	-1.53634400	0.17458400	-1.06768700
B	-1.53634400	-0.17458400	1.06768700
O	-1.54685300	-1.12252300	-1.66639400
O	-2.81630500	0.79340000	-1.20766900
O	-2.81630500	-0.79339900	1.20766800
O	-1.54685300	1.12252300	1.66639400
C	-0.40507100	2.35623800	-0.81026500
C	0.91518900	0.46046800	-1.31794200
C	0.71893800	3.12226100	-0.68169800
H	-1.40570200	2.74540700	-0.68664800
C	2.06211200	1.22074800	-1.22355800
H	0.92493900	-0.58715900	-1.58639400
C	2.01726600	2.58325400	-0.88899800
H	0.59387300	4.17676100	-0.46307400
H	3.01124400	0.71801200	-1.37205000
C	3.23107500	3.39682200	-0.74884100
C	4.40003100	3.09034700	-1.47211300
C	3.26499700	4.50750100	0.11593700
C	5.55162900	3.85853200	-1.33341800
H	4.39410800	2.26162400	-2.17365000
C	4.41707500	5.27690900	0.25088400
H	2.39012300	4.74961100	0.71162300
H	6.43711700	3.60541000	-1.90994000
H	4.41878900	6.12395600	0.93134400
N	-0.33277300	1.01141200	-1.12985600
C	-0.40507200	-2.35623800	0.81026500
C	0.91518900	-0.46046800	1.31794200

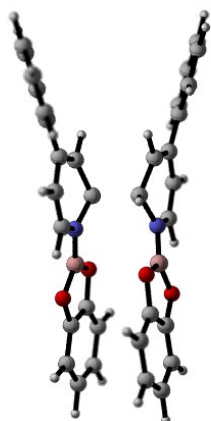
C	0.71893800	-3.12226100	0.68169800
H	-1.40570200	-2.74540600	0.68664800
C	2.06211200	-1.22074900	1.22355800
H	0.92493900	0.58715900	1.58639400
C	2.01726500	-2.58325400	0.88899800
H	0.59387200	-4.17676100	0.46307400
H	3.01124400	-0.71801200	1.37205000
C	3.23107500	-3.39682200	0.74884100
C	3.26499700	-4.50750000	-0.11593700
C	4.40003100	-3.09034700	1.47211300
C	4.41707400	-5.27690900	-0.25088500
H	2.39012300	-4.74961000	-0.71162400
C	5.55162900	-3.85853300	1.33341800
H	4.39410700	-2.26162500	2.17365100
H	4.41878900	-6.12395600	-0.93134400
H	6.43711600	-3.60541000	1.90994100
N	-0.33277400	-1.01141200	1.12985600
C	5.56816400	4.95747400	-0.47155700
H	6.46686400	5.55785200	-0.36539800
C	5.56816400	-4.95747400	0.47155700
H	6.46686300	-5.55785300	0.36539900
C	-3.45111800	-2.49847000	-2.46698400
C	-4.84220600	-2.47544000	-2.66880800
C	-5.59839000	-1.33938300	-2.37498100
C	-4.99833600	-0.17296700	-1.87039700
C	-3.62824100	-0.20107100	-1.68918300
C	-2.86961000	-1.34576300	-1.97365200
H	-2.85453400	-3.37879100	-2.68205600
H	-5.33483200	-3.36232000	-3.05609400
H	-6.67239000	-1.35469100	-2.53485100
H	-5.57420000	0.71203300	-1.62326300
C	-4.99833600	0.17296700	1.87039600
C	-5.59839100	1.33938300	2.37498100
C	-4.84220600	2.47544000	2.66880900
C	-3.45111800	2.49847000	2.46698400
C	-2.86961000	1.34576300	1.97365200
C	-3.62824100	0.20107100	1.68918300
H	-5.57420000	-0.71203300	1.62326300
H	-6.67239000	1.35469100	2.53485100
H	-5.33483200	3.36232000	3.05609500
H	-2.85453400	3.37879100	2.68205600



'2B

B	1.52769000	-0.54678500	-1.35703800
B	1.52752400	0.54700900	1.35724900
O	1.60320000	0.69323200	-1.99526100
O	2.79261800	-1.12202000	-1.19433400
O	2.79248000	1.12203400	1.19399100
O	1.60306900	-0.69279400	1.99588900
C	0.33524800	-2.41764000	-0.32486000
C	-0.89292700	-0.34145700	-0.71365700
C	-0.81200100	-3.07580200	-0.06911100
H	1.31437200	-2.85081100	-0.15754100
C	-2.11204600	-1.20311700	-0.87478100
H	-0.87759500	0.46344800	-1.45173300
C	-2.08937000	-2.49813700	-0.48871200
H	-0.77154000	-4.08324900	0.32555000
H	-3.02811900	-0.72596500	-1.20452700
C	-3.29885700	-3.35309000	-0.52492700
C	-4.25542300	-3.21189600	-1.54269300
C	-3.52288600	-4.31812700	0.46938400
C	-5.40423400	-3.99912900	-1.55771400
H	-4.07984100	-2.49457300	-2.33868800
C	-4.67278200	-5.10557300	0.45550800
H	-2.80350700	-4.43463900	1.27467000
H	-6.12832500	-3.87802300	-2.35876100
H	-4.83082100	-5.84005600	1.24049300
N	0.33579600	-1.13670800	-0.88000300
C	0.33492500	2.41777700	0.32509200
C	-0.89305400	0.34150700	0.71394800
C	-0.81237600	3.07580300	0.06920600
H	1.31401400	2.85103700	0.15780300
C	-2.11228200	1.20303900	0.87492000
H	-0.87769300	-0.46335700	1.45206900
C	-2.08971400	2.49803100	0.48875000
H	-0.77199000	4.08322700	-0.32552000

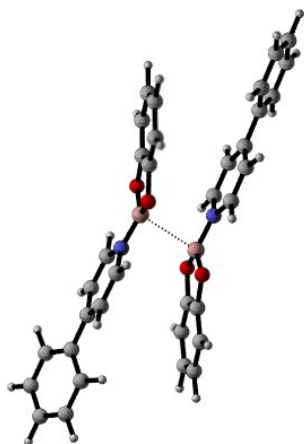
H	-3.02832200	0.72582200	1.20466300
C	-3.29929400	3.35285800	0.52482300
C	-3.52336500	4.31779600	-0.46957500
C	-4.25591200	3.21163600	1.54253600
C	-4.67334700	5.10511800	-0.45583300
H	-2.80394600	4.43432500	-1.27482400
C	-5.40480900	3.99874500	1.55742400
H	-4.08030500	2.49438900	2.33859500
H	-4.83141500	5.83952400	-1.24088400
H	-6.12894000	3.87761900	2.35843200
N	0.33556500	1.13689900	0.88034400
C	-5.61881000	-4.94991400	-0.55813200
H	-6.51254800	-5.56718200	-0.57254300
C	-5.61942400	4.94943200	0.55775600
H	-6.51323100	5.56660300	0.57206300
C	3.58312200	2.01589400	-2.72301200
C	4.98656300	1.98346200	-2.76397100
C	5.70459900	0.88838200	-2.27562400
C	5.05282500	-0.22762000	-1.72604000
C	3.67280700	-0.18460900	-1.69737700
C	2.95415000	0.91206800	-2.18008000
H	3.01505200	2.86285400	-3.09198200
H	5.52198600	2.83062800	-3.18152400
H	6.78944400	0.89831100	-2.31839400
H	5.59567600	-1.07648400	-1.32626500
C	5.05272800	0.22758300	1.72543300
C	5.70452400	-0.88829400	2.27524100
C	4.98649800	-1.98312600	2.76415900
C	3.58304300	-2.01542500	2.72357400
C	2.95404800	-0.91172200	2.18041800
C	3.67269800	0.18470700	1.69714400
H	5.59556300	1.07624600	1.32520900
H	6.78937900	-0.89832700	2.31773100
H	5.52193900	-2.83020100	3.18187200
H	3.01497900	-2.86219300	3.09299500



³2B

B	-1.65574200	0.94833400	-1.13852300
B	-1.65572500	-0.94832100	1.13848900
O	-1.94444800	-0.28305700	-1.72671400
O	-2.79980600	1.72989000	-0.98401600
O	-2.79978400	-1.72989200	0.98402600
O	-1.94442300	0.28306700	1.72668700
C	-0.19678300	2.57383800	-0.06574300
C	0.76293100	0.44790500	-0.72618700
C	1.05760100	3.09292300	0.16028500
H	-1.10738100	3.10056100	0.18622800
C	2.05647900	1.13681000	-0.83013300
H	0.60926800	-0.32727200	-1.48144400
C	2.22380200	2.42198400	-0.29884200
H	1.12623100	4.07418000	0.61358600
H	2.90495500	0.53184000	-1.11945200
C	3.54754600	3.05414800	-0.21640800
C	4.58931700	2.67069600	-1.08566900
C	3.82996600	4.05017200	0.73992600
C	5.84763600	3.25893400	-1.00516400
H	4.39749100	1.92584800	-1.85121900
C	5.08914900	4.63547700	0.82065900
H	3.06381200	4.34537100	1.44992200
H	6.62799900	2.94903200	-1.69509900
H	5.27950900	5.39381600	1.57549600
N	-0.36564000	1.35147800	-0.69886500
C	-0.19678200	-2.57383100	0.06570500
C	0.76293300	-0.44788000	0.72608900
C	1.05759100	-3.09291700	-0.16032600
H	-1.10738300	-3.10055900	-0.18624500
C	2.05648400	-1.13678400	0.83003700
H	0.60927400	0.32730500	1.48134000
C	2.22380200	-2.42196600	0.29879700
H	1.12621200	-4.07418600	-0.61360200

H	2.90496000	-0.53180000	1.11932700
C	3.54754700	-3.05414300	0.21640200
C	3.82997800	-4.05018300	-0.73991000
C	4.58930000	-2.67069600	1.08568500
C	5.08915900	-4.63550100	-0.82060900
H	3.06383800	-4.34538600	-1.44991900
C	5.84761600	-3.25894500	1.00521500
H	4.39746200	-1.92584300	1.85122700
H	5.27952700	-5.39385300	-1.57543100
H	6.62796500	-2.94904500	1.69516700
N	-0.36562900	-1.35145900	0.69880600
C	6.10857600	4.24509200	-0.05165100
H	7.09211100	4.70132800	0.01303500
C	6.10856900	-4.24511600	0.05171900
H	7.09209900	-4.70136500	-0.01293700
C	-4.13186200	-1.29732700	-2.35418300
C	-5.51166500	-1.03967000	-2.36156100
C	-6.02849000	0.17865100	-1.91077200
C	-5.19121800	1.19711400	-1.43086800
C	-3.83578900	0.93188600	-1.43131000
C	-3.31923200	-0.28523400	-1.88207800
H	-3.71829300	-2.24197500	-2.68906700
H	-6.18968200	-1.80678700	-2.72267100
H	-7.10179100	0.34060000	-1.92291200
H	-5.58056400	2.13722600	-1.05781200
C	-5.19118700	-1.19714000	1.43095200
C	-6.02845700	-0.17867200	1.91085000
C	-5.51163400	1.03966700	2.36159100
C	-4.13183200	1.29733600	2.35417300
C	-3.31920500	0.28524000	1.88207100
C	-3.83576100	-0.93189600	1.43134600
H	-5.58053500	-2.13726300	1.05792600
H	-7.10175600	-0.34063200	1.92302200
H	-6.18964800	1.80678500	2.72270100
H	-3.71826300	2.24199400	2.68903000

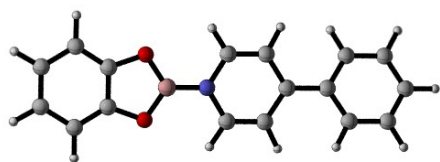


2B-TS'

Imaginary frequency: -201.78

C	-2.06664600	-2.15713500	-0.34954000
C	-1.94262500	-2.13361500	1.04440000
C	-2.93786300	-2.61896900	1.87297800
C	-4.08757300	-3.13630400	1.25108600
C	-4.21444000	-3.15422900	-0.13948500
C	-3.19624300	-2.65738100	-0.97117900
H	-2.82774000	-2.60005100	2.95241800
H	-4.88949300	-3.53249000	1.86754900
H	-5.11650600	-3.55645200	-0.59087300
H	-3.28422600	-2.66592700	-2.05256000
O	-0.93255400	-1.62925100	-0.92945800
O	-0.73216700	-1.57789900	1.39758700
B	-0.10862400	-1.27365000	0.16448400
C	1.94260200	2.13368700	1.04436800
C	2.06661400	2.15720400	-0.34957200
C	3.19618300	2.65750300	-0.97122000
C	4.21435800	3.15441000	-0.13953500
C	4.08750000	3.13648700	1.25103700
C	2.93781900	2.61909700	1.87293900
H	3.28415900	2.66604400	-2.05260200
H	5.11640000	3.55667700	-0.59093100
H	4.88940200	3.53271900	1.86749300
H	2.82770300	2.60018100	2.95237900
O	0.73217400	1.57791100	1.39756200
O	0.93254700	1.62925900	-0.92947800
B	0.10864700	1.27360400	0.16446700
C	1.95225100	-1.27623200	-1.21028700
C	3.31216500	-1.19945100	-1.34393400
C	4.17248200	-1.11488500	-0.22122400
C	3.52530600	-1.17585800	1.03983600
C	2.16528700	-1.26980800	1.15326300

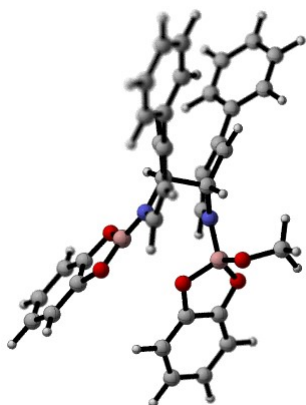
H	1.27890400	-1.32600300	-2.05507400
H	3.71767700	-1.17442100	-2.34981000
H	4.10997000	-1.19160300	1.95344500
H	1.65403500	-1.34074400	2.10365300
N	1.33951900	-1.27504400	0.03595100
C	5.62743900	-0.98847900	-0.34938800
C	6.39256200	-0.34779900	0.64852800
C	6.31482500	-1.50050700	-1.47062400
C	7.77513700	-0.23295900	0.53269700
H	5.89055500	0.10002300	1.50088600
C	7.69656200	-1.38124700	-1.58491200
H	5.76329900	-2.02764300	-2.24396700
C	8.43815400	-0.74851400	-0.58353400
H	8.33713500	0.27345800	1.31343900
H	8.19936500	-1.79500900	-2.45540500
H	9.51707400	-0.65750300	-0.67313900
C	-2.16526500	1.26977600	1.15324700
C	-3.52528500	1.17582600	1.03982000
C	-4.17245600	1.11482100	-0.22124100
C	-3.31213700	1.19934800	-1.34395000
C	-1.95222200	1.27612700	-1.21029900
H	-1.65401600	1.34073700	2.10363600
H	-4.10995100	1.19159700	1.95342600
H	-3.71764500	1.17428400	-2.34982600
H	-1.27887200	1.32586700	-2.05508500
N	-1.33949700	1.27498000	0.03593900
C	-5.62741300	0.98841900	-0.34940500
C	-6.31479200	1.50041100	-1.47066300
C	-6.39254300	0.34777700	0.64852900
C	-7.69653000	1.38115200	-1.58495200
H	-5.76326100	2.02751800	-2.24402200
C	-7.77511800	0.23293700	0.53269600
H	-5.89054100	-0.10001700	1.50090500
C	-8.43812800	0.74845600	-0.58355500
H	-8.19932700	1.79488500	-2.45546200
H	-8.33712100	-0.27345100	1.31345400
H	-9.51704800	0.65744500	-0.67316300



1C

C	-3.93447900	0.69461600	0.07369400
C	-3.93449400	-0.69465700	-0.07352700

C	-5.10717900	-1.42327700	-0.15098500
C	-6.30505800	-0.69517400	-0.07386900
C	-6.30504200	0.69520400	0.07390600
C	-5.10714300	1.42327400	0.15108700
H	-5.09468600	-2.50194700	-0.26555500
H	-7.25038400	-1.22662600	-0.13051100
H	-7.25035700	1.22668200	0.13050900
H	-5.09461600	2.50194300	0.26565400
O	-2.63033400	1.15076100	0.12175900
O	-2.63035000	-1.15082500	-0.12156100
B	-1.85375800	-0.00002900	0.00005300
C	0.30748000	1.19233900	0.12519700
C	1.66689300	1.19830000	0.11968100
C	2.44168600	0.00006000	-0.00013800
C	1.66692800	-1.19820500	-0.12007100
C	0.30751600	-1.19229000	-0.12558000
H	-0.28675800	2.09014100	0.23559100
H	2.15876100	2.15637000	0.24803300
H	2.15885800	-2.15622700	-0.24856100
H	-0.28669800	-2.09009400	-0.23610700
N	-0.42925200	0.00000800	-0.00010200
C	3.90014900	0.00003400	-0.00000400
C	4.64083100	-1.16638000	0.30669900
C	4.64095100	1.16639700	-0.30663200
C	6.03160900	-1.16464800	0.30496500
H	4.11926600	-2.07804700	0.58217800
C	6.03173600	1.16456600	-0.30471100
H	4.11950400	2.07809200	-0.58223400
C	6.74184700	-0.00006700	0.00017900
H	6.56616500	-2.07817500	0.55379500
H	6.56639000	2.07804300	-0.55351500
H	7.82819500	-0.00010800	0.00023900

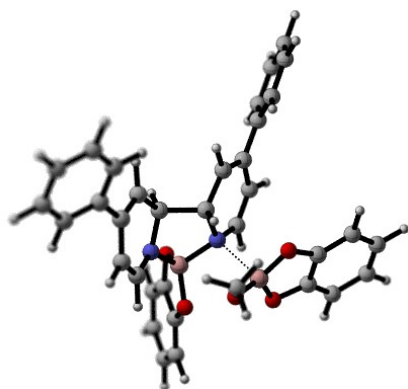


13B

C	2.90319100	1.05628800	2.34874100
C	3.32126000	2.19405100	1.64697500

C	4.50755000	2.83949800	1.94715800
C	5.28015400	2.30025700	2.99007100
C	4.86391400	1.16419200	3.68803900
C	3.65610600	0.51724100	3.37598300
H	4.82071200	3.72047400	1.39580500
H	6.22096900	2.77672200	3.25300400
H	5.48610100	0.76702600	4.48572100
H	3.32358700	-0.36891100	3.90672300
O	1.69406100	0.63428300	1.85924500
O	2.38631100	2.51610800	0.69765500
B	1.39449700	1.52526800	0.81864800
C	0.47928100	-2.25085600	0.20458000
C	-0.55551900	-2.82073100	0.90060100
C	-1.90414700	-2.53173500	0.45060200
C	-2.09632800	-1.48898800	-0.40286100
C	-0.95690800	-0.53812500	-0.67815100
H	1.49289300	-2.62626700	0.30530700
H	-0.35839200	-3.65168900	1.56807100
H	-3.07267500	-1.27040300	-0.82512800
H	-1.08053900	-0.04617900	-1.64510400
N	0.31947400	-1.26365600	-0.71299600
C	-3.02523400	-3.41530000	0.86354400
C	-4.07540700	-3.73676100	-0.01532900
C	-3.07457800	-3.95548000	2.16114900
C	-5.13414300	-4.54839400	0.38854900
H	-4.04149900	-3.35755700	-1.03257100
C	-4.13299400	-4.76805000	2.56743700
H	-2.28029300	-3.71442300	2.86194500
C	-5.17103800	-5.06985200	1.68410000
H	-5.92876700	-4.78451100	-0.31622400
H	-4.14738600	-5.16453600	3.58060300
H	-5.99460800	-5.70681200	1.99846600
C	-0.93861100	0.61220500	0.40648700
C	-2.25978800	1.34290200	0.43697100
C	-2.47856500	2.40692100	-0.37252800
C	-1.34960200	2.93457300	-1.14039100
C	-0.09405700	2.55045800	-0.82152100
H	-0.73744800	0.14316500	1.37258200
H	-3.03458200	0.97472000	1.10234200
H	-1.51028500	3.66179700	-1.92824300
H	0.78762400	2.98308200	-1.28219200
N	0.14670400	1.58637700	0.15205300
C	-3.79284700	3.09436700	-0.42772800
C	-3.87873800	4.48467100	-0.62240200

C	-4.99564600	2.37761900	-0.28979000
C	-5.11282900	5.13327800	-0.66155300
H	-2.96366900	5.06155100	-0.72096900
C	-6.22923200	3.02473800	-0.32469700
H	-4.95459400	1.29804900	-0.17707500
C	-6.29588800	4.40769900	-0.51133800
H	-5.14913000	6.21091900	-0.80556100
H	-7.14308800	2.44435300	-0.21962800
H	-7.25864700	4.91201400	-0.54620600
C	3.56429100	-1.76877100	-1.83541700
C	3.66393300	-0.45188100	-1.33422900
C	4.90039000	0.12145300	-1.07821900
C	6.05487500	-0.64590100	-1.33190100
C	5.95718600	-1.94493500	-1.82574300
C	4.69956700	-2.52609100	-2.08367700
H	4.96794100	1.13281100	-0.68864500
H	7.03370000	-0.21232600	-1.13724400
H	6.85995000	-2.52201100	-2.01645600
O	2.27384900	-2.12878100	-1.99436900
O	2.43604800	0.08488600	-1.15689800
B	1.43746500	-0.90303800	-1.73203500
O	0.88349300	-0.32430800	-2.92894300
C	0.22276400	-1.18419100	-3.82078000
H	0.87883700	-1.99494400	-4.17178700
H	-0.67087300	-1.65444700	-3.37475900
H	-0.10226800	-0.59844700	-4.69196800
H	4.60911100	-3.53913500	-2.46715600



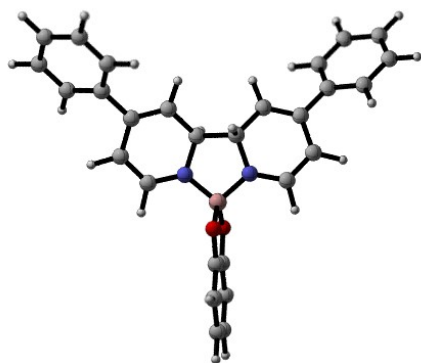
3B-TS

Imaginary frequency: -165.20

C	-1.24883500	-3.12697100	2.17884700
C	-1.19364200	-3.76779300	0.92425600
C	-1.76528500	-5.01332900	0.72612100
C	-2.40382200	-5.62661100	1.82289600
C	-2.45794700	-4.99598700	3.06451600
C	-1.87709000	-3.72689900	3.25983200

H	-1.72006700	-5.49084300	-0.24850000
H	-2.86032900	-6.60553500	1.69298500
H	-2.95557800	-5.48644400	3.89858000
H	-1.91451100	-3.22565700	4.22314800
O	-0.63595500	-1.92508400	2.12233400
O	-0.52899300	-2.99878600	0.02839100
B	-0.10913800	-1.77476000	0.72615900
C	-1.81246800	0.10257400	0.72107300
C	-2.02093100	1.37504200	1.11086200
C	-0.97598300	2.38305800	0.92567400
C	0.20001100	1.99210700	0.38837800
C	0.50775600	0.57360800	0.02079300
H	-2.58609400	-0.64801800	0.84108700
H	-2.98970900	1.66127700	1.50495200
H	1.02126400	2.69735000	0.27569600
H	0.91130500	0.54265400	-0.99872900
N	-0.65253900	-0.38215500	0.09467600
C	-1.21530500	3.78607300	1.34363600
C	-0.66434800	4.86793900	0.63263400
C	-2.00184400	4.08024500	2.47220900
C	-0.87322600	6.18344700	1.04203200
H	-0.08622400	4.66640000	-0.26464800
C	-2.21346200	5.39639500	2.88214000
H	-2.43089800	3.26369700	3.04560900
C	-1.64977300	6.45695000	2.17077600
H	-0.43899700	6.99974800	0.46878000
H	-2.81911800	5.59287000	3.76418800
H	-1.81885700	7.48362500	2.48683600
C	1.61581900	-0.09230900	0.93300600
C	3.03388000	0.33973700	0.68279300
C	3.90835700	-0.43091000	-0.01494500
C	3.49254800	-1.74829600	-0.47143500
C	2.26316900	-2.21196400	-0.09574700
H	1.32848600	0.12829600	1.97223900
H	3.34781200	1.28908200	1.10925000
H	4.14244000	-2.35558800	-1.08994600
H	1.90381500	-3.19025400	-0.40219800
N	1.39830600	-1.52645800	0.69147700
C	5.29964200	0.03007200	-0.26149800
C	6.37567600	-0.87535900	-0.24653300
C	5.58801400	1.38214000	-0.52000200
C	7.68467900	-0.44535600	-0.46270100
H	6.17688400	-1.92300900	-0.04011500
C	6.89558600	1.81456200	-0.73484500

H	4.76691200	2.09152300	-0.57128500
C	7.95350700	0.90272200	-0.70762700
H	8.49867200	-1.16674000	-0.43602800
H	7.08783400	2.86610300	-0.93700700
H	8.97335500	1.23788600	-0.88177800
C	-2.86173300	0.68284600	-2.42502800
C	-3.43726200	-0.54211700	-2.04861000
C	-4.81109400	-0.70384500	-1.98549600
C	-5.60909400	0.40688400	-2.31607300
C	-5.03573200	1.62249900	-2.69162000
C	-3.63862100	1.77935000	-2.75301100
H	-5.24470400	-1.65448800	-1.69039900
H	-6.69161900	0.31278700	-2.27488600
H	-5.67548400	2.46617100	-2.93894300
O	-1.50109400	0.57241400	-2.41971800
O	-2.46332600	-1.45928200	-1.79281700
B	-1.22466600	-0.76734500	-1.98065600
O	-0.11833000	-1.43918700	-2.42164100
C	0.84365500	-0.85821000	-3.28183600
H	0.62777400	0.19502100	-3.49348200
H	1.83404400	-0.94366800	-2.82131100
H	0.85328400	-1.40951100	-4.23286900
H	-3.18028100	2.72171400	-3.03701600



INT-B

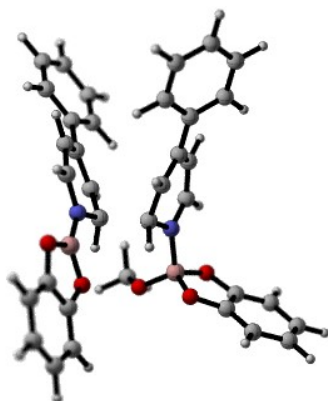
C	-0.22952600	4.06780000	-0.66759900
C	0.23213800	4.06727500	0.66796100
C	0.46555200	5.25575200	1.34358800
C	0.22950400	6.46586200	0.65923900
C	-0.22547100	6.46636400	-0.65760900
C	-0.46223700	5.25675300	-1.34260300
H	0.82066300	5.24349600	2.37067800
H	0.40653000	7.40966300	1.17120600
H	-0.40193600	7.41054700	-1.16906200
H	-0.81735500	5.24524100	-2.36969900
O	-0.38816400	2.80524700	-1.11339600

O	0.39002400	2.80441600	1.11304300
B	0.00051900	1.86880200	-0.00046100
C	-0.63021900	-0.51343800	0.44653300
C	-1.71697800	-1.48069900	0.05238000
C	-3.01949800	-1.16880500	0.28351400
C	-3.36434700	0.17202200	0.73479100
C	-2.40213800	1.14164700	0.63138900
H	-1.42522000	-2.45760200	-0.32608000
H	-4.39909300	0.45278500	0.89207600
H	-2.65065500	2.19797700	0.71211500
N	-1.10956000	0.87388300	0.35300500
C	-4.10277900	-2.15387800	0.02823300
C	-5.22937800	-2.21731200	0.86760900
C	-4.04067500	-3.05768400	-1.04767300
C	-6.24074400	-3.15348100	0.65222300
H	-5.29625700	-1.53534200	1.71063600
C	-5.05002600	-3.99414200	-1.26474400
H	-3.19593200	-3.00375400	-1.72838100
C	-6.15775400	-4.04936600	-0.41524700
H	-7.09620800	-3.18439400	1.32396200
H	-4.97671000	-4.67649700	-2.10904000
H	-6.94799200	-4.77662200	-0.58704400
C	2.40230900	1.13992500	-0.63364000
C	3.36387800	0.16963600	-0.73687100
C	3.01856300	-1.17056300	-0.28408000
C	1.71598200	-1.48152700	-0.05203100
C	0.62967300	-0.51404900	-0.44690800
H	2.65140200	2.19605000	-0.71530000
H	4.39867700	0.44964000	-0.89516000
H	1.42387300	-2.45778600	0.32782000
N	1.10974900	0.87308100	-0.35428700
C	4.10148400	-2.15587200	-0.02817800
C	5.22757700	-2.22090400	-0.86810900
C	4.03951800	-3.05832300	1.04886900
C	6.23859600	-3.15730900	-0.65213000
H	5.29433200	-1.54001100	-1.71201800
C	5.04852700	-3.99501700	1.26653300
H	3.19516800	-3.00313300	1.72996300
C	6.15575400	-4.05183600	0.41649000
H	7.09367200	-3.18948300	-1.32430500
H	4.97534000	-4.67629600	2.11170900
H	6.94572600	-4.77927300	0.58874100
H	0.29261900	-0.71468300	-1.48850500
H	-0.29314400	-0.71356900	1.48822400

³INT-B*

C	0.01671100	3.55581600	-0.70408900
C	-0.01669500	3.55574800	0.70416100
C	-0.03704100	4.74107400	1.42113200
C	-0.01871400	5.94919200	0.69666200
C	0.01901500	5.94925900	-0.69635400
C	0.03719300	4.74121000	-1.42094300
H	-0.06624600	4.72845800	2.50701600
H	-0.03339400	6.89287700	1.23716800
H	0.03381300	6.89299500	-1.23676700
H	0.06639300	4.72869700	-2.50682800
O	0.02107800	2.28677100	-1.18259000
O	-0.02125600	2.28665500	1.18253600
B	-0.00004500	1.38369100	-0.00007100
C	-1.46564000	-0.52207200	0.86845700
C	-2.60522200	-1.26789400	0.92755700
C	-3.70395800	-1.06230000	0.02222600
C	-3.46640000	-0.00779700	-0.92785500
C	-2.30459400	0.70676900	-0.94907300
H	-2.66778900	-2.01570800	1.71102300
H	-4.20769900	0.23165600	-1.68286100
H	-2.12068700	1.49121500	-1.67185500
N	-1.26352500	0.47755800	-0.06813400
C	-4.92299400	-1.83443900	0.06494400
C	-6.07384300	-1.48153700	-0.70013400
C	-5.05680400	-3.00063000	0.87512700
C	-7.24436500	-2.22594900	-0.65515500
H	-6.05162000	-0.59096100	-1.32065300
C	-6.23123700	-3.73893800	0.91417300
H	-4.21185700	-3.34265300	1.46475800
C	-7.34680600	-3.36736000	0.15142600
H	-8.09626200	-1.90797400	-1.25445800
H	-6.27764500	-4.62514900	1.54537900
H	-8.26508300	-3.94800700	0.18454800
C	2.30410700	0.70617200	0.94958500

C	3.46589500	-0.00842900	0.92846300
C	3.70394400	-1.06219200	-0.02231500
C	2.60573600	-1.26699800	-0.92846600
C	1.46615400	-0.52117200	-0.86942600
H	2.11982100	1.49007200	1.67286400
H	4.20677800	0.23039400	1.68407800
H	2.66875100	-2.01415300	-1.71252500
N	1.26354500	0.47770400	0.06786200
C	4.92296200	-1.83436500	-0.06493600
C	6.07342500	-1.48205800	0.70099500
C	5.05713700	-2.99999300	-0.87586700
C	7.24393200	-2.22649700	0.65611100
H	6.05092000	-0.59190700	1.32211600
C	6.23155300	-3.73833500	-0.91481200
H	4.21247600	-3.34156600	-1.46617000
C	7.34673800	-3.36734800	-0.15121800
H	8.09553200	-1.90898500	1.25608100
H	6.27824700	-4.62410800	-1.54661000
H	8.26500300	-3.94801900	-0.18426200
H	0.64749600	-0.67598200	-1.56268600
H	-0.64657600	-0.67751300	1.56109300

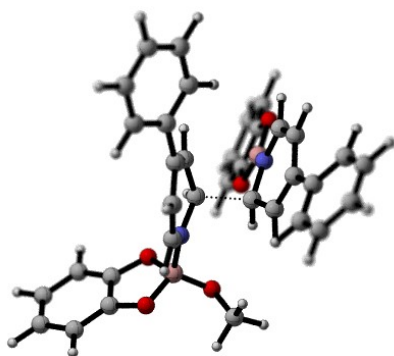


³B

C	-3.32765400	3.37784000	-0.07365000
C	-2.63222200	4.43497900	0.52573900
C	-3.28591400	5.54839500	1.02315200
C	-4.68588200	5.56997700	0.90059600
C	-5.37897900	4.51334200	0.30375700
C	-4.70553000	3.38741700	-0.19884200
H	-2.73613800	6.36210200	1.48538100
H	-5.23698900	6.42635400	1.28001400
H	-6.46192500	4.55924500	0.22653900
H	-5.22890500	2.55711300	-0.66102200
O	-2.43882900	2.41465700	-0.47607100
O	-1.28543500	4.16102000	0.51668300
B	-1.17582600	2.90196000	-0.10891500

C	-0.39374300	-0.22993400	0.22036600
C	0.53196800	-0.17527300	1.37141300
C	1.59071300	-1.03567000	1.46104300
C	1.67390300	-2.10047800	0.50115900
C	0.58364800	-2.34444800	-0.31304900
H	0.36281400	0.58041100	2.13110300
H	2.52347700	-2.77294800	0.48185100
H	0.50903700	-3.25592000	-0.89770100
N	-0.48784800	-1.53987300	-0.37562200
C	2.57774100	-0.93542000	2.56499200
C	3.12268500	-2.08687400	3.15937800
C	2.99451200	0.31728400	3.04896100
C	4.03927500	-1.99156700	4.20577100
H	2.80259900	-3.06407800	2.80875300
C	3.90951600	0.41291800	4.09637700
H	2.61407100	1.21517000	2.57115500
C	4.43697700	-0.74040700	4.68137000
H	4.43981600	-2.89792200	4.65458800
H	4.22240600	1.39349600	4.44832800
H	5.15443200	-0.66499500	5.49523400
C	1.25267500	2.74406600	0.13845600
C	2.47642700	2.28319300	-0.33657100
C	2.56734900	1.24681900	-1.27798200
C	1.32467300	0.62386700	-1.66713200
C	0.06374100	0.92027100	-0.99275300
H	1.17342000	3.56409700	0.84200200
H	3.37198100	2.73814900	0.07547000
H	1.29810100	-0.09851700	-2.47184400
N	0.04107400	2.22780200	-0.32733700
C	3.84760100	0.83358800	-1.83887200
C	4.98406200	1.68321300	-1.83883300
C	4.01268000	-0.44047200	-2.44110600
C	6.19740600	1.28219400	-2.38310400
H	4.89569100	2.68643900	-1.43105900
C	5.22796800	-0.83523600	-2.99081800
H	3.18178500	-1.13817100	-2.42619400
C	6.33637600	0.01745500	-2.97072100
H	7.04257500	1.96833600	-2.36509900
H	5.31459100	-1.82673200	-3.43208700
H	7.28407200	-0.29174700	-3.40493700
H	-0.79664900	0.83275100	-1.65902000
H	-1.40105300	0.10591400	0.47484100
C	-2.79339400	-3.95591500	-0.58002000
C	-3.48191300	-2.93492700	0.11057100

C	-4.54137300	-3.23613500	0.95333500
C	-4.90911600	-4.58842000	1.10021900
C	-4.22920300	-5.59478100	0.41756200
C	-3.15286400	-5.28643600	-0.43883600
H	-5.06505100	-2.44365300	1.48083000
H	-5.73648300	-4.84538700	1.75836800
H	-4.52748300	-6.63319700	0.54507200
H	-2.61386400	-6.06200700	-0.97649000
O	-1.80325300	-3.43387600	-1.34314200
O	-2.96640700	-1.72196200	-0.17947700
B	-1.83591000	-1.95501200	-1.11943300
C	-1.33241300	-1.57973900	-3.47108300
H	-1.56495700	-0.86977200	-4.27524600
H	-0.23806600	-1.57954800	-3.33027100
H	-1.62248800	-2.58852400	-3.80093000
O	-2.02918800	-1.18669300	-2.31677300



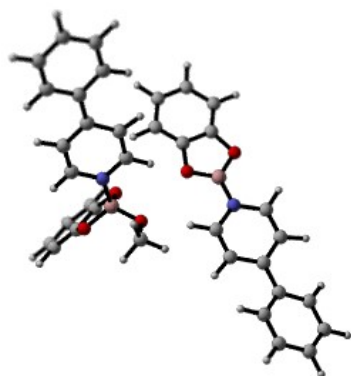
2b-TS

Imaginary frequency: -179.82

C	-3.29563000	3.36338700	-0.08356800
C	-2.60076000	4.42266300	0.51251300
C	-3.25560500	5.53342800	1.01429100
C	-4.65629600	5.54978100	0.89963900
C	-5.34885800	4.49081900	0.30623800
C	-4.67421000	3.36765400	-0.20083500
H	-2.70623900	6.34892100	1.47383100
H	-5.20844000	6.40390900	1.28259000
H	-6.43238600	4.53275300	0.23528500
H	-5.19694900	2.53548200	-0.66033000
O	-2.40530900	2.40391700	-0.49190500
O	-1.25289400	4.15345900	0.49565900
B	-1.14265000	2.89571800	-0.13149600
C	-0.39141300	-0.25824200	0.24552000
C	0.54175600	-0.19179000	1.37534500
C	1.58217400	-1.07447200	1.48658200
C	1.63025900	-2.17224400	0.56157300
C	0.54472200	-2.39486700	-0.26166800

H	0.40740800	0.60124000	2.10340200
H	2.45840400	-2.87124700	0.56361200
H	0.45035800	-3.30991700	-0.83729400
N	-0.50170100	-1.55683000	-0.35157100
C	2.58173100	-0.95727800	2.57599800
C	3.11238500	-2.09927100	3.20156100
C	3.02688800	0.30251100	3.01559400
C	4.04116600	-1.98776600	4.23533700
H	2.77099600	-3.08133400	2.88640400
C	3.95428500	0.41397500	4.05030700
H	2.65945000	1.19233500	2.51311100
C	4.46662300	-0.72970900	4.66700200
H	4.42967300	-2.88676200	4.70887600
H	4.28918700	1.39926400	4.36706300
H	5.19390100	-0.64179600	5.47079800
C	1.28957300	2.75446600	0.09331700
C	2.50989600	2.28120100	-0.36954200
C	2.59787500	1.22664100	-1.29459700
C	1.35230500	0.61141900	-1.68253600
C	0.10100000	0.92941200	-1.02723300
H	1.20941400	3.58395600	0.78534600
H	3.40682900	2.73965700	0.03546600
H	1.32516000	-0.12973900	-2.47007600
N	0.07659800	2.22624700	-0.35891600
C	3.87793700	0.79257100	-1.83822800
C	5.02370700	1.63005700	-1.84203000
C	4.03515500	-0.49301300	-2.41864500
C	6.23704800	1.20798900	-2.36983200
H	4.94303600	2.64049100	-1.45076400
C	5.25078400	-0.90901300	-2.95144700
H	3.19715200	-1.18216300	-2.40014200
C	6.36792600	-0.06755100	-2.93597700
H	7.08911900	1.88567500	-2.35569300
H	5.33074400	-1.90849000	-3.37571400
H	7.31593200	-0.39348500	-3.35707900
H	-0.77255300	0.81389900	-1.66953300
H	-1.38908500	0.11801800	0.47465900
C	-2.88859800	-3.89021100	-0.55588500
C	-3.55813400	-2.82480100	0.08414300
C	-4.65004000	-3.06158000	0.90558600
C	-5.07029500	-4.39477100	1.08297300
C	-4.40898700	-5.44529000	0.45042500
C	-3.29959000	-5.20217700	-0.38452200
H	-5.15853900	-2.23497900	1.39411800

H	-5.92370000	-4.60171000	1.72528700
H	-4.74788100	-6.46802900	0.60099400
H	-2.77484500	-6.01275700	-0.88319000
O	-1.86060600	-3.42706600	-1.30683400
O	-2.99140000	-1.64011700	-0.22817600
B	-1.84470700	-1.94209000	-1.12614600
C	-1.24083600	-1.64761200	-3.46416400
H	-1.40940100	-0.94676800	-4.29178500
H	-0.15496700	-1.68696200	-3.27386600
H	-1.55673300	-2.65125800	-3.78611400
O	-1.97081600	-1.20271300	-2.34962600

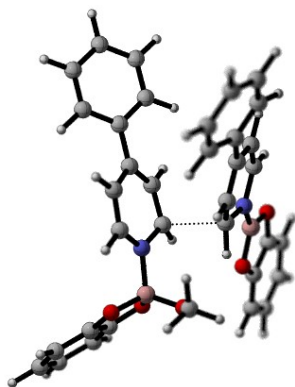


1C+2C

C	-0.12663700	-0.25091300	3.03309700
C	0.53508000	-0.99293800	4.01484600
C	-0.05068600	-1.27364100	5.23619200
C	-1.34685200	-0.77135900	5.43776800
C	-2.00337000	-0.02538300	4.45233900
C	-1.40014600	0.25523800	3.21641000
H	0.46855200	-1.85167900	5.99392300
H	-1.84767400	-0.96861900	6.38176900
H	-3.00558600	0.34676300	4.64496600
H	-1.87562000	0.83829400	2.43518100
O	0.68622600	-0.13296400	1.92727500
O	1.79054300	-1.35295300	3.54910600
B	1.84682500	-0.80040300	2.26750200
C	-2.15226400	-0.65380400	-0.73093600
C	-3.20445800	-1.52192700	-0.77686100
C	-4.47786300	-1.15427500	-1.33808400
C	-4.51136300	0.20151800	-1.82185300
C	-3.42990100	1.03081500	-1.74094200
H	-3.03870900	-2.52216000	-0.39087600
H	-5.41819800	0.61184800	-2.25327300
H	-3.45664900	2.05106700	-2.10296900
N	-2.22013400	0.64023100	-1.20851600
C	-5.60347900	-2.05288200	-1.41054300

C	-6.80582100	-1.71625500	-2.10385600
C	-5.59281700	-3.34168500	-0.79536100
C	-7.88546600	-2.58492000	-2.17272800
H	-6.88114200	-0.75983500	-2.61202400
C	-6.67751800	-4.20335100	-0.86961700
H	-4.72001400	-3.65998700	-0.23368800
C	-7.84498600	-3.84476700	-1.55864800
H	-8.77598300	-2.27777000	-2.71971500
H	-6.61603500	-5.17295200	-0.37708200
H	-8.69287700	-4.52267600	-1.61461100
C	4.14212800	-1.58360200	1.78221000
C	5.23168200	-1.65481100	0.97161000
C	5.26218000	-1.04781600	-0.32531100
C	4.05379900	-0.36308500	-0.68774000
C	2.97148800	-0.28923600	0.13269800
H	4.10124900	-2.05317800	2.75706200
H	6.08029500	-2.22764300	1.33030100
H	3.98134500	0.15752000	-1.63607400
N	2.97981700	-0.89891900	1.40105500
C	6.42026400	-1.12586500	-1.20207900
C	7.70527200	-1.47812900	-0.71581600
C	6.32259400	-0.85527100	-2.59091300
C	8.80832400	-1.55661800	-1.55822300
H	7.84576100	-1.66216200	0.34508200
C	7.42919100	-0.93315000	-3.42849600
H	5.35747500	-0.60967900	-3.02243400
C	8.68550900	-1.28558200	-2.92477500
H	9.77772300	-1.82265500	-1.14188900
H	7.30783800	-0.72482200	-4.48924500
H	9.54907100	-1.34629100	-3.58174500
H	2.05702300	0.23441500	-0.13594700
H	-1.18913700	-0.93383700	-0.32039800
C	-1.18739400	3.89888700	-1.03242900
C	-1.04253800	3.48404900	0.30903400
C	-0.99852400	4.41014400	1.34033700
C	-1.09863600	5.77637600	1.01007700
C	-1.23848200	6.18513300	-0.31447900
C	-1.28574800	5.24155800	-1.36061800
H	-0.88715200	4.08127000	2.37004200
H	-1.06419700	6.51884700	1.80456700
H	-1.31327400	7.24470100	-0.54952600
H	-1.39656200	5.54756900	-2.39752200
O	-1.22277300	2.83060800	-1.86360800
O	-0.96953000	2.13815800	0.39032000

B	-1.00484400	1.61720400	-1.01404000
C	0.45851200	0.52760200	-2.61985800
H	1.42191000	0.00262800	-2.66858200
H	-0.32021200	-0.16055500	-2.98522500
H	0.49539400	1.38903800	-3.30320300
O	0.23568900	0.92702500	-1.28817200



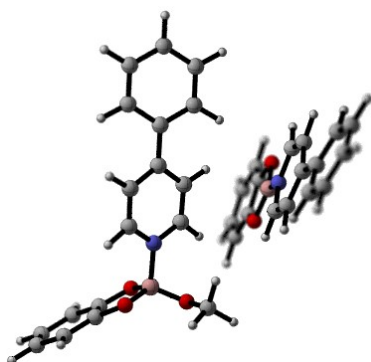
1b-TS

Imaginary frequency: -379.42

C	-2.52481500	-0.71092800	2.63136400
C	-2.83975000	-2.01047500	2.21173400
C	-4.04505800	-2.60673300	2.53744000
C	-4.94458800	-1.84986800	3.30942000
C	-4.62973600	-0.55498500	3.72716200
C	-3.40150800	0.04117800	3.39189100
H	-4.27899100	-3.61270800	2.20391400
H	-5.90356900	-2.28323900	3.58136800
H	-5.34728300	0.00735100	4.31891000
H	-3.14646500	1.04824200	3.70593700
O	-1.27358700	-0.37355200	2.18487900
O	-1.79524600	-2.52801000	1.49500500
B	-0.84256000	-1.49172400	1.44759200
C	-1.06103300	1.81535200	-0.25720800
C	-0.33870100	2.87946200	0.19730400
C	1.07903700	2.94791000	-0.07649700
C	1.64214000	1.84153100	-0.67390400
C	0.88603600	0.66044100	-0.92669000
H	-2.13997000	1.78192900	-0.15816700
H	-0.85740700	3.70915300	0.66350700
H	2.71154300	1.79624800	-0.86040300
H	1.26445300	-0.09880100	-1.59597500
N	-0.50369500	0.74448300	-0.90150600
C	1.87480300	4.13829000	0.27995000
C	3.02603100	4.50200600	-0.44893600
C	1.51192000	4.96066400	1.36600500
C	3.78302200	5.61696600	-0.09990400

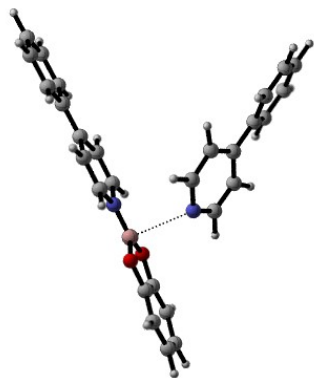
H	3.31116300	3.91346200	-1.31625900
C	2.26779900	6.07890100	1.71300500
H	0.64274800	4.70007700	1.96268200
C	3.41023100	6.41659600	0.98450900
H	4.66269500	5.87169300	-0.68708800
H	1.96494700	6.68635900	2.56326800
H	3.99792400	7.29097700	1.25307600
C	1.40591300	-0.57444100	0.86232600
C	2.75925400	-0.93311100	0.67944400
C	3.16439300	-2.15333500	0.16691600
C	2.08371400	-3.09976900	-0.10514700
C	0.80588300	-2.82705700	0.22031400
H	1.15875000	0.23206300	1.54186100
H	3.49320600	-0.16533700	0.91150000
H	2.29067500	-4.03068900	-0.62251600
H	-0.00919600	-3.51225700	0.02395700
N	0.43234900	-1.62932100	0.86382200
C	4.56416400	-2.49407600	-0.07891400
C	4.99496300	-3.84103200	-0.15916800
C	5.56489600	-1.50462900	-0.24675800
C	6.32896000	-4.17228900	-0.38194600
H	4.27316300	-4.63903300	-0.01243300
C	6.89667700	-1.83853300	-0.46184700
H	5.28161900	-0.45592600	-0.23497400
C	7.29820400	-3.17771800	-0.53381300
H	6.61515300	-5.22162000	-0.42886600
H	7.62958200	-1.04416300	-0.59121300
H	8.33923000	-3.43703400	-0.70961900
C	-3.45643700	0.54148200	-2.59036600
C	-3.73714500	-0.19762300	-1.42006200
C	-5.03796200	-0.37472700	-0.97510200
C	-6.07799100	0.20388200	-1.73022600
C	-5.80426300	0.93214700	-2.88667600
C	-4.48002900	1.11227400	-3.33336000
H	-5.23673000	-0.94002900	-0.06892600
H	-7.10717400	0.07909500	-1.40014300
H	-6.62128000	1.37214900	-3.45501200
O	-2.12908000	0.58325000	-2.82263200
O	-2.59040200	-0.65220400	-0.86394100
B	-1.44114900	-0.20582300	-1.73316200
O	-0.61752800	-1.25839500	-2.22446700
C	-1.21375700	-2.22232400	-3.05361300
H	-2.05295000	-2.73053100	-2.55397100
H	-1.59175700	-1.78242600	-3.98912600

H	-0.45580500	-2.97536600	-3.30435200
H	-4.25518500	1.68068700	-4.23193700



1b			
C	-0.62722800	4.35228700	-0.59796500
C	0.34103700	4.94381500	0.22431700
C	0.11566800	6.15252600	0.85953100
C	-1.13298500	6.76212700	0.64481100
C	-2.09854400	6.16972000	-0.17191900
C	-1.86020400	4.94184500	-0.81368400
H	0.87289300	6.60088100	1.49483600
H	-1.34832200	7.71138800	1.12822500
H	-3.05641100	6.66269100	-0.31421800
H	-2.60396400	4.46657900	-1.44469300
O	-0.14555500	3.16955700	-1.09976700
O	1.45977600	4.14950200	0.26825300
B	1.15126100	3.04265100	-0.55488300
C	-1.06544400	-0.27426800	0.12884400
C	-0.06664900	-0.28257500	1.08228100
C	0.02593900	-1.33195600	2.02489400
C	-0.94115500	-2.36264800	1.88973500
C	-1.90039000	-2.30717600	0.90606500
H	0.62148700	0.55287000	1.10683300
H	-0.91652300	-3.23310500	2.53612200
H	-2.63433000	-3.08937800	0.76042000
N	-1.98353000	-1.26896400	0.03080500
C	1.05403800	-1.35532100	3.07300400
C	0.86832900	-2.09095800	4.26510000
C	2.26337900	-0.63888300	2.93058800
C	1.83820600	-2.10677800	5.26245800
H	-0.06122000	-2.62956900	4.42488400
C	3.23206600	-0.66270800	3.92871100
H	2.46851100	-0.09235000	2.01463000
C	3.02937500	-1.39255600	5.10407700
H	1.65973000	-2.67441300	6.17307900
H	4.15882500	-0.11383100	3.78028300
H	3.78706200	-1.40492300	5.88335400

C	3.28945800	1.84563600	-0.18186800
C	4.13669200	0.82676900	-0.46716900
C	3.82439500	-0.24201300	-1.38271300
C	2.50672800	-0.13723800	-1.93395600
C	1.64764500	0.88074100	-1.66041800
H	3.53082900	2.63945200	0.51407300
H	5.08553400	0.83007500	0.06119600
H	2.14705800	-0.88514400	-2.63421300
N	2.00665400	1.95904500	-0.79466700
C	4.74355500	-1.30610100	-1.70041400
C	6.11184000	-1.28044900	-1.29640100
C	4.35349800	-2.45973700	-2.44418500
C	6.99435200	-2.30796800	-1.60311400
H	6.49267000	-0.42229500	-0.75005000
C	5.24412300	-3.47957100	-2.74985200
H	3.32193100	-2.56405700	-2.76736000
C	6.58130000	-3.42700600	-2.33587400
H	8.02884400	-2.23021000	-1.27021400
H	4.88583800	-4.33847100	-3.31598800
H	7.27509200	-4.22870100	-2.57556500
H	0.67982300	0.97745500	-2.13301900
H	-1.17832000	0.53410800	-0.58236600
C	-5.09617000	-2.35339200	-0.75707300
C	-5.34126300	-1.02534000	-0.35209400
C	-6.58643600	-0.64381700	0.12383700
C	-7.59706400	-1.62280000	0.18718100
C	-7.35355600	-2.93469700	-0.21529500
C	-6.08636600	-3.31973500	-0.69656600
H	-6.76617400	0.38148700	0.43425200
H	-8.58199700	-1.34546900	0.55609300
H	-8.14845000	-3.67482800	-0.15856400
H	-5.88363400	-4.33884600	-1.01434300
O	-3.80934500	-2.49491400	-1.17051400
O	-4.23313800	-0.26517500	-0.50081900
B	-3.18742500	-1.14641900	-1.06414100
C	-1.79372500	-1.40189700	-3.03545400
H	-1.57038200	-0.86619000	-3.96590200
H	-0.83871100	-1.60342000	-2.52235300
H	-2.25245900	-2.36821900	-3.29007500
O	-2.65710500	-0.60054200	-2.26262000

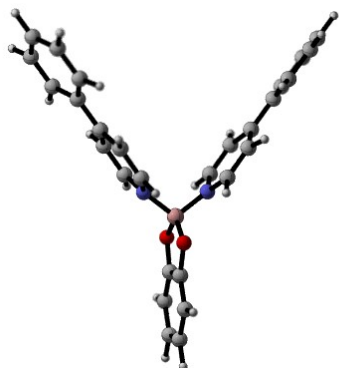


AB-TS1

Imaginary frequency: -24.80

C	-4.27451000	-1.49780800	-0.50999700
C	-4.18490700	-1.00993000	0.80416900
C	-5.30472600	-0.58572400	1.49882200
C	-6.54286100	-0.66202900	0.83314300
C	-6.63226500	-1.14722500	-0.47180500
C	-5.48858800	-1.57786100	-1.17021900
H	-5.22238200	-0.21329200	2.51536200
H	-7.44266500	-0.33554600	1.34867300
H	-7.60129700	-1.19398000	-0.96258800
H	-5.54592800	-1.95627300	-2.18609000
O	-3.03723400	-1.86089600	-0.95442000
O	-2.88551900	-1.04687000	1.22456400
B	-2.15475900	-1.52852100	0.10587600
C	0.05739400	-1.57874900	1.23038100
C	1.37239300	-1.90569600	1.23629600
C	2.04858900	-2.53966900	0.13081700
C	1.18425200	-2.73220700	-1.00299900
C	-0.13361100	-2.40830500	-1.01329400
H	-0.43042900	-1.08475500	2.06137400
H	1.92466800	-1.64180500	2.13354900
H	1.57497000	-3.16471000	-1.91975700
H	-0.77448400	-2.57450700	-1.87022400
N	-0.79057200	-1.85651700	0.12263000
C	3.43273400	-2.91923200	0.15361900
C	4.10316600	-3.47635700	-0.98226300
C	4.25421300	-2.77541000	1.31728200
C	5.44162700	-3.84038200	-0.95245800
H	3.55576600	-3.61745400	-1.91001100
C	5.59233500	-3.14164100	1.33442200
H	3.82131900	-2.37493400	2.22945000
C	6.21943500	-3.68183900	0.20305200
H	5.89174100	-4.25675100	-1.85398500
H	6.16101000	-3.00614800	2.25463800

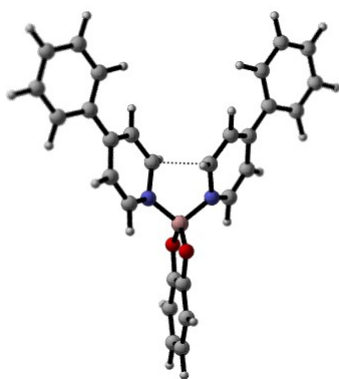
H	7.26807900	-3.96820700	0.22137000
C	-1.88709600	1.91948300	0.17435000
C	-1.00283700	2.96177500	0.41179300
C	0.17996200	3.07536400	-0.35166600
C	0.37992000	2.05953800	-1.31101600
C	-0.56780200	1.05877200	-1.47580600
H	-2.80337600	1.84045300	0.75687800
H	-1.25414800	3.70963500	1.15874400
H	1.28690000	2.02951000	-1.90729500
H	-0.39833800	0.26635100	-2.20152400
N	-1.70920200	0.96743900	-0.76368500
C	1.13636000	4.17676300	-0.15870500
C	1.25439700	4.84225400	1.08197000
C	1.97363100	4.61690900	-1.20786800
C	2.15480500	5.88810000	1.26055700
H	0.65457800	4.50847100	1.92365500
C	2.87457400	5.66156200	-1.02701300
H	1.89325300	4.14779500	-2.18412500
C	2.97423500	6.30968500	0.20861900
H	2.22734000	6.37038600	2.23314700
H	3.49928900	5.97847500	-1.85941500
H	3.67946300	7.12472700	0.34991200



INT-AB

C	-4.27303100	0.00153200	-0.67368800
C	-4.26257000	0.00152400	0.73561600
C	-5.44301100	0.00175900	1.46037200
C	-6.65671700	0.00200000	0.74489900
C	-6.66691000	0.00199700	-0.64827300
C	-5.46371500	0.00176500	-1.38130400
H	-5.42210400	0.00175300	2.54649300
H	-7.59626600	0.00218200	1.29274900
H	-7.61433300	0.00217300	-1.18237800
H	-5.45854900	0.00176500	-2.46761900
O	-3.00803800	0.00129600	-1.16613200
O	-2.99076300	0.00128800	1.20940900

B	-2.11536700	0.00091300	0.01470900
C	-0.58303100	-1.66587300	1.17895000
C	0.52343900	-2.46829000	1.19043100
C	1.13834500	-2.94028400	-0.01219900
C	0.48476000	-2.49207200	-1.20396800
C	-0.61421100	-1.68017500	-1.17187300
H	-1.07989300	-1.35494700	2.08999900
H	0.89414800	-2.78961200	2.15866200
H	0.85873800	-2.78334300	-2.18022900
H	-1.11993000	-1.35802100	-2.07402900
N	-1.18864300	-1.23929000	0.00855500
C	2.29797900	-3.80850400	-0.01952500
C	2.71818300	-4.50542300	-1.18810900
C	3.08988400	-4.02315100	1.14448200
C	3.82643200	-5.34194700	-1.18740800
H	2.14450500	-4.40657500	-2.10486100
C	4.19519400	-4.86370900	1.13782200
H	2.84723500	-3.49297500	2.06050500
C	4.58431300	-5.53876000	-0.02594900
H	4.10066900	-5.85673400	-2.10709700
H	4.77127600	-4.98646100	2.05378400
H	5.45195900	-6.19347700	-0.02893700
C	-0.58170500	1.66654300	1.17894300
C	0.52540800	2.46807500	1.19042200
C	1.14070700	2.93954900	-0.01222800
C	0.48670500	2.49191500	-1.20396600
C	-0.61293200	1.68090100	-1.17184700
H	-1.07879100	1.35602600	2.09001100
H	0.89633400	2.78911800	2.15865800
H	0.86077900	2.78298000	-2.18025200
H	-1.11893900	1.35923300	-2.07401500
N	-1.18763300	1.24041400	0.00856700
C	2.30107200	3.80681000	-0.01956700
C	3.09295000	4.02111500	1.14452400
C	2.72201900	4.50312300	-1.18824200
C	4.19890400	4.86082400	1.13786000
H	2.84973500	3.49135200	2.06063100
C	3.83090800	5.33880000	-1.18754300
H	2.14847900	4.40445300	-2.10509800
C	4.58873500	5.53531200	-0.02599700
H	4.77492900	4.98333600	2.05389000
H	4.10570600	5.85314800	-2.10731000
H	5.45687200	6.18937900	-0.02899100

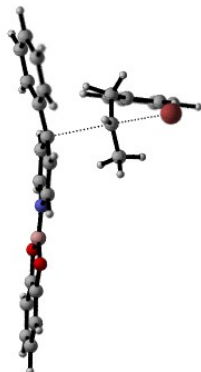


AB-TS2

Imaginary frequency: -416.93

C	-4.19855300	-0.57603400	-0.65940100
C	-4.23814300	-0.08698400	0.66251900
C	-5.44135700	0.07450400	1.33112300
C	-6.62706900	-0.26094700	0.64701200
C	-6.58825200	-0.74060500	-0.66068600
C	-5.36225000	-0.90521000	-1.33630300
H	-5.45903100	0.44914300	2.35091100
H	-7.58356300	-0.14195500	1.15141800
H	-7.51469600	-0.99326900	-1.17190500
H	-5.32007700	-1.27811800	-2.35600000
O	-2.92140300	-0.65873000	-1.09756800
O	-2.98869000	0.17449800	1.11017700
B	-2.04805000	-0.17226000	0.00754200
C	0.27112500	-0.76122800	0.79441200
C	1.39694200	-1.61458600	0.77673800
C	1.38844100	-2.85815100	0.16787400
C	0.10612700	-3.28209500	-0.37516100
C	-0.98752800	-2.48091100	-0.25980100
H	2.29814500	-1.24390600	1.25858500
H	0.00756300	-4.22760500	-0.89641600
H	-1.94280300	-2.76908000	-0.68300000
N	-0.99443100	-1.26264100	0.38072600
C	2.57562700	-3.71337400	0.11247200
C	2.46903500	-5.11698000	-0.04000400
C	3.88696800	-3.18575600	0.20403900
C	3.59480700	-5.93498900	-0.08250300
H	1.48416000	-5.57097600	-0.09316500
C	5.00895900	-4.00533300	0.16561400
H	4.02077300	-2.11026900	0.27733300
C	4.87836500	-5.39184100	0.02064200
H	3.46740200	-7.01063700	-0.19158300
H	5.99855300	-3.55703700	0.23304600
H	5.75707400	-6.03092500	-0.01848100

C	-1.37250000	2.28125100	0.25741000
C	-0.42474700	3.25182900	0.36634900
C	0.91400600	3.03162900	-0.15958200
C	1.13115700	1.79700400	-0.74682000
C	0.15709600	0.77330800	-0.76341000
H	-2.36521800	2.41667000	0.67072600
H	-0.67853600	4.17688300	0.87170000
H	2.08571200	1.57211200	-1.21599700
N	-1.17586100	1.06984200	-0.36431400
C	1.94544500	4.07019100	-0.11327100
C	1.60820900	5.44161900	-0.01644900
C	3.32624100	3.75960700	-0.16064800
C	2.58496900	6.43322800	0.01422700
H	0.56126700	5.72933500	0.00115600
C	4.29930700	4.75206000	-0.13314900
H	3.63317700	2.71796900	-0.19038400
C	3.94172400	6.10278500	-0.04459600
H	2.28248600	7.47698600	0.07885300
H	5.34991700	4.46926000	-0.16502200
H	4.70391700	6.87754200	-0.01459100
H	0.23958700	-0.00252500	-1.51873400
H	0.22230700	0.01119500	1.55620200

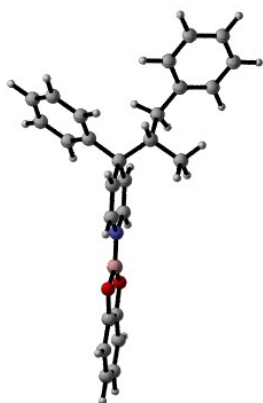


5A-TS

Imaginary frequency: -238.96

C	-5.59523700	0.49990300	0.60473600
C	-5.70137000	-0.05998000	-0.67566900
C	-6.87348800	0.01433800	-1.40740400
C	-7.95854900	0.67835600	-0.80865600
C	-7.85282000	1.23617100	0.46715800
C	-6.65718800	1.15539400	1.20251500
H	-6.94240700	-0.42186400	-2.39875900
H	-8.89568000	0.75789500	-1.35310200
H	-8.70873500	1.74442200	0.90311600
H	-6.56201800	1.58614600	2.19410400
O	-4.33525500	0.28299200	1.09992300

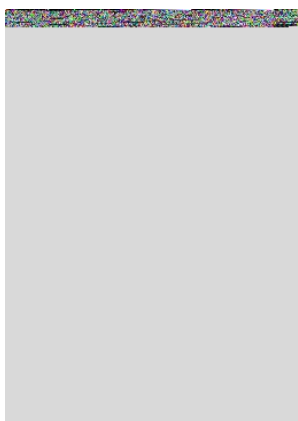
O	-4.51145800	-0.64534100	-1.02305300
B	-3.65971100	-0.42928900	0.08338000
C	-1.51172700	-0.60499200	1.29723600
C	-0.24946600	-1.07749700	1.39940800
C	0.42705800	-1.80651400	0.34700700
C	-0.42902500	-2.01977300	-0.81164900
C	-1.69718900	-1.57279200	-0.89911900
H	-1.98678700	-0.02176900	2.07640300
H	0.28223500	-0.82528500	2.31237000
H	-0.04934700	-2.56011900	-1.67309400
H	-2.31687100	-1.72448300	-1.77412900
N	-2.33095600	-0.85944900	0.16097700
C	1.59296000	-2.63312600	0.60342600
C	2.19464200	-2.72304600	1.88942600
C	2.23287000	-3.38325600	-0.42381300
C	3.33742300	-3.48669700	2.12111500
H	1.73505800	-2.21773300	2.73335500
C	3.37000100	-4.14202000	-0.18486100
H	1.83818300	-3.35473100	-1.43500300
C	3.94379500	-4.20781300	1.09201800
H	3.75133500	-3.52285600	3.12780600
H	3.82138200	-4.68916700	-1.01068700
H	4.83548900	-4.80212500	1.27389800
C	2.75829100	1.79434100	2.38180800
C	3.05557500	1.69749800	1.01633600
C	3.43746600	2.86450500	0.33305200
C	3.51437600	4.08505400	1.00397200
C	3.21525800	4.16846600	2.36695700
C	2.83606000	3.01611200	3.05532800
H	2.46737800	0.89759000	2.92542700
H	3.65924900	2.79314500	-0.73016500
H	3.81158400	4.97788900	0.45762700
H	3.27747300	5.12260600	2.88634800
H	2.60046400	3.06482600	4.11662800
C	2.99997000	0.35643400	0.30678800
C	1.92700500	0.17382500	-0.73642600
H	2.90319500	-0.44067900	1.06170600
H	3.95714900	0.16816700	-0.19264800
C	0.76161200	1.08611800	-0.88274500
H	0.17590300	0.82738300	-1.76587300
H	0.10630800	1.02608900	0.00385600
H	1.08443800	2.12703800	-0.97531100
Br	3.31533300	1.15915400	-2.89951000
H	2.03751300	-0.67542200	-1.38735600



5A

C	5.39714000	-0.63832900	0.66137100
C	5.46354900	-0.36302300	-0.70656300
C	6.65731500	-0.39701800	-1.40339400
C	7.80667500	-0.72328900	-0.66589200
C	7.74028800	-0.99858100	0.70316800
C	6.52132100	-0.96070900	1.39899300
H	6.69639700	-0.18142600	-2.46589100
H	8.76617700	-0.76158300	-1.17310100
H	8.64902100	-1.24741100	1.24321700
H	6.45748800	-1.17239800	2.46108000
O	4.08680300	-0.53043900	1.08746100
O	4.19697400	-0.07448000	-1.17802300
B	3.37191800	-0.18401300	-0.05908700
C	1.17889800	-0.10026900	1.07130700
C	-0.14274700	0.11086700	1.08643100
C	-0.96704200	0.50262900	-0.12705000
C	-0.02853700	0.58029800	-1.32328600
C	1.29186600	0.37608700	-1.27057600
H	1.72826100	-0.39038500	1.95988900
H	-0.65967100	-0.01740900	2.03265600
H	-0.46510000	0.84437700	-2.28264500
H	1.92823700	0.46223100	-2.14376300
N	1.96954900	0.03021300	-0.08440700
C	-1.61191400	1.90422100	0.04363000
C	-1.28536500	2.73862300	1.12026300
C	-2.50567300	2.40390100	-0.91936900
C	-1.84622500	4.01156900	1.24806000
H	-0.57333200	2.39485200	1.86397400
C	-3.06352400	3.67635800	-0.79934300
H	-2.76920600	1.80036300	-1.78366100
C	-2.74047000	4.48700100	0.29050900
H	-1.57547900	4.63306400	2.09802600
H	-3.75078400	4.03498800	-1.56161100

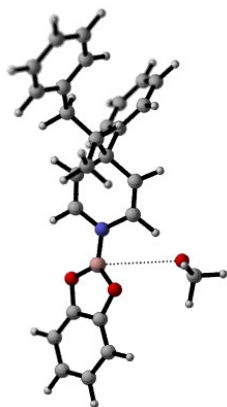
H	-3.17561700	5.47814400	0.38652400
C	-4.66329000	-2.68521000	0.78018300
C	-4.40272000	-1.35893400	0.41141300
C	-5.38208700	-0.67162900	-0.32180500
C	-6.57865200	-1.29132000	-0.68075100
C	-6.82174200	-2.61615600	-0.31041300
C	-5.85966600	-3.31099300	0.42289400
H	-3.92177200	-3.23215600	1.35853000
H	-5.20381900	0.36384100	-0.60519900
H	-7.32536100	-0.73791900	-1.24483600
H	-7.75494700	-3.09963900	-0.58705500
H	-6.04005900	-4.34047800	0.72207300
C	-3.10367900	-0.67281400	0.78194900
C	-2.09034500	-0.58136600	-0.39182700
H	-2.63825000	-1.21001400	1.61768600
H	-3.32690800	0.33855000	1.14111900
C	-1.50431200	-1.95986500	-0.72242900
H	-0.84111500	-1.91431300	-1.59174100
H	-0.92106300	-2.35314400	0.11875600
H	-2.30624400	-2.67200400	-0.94271600
H	-2.64787600	-0.24450600	-1.27537700



³⁵A*

C	5.41052500	-0.82000100	0.58973300
C	5.51294800	-0.15161300	-0.63282300
C	6.73672200	0.17047200	-1.19055100
C	7.87746900	-0.20832600	-0.46515600
C	7.77468900	-0.87758800	0.75822700
C	6.52608700	-1.19920900	1.31370000
H	6.80407500	0.68968400	-2.14068300
H	8.85954000	0.02496600	-0.86582000
H	8.67805500	-1.15586300	1.29293300
H	6.43360500	-1.71780300	2.26209700
O	4.07685000	-1.00571200	0.89887800
O	4.24727000	0.09766000	-1.12687000

B	3.38543900	-0.43364600	-0.16997000
C	1.14851300	-0.89955200	0.76375800
C	-0.17968900	-0.71419200	0.82093100
C	-0.98157300	0.01349100	-0.26130200
C	-0.10667500	-0.03205200	-1.50285300
C	1.30978300	0.29450700	-1.31172100
H	1.68987800	-1.44277500	1.53017300
H	-0.70889700	-1.11512200	1.68060700
H	-0.37804600	-0.72945800	-2.29713300
H	1.83228400	1.12506700	-1.77203000
N	1.96622100	-0.37869900	-0.26472000
C	-1.22390400	1.50362800	0.09117200
C	-0.89085000	2.05591000	1.33336500
C	-1.79443900	2.34922600	-0.87509900
C	-1.13181500	3.40475200	1.60936400
H	-0.42914400	1.42927300	2.08983300
C	-2.03638600	3.69494900	-0.60346700
H	-2.03792100	1.95133300	-1.85689500
C	-1.70721000	4.22983500	0.64429000
H	-0.86390700	3.80840900	2.58260100
H	-2.47588400	4.32836900	-1.36999400
H	-1.89274700	5.27914700	0.85775600
C	-5.37441700	-2.08360200	0.77148600
C	-4.76701800	-0.88320400	0.38097500
C	-5.53723300	0.04601700	-0.33507900
C	-6.86827500	-0.21855900	-0.65539000
C	-7.45901600	-1.42214100	-0.26274800
C	-6.70741600	-2.35384600	0.45335500
H	-4.79769900	-2.81307800	1.33619000
H	-5.08708600	0.99023100	-0.63513200
H	-7.44749800	0.51780200	-1.20695000
H	-8.49706600	-1.62864700	-0.50964400
H	-7.15766700	-3.29179900	0.76856000
C	-3.32008200	-0.57816800	0.71380900
C	-2.36241800	-0.70964800	-0.50283800
H	-2.98562800	-1.25056000	1.51439100
H	-3.25788100	0.43966500	1.11295800
C	-2.21234400	-2.18761900	-0.89787400
H	-1.63511500	-2.32044200	-1.81741200
H	-1.71071900	-2.75864100	-0.10803300
H	-3.19850300	-2.63365000	-1.06238100
H	-2.83560400	-0.18336900	-1.34274100

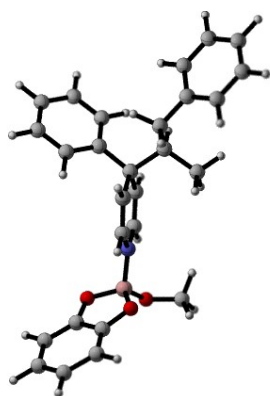


6A-TS

Imaginary frequency: -37.23

C	5.02780400	-0.65572200	-1.15434600
C	5.09817800	-0.78613100	0.23815500
C	6.25865400	-1.19405800	0.87260000
C	7.36061300	-1.48624400	0.05221500
C	7.28773900	-1.36448400	-1.33875600
C	6.10665300	-0.94011300	-1.97214100
H	6.30065300	-1.26495300	1.95433600
H	8.29139300	-1.80871500	0.51203700
H	8.16045800	-1.59503700	-1.94454400
H	6.03869100	-0.83377300	-3.05047900
O	3.77199800	-0.21893600	-1.50080200
O	3.89393200	-0.45968500	0.79054600
B	3.08451100	-0.07742800	-0.27385800
C	1.09473800	0.79520300	0.94342900
C	-0.23431200	0.97835200	0.98868700
C	-1.22822500	0.65534000	-0.12622200
C	-0.43050200	0.26243800	-1.35530700
C	0.89968700	0.08491400	-1.35528100
H	1.85392200	1.21759400	1.69560500
H	-0.64348500	1.44431200	1.88293400
H	-0.96275800	0.09161500	-2.28800400
H	1.42899900	-0.22750100	-2.25038700
N	1.70477500	0.26735700	-0.22792500
C	-2.07113900	1.93171700	-0.38047700
C	-3.00660500	2.38515700	0.56788300
C	-1.88788000	2.72151500	-1.52452300
C	-3.73734000	3.55666800	0.37078300
H	-3.15815100	1.82602000	1.48679700
C	-2.62045000	3.89240600	-1.73052100
H	-1.14284500	2.42230400	-2.25504400
C	-3.55469300	4.31663700	-0.78623900
H	-4.44807000	3.87918900	1.12888400

H	-2.45069900	4.47861400	-2.63134500
H	-4.12343300	5.23042100	-0.94189500
C	-5.45482000	-1.05563400	0.39115200
C	-4.40951000	-1.68034700	-0.30785500
C	-4.49929600	-3.06261700	-0.52323000
C	-5.58927200	-3.79895500	-0.05387400
C	-6.61827700	-3.16306700	0.64163100
C	-6.54614900	-1.78521700	0.86167400
H	-5.40700700	0.01805600	0.56112300
H	-3.70265300	-3.56608900	-1.06654300
H	-5.63379300	-4.87076200	-0.23405600
H	-7.46879000	-3.73359100	1.00708400
H	-7.34418100	-1.27695700	1.39833500
C	-3.22849500	-0.87117700	-0.79927800
C	-2.18732100	-0.53376900	0.30441100
H	-3.60069200	0.06395200	-1.23425100
H	-2.72454600	-1.41732700	-1.60661700
C	-1.40734000	-1.78455300	0.72498900
H	-0.69246000	-1.54482000	1.51679500
H	-2.08801200	-2.56210400	1.09093200
H	-0.84195800	-2.19451600	-0.12073100
H	-2.74378300	-0.18920700	1.18623400
C	3.41415700	1.21812600	3.47103100
H	2.75654100	0.30873700	3.63990100
H	4.45774100	0.77280400	3.47446300
H	3.36175500	1.76066100	4.46450400
O	3.10302000	1.96217100	2.39340100

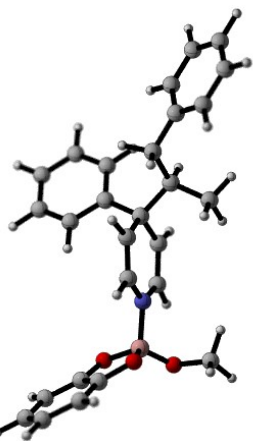


6A

C	5.00985000	0.35003700	-0.10660100
C	4.79542700	-0.88840500	-0.75594700
C	5.60986600	-1.30190200	-1.79841200
C	6.66406300	-0.45376500	-2.19759200
C	6.87567900	0.76691400	-1.56095700
C	6.04530900	1.18612400	-0.50138200
H	5.43258100	-2.25624600	-2.28807500

H	7.31605400	-0.76106700	-3.01303000
H	7.69360500	1.40960400	-1.88151600
H	6.20239500	2.13710000	0.00090600
O	4.10180100	0.54880500	0.86371400
O	3.72905100	-1.52648700	-0.22656700
B	3.25578800	-0.69127600	0.93696500
C	0.94279300	0.00688100	1.79204300
C	-0.35047200	0.37928000	1.68618900
C	-1.10872800	0.46066200	0.36708500
C	-0.13776900	0.05608200	-0.73034100
C	1.14281900	-0.31718500	-0.50696300
H	1.44393400	-0.02262600	2.75437100
H	-0.88591300	0.66382400	2.58987800
H	-0.49619900	0.05205500	-1.75727800
H	1.78663100	-0.61942900	-1.32616200
N	1.74162800	-0.37167100	0.73124200
C	-1.60663800	1.92620300	0.19998000
C	-2.61334700	2.45849500	1.02606900
C	-1.02097300	2.79190600	-0.73378500
C	-3.02710200	3.78604000	0.91104100
H	-3.07767600	1.83288000	1.78397700
C	-1.43491300	4.11972100	-0.85922100
H	-0.21436000	2.41325900	-1.35431000
C	-2.44385700	4.62603700	-0.03976800
H	-3.80670700	4.16544400	1.56904200
H	-0.95803500	4.76232400	-1.59668200
H	-2.76476400	5.66125000	-0.13237300
C	-5.61199300	-0.31302100	-0.18229300
C	-4.57952400	-1.02473300	-0.81451700
C	-4.88115500	-2.29171800	-1.33355400
C	-6.16338600	-2.83391300	-1.22171900
C	-7.17689000	-2.11440500	-0.58753900
C	-6.89461700	-0.84834800	-0.06819900
H	-5.40032600	0.67642000	0.21798500
H	-4.09817100	-2.85775200	-1.83328600
H	-6.36986900	-3.81947600	-1.63330100
H	-8.17675900	-2.53318100	-0.50096600
H	-7.67735900	-0.27444300	0.42315300
C	-3.19233500	-0.42919000	-0.91970800
C	-2.36320300	-0.51283600	0.39214600
H	-3.28346300	0.62277000	-1.21505600
H	-2.63869500	-0.93506800	-1.72005200
C	-1.95579700	-1.95969300	0.69122800
H	-1.41019400	-2.01995600	1.63754900

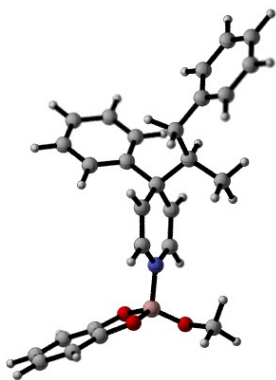
H	-2.83570800	-2.61115200	0.75345000
H	-1.29197000	-2.34302100	-0.09255400
H	-3.01573500	-0.18159500	1.21269100
C	2.98570700	-2.60842000	2.40540900
H	1.88378400	-2.65931300	2.36168600
H	3.37879700	-3.30698000	1.65045100
H	3.29935200	-2.96259500	3.39792700
O	3.47434000	-1.30682300	2.22184000



^{36A*}

C	4.83723300	0.31912100	-0.12021600
C	4.68781000	-0.87916300	-0.85199900
C	5.47052900	-1.14334300	-1.96433600
C	6.42339900	-0.17765000	-2.34811800
C	6.56972000	1.00648200	-1.62858700
C	5.77218700	1.27157400	-0.49735100
H	5.34525500	-2.07005400	-2.51818500
H	7.04852800	-0.36323800	-3.21906800
H	7.30952400	1.74079800	-1.94069300
H	5.87823500	2.19155500	0.07088000
O	3.97677000	0.35870000	0.91764600
O	3.71174200	-1.64772100	-0.31372300
B	3.22992700	-0.92609800	0.90522200
C	0.94817200	-0.25069300	1.82369800
C	-0.41661100	0.11788100	1.72197000
C	-1.11029600	0.26110300	0.40103400
C	-0.23802900	-0.22335300	-0.72085300
C	1.08871000	-0.60595000	-0.51627600
H	1.49993800	-0.22845000	2.75287000
H	-0.95963800	0.41738400	2.61320600
H	-0.61356200	-0.15362200	-1.73615500
H	1.73680200	-0.91479200	-1.32452100
N	1.66216900	-0.61152300	0.72051600
C	-1.32180500	1.79377600	0.31507300
C	-2.51546800	2.43750600	0.73843000

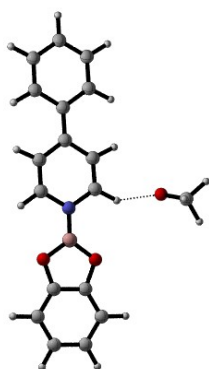
C	-0.27373700	2.63348900	-0.13775200
C	-2.64694400	3.82614700	0.68824600
H	-3.34606400	1.85609400	1.12587000
C	-0.40721700	4.01226700	-0.17502700
H	0.65556700	2.17775400	-0.46738000
C	-1.60526800	4.63480100	0.23254100
H	-3.58242300	4.27877700	1.01596000
H	0.42606200	4.61593400	-0.52974300
H	-1.71297100	5.71596000	0.19465500
C	-5.65651700	0.09245800	-0.32482900
C	-4.69876800	-0.78578600	-0.86062000
C	-5.13935900	-2.04127400	-1.30453600
C	-6.48150200	-2.41439500	-1.21093400
C	-7.41895300	-1.53199400	-0.66897100
C	-6.99845200	-0.27540200	-0.22695500
H	-5.33868700	1.07742200	0.00908600
H	-4.41674000	-2.73320600	-1.73178100
H	-6.79504300	-3.39411200	-1.56477200
H	-8.46567000	-1.81796900	-0.59697400
H	-7.71982500	0.42441000	0.18952800
C	-3.24241700	-0.38406700	-0.93949900
C	-2.46481200	-0.54997500	0.39843000
H	-3.17211100	0.66183800	-1.25865600
H	-2.74292100	-0.98584000	-1.70797700
C	-2.24343800	-2.03440200	0.72538100
H	-1.72436100	-2.14820200	1.68196100
H	-3.20108300	-2.56408900	0.78748300
H	-1.63102000	-2.51711800	-0.04469100
H	-3.09247300	-0.13521400	1.19801200
C	2.96057300	-2.93978000	2.23574600
H	1.85833300	-2.98000000	2.23583500
H	3.32391500	-3.57773000	1.41563000
H	3.31388700	-3.36534600	3.18491400
O	3.44414900	-1.62523800	2.13268200



7A

C	4.80244700	0.28979400	0.23506000
C	4.72472400	-0.58888300	-0.87073200
C	5.52372300	-0.40966000	-1.99121200
C	6.40748000	0.67934200	-1.98686100
C	6.47918300	1.55614600	-0.89487400
C	5.67088600	1.37665500	0.23415300
H	5.46024500	-1.09174700	-2.83324700
H	7.04793000	0.84610000	-2.84851200
H	7.17665100	2.38857700	-0.92325200
H	5.71876300	2.04546000	1.08752000
O	3.94741700	-0.08614100	1.20199700
O	3.78889800	-1.54065900	-0.65623600
B	3.24477600	-1.29852000	0.70717800
C	1.00270700	-0.50398800	1.66427300
C	-0.25307800	0.00403500	1.62447400
C	-1.00607700	0.27259600	0.34185600
C	-0.14718200	-0.15138600	-0.82181900
C	1.10250000	-0.66706200	-0.68270900
H	1.52919700	-0.68013900	2.59517200
H	-0.74697200	0.24673900	2.56059100
H	-0.55363900	-0.05775700	-1.82386600
H	1.70314000	-0.97019800	-1.53190300
N	1.70423800	-0.85362000	0.53403800
C	-1.31494300	1.79821000	0.31108000
C	-2.18249300	2.36617600	1.25909100
C	-0.70367900	2.65301900	-0.61490500
C	-2.44610800	3.73531700	1.26426500
H	-2.65811300	1.74189400	2.01040600
C	-0.96962500	4.02416200	-0.61424100
H	-0.00416200	2.24988200	-1.34022600
C	-1.84362100	4.57203700	0.32293100
H	-3.12173000	4.14810900	2.00885800
H	-0.48431600	4.66256800	-1.34772600
H	-2.04894000	5.63888900	0.32587300
C	-5.56100800	0.10288200	-0.04051900
C	-4.66944200	-0.68270800	-0.78665100
C	-5.15671800	-1.85324800	-1.38251600
C	-6.49239700	-2.23341100	-1.23470200
C	-7.36622700	-1.44474200	-0.48592000
C	-6.89540400	-0.27266700	0.11058600
H	-5.20482400	1.02385900	0.41690500
H	-4.48420400	-2.47092000	-1.97387100
H	-6.84919600	-3.14441500	-1.70826300
H	-8.40655400	-1.73715400	-0.37159700

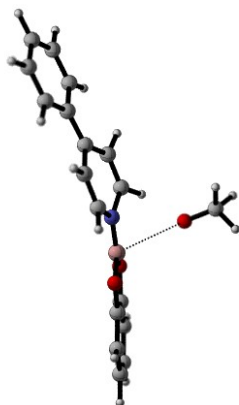
H	-7.57036500	0.35331600	0.68871600
C	-3.21986500	-0.26419700	-0.93206100
C	-2.36856500	-0.55539700	0.33187100
H	-3.17972000	0.80851600	-1.15303800
H	-2.77954900	-0.78307600	-1.79246200
C	-2.13716800	-2.06113500	0.51382900
H	-1.60000200	-2.27824100	1.44232800
H	-3.09663900	-2.58664100	0.54766600
H	-1.55393600	-2.47785200	-0.31583200
H	-2.93967100	-0.20197800	1.19913100
C	2.92171500	-3.64151500	1.26105400
H	1.83922600	-3.68075500	1.05749300
H	3.45111900	-3.99618600	0.36641000
H	3.13658300	-4.32521100	2.08893900
O	3.34562700	-2.34894200	1.63984100



1D

C	-0.34278400	0.78084900	-0.11064600
C	-1.69258900	0.73953100	-0.10340600
C	-2.49194000	-0.47614200	-0.01609800
C	-1.67071400	-1.65392500	0.05747700
C	-0.31462200	-1.63940900	0.05375500
H	0.17756700	1.74357200	-0.19405400
H	-2.14622700	1.72387100	-0.17749800
H	-2.13102500	-2.63843000	0.12340100
H	0.28165700	-2.54309000	0.11136800
N	0.44194500	-0.42623300	-0.02584600
C	-3.91434800	-0.50964300	-0.00750400
C	-4.72228700	0.68340000	-0.06716300
C	-4.68510000	-1.72755700	0.06108300
C	-6.10651400	0.65139500	-0.05905300
H	-4.22486700	1.64729300	-0.11838400
C	-6.07114000	-1.74009700	0.06809300
H	-4.16633500	-2.68264900	0.10774200
C	-6.82699500	-0.55639200	0.00842000
H	-6.64821600	1.59878200	-0.10623500

H	-6.58333100	-2.70450600	0.12150500
H	-7.91553700	-0.57296700	0.01446800
C	3.96624300	0.16112300	-0.05841200
C	3.91347900	-1.24215900	0.03704700
C	5.06684600	-2.01086500	0.09166500
C	6.30199800	-1.32827500	0.04764100
C	6.35340800	0.06154200	-0.04698500
C	5.17727800	0.83801200	-0.10203900
H	5.01169400	-3.09328600	0.16546700
H	7.22670700	-1.90102500	0.08871400
H	7.31921400	0.56242300	-0.07897000
H	5.20181500	1.92056800	-0.17483200
O	2.71106700	0.66905700	-0.09551300
O	2.61688200	-1.64949800	0.06220500
B	1.82973500	-0.44602500	-0.02117300
C	0.23404900	4.69487000	0.46915100
H	0.28893300	4.31894300	1.55143400
H	1.24080600	5.25780300	0.37894500
H	-0.49772500	5.58221200	0.57698500
O	-0.04332700	3.81002700	-0.47186900

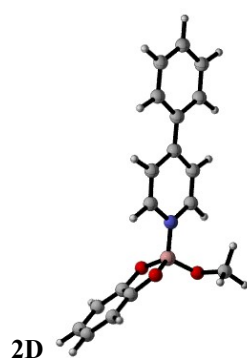


1D-TS

Imaginary frequency: -38.49

C	0.46196500	1.05534800	0.13086100
C	1.80818300	0.99825300	0.23047000
C	2.61777900	-0.15259300	-0.16555100
C	1.84752100	-1.11530200	-0.92153100
C	0.49892200	-1.07152100	-1.03087100
H	-0.16759800	1.95209900	0.23983900
H	2.30179700	1.91851800	0.53867300
H	2.35421700	-1.89529300	-1.48859300
H	-0.07091600	-1.76495100	-1.64064100
N	-0.27395400	-0.09622600	-0.32687200
C	4.00824800	-0.27630000	0.07734200
C	4.77252900	0.70994800	0.80794900
C	4.80081800	-1.40173900	-0.36680900

C	6.13576400	0.59631000	1.02144700
H	4.25483900	1.57316500	1.21782100
C	6.16419600	-1.49632700	-0.14328200
H	4.30904700	-2.21851600	-0.89066100
C	6.88033800	-0.50180300	0.54933400
H	6.64171500	1.38705600	1.58152200
H	6.69228500	-2.37905400	-0.51430500
H	7.95108100	-0.58647500	0.72699900
C	-3.68943400	-0.13059200	0.71274900
C	-3.68115600	-1.12649800	-0.28320700
C	-4.81629900	-1.85868200	-0.59063300
C	-5.99232400	-1.56568800	0.13141100
C	-6.00277100	-0.57653000	1.11495400
C	-4.84427600	0.16332000	1.42344600
H	-4.79229200	-2.62574000	-1.35987000
H	-6.90346200	-2.11943400	-0.08818400
H	-6.92468000	-0.36546500	1.65421400
H	-4.84229000	0.94429100	2.17710600
O	-2.45869400	0.40912200	0.83569000
O	-2.43624900	-1.21680200	-0.82155000
B	-1.64654100	-0.22922800	-0.13575200
C	-1.52531200	3.89782200	-1.33618300
H	-0.58362100	3.70721700	-1.95191100
H	-2.34185700	3.88196500	-2.14684600
H	-1.44074400	5.03089900	-1.13211200
O	-1.72446800	3.11954000	-0.28008400



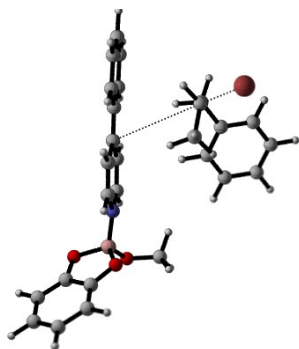
C	0.63492300	-1.47595200	-0.53657100
C	1.96138400	-1.20787400	-0.59169800
C	2.56660500	0.01298600	-0.05469200
C	1.53286500	0.91792800	0.45947400
C	0.21474300	0.61032400	0.49647000
H	0.21264900	-2.37836300	-0.96805100
H	2.58705900	-1.94711800	-1.08893600
H	1.81305000	1.90302700	0.82784200
H	-0.52292800	1.30355500	0.88753100

N	-0.31856100	-0.62161800	0.06138400
C	3.94292000	0.28340400	-0.04551600
C	4.95261400	-0.63469300	-0.56269700
C	4.52352000	1.51287200	0.48427900
C	6.30434700	-0.34871300	-0.55989500
H	4.63237200	-1.59432500	-0.96483500
C	5.88064700	1.77156900	0.47408700
H	3.86140900	2.26317400	0.91279500
C	6.82709300	0.86106600	-0.04891300
H	6.99149800	-1.09707400	-0.96905700
H	6.22838300	2.72203100	0.89262700
H	7.89487800	1.07515600	-0.05044500
C	-3.56321700	0.32495000	-0.83727000
C	-3.57899100	0.44984200	0.58020900
C	-4.58333600	1.16440200	1.21940900
C	-5.59283700	1.76705100	0.43467600
C	-5.57694600	1.64955100	-0.95232500
C	-4.55615800	0.92419900	-1.60567700
H	-4.58048800	1.25477100	2.30383300
H	-6.38723000	2.32944100	0.92520300
H	-6.36036200	2.12045600	-1.54641800
H	-4.53520900	0.82877600	-2.68924400
O	-2.51724600	-0.38958400	-1.24724800
O	-2.53132500	-0.17678600	1.12817700
B	-1.79304100	-0.92266300	0.00588800
C	-1.69092800	-3.04106200	1.18398000
H	-0.59629500	-3.06146700	1.31370500
H	-2.12500700	-2.60841900	2.10196200
H	-2.04293900	-4.08384100	1.10528300
O	-2.08532900	-2.34816000	0.03445900

³²D*

C	0.60796200	1.48199500	0.54991500
C	1.95553700	1.20055900	0.60588300
C	2.51353400	0.01111600	0.02691000
C	1.53524200	-0.84729600	-0.58459800
C	0.19295000	-0.53670100	-0.60384500

H	0.18284300	2.38381300	0.97602000
H	2.60870200	1.94585400	1.04969600
H	1.83709600	-1.80570500	-0.99562500
H	-0.54504000	-1.18293400	-1.06339200
N	-0.31898400	0.63837500	-0.06195500
C	3.93377900	-0.29277600	0.05250400
C	4.83381200	0.46986600	0.84672700
C	4.46914300	-1.36025800	-0.71951700
C	6.23304900	0.16733100	0.86956100
H	4.44304900	1.21434900	1.53566500
C	5.87154100	-1.64924100	-0.70256400
H	3.82897800	-1.88798900	-1.42183000
C	6.73287300	-0.88455500	0.09260100
H	6.90633800	0.76654700	1.48549400
H	6.26135000	-2.47349400	-1.30284100
H	7.80381600	-1.11078000	0.10765800
C	-3.52532200	-0.30884100	0.85345400
C	-3.54846400	-0.47080200	-0.55159900
C	-4.52281600	-1.25267500	-1.16913700
C	-5.48826000	-1.88410900	-0.35162900
C	-5.46564900	-1.72839700	1.03151500
C	-4.47735000	-0.93186300	1.65822900
H	-4.52913500	-1.36839300	-2.25058200
H	-6.25751100	-2.50224600	-0.81510000
H	-6.21786000	-2.22492500	1.64483100
H	-4.45138400	-0.80130600	2.73744900
O	-2.51088000	0.48067200	1.23335100
O	-2.53763200	0.20526400	-1.13083300
B	-1.82257700	0.96804400	-0.02822400
C	-1.67003500	3.04204900	-1.28156100
H	-0.57793800	3.01406400	-1.43254400
H	-2.14167100	2.60141000	-2.17674500
H	-1.97691000	4.09971800	-1.22522300
O	-2.06625100	2.39791000	-0.10442300

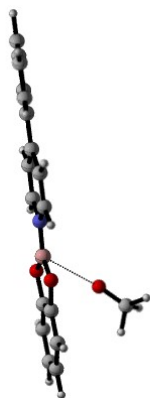


2D-TS

Imaginary frequency: -58.82

C	-1.55779900	0.25773500	-1.69021500
C	-0.44752500	1.02917400	-1.80789100
C	0.05396400	1.89217400	-0.73455900
C	-0.82288400	1.82548500	0.44041300
C	-1.92827500	1.04349400	0.50570200
H	-1.91657500	-0.35987600	-2.50745000
H	0.07140200	0.99411100	-2.76325000
H	-0.60716100	2.43956600	1.31209300
H	-2.55767300	1.01644100	1.38852000
N	-2.35224400	0.19546000	-0.53225700
C	1.21774200	2.67045400	-0.82319200
C	2.05341800	2.73815700	-2.01877900
C	1.73530800	3.48090900	0.27446500
C	3.21205800	3.49286000	-2.08365000
H	1.74280800	2.19818200	-2.91084400
C	2.89918800	4.22051700	0.17914600
H	1.18157600	3.51263800	1.21068500
C	3.68311900	4.25762800	-0.99718900
H	3.77562900	3.49245100	-3.02124200
H	3.21507500	4.80134800	1.05045400
H	4.60076100	4.83900900	-1.05732400
C	-5.81441400	0.24774400	-0.11840400
C	-5.37061200	-0.43189300	1.04800200
C	-6.20630400	-0.58298300	2.14554300
C	-7.51155900	-0.04603000	2.08036300
C	-7.94708100	0.62357300	0.94006700
C	-7.09806000	0.77899600	-0.17717700
H	-5.85178700	-1.10325700	3.03273000
H	-8.17871800	-0.15821600	2.93443000
H	-8.95594500	1.03408700	0.90374200
H	-7.42940200	1.30175600	-1.07162200
O	-4.85804400	0.28587600	-1.04777200
O	-4.10283300	-0.84640500	0.90737600
B	-3.67886400	-0.54342900	-0.52903400
C	-2.78274000	-2.76031900	-0.94321100
H	-1.72215400	-2.45855900	-0.98228100
H	-2.98936300	-3.09668500	0.08670200
H	-2.91461800	-3.62487600	-1.61411200
O	-3.65016100	-1.74086900	-1.35094900
C	1.89716500	-1.95408700	-1.23395600
C	3.19047600	-1.61139000	-0.80701800
C	4.15882400	-2.62335100	-0.72894000
C	3.84858600	-3.94290600	-1.06580900
C	2.55776600	-4.27299900	-1.48732600

C	1.58531400	-3.27478400	-1.56837800
H	1.13011600	-1.18485500	-1.31401600
H	5.15815900	-2.37104400	-0.38421000
H	4.61578300	-4.71283300	-0.99877000
H	2.31249900	-5.30084400	-1.74959200
H	0.57468100	-3.51531400	-1.89038500
C	3.52466000	-0.17972000	-0.44558000
C	3.35914200	0.20907700	1.02419700
H	2.87494700	0.51416200	-0.99783900
H	4.54974300	0.05985000	-0.74899800
C	2.07479000	-0.20682700	1.70908600
H	2.07199600	0.11843500	2.75392700
H	1.23057300	0.27105400	1.19462100
H	1.93409100	-1.29117700	1.67853200
Br	4.94013900	-0.57763700	2.11255400
H	3.54141200	1.27772800	1.13358200

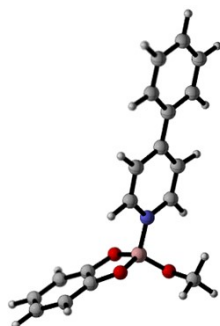


1C-TS

Imaginary frequency: -58.14

C	-0.73102500	0.82334800	-0.69916800
C	-2.08369200	0.92112400	-0.64922500
C	-2.92151900	-0.07468600	-0.03306600
C	-2.17916700	-1.15808100	0.55592000
C	-0.82534100	-1.23916700	0.50792100
H	-0.09914300	1.57358600	-1.15685300
H	-2.52412200	1.79492000	-1.11770600
H	-2.69495900	-1.94481300	1.09671700
H	-0.26641500	-2.04434200	0.96783500
N	-0.03900500	-0.27001700	-0.14324400
C	-4.36159800	0.00756800	0.00041000
C	-5.17639400	-1.07636800	0.44286300
C	-5.06904600	1.17651900	-0.40863200
C	-6.56178000	-0.99347700	0.47445600
H	-4.70941000	-2.00869300	0.74556900
C	-6.45488400	1.24960100	-0.37549800
H	-4.51513800	2.05052500	-0.73705900

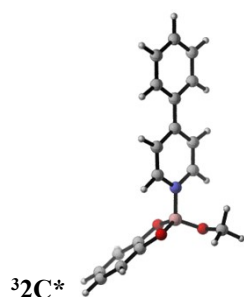
C	-7.22842900	0.16870500	0.06638900
H	-7.13412900	-1.85432200	0.81730700
H	-6.94213200	2.17001500	-0.69396700
H	-8.31331900	0.22995200	0.09167100
C	3.46228200	0.03949000	-0.73548600
C	3.41786600	-1.14838500	-0.00467400
C	4.55999700	-1.86946300	0.30410100
C	5.77658600	-1.33863500	-0.14668500
C	5.82314500	-0.13123400	-0.85752600
C	4.65856400	0.58604300	-1.16313800
H	4.50698100	-2.79217100	0.87371900
H	6.70117000	-1.86553600	0.07656900
H	6.78612400	0.26824700	-1.16549900
H	4.67808200	1.54272800	-1.66940300
O	2.18182700	0.49093700	-0.95529100
O	2.10567100	-1.43167700	0.32891400
B	1.38024000	-0.38171700	-0.23738200
C	4.42832400	2.30487700	1.89472000
H	4.08295000	1.98900700	2.92248200
H	5.34761100	1.67185300	1.72176200
H	4.85961000	3.33837300	2.05533600
O	3.51309500	2.21482900	0.91625700



2C

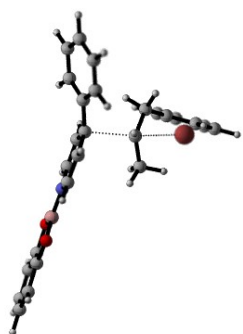
C	-0.58077700	-1.46068400	0.61867200
C	-1.91471700	-1.17552300	0.67191900
C	-2.48141400	-0.03179200	0.00577300
C	-1.49857800	0.75438400	-0.69445200
C	-0.17418800	0.42108500	-0.70923400
H	-0.15407400	-2.32598400	1.11266900
H	-2.54359300	-1.85541700	1.23685400
H	-1.78884300	1.64784000	-1.23686700
H	0.56146600	1.00964500	-1.24340200
N	0.33025400	-0.68864200	-0.06961200
C	-3.88600400	0.28976500	0.03428900
C	-4.42888700	1.41339700	-0.66270600
C	-4.83669800	-0.49324900	0.75970600

C	-5.78188600	1.71728600	-0.63409800
H	-3.77060500	2.05514700	-1.23997500
C	-6.18786400	-0.18101700	0.78213800
H	-4.50128800	-1.36121300	1.31882000
C	-6.69052800	0.92881500	0.08711000
H	-6.13878000	2.58640900	-1.18562600
H	-6.86584600	-0.81390400	1.35375500
H	-7.75021300	1.17045100	0.10715700
C	3.46743100	0.35804400	0.85384900
C	3.52157000	0.45723400	-0.55487900
C	4.45851500	1.26281600	-1.18194100
C	5.36152100	1.98451700	-0.37403400
C	5.30844400	1.88933600	1.01477800
C	4.35368700	1.06962500	1.64982800
H	4.48822700	1.32969700	-2.26647800
H	6.10574300	2.62279800	-0.84600400
H	6.01280400	2.45362800	1.62287500
H	4.30391800	0.98897800	2.73240100
O	2.48200200	-0.47350600	1.24059700
O	2.55954800	-0.30517400	-1.12412300
B	1.86945400	-1.03058400	-0.00473600
C	1.75115900	-3.14167800	-1.19904200
H	0.67787500	-3.09121600	-1.45049900
H	2.31351800	-2.74972100	-2.06054100
H	2.01685200	-4.19978000	-1.06718600
O	2.05958400	-2.45483200	-0.01435400



C	0.57247100	1.44961900	0.64332100
C	1.90603400	1.16397700	0.68871200
C	2.47150600	0.03022700	0.00516100
C	1.48771200	-0.74777700	-0.70268900
C	0.16379800	-0.41525900	-0.71332800
H	0.14652300	2.30539900	1.15402300
H	2.53464800	1.83234500	1.26731000
H	1.77774000	-1.63216200	-1.25964800
H	-0.57053700	-0.99868900	-1.25446000
N	-0.33980100	0.68782100	-0.05768400

C	3.87718500	-0.29035500	0.02532300
C	4.83293600	0.50370900	0.73046100
C	4.41353600	-1.42312400	-0.66037200
C	6.18468500	0.19264800	0.74520800
H	4.50271800	1.38216100	1.27600100
C	5.76711900	-1.72596700	-0.63983900
H	3.74986600	-2.07600500	-1.21853100
C	6.68108300	-0.92658800	0.06166900
H	6.86762500	0.83460900	1.30032700
H	6.11948300	-2.60326600	-1.18095900
H	7.74103500	-1.16729700	0.07548000
C	-3.44421400	-0.38540500	0.89683500
C	-3.52730800	-0.43463900	-0.60076600
C	-4.49348000	-1.19453100	-1.24069700
C	-5.37871100	-1.94370800	-0.46301500
C	-5.23791800	-1.96901400	1.05377100
C	-4.27765600	-1.15836800	1.68121300
H	-4.56908400	-1.17692800	-2.32674500
H	-6.23821900	-2.42761500	-0.91921700
H	-5.77168500	-2.72884100	1.61841100
H	-4.16842100	-1.14701100	2.76409900
O	-2.47852600	0.46771600	1.25590600
O	-2.55648600	0.33470300	-1.12438000
B	-1.86641900	1.03985300	0.01040600
C	-1.75761000	3.17010300	-1.14483000
H	-0.68590000	3.11478500	-1.39924400
H	-2.32714300	2.80487600	-2.01256100
H	-2.01331000	4.22589200	-0.98311200
O	-2.06894500	2.45638500	0.02519300



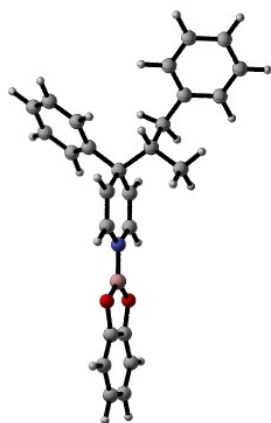
2C-TS

Imaginary frequency: -313.72

C	-5.57762500	-0.49739700	-0.52949500
C	-5.64163300	0.11749300	0.72161500
C	-6.79272400	0.10899000	1.48715500
C	-7.90109600	-0.55358100	0.93810700
C	-7.83701400	-1.16984200	-0.31623100

C	-6.66152100	-1.15358900	-1.08236600
H	-6.82998500	0.58929700	2.45889400
H	-8.82789400	-0.58764400	1.50261800
H	-8.71502700	-1.67387000	-0.70849600
H	-6.59994000	-1.62883600	-2.05537300
O	-4.30625900	-0.32685400	-1.05775200
O	-4.41247300	0.69042600	1.01234600
B	-3.62935500	0.39800800	-0.09121300
C	-1.50938300	0.48536400	-1.35416800
C	-0.21664900	0.86846600	-1.49573900
C	0.50502500	1.56447300	-0.45118900
C	-0.32955700	1.92609900	0.68318500
C	-1.62283300	1.54295500	0.78350500
H	-2.04212700	-0.07269200	-2.11411400
H	0.29421900	0.58801500	-2.41007200
H	0.08609700	2.52931700	1.48247400
H	-2.24846700	1.80357100	1.62806500
N	-2.25622300	0.80371500	-0.21957300
C	1.65833600	2.44595700	-0.78800700
C	1.92310700	2.81212900	-2.11979500
C	2.50536400	2.95590300	0.21633400
C	2.99329900	3.64921400	-2.43755000
H	1.26818300	2.47246800	-2.91600800
C	3.57206400	3.79044500	-0.10275900
H	2.36253900	2.67029500	1.25476600
C	3.82332800	4.14206400	-1.43185000
H	3.16991700	3.92121600	-3.47474100
H	4.21714500	4.15687400	0.69065400
H	4.65820500	4.79194400	-1.67828300
C	2.58447300	-2.43049300	-2.19957800
C	2.94755400	-1.95784700	-0.93245700
C	3.50307400	-2.86081600	-0.01231000
C	3.68535200	-4.19936300	-0.35880300
C	3.31818900	-4.66042900	-1.62592600
C	2.76674500	-3.77092300	-2.54781600
H	2.16422700	-1.73956000	-2.92872300
H	3.78151800	-2.50161400	0.97595600
H	4.11969900	-4.88497100	0.36443400
H	3.46433700	-5.70403700	-1.89275800
H	2.48216600	-4.11621400	-3.53878000
C	2.77116600	-0.49079900	-0.57400800
C	1.68327900	-0.16826700	0.43815400
H	2.58813100	0.06833400	-1.50201700
H	3.70708600	-0.09322100	-0.16956200

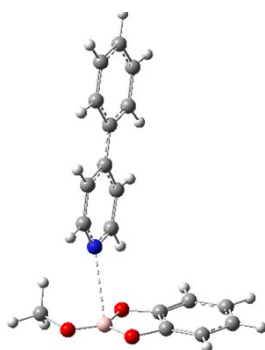
C	0.63732500	-1.17783300	0.78132800
H	-0.10570200	-0.76270000	1.46714000
H	0.14205000	-1.56409100	-0.11790600
H	1.10614600	-2.03208200	1.28014700
Br	3.33708200	-0.43510300	2.84069700
H	1.92394800	0.56396900	1.19760700



3C

C	5.37067700	-0.62286000	0.65684300
C	5.43151800	-0.35225200	-0.71475900
C	6.61674900	-0.39924700	-1.42710000
C	7.75828400	-0.73514500	-0.69032000
C	7.69732400	-1.00663900	0.68731800
C	6.49172800	-0.95587200	1.39637600
H	6.65349600	-0.18801600	-2.48982300
H	8.71609900	-0.78691400	-1.19777000
H	8.60928800	-1.26268000	1.21679200
H	6.43455900	-1.16351600	2.45890000
O	4.05505400	-0.49663800	1.08351400
O	4.15528900	-0.05150100	-1.17217000
B	3.36688800	-0.15178300	-0.05308900
C	1.18099500	-0.03040700	1.09732200
C	-0.15166300	0.20420700	1.11752500
C	-0.95299200	0.55975900	-0.09644000
C	-0.05091900	0.65556900	-1.28899100
C	1.28843500	0.43775300	-1.24772500
H	1.74615400	-0.30853000	1.97852700
H	-0.66803600	0.10876500	2.06660700
H	-0.49287200	0.93188300	-2.24079400
H	1.92953800	0.52940500	-2.11600900
N	1.92749900	0.08584500	-0.07050000
C	-1.65371100	1.94488300	0.04454300
C	-1.35678500	2.80229100	1.11206000
C	-2.55192600	2.38575900	-0.94049400
C	-1.97190700	4.05151800	1.21494900

H	-0.64374400	2.50346800	1.87425100
C	-3.16086400	3.63592600	-0.83955200
H	-2.78666900	1.76070000	-1.79743000
C	-2.87652500	4.47259900	0.24155900
H	-1.73716500	4.69467900	2.05807500
H	-3.85607800	3.95600400	-1.61014000
H	-3.35183700	5.44566200	0.31956500
C	-4.51956200	-2.77126300	0.73559100
C	-4.32152100	-1.41697800	0.42430600
C	-5.32839700	-0.73485600	-0.28075300
C	-6.49838100	-1.38667900	-0.66238300
C	-6.68243600	-2.73621900	-0.34615800
C	-5.69075600	-3.42589600	0.35674800
H	-3.75763300	-3.31049400	1.29375800
H	-5.19541900	0.31891000	-0.51683300
H	-7.27110200	-0.84326800	-1.19860100
H	-7.59563600	-3.24515700	-0.64035200
H	-5.83351700	-4.47122800	0.61506400
C	-3.05399000	-0.69444400	0.82504200
C	-2.04922300	-0.59806100	-0.35454900
H	-2.58103900	-1.22067200	1.66338400
H	-3.30446800	0.31334400	1.17272900
C	-1.40734500	-1.95430900	-0.67540500
H	-0.75642100	-1.90526200	-1.55404500
H	-0.81681500	-2.33297200	0.16714500
H	-2.18919800	-2.68871800	-0.88749600
H	-2.60199000	-0.26711900	-1.24065000



3C-TS

Imaginary frequency: -26.10

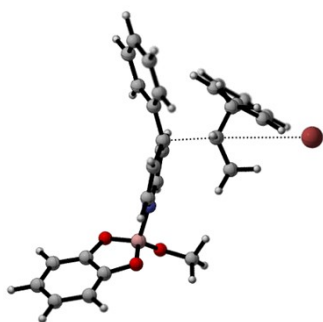
C	1.34605900	2.20420900	0.55136500
C	2.60625200	1.65814000	0.65074100
C	2.94581700	0.42848300	-0.01752800
C	1.83704000	-0.11578800	-0.75817200
C	0.61502300	0.51809400	-0.79147700
H	1.12926900	3.13762000	1.07701900
H	3.34041300	2.17832500	1.26005800

H	1.94603300	-1.04172100	-1.31640000
H	-0.20154800	0.07601600	-1.36627100
N	0.30660500	1.68274200	-0.15651700
C	4.24290000	-0.18383700	0.04603400
C	4.53985000	-1.44012000	-0.58570100
C	5.34833300	0.41109600	0.74548400
C	5.79321100	-2.02481600	-0.52086100
H	3.75663800	-1.96152200	-1.12895900
C	6.59735800	-0.18364400	0.80171000
H	5.21083100	1.36653900	1.24412800
C	6.85619600	-1.41577200	0.17223500
H	5.95337600	-2.98162400	-1.01971000
H	7.39594100	0.32095500	1.34726200
H	7.83882000	-1.87913800	0.21967900
C	-4.32557200	-0.57984200	0.72284000
C	-3.63120100	-0.77757900	-0.47662800
C	-3.51696400	-2.02784300	-1.05653000
C	-4.13646500	-3.09657900	-0.38780600
C	-4.83266400	-2.89978400	0.80781500
C	-4.93920700	-1.62544800	1.38945000
H	-2.96503700	-2.16829600	-1.98002600
H	-4.06541800	-4.09596800	-0.80834800
H	-5.29742000	-3.74815500	1.30311700
H	-5.47197600	-1.46073500	2.32056100
O	-4.27784400	0.74838700	1.06746400
O	-3.13511600	0.42408200	-0.91967000
B	-3.52979500	1.36140000	0.04782200
C	-2.43143200	3.25440500	-0.96051200
H	-1.41723100	2.85848100	-0.80628900
H	-2.78258700	3.02976300	-1.97511700
H	-2.45724000	4.33656100	-0.80478700
O	-3.32420600	2.68083800	0.01418400

4C

C	-2.89932700	1.13241800	-0.00011100
C	-1.52139100	1.19482500	-0.00017800
C	-0.71838200	-0.00000500	-0.00003100
C	-1.52136100	-1.19482700	0.00005200
C	-2.89933800	-1.13238300	0.00010300
H	-3.46790100	2.06728400	-0.00023400
H	-1.05351600	2.17602800	-0.00045500
H	-1.05353500	-2.17605300	0.00005300

H	-3.46785500	-2.06729600	0.00019000
N	-3.65053900	-0.00002400	0.00007100
C	0.71707200	0.00002800	0.00004500
C	1.49506300	-1.21018300	-0.00004500
C	1.49509700	1.21021000	0.00017200
C	2.87904400	-1.20304200	-0.00010900
H	0.98542000	-2.16993800	-0.00004900
C	2.87907900	1.20302000	0.00011100
H	0.98550700	2.16999100	0.00042200
C	3.61225900	-0.00002300	-0.00006600
H	3.40945100	-2.15666500	-0.00018600
H	3.40951800	2.15662500	0.00023100
H	4.69979500	-0.00003500	-0.00013800

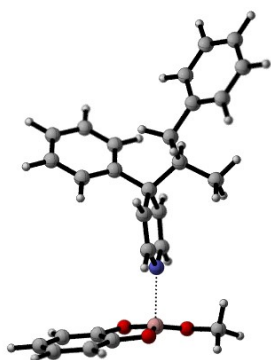


4C-TS

Imaginary frequency: -248.39

C	1.14439600	0.03290600	1.20249800
C	0.07118600	0.84717100	0.96082500
C	-0.22265300	1.32785100	-0.36930900
C	0.79970900	0.99226500	-1.33634400
C	1.85908000	0.18693800	-1.01174900
H	1.34606600	-0.38250500	2.18302900
H	-0.60844100	1.06336900	1.77687200
H	0.74026800	1.38750800	-2.34498700
H	2.62370500	-0.08428800	-1.72933900
N	2.05032800	-0.30687600	0.24117400
C	-0.93025400	2.64024400	-0.55593400
C	-1.07226200	3.53730100	0.51583800
C	-1.41125400	3.04786400	-1.81312700
C	-1.69159700	4.77646800	0.34633100
H	-0.66896300	3.27447100	1.48844500
C	-2.02749100	4.28556100	-1.98495200
H	-1.31792800	2.38622800	-2.66918300
C	-2.17625900	5.15754500	-0.90440200
H	-1.78312400	5.44868800	1.19600500
H	-2.39691400	4.56641600	-2.96800100
H	-2.65879300	6.12213600	-1.03834800
C	5.39824300	-0.07810400	0.60501400

C	5.28483500	-0.86599800	-0.55839600
C	6.29919300	-0.91106500	-1.50007700
C	7.45466100	-0.14151200	-1.25969700
C	7.56795300	0.63929200	-0.11068100
C	6.53325600	0.68168600	0.84367300
H	6.19873700	-1.52472100	-2.39100400
H	8.26584800	-0.15982600	-1.98377100
H	8.46814400	1.22647900	0.05615900
H	6.61213400	1.28598600	1.74288500
O	4.29097700	-0.19310600	1.37343200
O	4.08751300	-1.50951500	-0.58327400
B	3.38886300	-1.13502000	0.67382400
C	2.32778300	-3.29808400	0.97345900
H	1.34413200	-3.02010200	0.56182000
H	2.91062500	-3.76773100	0.16840300
H	2.16534900	-4.03915500	1.76503900
O	3.00619600	-2.19665500	1.53362400
C	-3.33366700	1.02363300	2.05627100
C	-3.45010100	0.02852700	1.07367200
C	-3.86391300	-1.25457500	1.46800400
C	-4.10846000	-1.53542400	2.81372800
C	-3.95962300	-0.54518800	3.78708200
C	-3.58001200	0.74175300	3.40185900
H	-3.05796200	2.03314000	1.76027600
H	-4.04046500	-2.00707000	0.69968600
H	-4.43032500	-2.53439900	3.09920200
H	-4.15301900	-0.76922300	4.83392400
H	-3.48304200	1.52955700	4.14625000
C	-3.18537600	0.33936700	-0.38786700
C	-1.84372500	-0.01978000	-0.97491500
H	-3.42767100	1.38491700	-0.60682200
H	-3.87305500	-0.29932800	-0.99927100
C	-1.35615800	-1.41241700	-0.78153400
H	-0.39757500	-1.59359600	-1.27622500
H	-1.28485300	-1.69232200	0.27427800
H	-2.12826900	-2.06692100	-1.24285600
Br	-4.59259200	-2.58336900	-1.91824200
H	-1.76294100	0.32229600	-2.00720100

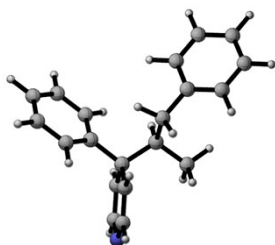


7A-TS

Imaginary frequency: -73.06

C	-4.81670700	0.35013500	-0.17831000
C	-4.71581200	-0.47996600	0.94640300
C	-5.13691200	-0.06687100	2.19782900
C	-5.67491600	1.22796500	2.29563300
C	-5.77590800	2.05588600	1.17528300
C	-5.34491600	1.62630800	-0.09135800
H	-5.05827500	-0.72144100	3.06029500
H	-6.01870800	1.58721700	3.26159000
H	-6.19684100	3.05188700	1.28111200
H	-5.42119100	2.26054400	-0.96871300
O	-4.34005300	-0.30396500	-1.28463400
O	-4.16402300	-1.68622100	0.58295100
B	-3.86847200	-1.54230100	-0.79726900
C	-1.00232800	-0.66215600	-1.66322200
C	0.26310200	-0.14303400	-1.66278900
C	1.00208000	0.20581600	-0.39394700
C	0.14039600	-0.14447700	0.78990900
C	-1.10658000	-0.68805800	0.65784800
H	-1.51951400	-0.88065300	-2.59413400
H	0.75973500	0.05597600	-2.60852700
H	0.53495700	0.03371600	1.78590100
H	-1.70083300	-0.94339100	1.53157600
N	-1.70534300	-0.94584700	-0.53624800
C	1.30428500	1.73241200	-0.45894900
C	2.17499600	2.24295400	-1.43628800
C	0.68479400	2.64179600	0.40812400
C	2.43447900	3.60993100	-1.52603700
H	2.65662700	1.57449800	-2.14455900
C	0.94533400	4.01129200	0.32129000
H	-0.01639700	2.28341600	1.15480400
C	1.82319000	4.50229100	-0.64329700
H	3.11327600	3.97725100	-2.29129100
H	0.45295600	4.69275500	1.00994700
H	2.02490600	5.56760400	-0.71245900

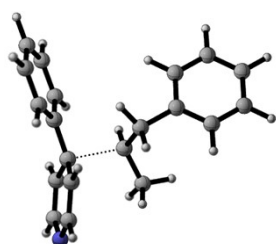
C	5.54834000	0.10721600	0.05253900
C	4.65862800	-0.65371600	0.82600800
C	5.15394800	-1.78832800	1.48166400
C	6.49565900	-2.15806100	1.36504300
C	7.36758900	-1.39451300	0.58856800
C	6.88881000	-0.25781700	-0.06720600
H	5.18510200	1.00046100	-0.45197400
H	4.48299200	-2.38532700	2.09555400
H	6.85870000	-3.04104800	1.88471800
H	8.41256300	-1.67876800	0.49851800
H	7.56212000	0.34879700	-0.66749900
C	3.20227100	-0.24786700	0.93519800
C	2.36991000	-0.61309500	-0.32195200
H	3.14617600	0.83382800	1.10199800
H	2.75776800	-0.72853400	1.81526100
C	2.14770800	-2.12782100	-0.42360100
H	1.63020500	-2.39933800	-1.34900900
H	3.10967900	-2.64987400	-0.40967500
H	1.54994800	-2.49977100	0.41671900
H	2.95050700	-0.30419600	-1.19958700
C	-3.24410700	-3.83283300	-1.14551100
H	-2.21088100	-3.78452700	-0.77789500
H	-3.89279000	-4.16715800	-0.32730300
H	-3.29648400	-4.55689700	-1.96342800
O	-3.65849000	-2.57568000	-1.65645400



8A

C	-3.06915500	-2.06181200	-1.24843500
C	-2.10346300	-1.09451000	-1.33641400
C	-1.32365400	-0.61250200	-0.13715000
C	-1.77780700	-1.37964500	1.07662800
C	-2.74650600	-2.34332000	1.01572200
H	-3.61738700	-2.36005600	-2.14112600
H	-1.89260600	-0.63048000	-2.29661700
H	-1.30565200	-1.16120700	2.03051400
H	-3.03064700	-2.88050900	1.91980600
N	-3.42246500	-2.71123800	-0.10830200
C	-1.60575300	0.91271700	0.00028200
C	-1.16564900	1.80960300	-0.98778500

C	-2.34591900	1.43053300	1.07126800
C	-1.43546400	3.17446200	-0.89515800
H	-0.61011000	1.44622400	-1.84784700
C	-2.61586000	2.79766800	1.16748200
H	-2.72470200	0.76022800	1.83611800
C	-2.15981100	3.67724600	0.18730200
H	-1.08128100	3.84491500	-1.67398500
H	-3.18907400	3.17082800	2.01224000
H	-2.37030600	4.74066100	0.26084200
C	2.93839600	1.00865600	-0.28677700
C	2.54812700	-0.11987100	0.45025200
C	3.53696100	-1.03567000	0.83239900
C	4.87502200	-0.83636400	0.48514300
C	5.24742400	0.28814800	-0.25175000
C	4.27290800	1.21239500	-0.63583100
H	2.18600100	1.73820900	-0.58003100
H	3.25643700	-1.91139600	1.41360900
H	5.62574800	-1.55911700	0.79447000
H	6.28833400	0.44668500	-0.52077900
H	4.55406100	2.09634400	-1.20276100
C	1.09084200	-0.32890800	0.81031300
C	0.23542300	-0.85138100	-0.37430100
H	0.67342800	0.62062400	1.16480200
H	1.02148800	-1.03726400	1.64494400
C	0.55921700	-2.31698700	-0.69102700
H	0.02264000	-2.66510400	-1.57892100
H	1.63191500	-2.43344800	-0.87644700
H	0.28616800	-2.97366900	0.14302800
H	0.50113000	-0.25655500	-1.25671300

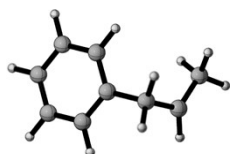


8A-TS

Imaginary frequency: -438.09

C	3.10283500	-2.23560100	1.11454600
C	2.49394000	-0.99838700	1.20399400
C	1.81784100	-0.42674200	0.06213200
C	2.01940200	-1.18343900	-1.15153200
C	2.64355000	-2.41512100	-1.11494200
H	3.58556700	-2.66224700	1.99331100
H	2.52726200	-0.45383400	2.14276700

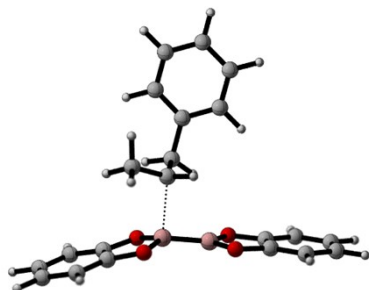
H	1.62563500	-0.81515700	-2.09365300
H	2.74309000	-2.99486100	-2.03212500
N	3.18724400	-2.97283200	-0.01206500
C	1.71482500	1.07860900	0.00026500
C	1.35743000	1.83449200	1.13076700
C	2.01918800	1.77609900	-1.17914600
C	1.29018900	3.22540000	1.07949900
H	1.12626900	1.33363500	2.06669100
C	1.94841400	3.16961100	-1.23437500
H	2.34272200	1.22997200	-2.05912400
C	1.58079700	3.90223400	-0.10707800
H	1.01088800	3.78138900	1.97070000
H	2.19331400	3.68044200	-2.16191100
H	1.52858000	4.98667500	-0.14793500
C	-2.95842600	0.92648000	0.22626100
C	-2.49036500	-0.22903300	-0.41666800
C	-3.40911000	-1.24337300	-0.71728700
C	-4.75860200	-1.10907900	-0.38498800
C	-5.21125700	0.04506700	0.25570300
C	-4.30561000	1.06429200	0.55933700
H	-2.25786500	1.72544400	0.46097600
H	-3.06573700	-2.14216300	-1.22486400
H	-5.45650400	-1.90510400	-0.63181200
H	-6.26173500	0.15217200	0.51255200
H	-4.65009500	1.97010900	1.05185700
C	-1.01330100	-0.37571500	-0.74884500
C	-0.22000500	-0.86228600	0.45334600
H	-0.62665100	0.59340700	-1.08415200
H	-0.89009200	-1.08244100	-1.57856900
C	-0.34057500	-2.32220400	0.79293400
H	0.25982300	-2.58921500	1.66643400
H	-1.38816400	-2.56858800	1.02014100
H	-0.02942700	-2.95571900	-0.04569100
H	-0.31454400	-0.20190100	1.31531500



R[•]

C	-0.83022600	-1.27422400	-0.02750900
C	0.00800400	-0.27269400	0.48125400
C	-0.48331800	1.03781900	0.54571000
C	-1.77509800	1.34136400	0.11190000
C	-2.59928100	0.33505500	-0.39394900
C	-2.12228100	-0.97591600	-0.46031000

H	-0.46653700	-2.29846300	-0.08040000
H	0.14948100	1.82629300	0.94772900
H	-2.13900200	2.36389100	0.17478700
H	-3.60636000	0.56870200	-0.72896400
H	-2.75890700	-1.76830000	-0.84601900
C	1.43865100	-0.59708200	0.90725100
C	2.40144000	-0.54083700	-0.24606100
H	1.45858500	-1.59676100	1.36051800
H	1.74920800	0.11492200	1.68464200
C	2.94534600	0.75599100	-0.74580400
H	3.79001000	0.60512600	-1.42743700
H	2.18731000	1.33948800	-1.29878500
H	3.28497700	1.39668700	0.08038500
H	2.45181100	-1.40843800	-0.90134000

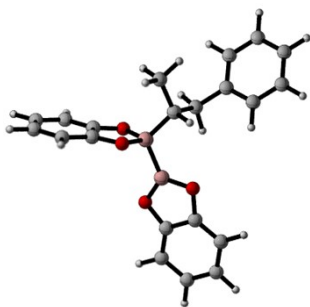


9A-TS

Imaginary frequency: -182.48

C	-3.30569700	-1.12186900	0.56089400
C	-3.21291700	-0.69118300	-0.76990800
C	-4.34076200	-0.40980800	-1.52786300
C	-5.58103700	-0.57976100	-0.89931400
C	-5.67389800	-1.01077500	0.43153600
C	-4.53043400	-1.28947800	1.19115900
H	-4.25700300	-0.07859600	-2.55767900
H	-6.48997100	-0.37405800	-1.45722200
H	-6.65345600	-1.13211000	0.88482300
H	-4.59015700	-1.62411200	2.22152900
O	-2.05252400	-1.32596200	1.06155700
O	-1.89917300	-0.61802900	-1.13397900
B	-1.14852500	-0.96931800	0.02350600
C	2.44853000	-2.13271000	-0.73784400
C	2.32018700	-2.53989100	0.59036700
C	3.35240500	-3.16566300	1.26885200
C	4.54038500	-3.36898600	0.55189500
C	4.66889200	-2.95965000	-0.78097300
C	3.61494000	-2.32864300	-1.45756100
H	3.24069500	-3.47970200	2.30127400
H	5.37781400	-3.85566700	1.04327700

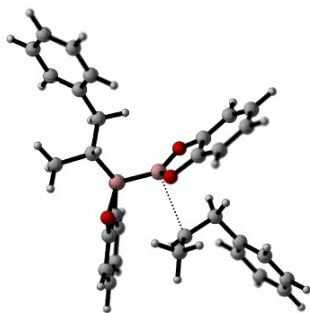
H	5.60405600	-3.13452500	-1.30487400
H	3.70192800	-2.00902600	-2.49068700
O	1.26705600	-1.54610500	-1.14280000
O	1.05822500	-2.21524400	1.04016200
B	0.41406200	-1.60754800	-0.03847400
C	2.29452700	2.82444900	0.02677400
C	0.93805800	2.91491500	-0.31785100
C	0.33891100	4.18155300	-0.34018500
C	1.07354000	5.32700500	-0.02835500
C	2.42260000	5.22292300	0.31402700
C	3.03175100	3.96644200	0.33919900
H	2.77804300	1.84975100	0.04118200
H	-0.70944900	4.27194100	-0.61596800
H	0.59214900	6.30117300	-0.05844300
H	2.99630300	6.11387800	0.55484500
H	4.08368300	3.87572200	0.59760300
C	0.13706700	1.65808600	-0.62903600
C	-0.35889100	1.00140600	0.64790400
H	0.76420500	0.95868500	-1.19198600
H	-0.71822700	1.90548900	-1.26714800
C	-1.51730600	1.63758400	1.36607000
H	-1.81673600	1.06067500	2.24465500
H	-1.23381800	2.64612400	1.70720300
H	-2.38951500	1.75535400	0.71177100
H	0.43799000	0.66037400	1.31243200



9A

C	2.11046100	2.29572300	-0.79196100
C	1.89386400	2.39594100	0.61601600
C	2.61964800	3.30401800	1.39934900
C	3.55254000	4.09569600	0.74376500
C	3.76791200	3.99537000	-0.65456200
C	3.05668900	3.09990700	-1.44153800
H	2.44896500	3.37144700	2.46823600
H	4.13719900	4.81224200	1.31311900
H	4.51093700	4.63821000	-1.11720200
H	3.21377500	3.01436200	-2.51123800
O	1.31709300	1.38216600	-1.31972000

O	0.96156000	1.54612000	1.00311800
B	0.49180700	0.77408900	-0.20576200
C	2.11714600	-2.73103900	0.37139700
C	0.95573000	-3.10174900	-0.30621900
C	0.66997100	-4.42242600	-0.60675600
C	1.61169700	-5.37639400	-0.19419900
C	2.77744400	-5.00473600	0.48615500
C	3.05421300	-3.66256400	0.78478400
H	-0.23722200	-4.69858800	-1.13387100
H	1.43025400	-6.42566500	-0.40810800
H	3.48444000	-5.77093400	0.79080900
H	3.95383500	-3.36313000	1.31217800
O	2.12658800	-1.36013600	0.52824300
O	0.21918200	-1.96813600	-0.58463000
B	0.95219100	-0.89941600	-0.06682100
C	-3.90444500	-0.73961500	-0.37478900
C	-3.42696300	0.29692300	0.44214200
C	-4.35473500	1.20478200	0.96877000
C	-5.71797300	1.08578400	0.68868300
C	-6.17760100	0.05123100	-0.12662300
C	-5.26410800	-0.86309800	-0.65765300
H	-3.19761200	-1.45789800	-0.78549000
H	-4.00447200	2.01144500	1.60922100
H	-6.42006800	1.80084500	1.11045500
H	-7.23810100	-0.04507400	-0.34440300
H	-5.61294200	-1.67645100	-1.28928600
C	-1.94301800	0.42074100	0.72551000
C	-1.12258300	0.96504700	-0.47266400
H	-1.55870300	-0.56848200	1.00465900
H	-1.78505700	1.07304400	1.59389300
C	-1.48404200	2.42053200	-0.80685300
H	-0.95028100	2.76927500	-1.69732300
H	-2.55840500	2.52648000	-0.99945500
H	-1.23275100	3.09548100	0.02182900
H	-1.35023000	0.33947000	-1.34771300

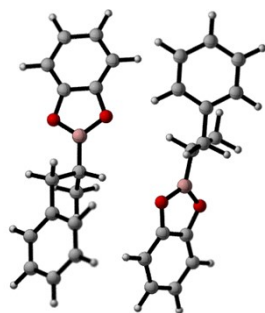


11A-TS

Imaginary frequency: -128.05

C	4.96695100	-0.13780000	-1.40156300
C	4.28211000	0.72657800	-0.53507400
C	5.02022500	1.59501200	0.28070500
C	6.41350700	1.61409900	0.21611300
C	7.08695200	0.75629600	-0.65587600
C	6.35951300	-0.11947100	-1.46537300
H	4.40369700	-0.81964200	-2.03468500
H	4.50059800	2.27104400	0.95553900
H	6.97260200	2.30244400	0.84419400
H	8.17213300	0.77163400	-0.70637800
H	6.87679300	-0.78609500	-2.15010100
C	2.75243900	0.69145900	-0.45224800
C	2.43467500	-0.41736100	0.49398700
H	2.32692000	0.49747300	-1.44117200
H	2.37535300	1.65345500	-0.09568200
C	2.33382000	-0.25158600	1.95843300
H	1.35717300	-0.62112000	2.31485600
H	3.08829500	-0.87176400	2.46661300
H	2.42973500	0.79127400	2.27082700
H	2.62877600	-1.41750200	0.12251200
C	-5.15051300	0.97744100	0.05280400
C	-4.74511800	-0.18763300	-0.61644800
C	-5.74047400	-1.03510600	-1.12100800
C	-7.09511000	-0.73487800	-0.96065600
C	-7.48102100	0.42627200	-0.29041800
C	-6.50111800	1.28352600	0.21612400
H	-4.39414500	1.65414800	0.44600600
H	-5.44805200	-1.94003100	-1.64926100
H	-7.84831800	-1.40824700	-1.36274200
H	-8.53446500	0.66389500	-0.16641400
H	-6.78992600	2.19445400	0.73503200
C	-3.27218200	-0.51023100	-0.77360500
C	-2.59615600	-1.04471700	0.51742200
H	-2.75023600	0.39216400	-1.11534800
H	-3.14156600	-1.25372600	-1.56977500
C	-3.18324200	-2.40722700	0.93425800
H	-2.75019900	-2.75069800	1.87873200
H	-4.27162500	-2.35139800	1.05896800
H	-2.97515400	-3.17207700	0.17463600
H	-2.79976000	-0.32799300	1.32711600
C	0.54373500	-2.77346500	0.90051100
C	0.40891200	-2.75299700	-0.51495200
C	1.23678300	-3.53456700	-1.32775300
C	2.19438700	-4.33134600	-0.69845100

C	2.31389500	-4.36657900	0.70519200
C	1.48487100	-3.59790200	1.52390400
H	1.12476900	-3.51284700	-2.40705500
H	2.85803400	-4.94401800	-1.30227300
H	3.06521700	-5.00731800	1.15798300
H	1.56451200	-3.62408700	2.60615900
O	-0.32213400	-1.93625000	1.47381100
O	-0.56898200	-1.93574300	-0.88617400
B	-0.96233800	-1.16826100	0.34169300
C	-0.26022600	2.58149400	-0.53218400
C	-0.24385000	2.63548700	0.86334700
C	-0.18304400	3.83731200	1.55006600
C	-0.13809800	5.00405400	0.77270000
C	-0.15381400	4.94999100	-0.62627300
C	-0.21576100	3.72689100	-1.31027900
H	-0.17670700	3.86746300	2.63477900
H	-0.09259400	5.96917700	1.26898300
H	-0.11999200	5.87391600	-1.19627800
H	-0.23313400	3.67354200	-2.39386100
O	-0.32218700	1.26497200	-0.92814700
O	-0.29371100	1.35397300	1.36051800
B	-0.35784300	0.49597900	0.24782600

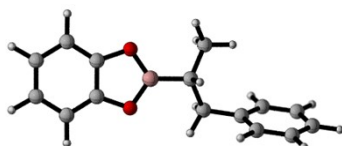


11A

C	3.34937800	-1.15522300	1.59806500
C	2.92128700	-2.47809200	1.40620500
C	3.84749400	-3.50933000	1.60531400
C	5.16400000	-3.23326000	1.98278200
C	5.57639300	-1.91413300	2.16966200
C	4.66265500	-0.87453500	1.97616600
H	2.64527700	-0.33966400	1.44876100
H	3.53264900	-4.54145200	1.46717200
H	5.86458900	-4.05075900	2.13339100
H	6.59860400	-1.69629500	2.46775600
H	4.97094000	0.15714900	2.12707800
C	1.49236100	-2.76916500	0.99265200
C	1.17494300	-2.42193800	-0.49678700
H	0.80940000	-2.20183300	1.63736200

H	1.27495700	-3.83162100	1.16571300
C	1.99612700	-3.26878200	-1.48416900
H	1.79042400	-2.98102800	-2.52100600
H	3.07090600	-3.15293500	-1.30815900
H	1.75348000	-4.33420700	-1.38924700
H	1.44350300	-1.36271400	-0.63315800
C	-3.16768700	1.50834500	2.26829100
C	-3.01044700	2.54080800	1.33089600
C	-4.16204300	3.17774800	0.85086500
C	-5.43286200	2.79440200	1.28599400
C	-5.57391400	1.76395500	2.21563900
C	-4.43432900	1.12175800	2.70786800
H	-2.28623100	1.00677100	2.66263500
H	-4.06157100	3.98670700	0.13063300
H	-6.31154600	3.30503100	0.90018100
H	-6.56106000	1.46750000	2.56022100
H	-4.53144500	0.32565300	3.44189600
C	-1.62865600	2.93997900	0.85316200
C	-0.99675200	1.94160800	-0.16263200
H	-0.96593000	3.02888000	1.72477400
H	-1.66908000	3.93609700	0.39536600
C	-1.81759200	1.85302700	-1.47053600
H	-1.39102000	1.11322000	-2.15773400
H	-2.85158400	1.55551700	-1.26603200
H	-1.83985600	2.81828700	-1.99110300
H	-0.98892500	0.94369700	0.29470900
C	2.67280800	2.21863300	-0.81844700
C	2.24788400	3.51092700	-1.12650700
C	3.12704600	4.48705200	-1.56225000
C	4.47303900	4.10983900	-1.68011100
C	4.89798100	2.81274600	-1.37041000
C	3.99698200	1.83195300	-0.92893300
H	2.78608400	5.48927300	-1.79949700
H	5.19928000	4.84253700	-2.01967600
H	5.94830200	2.55642500	-1.47355100
H	4.31476700	0.82466400	-0.68118700
O	1.58038700	1.47330400	-0.41303700
O	0.88564200	3.59823900	-0.92280600
B	0.48536000	2.33589000	-0.48849200
C	-2.34386100	-3.15544100	-1.52311500
C	-2.54701500	-2.14983500	-0.57779100
C	-3.81116700	-1.69066800	-0.25071200
C	-4.88546500	-2.29400200	-0.92201000
C	-4.68314400	-3.30399000	-1.86964000

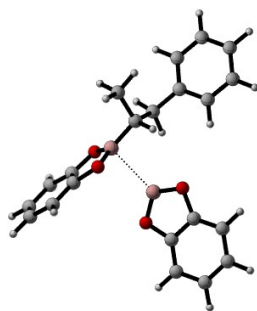
C	-3.39530000	-3.75788400	-2.19148200
H	-3.95762400	-0.90585800	0.48424900
H	-5.89662100	-1.96606800	-0.69925100
H	-5.53988100	-3.74734900	-2.36875500
H	-3.22521900	-4.53911800	-2.92484500
O	-0.98943800	-3.39850800	-1.63852800
O	-1.32133000	-1.74594800	-0.08458400
B	-0.37106500	-2.52433300	-0.74855300



P

C	3.13536400	0.61394600	-0.19794900
C	2.87399100	-0.72120600	0.11116400
C	3.88814500	-1.63012500	0.35721100
C	5.20038000	-1.14006400	0.27921000
C	5.46256700	0.19929500	-0.03099300
C	4.42467000	1.11042100	-0.27729700
H	3.67289400	-2.66604600	0.59712600
H	6.02924800	-1.81703300	0.46417600
H	6.49136300	0.54347800	-0.08239000
H	4.61579900	2.15083100	-0.51815900
O	1.93802100	1.27368700	-0.38755500
O	1.50829400	-0.92035500	0.11954300
B	0.94488500	0.31582300	-0.19463800
C	-3.43185300	-1.02568500	-0.79788700
C	-2.91591600	-0.33433800	0.30856900
C	-3.81262700	0.36421500	1.12712700
C	-5.18141600	0.37815600	0.84959100
C	-5.67872100	-0.31131400	-0.25636900
C	-4.79735700	-1.01537700	-1.08036300
H	-2.75443900	-1.58417300	-1.44131700
H	-3.43441600	0.89999000	1.99511800
H	-5.85810900	0.92613700	1.50043200
H	-6.74363400	-0.30458700	-0.47315900
H	-5.17509200	-1.56213200	-1.94073600
C	-1.42737400	-0.34263600	0.59293600
C	-0.59647900	0.57971900	-0.34561200
H	-1.04751900	-1.36765600	0.50460100
H	-1.25408200	-0.03914300	1.63390000
C	-0.95364700	2.06999200	-0.18984200
H	-0.37358800	2.69000700	-0.88103500
H	-2.01698500	2.24458100	-0.38411800

H	-0.73805800	2.42392700	0.82618200
H	-0.84667900	0.28606200	-1.38030700

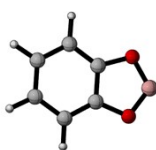


10a-TS

Imaginary frequency: -72.61

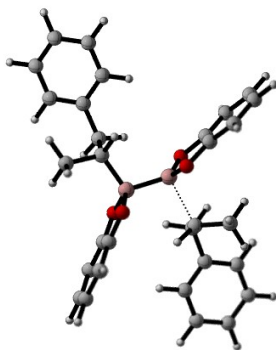
C	2.26301200	-2.13246500	0.73154500
C	1.91967200	-2.61682600	-0.53272600
C	2.82351400	-3.30653800	-1.32320600
C	4.10582700	-3.49823300	-0.78922200
C	4.44985400	-3.01223700	0.47798600
C	3.52688900	-2.31208800	1.26789700
H	2.54614800	-3.67734500	-2.30431000
H	4.84694600	-4.03588700	-1.37347900
H	5.45288800	-3.17996600	0.85935100
H	3.78211100	-1.92957200	2.25053800
O	1.17437900	-1.49447700	1.28221700
O	0.60901000	-2.29480300	-0.80079300
B	0.15397900	-1.58160600	0.31680600
C	2.15719700	2.59137900	-0.39430800
C	0.91350600	3.00474700	0.08083100
C	0.66594100	4.31240600	0.45697700
C	1.73878500	5.20783300	0.33628500
C	2.98795100	4.79291900	-0.14060400
C	3.22365200	3.46322700	-0.51950400
H	-0.30632600	4.62209300	0.82490800
H	1.59439900	6.24601600	0.62007100
H	3.79480200	5.51537500	-0.22007500
H	4.18670800	3.12978700	-0.89072900
O	2.10070900	1.23376800	-0.69294800
O	0.04917300	1.91345200	0.09146000
B	0.81294200	0.86747400	-0.38110000
C	-3.77413000	0.84783300	-0.06538400
C	-3.57624200	-0.48730100	-0.45049700
C	-4.70164000	-1.30820500	-0.59651300
C	-5.98777400	-0.81552800	-0.36303600
C	-6.16931200	0.51322300	0.02070200
C	-5.05592400	1.34439900	0.16833900
H	-2.91109800	1.50148200	0.04537400

H	-4.56898700	-2.34393100	-0.90190400
H	-6.84686700	-1.47062200	-0.48459300
H	-7.16903400	0.90010200	0.20011400
H	-5.18762600	2.38313800	0.46137700
C	-2.17505700	-1.01142800	-0.69058900
C	-1.35898600	-1.24899400	0.60819300
H	-1.63273000	-0.29569600	-1.32266700
H	-2.22045700	-1.94774300	-1.26086000
C	-1.96206300	-2.38668500	1.46884600
H	-1.40737200	-2.51271800	2.40506100
H	-3.00674800	-2.17211000	1.72018600
H	-1.93817400	-3.34405200	0.93287600
H	-1.39739000	-0.32982800	1.20865800



10a

C	-0.32782900	-0.69712000	0.00007100
C	-0.32783200	0.69701800	0.00007600
C	0.84359500	1.43304800	0.00005100
C	2.03943800	0.70008600	-0.00004100
C	2.03948200	-0.69998000	-0.00000600
C	0.84371900	-1.43302600	0.00004600
H	0.83087600	2.51767900	-0.00000700
H	2.98551800	1.23326100	-0.00025400
H	2.98559200	-1.23310000	-0.00022800
H	0.83113800	-2.51767600	-0.00000200
O	-1.64241800	-1.14942100	0.00000600
O	-1.64251300	1.14942400	0.00002000
B	-2.40342000	-0.00007000	-0.00017900



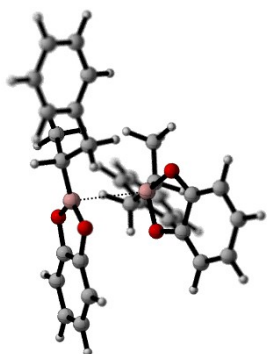
ts-1

Imaginary frequency: -209.51

C	-4.77688600	0.20036500	-0.78334800
C	-4.05581700	-0.93979100	-1.17088200
C	-4.77000100	-2.02153900	-1.70360700
C	-6.15885100	-1.97143800	-1.84226200

C	-6.86142200	-0.83207400	-1.44870900
C	-6.16360400	0.25612500	-0.91902100
H	-4.24063600	1.05597300	-0.37761500
H	-4.22935100	-2.91107400	-2.02002200
H	-6.69043300	-2.82237900	-2.26123400
H	-7.94206400	-0.78957400	-1.55730800
H	-6.70013600	1.15188800	-0.61593900
C	-2.54995000	-0.98830500	-1.00260800
C	-2.09780100	-1.24758600	0.45845000
H	-2.12216500	-0.04226200	-1.35186700
H	-2.13313400	-1.77413300	-1.64460100
C	-2.47050500	-2.66122400	0.93349400
H	-2.23526100	-2.80216600	1.99303700
H	-3.54343900	-2.84621600	0.80044400
H	-1.93568500	-3.43293500	0.36347800
H	-2.60363400	-0.52301300	1.11157300
C	4.49280200	-0.45010100	-1.19464900
C	3.82173900	0.77754500	-1.29407500
C	4.56814100	1.91842900	-1.61870600
C	5.94393500	1.83745300	-1.84165800
C	6.59884700	0.60922900	-1.74107200
C	5.86717400	-0.53550800	-1.41728400
H	3.93132100	-1.34787000	-0.94451300
H	4.06336800	2.87793700	-1.70728700
H	6.50240100	2.73401100	-2.09873800
H	7.66934100	0.54341500	-1.91652500
H	6.36756800	-1.49773000	-1.34126300
C	2.32436600	0.87123600	-1.02731000
C	2.02541800	0.89640300	0.46089300
H	1.81236600	0.02218500	-1.49117800
H	1.92615000	1.77868300	-1.49405900
C	2.41731800	2.12316700	1.23616100
H	2.11730400	2.05215300	2.28470300
H	3.51044700	2.25799200	1.20510200
H	1.97436500	3.03252800	0.81125000
H	2.22986800	-0.04307200	0.97769200
C	-0.87339500	2.72421500	1.47322000
C	-0.93332200	2.81650600	0.07626700
C	-1.33075100	3.98082200	-0.56423500
C	-1.67747800	5.06525700	0.25396300
C	-1.61712400	4.97398600	1.65052900
C	-1.20763400	3.79515700	2.28904400
H	-1.37413900	4.03966100	-1.64692800
H	-2.00076800	5.99428700	-0.20672200

H	-1.89366000	5.83415900	2.25351000
H	-1.15666200	3.71394600	3.36989300
O	-0.45433900	1.47489600	1.83050600
O	-0.55538000	1.62282400	-0.47470800
B	-0.19549700	0.77439900	0.61586400
C	1.06854800	-2.62397300	0.19729700
C	0.92782500	-2.49544300	1.61188400
C	1.64303800	-3.32035600	2.49064200
C	2.48712400	-4.26583500	1.92237100
C	2.62498700	-4.39497700	0.51794700
C	1.92404200	-3.58106600	-0.36448400
H	1.52853300	-3.21448600	3.56395300
H	3.05767800	-4.92706900	2.56778200
H	3.29625900	-5.15260200	0.12449600
H	2.01776700	-3.67651700	-1.44102000
O	0.30425600	-1.74209300	-0.42388100
O	0.06974600	-1.53635800	1.90542900
B	-0.45698500	-0.96239000	0.61646300



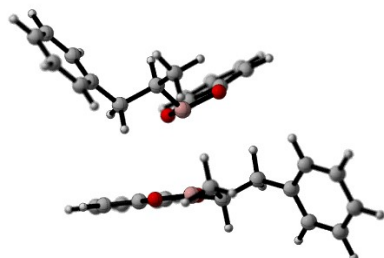
ts-2

Imaginary frequency: -26.39

C	5.03891800	-1.23174700	-0.68943800
C	3.96982500	-1.78892800	0.02925100
C	4.14442200	-3.06364500	0.58491900
C	5.34341400	-3.76221000	0.42674300
C	6.39539800	-3.19503400	-0.29309400
C	6.23853700	-1.92378800	-0.85110300
H	4.92806600	-0.23900700	-1.12166800
H	3.33152600	-3.51070400	1.15291600
H	5.45523300	-4.74897300	0.86941400
H	7.33041200	-3.73555800	-0.41553500
H	7.05431100	-1.46926500	-1.40813200
C	2.66829900	-1.02939900	0.18675900
C	1.77617600	-1.02406600	-1.08810100
H	2.89095400	0.00878000	0.46418300
H	2.08960600	-1.45116900	1.01724700
C	1.30836800	-2.43641500	-1.48067300

H	0.69208400	-2.41308900	-2.38625100
H	2.16001100	-3.10007100	-1.66919600
H	0.70688400	-2.88932300	-0.68294500
H	2.40281700	-0.64262200	-1.91778500
C	-5.50494400	-0.74705600	0.83735600
C	-4.40780900	-1.16316400	0.06794300
C	-4.56578300	-2.29166400	-0.74750500
C	-5.77640300	-2.98680600	-0.79126600
C	-6.85690600	-2.56175500	-0.01777400
C	-6.71661700	-1.43646000	0.79797500
H	-5.40695300	0.13258700	1.47096500
H	-3.72959000	-2.62689200	-1.35728400
H	-5.87464100	-3.85955900	-1.43222400
H	-7.80097200	-3.09929400	-0.05186400
H	-7.55385800	-1.09268100	1.40051400
C	-3.09293800	-0.41258100	0.13168900
C	-2.24358200	-0.72070100	1.39483100
H	-3.29441000	0.66574900	0.10118100
H	-2.49471600	-0.64235100	-0.75781000
C	-1.77337100	-2.18269800	1.46325000
H	-1.19588200	-2.36807000	2.37525200
H	-2.62136300	-2.87621500	1.45031500
H	-1.12885900	-2.42200200	0.60944800
H	-2.90406200	-0.55130800	2.26622000
C	-0.18086100	2.31323700	1.99371000
C	0.57229400	1.35048700	2.67108000
C	1.68952500	1.68777000	3.41553300
C	2.02840400	3.04915700	3.46518500
C	1.27121600	4.01341500	2.79182400
C	0.14288000	3.65846400	2.03562500
H	2.26879300	0.93177400	3.93529400
H	2.89608500	3.35746800	4.04137200
H	1.55814800	5.05925800	2.85687800
H	-0.45567200	4.39817000	1.51344300
O	-1.21952300	1.69651800	1.33800000
O	0.01629100	0.11073900	2.46224100
B	-1.08471900	0.32330300	1.61647300
C	-0.28886900	1.27958100	-2.62994000
C	0.56687700	2.12122100	-1.81099800
C	0.79684400	3.46866400	-2.14938300
C	0.15288700	3.94973700	-3.27531700
C	-0.68654200	3.12076300	-4.08262700
C	-0.90738700	1.78640700	-3.78716400
H	1.43703800	4.08621000	-1.52985800

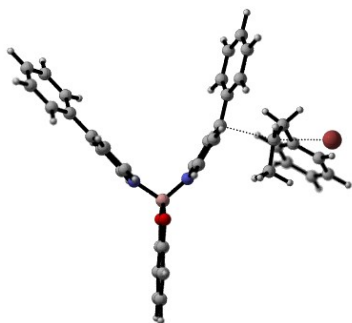
H	0.28222900	4.98904200	-3.56225000
H	-1.16412800	3.56071800	-4.95299600
H	-1.54007800	1.15062500	-4.39604800
O	-0.37133000	0.07797100	-2.13427600
O	1.03683000	1.45969100	-0.79665200
B	0.55856300	-0.00455800	-0.90308300



11A

C	-5.02400900	-1.36919700	0.56464500
C	-3.90534000	-1.90621400	-0.09101900
C	-4.01167800	-3.19954000	-0.62053300
C	-5.19222700	-3.93550000	-0.49762100
C	-6.29430200	-3.38777100	0.15971200
C	-6.20571900	-2.09853800	0.69071200
H	-4.96641300	-0.36292000	0.97528400
H	-3.15905600	-3.63157900	-1.13981700
H	-5.25052000	-4.93607300	-0.91904900
H	-7.21523900	-3.95724500	0.25450600
H	-7.06080400	-1.65914400	1.19879500
C	-2.62371300	-1.10689300	-0.20872700
C	-1.77989900	-1.05936500	1.09797200
H	-2.86833400	-0.07905100	-0.50530700
H	-2.00197700	-1.51797400	-1.01333000
C	-1.28379900	-2.45135900	1.52750300
H	-0.71004500	-2.39688400	2.45931200
H	-2.11953600	-3.14265000	1.68583600
H	-0.63035200	-2.89071700	0.76330700
H	-2.44665900	-0.68450200	1.89882800
C	5.56428600	-0.78782300	-0.74884200
C	4.42327600	-1.16449400	-0.02423900
C	4.51178300	-2.29026700	0.80530200
C	5.69794500	-3.02077600	0.90588000
C	6.82282600	-2.63482500	0.17641400
C	6.75174600	-1.51276800	-0.65264400
H	5.52034700	0.08899800	-1.39239300
H	3.64050300	-2.59505000	1.38087100
H	5.74232100	-3.89056500	1.55677400
H	7.74786100	-3.20008000	0.25499900
H	7.62401300	-1.19923400	-1.22101100

C	3.13589900	-0.37495800	-0.14975500
C	2.33619300	-0.66148600	-1.45092200
H	3.36780700	0.69686400	-0.11155500
H	2.48969000	-0.58379700	0.71125000
C	1.83259900	-2.11185300	-1.54211000
H	1.29732600	-2.28455000	-2.48190200
H	2.66119700	-2.82608200	-1.48561100
H	1.13896200	-2.33139700	-0.72180500
H	3.03655300	-0.50484700	-2.29238800
C	0.26372600	2.38734100	-1.98317600
C	-0.49206800	1.43788900	-2.67461200
C	-1.63080900	1.78336300	-3.38125000
C	-1.98916700	3.14060600	-3.37565400
C	-1.22898000	4.09238700	-2.68795500
C	-0.07756300	3.72862000	-1.97156800
H	-2.21204500	1.03715300	-3.91275000
H	-2.87449800	3.45590600	-3.92032300
H	-1.53118400	5.13569600	-2.71123100
H	0.52397600	4.45852900	-1.43922800
O	1.32596500	1.76112700	-1.37278100
O	0.08652400	0.19922700	-2.51881300
B	1.20409600	0.40202000	-1.69976500
C	0.13801200	1.34025600	2.66573300
C	-0.69262600	2.13412700	1.77555000
C	-0.97948000	3.48291100	2.06153000
C	-0.41657600	4.01289100	3.20874000
C	0.39641700	3.23105000	4.08702200
C	0.67195200	1.89664300	3.84282500
H	-1.59852900	4.06415200	1.38778100
H	-0.59132500	5.05535400	3.45778900
H	0.80881300	3.70812800	4.97107800
H	1.28493300	1.29634900	4.50553800
O	0.28553100	0.12994000	2.20972800
O	-1.08400100	1.43291300	0.75470400
B	-0.57853200	-0.01705600	0.93367600

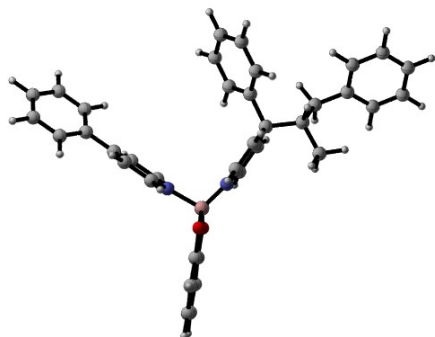


1F-TS

Imaginary frequency: -244.28

C	1.90046700	4.33099400	-0.46315800
C	2.01732100	4.29253100	0.93774200
C	2.15148800	5.45313500	1.68007300
C	2.16800000	6.67679700	0.98395200
C	2.05241100	6.71475800	-0.40450600
C	1.91566500	5.53055100	-1.15358300
H	2.23648900	5.41097400	2.76185200
H	2.27010400	7.60364500	1.54281800
H	2.06519600	7.67097100	-0.92156100
H	1.82118500	5.54739000	-2.23530500
O	1.77714900	3.07128100	-0.97084300
O	1.97396400	3.00669500	1.38952400
B	1.85696700	2.17214400	0.18731200
C	0.37908400	0.53594800	1.44100700
C	-0.34551100	-0.61385600	1.48698100
C	-0.88651500	-1.23469300	0.29756800
C	-0.55742100	-0.51853800	-0.91146600
C	0.15901200	0.63909600	-0.90210200
H	-0.52544900	-1.05380500	2.46215500
H	-0.94559200	-0.85769800	-1.86673700
H	0.34753800	1.20835900	-1.80509500
N	0.68128700	1.19258900	0.25623700
C	-1.24749100	-2.65837500	0.27907100
C	-1.22576600	-3.41340700	-0.91681600
C	-1.64081600	-3.34682600	1.45288100
C	-1.58653900	-4.76077400	-0.93932200
H	-0.88286700	-2.95159400	-1.83715200
C	-1.99660600	-4.68898300	1.42700700
H	-1.69702700	-2.81384300	2.39715800
C	-1.97533200	-5.41402800	0.22924300
H	-1.55096600	-5.30387900	-1.88165800
H	-2.30464000	-5.17364100	2.35064100
H	-2.25795200	-6.46336400	0.21197400
C	3.73557000	0.70895800	1.16506400
C	4.65738200	-0.30715700	1.08968800
C	5.05817800	-0.84949900	-0.15903900
C	4.44580900	-0.25588900	-1.29422100
C	3.53549400	0.76463900	-1.16439400
H	3.42723600	1.14285300	2.10807400
H	5.05790400	-0.70149600	2.01745300
H	4.72610300	-0.56509200	-2.29564500
N	3.15774400	1.26056100	0.05404100
C	6.03982100	-1.92944300	-0.27117000
C	6.98855200	-2.17650300	0.74836000

C	6.08282600	-2.77196000	-1.40648200
C	7.92183300	-3.20160800	0.63729400
H	7.01348000	-1.53466000	1.62405900
C	7.01879500	-3.79522700	-1.51473700
H	5.34812800	-2.64439800	-2.19585100
C	7.94816300	-4.02154400	-0.49515200
H	8.64154900	-3.35664500	1.43791100
H	7.01444200	-4.43043900	-2.39754700
H	8.67705500	-4.82303200	-0.57991700
H	3.09015700	1.25747900	-2.01978000
H	0.75134300	1.01771200	2.33772700
C	-4.28084700	-0.23636100	-2.90321900
C	-4.75916900	-0.34917800	-1.59160600
C	-5.92513100	0.35298200	-1.24263700
C	-6.58290000	1.14270400	-2.18545000
C	-6.09503000	1.24890600	-3.49124000
C	-4.93915900	0.55481600	-3.84828400
H	-3.38266300	-0.78035900	-3.19045800
H	-6.29492300	0.27074800	-0.22142500
H	-7.48455000	1.67908700	-1.89739300
H	-6.61159600	1.86689000	-4.22269000
H	-4.54781400	0.62666400	-4.86106400
C	-4.05469600	-1.23600100	-0.57910300
C	-3.35552300	-0.54307000	0.56403700
H	-3.33714800	-1.87884500	-1.11490300
H	-4.78194000	-1.91890200	-0.12611800
C	-3.10344200	0.92170300	0.58084600
H	-2.48371300	1.20359300	1.43506300
H	-2.60778400	1.24778700	-0.34521600
H	-4.04883300	1.46999400	0.65692600
Br	-5.69630100	-0.47979500	2.33601600
H	-3.24673500	-1.10979000	1.47441300

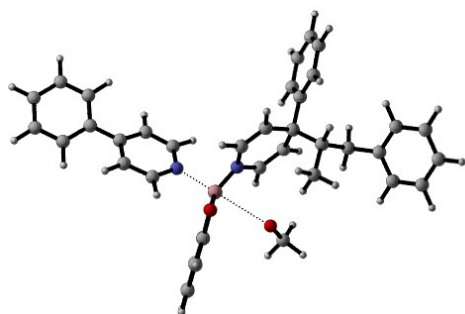


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C	-2.57107800	4.01865200	-0.71640500
C	-2.49222600	4.02543800	0.68453900
C	-3.03150100	5.05636000	1.43332500

C	-3.66404300	6.10158200	0.73596100
C	-3.74206100	6.09501000	-0.65651000
C	-3.19088000	5.04278600	-1.41015500
H	-2.96137200	5.05308200	2.51668500
H	-4.09619700	6.92645800	1.29567200
H	-4.23423800	6.91488200	-1.17229800
H	-3.24167600	5.02940300	-2.49454500
O	-1.96017400	2.90127900	-1.22550300
O	-1.82724900	2.91319400	1.13276600
B	-1.54147900	2.13568900	-0.06218500
C	-2.86951900	0.20651500	1.18027200
C	-3.62988800	-0.94703200	1.26434000
C	-4.15743200	-1.53200400	0.09927300
C	-3.87614500	-0.88223100	-1.11466700
C	-3.10882500	0.27099800	-1.12542900
H	-3.83813100	-1.37164000	2.24016100
H	-4.23577800	-1.28458000	-2.05525400
H	-2.87849700	0.81004800	-2.03684600
N	-2.60519100	0.80361400	0.00303400
C	-4.97386900	-2.76521300	0.15101800
C	-6.04558100	-2.95450800	-0.73824900
C	-4.69385300	-3.77192400	1.09081900
C	-6.81607400	-4.11400900	-0.68602800
H	-6.29659600	-2.17613000	-1.45314400
C	-5.46102400	-4.93397200	1.13700100
H	-3.85074400	-3.65872800	1.76626000
C	-6.52554100	-5.10811900	0.25041800
H	-7.64815800	-4.23819200	-1.37328800
H	-5.22239700	-5.70721800	1.86173400
H	-7.12490600	-6.01332400	0.28884700
C	0.55857600	1.23636000	1.01169300
C	1.68224800	0.49653200	1.01071100
C	2.30413700	-0.10563200	-0.23886000
C	1.53088100	0.43457200	-1.43607900
C	0.40664900	1.16341700	-1.34194900
H	0.16248000	1.66315600	1.92800300
H	2.18342300	0.33842600	1.96140300
H	1.91441700	0.20460700	-2.42694300
N	-0.15718500	1.56710500	-0.13313100
C	2.19290700	-1.65593600	-0.26032200
C	1.50829200	-2.36126000	0.73726300
C	2.74409500	-2.40002700	-1.31835900
C	1.39469900	-3.75317500	0.69700900
H	1.05016200	-1.80835800	1.55171600

C	2.62768800	-3.78883300	-1.36771400
H	3.26712800	-1.89197500	-2.12414900
C	1.95497500	-4.47607000	-0.35501000
H	0.86338400	-4.27163900	1.49209600
H	3.06394900	-4.33532700	-2.20053400
H	1.86664400	-5.55887500	-0.38977900
C	7.01271300	0.73818600	1.11343300
C	6.17332700	-0.22956400	0.54598600
C	6.75092100	-1.19359000	-0.29466800
C	8.11913700	-1.18734300	-0.56392300
C	8.94227100	-0.21294700	0.00577300
C	8.38368600	0.74983100	0.84681300
H	6.58681200	1.48919900	1.77530100
H	6.11706300	-1.96084000	-0.73491300
H	8.54499000	-1.94713900	-1.21481200
H	10.00928700	-0.20770300	-0.20118600
H	9.01466200	1.51055100	1.29990500
C	4.68292300	-0.24804300	0.81774600
C	3.82773600	0.31055300	-0.35221400
H	4.47495700	0.33302100	1.72478400
H	4.37551000	-1.27946100	1.02584100
C	4.00299300	1.82833500	-0.48538000
H	3.45151800	2.21784200	-1.34645000
H	3.62762900	2.34624700	0.40530900
H	5.06069000	2.08365500	-0.61012400
H	4.20819400	-0.14654000	-1.27575600
H	-2.46624800	0.70222000	2.05551300
H	-0.11245600	1.52345800	-2.22452400



2F-TS

Imaginary frequency: -188.16

C	-1.67268600	-3.46803300	0.56706100
C	-1.82554000	-3.36762200	-0.82530200
C	-2.28973500	-4.42951000	-1.57912600
C	-2.60264200	-5.62123200	-0.89762000
C	-2.45414500	-5.72010300	0.48536900
C	-1.98672800	-4.63137700	1.24609200
H	-2.39834900	-4.34047300	-2.65570700

H	-2.96130300	-6.47779000	-1.46381400
H	-2.69807400	-6.65320900	0.98833300
H	-1.85866400	-4.69868400	2.32252600
O	-1.24861700	-2.27654100	1.08052900
O	-1.50488200	-2.10973900	-1.24274700
B	-1.12831100	-1.41265900	-0.05746800
C	-2.97876800	0.74136600	-0.57802000
C	-4.17683300	1.43798600	-0.58705700
C	-5.22880900	1.04479100	0.26572200
C	-4.97308900	-0.06286600	1.09872300
C	-3.74306600	-0.70240600	1.04803400
H	-4.30247000	2.26634100	-1.27685700
H	-5.71857500	-0.40510900	1.80937900
H	-3.50836800	-1.55002400	1.68362900
N	-2.75564800	-0.31341300	0.22428800
C	-6.52339400	1.75368500	0.28640100
C	-7.71968400	1.07551300	0.59578800
C	-6.60558800	3.13111900	-0.00082800
C	-8.94070900	1.74418300	0.61658900
H	-7.69287400	0.00716700	0.78984500
C	-7.82718400	3.79864700	0.02175600
H	-5.69732200	3.68771100	-0.21298600
C	-9.00411000	3.11068200	0.33032100
H	-9.84914600	1.19335900	0.84807900
H	-7.85943300	4.86384600	-0.19394900
H	-9.95742000	3.63223900	0.34684900
C	0.79799600	-0.33428800	-1.20165900
C	1.90259000	0.43024200	-1.21125100
C	2.42398800	1.17804200	0.00315300
C	1.30505800	1.20547400	1.03603400
C	0.18798600	0.46468700	0.93796500
H	0.53086100	-0.96458000	-2.03752700
H	2.53267700	0.38958600	-2.09498800
H	1.43750200	1.83433200	1.91332900
N	-0.11408000	-0.35074400	-0.14532600
C	2.78198100	2.65028800	-0.33388000
C	2.38243300	3.23688500	-1.54336200
C	3.45539800	3.47479400	0.58535800
C	2.66073000	4.57343500	-1.83681300
H	1.83142200	2.62855800	-2.25456600
C	3.73168000	4.81304200	0.30167400
H	3.76465300	3.07166300	1.54557600
C	3.34080500	5.37147100	-0.91674600
H	2.33954300	4.99207500	-2.78876100

H	4.25427900	5.42113100	1.03762200
H	3.55834000	6.41331500	-1.14159900
C	6.70953900	-1.29802300	0.07996200
C	6.18038800	0.00072700	0.06779000
C	6.96736100	1.03487300	0.59981200
C	8.23320300	0.78241000	1.12851400
C	8.74421700	-0.51781700	1.13598100
C	7.97570600	-1.55697200	0.60909400
H	6.11702600	-2.11252300	-0.32945600
H	6.57651000	2.05069000	0.59278800
H	8.82406800	1.60247100	1.53161200
H	9.73159900	-0.71762600	1.54621800
H	8.36171200	-2.57400200	0.60751800
C	4.80595000	0.29232200	-0.49363400
C	3.69583300	0.42494000	0.58766400
H	4.51788200	-0.50279600	-1.18987400
H	4.85741200	1.22408300	-1.07200000
C	3.33667400	-0.94415500	1.18557000
H	2.70839100	-0.82234100	2.07394800
H	2.78174600	-1.58813100	0.48506400
H	4.24963200	-1.46641000	1.49910400
H	4.10655900	1.04715800	1.39647900
H	-2.14978400	1.01532200	-1.22398000
H	-0.56469800	0.47905100	1.72120900
O	1.22363000	-2.98823800	-0.55899400
C	1.68674800	-3.58799200	-1.66819400
H	2.08989400	-2.89215600	-2.46842600
H	2.55312300	-4.29292900	-1.49103000
H	0.93893000	-4.22802300	-2.22090200

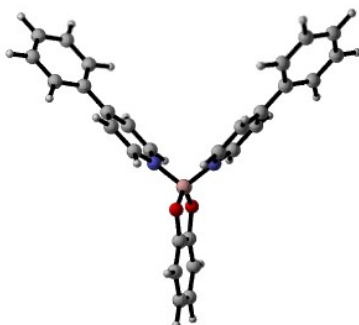


³INT-AB-HV*

C	-0.00151300	-3.55565900	-0.70288500
C	-0.03415000	-3.55946400	0.70537400
C	-0.06700700	-4.74657800	1.41889200
C	-0.06265400	-5.95267900	0.69085600
C	-0.02569300	-5.94900400	-0.70217900
C	0.00567700	-4.73911300	-1.42321600

H	-0.09525000	-4.73681200	2.50483100
H	-0.08781800	-6.89773800	1.22856300
H	-0.02197100	-6.89123500	-1.24539900
H	0.03464900	-4.72375300	-2.50906900
O	0.01875900	-2.28534000	-1.17754100
O	-0.02209800	-2.29181000	1.18760100
B	-0.00139200	-1.38564300	0.00753700
C	2.32290400	-0.74228600	0.92558500
C	3.48493400	-0.02819300	0.90485300
C	3.70931600	1.05020500	-0.02133600
C	2.59213100	1.28663600	-0.89616100
C	1.44642200	0.55108400	-0.82756200
H	2.15878700	-1.55943000	1.61612100
H	4.25795700	-0.32299800	1.60649000
H	2.62269700	2.08711100	-1.62762700
H	0.60378000	0.74766900	-1.48024300
N	1.26136700	-0.47874500	0.07923600
C	4.93156300	1.81685300	-0.06826800
C	5.20360100	2.75407200	-1.10863300
C	5.94860200	1.68807200	0.92369100
C	6.38018600	3.48885100	-1.14901300
H	4.48394300	2.88921800	-1.91016400
C	7.12252000	2.42677100	0.87523200
H	5.80066000	1.00973000	1.75832200
C	7.36197500	3.34055300	-0.15987700
H	6.53920800	4.18676700	-1.96971800
H	7.86364700	2.29319400	1.66195400
H	8.28248700	3.91752200	-0.19472500
C	-1.48600800	0.48681900	0.91063600
C	-2.62166400	1.23892600	0.96567000
C	-3.69681300	1.07393300	0.02442000
C	-3.44158800	0.05088700	-0.95505600
C	-2.28440100	-0.67136500	-0.97079200
H	-0.68521500	0.60998600	1.63067900
H	-2.70090900	1.95846800	1.77372800
H	-4.16450300	-0.15705300	-1.73675200
H	-2.08695100	-1.43270300	-1.71444800
N	-1.26598200	-0.48063800	-0.05525500
C	-4.91111900	1.85374300	0.06181500
C	-5.05735300	2.99384100	0.90627500
C	-6.04455700	1.53491600	-0.74314500
C	-6.22720200	3.73966800	0.93982700
H	-4.22522100	3.31007000	1.52771900
C	-7.21060600	2.28660500	-0.70332800

H	-6.01282400	0.66471200	-1.39154600
C	-7.32554900	3.40187200	0.13742500
H	-6.28344200	4.60524100	1.59827600
H	-8.04921400	1.99496500	-1.33394400
H	-8.24024100	3.98837500	0.16630900



1E

C	0.00567900	-4.05241700	-0.70135400
C	-0.00584000	-4.05241900	0.70134600
C	-0.01188000	-5.23202400	1.42379200
C	-0.00592200	-6.43675000	0.69717300
C	0.00563100	-6.43674900	-0.69718700
C	0.01165500	-5.23202100	-1.42380300
H	-0.02080700	-5.21979300	2.50926700
H	-0.01040600	-7.38020800	1.23592500
H	0.01006400	-7.38020600	-1.23594100
H	0.02058300	-5.21978800	-2.50927800
O	0.00959800	-2.76771600	-1.18226500
O	-0.00968600	-2.76771800	1.18226000
B	-0.00002400	-1.91652600	-0.00000100
C	1.74744300	-0.46808200	1.18897100
C	2.68904100	0.53063500	1.22500100
C	3.20922900	1.09791900	0.03197500
C	2.69832500	0.54654000	-1.17222800
C	1.75213400	-0.44836500	-1.15597100
H	3.06545000	0.84400000	2.19264400
H	3.03447400	0.91629600	-2.13464400
H	1.36334200	-0.89470900	-2.06283400
N	1.25206200	-0.96208400	0.01113800
C	4.21517800	2.16551000	0.04516100
C	5.09831900	2.35625300	-1.03957100
C	4.33636700	3.04142900	1.14568700
C	6.05208800	3.36926100	-1.02264600
H	5.06017200	1.68153000	-1.88963000
C	5.29145100	4.05337600	1.15993800
H	3.65192500	2.94914700	1.98377100
C	6.15675000	4.22583700	0.07651500

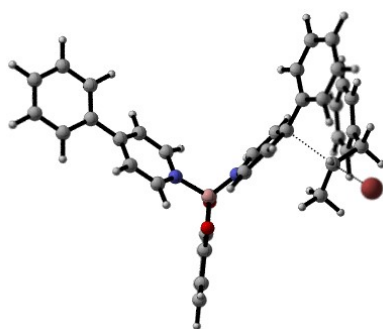
H	6.72499200	3.48439800	-1.86846300
H	5.35393200	4.71797600	2.01777500
H	6.90191400	5.01621200	0.08841600
C	-1.75215600	-0.44832300	1.15596900
C	-2.69831500	0.54661300	1.17222900
C	-3.20917700	1.09803300	-0.03197300
C	-2.68898400	0.53076000	-1.22500100
C	-1.74741700	-0.46798800	-1.18897200
H	-1.36339300	-0.89469700	2.06283000
H	-3.03447200	0.91636200	2.13464500
H	-3.06536200	0.84416000	-2.19264400
N	-1.25208000	-0.96203500	-0.01114000
C	-4.21509400	2.16565400	-0.04515700
C	-5.09826500	2.35638600	1.03955300
C	-4.33622100	3.04161400	-1.14565700
C	-6.05200400	3.36942200	1.02263100
H	-5.06016400	1.68163200	1.88959000
C	-5.29127400	4.05358900	-1.15990500
H	-3.65175400	2.94934000	-1.98372100
C	-6.15660400	4.22603800	-0.07650500
H	-6.72493300	3.48455000	1.86842900
H	-5.35370800	4.71822000	-2.01772100
H	-6.90174500	5.01643500	-0.08840400
H	-1.37308700	-0.94709800	-2.08518600
H	1.37312100	-0.94720300	2.08518200

³¹E*

C	0.07049200	3.36533800	-0.71801800
C	-0.07049200	3.36533600	0.71801900
C	-0.16007300	4.56751200	1.43778700
C	-0.07997300	5.74200700	0.70893700
C	0.07998200	5.74201000	-0.70892700
C	0.16007700	4.56751800	-1.43778200
H	-0.27635100	4.55701400	2.51576700
H	-0.13623800	6.69556500	1.22507500
H	0.13625000	6.69556900	-1.22506100
H	0.27635600	4.55702300	-2.51576100

O	0.08784500	2.14321100	-1.18568400
O	-0.08785000	2.14320600	1.18567900
B	-0.00000200	1.15604500	-0.00000400
C	-1.50227100	-0.68642700	0.79006100
C	-2.68530400	-1.35341000	0.84733000
C	-3.78898500	-1.04006300	-0.01835100
C	-3.51028600	0.01823200	-0.95142500
C	-2.31188400	0.66024200	-0.99207000
H	-2.78202900	-2.12345700	1.60460700
H	-4.24999300	0.30512800	-1.69080900
H	-2.09927600	1.43102100	-1.72096600
N	-1.25682900	0.33951200	-0.13216500
C	-5.06201100	-1.72820400	0.03941000
C	-6.22273300	-1.21174300	-0.59825400
C	-5.21986900	-2.95562500	0.73870300
C	-7.44264800	-1.87239200	-0.53821700
H	-6.17112900	-0.26239700	-1.12213100
C	-6.44315600	-3.61002400	0.79615200
H	-4.36166900	-3.41527800	1.21859000
C	-7.57083200	-3.07896200	0.15935200
H	-8.30770900	-1.43794400	-1.03400500
H	-6.51786000	-4.55102000	1.33623000
H	-8.52638800	-3.59353400	0.20492500
C	2.31186800	0.66022200	0.99208500
C	3.51027100	0.01821100	0.95144400
C	3.78898500	-1.04005900	0.01834700
C	2.68531900	-1.35338100	-0.84736300
C	1.50228600	-0.68639800	-0.79009800
H	2.09924800	1.43098200	1.72099600
H	4.24996400	0.30508700	1.69085000
H	2.78205700	-2.12340700	-1.60466000
N	1.25682900	0.33951700	0.13215100
C	5.06201000	-1.72820200	-0.03940800
C	6.22272200	-1.21175800	0.59828900
C	5.21987900	-2.95560500	-0.73872900
C	7.44263700	-1.87240800	0.53825700
H	6.17111000	-0.26242600	1.12218900
C	6.44316500	-3.61000500	-0.79617300
H	4.36168600	-3.41524400	-1.21864300
C	7.57083100	-3.07896100	-0.15933900
H	8.30769000	-1.43797400	1.03407200
H	6.51787700	-4.55098800	-1.33627200
H	8.52638700	-3.59353300	-0.20490800
H	0.67848500	-0.91644100	-1.45442700

H	-0.67845700	-0.91649000	1.45436800
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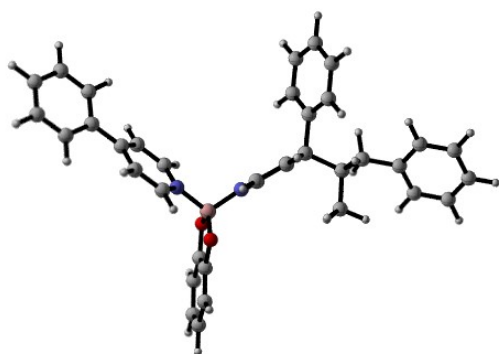


1E-TS

Imaginary frequency: -269.41

C	-1.94560200	3.80137800	0.89396300
C	-1.96042000	3.90126500	-0.50377800
C	-2.16616500	5.11026200	-1.14080900
C	-2.36453000	6.24054600	-0.32826400
C	-2.35202400	6.14075200	1.06255000
C	-2.13963600	4.90611300	1.70114400
H	-2.16763100	5.17649900	-2.22371600
H	-2.52718100	7.20644100	-0.79678900
H	-2.50584300	7.02951400	1.66703300
H	-2.12328700	4.81641300	2.78231100
O	-1.71366400	2.50115700	1.27889900
O	-1.74181900	2.66929200	-1.07449600
B	-1.64600200	1.75263900	0.04251000
C	-0.07284700	0.23973800	-1.22138900
C	0.92439100	-0.67900200	-1.30920400
C	1.70369600	-1.05105400	-0.15190900
C	1.23729800	-0.49199800	1.08557200
C	0.23596000	0.43431900	1.10892800
H	1.16327900	-1.10992200	-2.27488000
H	1.73741500	-0.74064500	2.01333400
H	-0.07764300	0.92997000	2.01893400
N	-0.43604600	0.81941700	-0.02674800
C	2.43767400	-2.34463400	-0.17031000
C	2.26336800	-3.25360900	0.88609800
C	3.27603700	-2.71606500	-1.23750300
C	2.91997600	-4.48235800	0.89381600
H	1.60051700	-2.99649800	1.70568700
C	3.93712700	-3.94162000	-1.22300900
H	3.47312700	-2.03500300	-2.06114900
C	3.76641900	-4.83010500	-0.15897100
H	2.76783300	-5.16757300	1.72342600
H	4.59971400	-4.19426800	-2.04547100
H	4.28682000	-5.78357700	-0.15253400

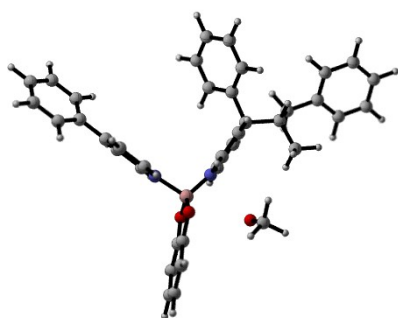
C	-3.60980100	0.55876500	-1.17996100
C	-4.65081300	-0.34648700	-1.27432800
C	-5.06340600	-1.07105000	-0.14305100
C	-4.37358900	-0.81836600	1.05819500
C	-3.33941300	0.09545300	1.08532900
H	-3.26482100	1.15333200	-2.01684700
H	-5.12699800	-0.50282400	-2.23508400
H	-4.66593000	-1.31249400	1.97718900
N	-2.95794900	0.76758900	-0.01962300
C	-6.16855600	-2.04434500	-0.20898700
C	-7.25258000	-1.83811100	-1.07842700
C	-6.15576200	-3.19652900	0.59452500
C	-8.29577900	-2.75755300	-1.13956700
H	-7.29479800	-0.93788500	-1.68385200
C	-7.19619000	-4.11880000	0.52577900
H	-5.31097800	-3.38811700	1.24907000
C	-8.26982400	-3.90140300	-0.33959100
H	-9.13269600	-2.57796100	-1.80753400
H	-7.16533500	-5.01146500	1.14309300
H	-9.08224800	-4.61998400	-0.39040500
H	-2.79531600	0.33640400	1.99022100
H	-0.63181200	0.56935700	-2.08878000
C	4.42410800	-1.33483200	2.37019200
C	4.41741900	-0.09548500	1.71967200
C	4.12172300	1.04862000	2.47357900
C	3.78566700	0.95035600	3.82340100
C	3.75708500	-0.29690100	4.45111100
C	4.09171500	-1.43860800	3.72169600
H	4.67625600	-2.22692100	1.80696500
H	4.15641900	2.02511100	2.00037700
H	3.55239400	1.84964400	4.38732500
H	3.49499100	-0.37466900	5.50279600
H	4.09546900	-2.41315200	4.20295500
C	4.69761200	-0.02058500	0.23164200
C	3.50995700	0.35189300	-0.62303600
H	5.10244300	-0.97059700	-0.12272100
H	5.47493900	0.73151100	0.03585200
C	2.92651000	1.71963000	-0.53962800
H	2.16673500	1.87363600	-1.30764900
H	2.48298900	1.91180600	0.44554000
H	3.71465600	2.46606000	-0.69845200
Br	5.00611800	0.47543900	-3.11439000
H	3.40340600	-0.16586600	-1.55859400



2E

C	1.56458100	-3.81526000	0.85212800
C	1.52607000	-3.87554900	-0.54676100
C	1.56855000	-5.08025400	-1.22636400
C	1.66532500	-6.24408100	-0.44800800
C	1.70889300	-6.18343000	0.94857300
C	1.65660600	-4.95616800	1.62856100
H	1.53183800	-5.11655800	-2.31004400
H	1.70748800	-7.20921800	-0.94315600
H	1.78327900	-7.10226900	1.52186100
H	1.68550000	-4.89942000	2.71159600
O	1.48046900	-2.50372100	1.27346300
O	1.43076300	-2.60503400	-1.07474400
B	1.43170500	-1.72163000	0.06548500
C	-0.25431000	-0.19625100	-1.11604100
C	-1.40337400	0.52452900	-1.20612300
C	-2.33795700	0.74702000	-0.05147600
C	-1.80414500	0.04364100	1.16025400
C	-0.65332400	-0.68187600	1.16325800
H	-1.65645400	0.97529900	-2.16036200
H	-2.37662600	0.09469900	2.08017200
H	-0.30546600	-1.22357900	2.03406200
N	0.14844100	-0.79733200	0.05242800
C	-2.43232500	2.28835800	0.16072700
C	-1.92882300	2.90238400	1.31470700
C	-2.99127600	3.10210000	-0.83780600
C	-2.01167100	4.28641000	1.48242400
H	-1.47065100	2.30460700	2.09668600
C	-3.06897100	4.48432500	-0.67258800
H	-3.37573500	2.66527600	-1.75518300
C	-2.58283200	5.08283000	0.49139100
H	-1.62737200	4.73842600	2.39249600
H	-3.51083500	5.09288000	-1.45637700
H	-2.64714700	6.15898400	0.62157000
C	3.43589500	-0.62830900	-1.15722400
C	4.55948300	0.17223600	-1.23387100

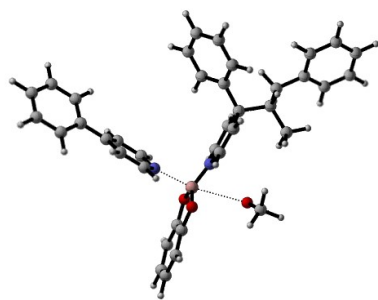
C	5.01161700	0.88176800	-0.10367300
C	4.25825700	0.72093600	1.07837100
C	3.14166300	-0.08952900	1.09068400
H	3.07224800	-1.20752900	-1.99740600
H	5.07509100	0.25596600	-2.18342400
H	4.56630000	1.19951900	2.00055200
N	2.72566800	-0.75157400	-0.01347400
C	6.21120700	1.73601600	-0.14950100
C	7.28183900	1.42331100	-1.00784100
C	6.30860400	2.87915700	0.66565000
C	8.41717100	2.22775800	-1.04457000
H	7.24498300	0.52673300	-1.61955300
C	7.43993600	3.68850000	0.61684300
H	5.48220800	3.15819800	1.31286900
C	8.49794300	3.36355400	-0.23545400
H	9.24194400	1.96481500	-1.69988500
H	7.49472600	4.57559200	1.24052400
H	9.38250500	3.99260000	-0.26828500
H	2.56396200	-0.25896100	1.99166600
H	0.39585600	-0.34706000	-1.96950600
C	-6.98107000	-0.90834300	0.50593700
C	-6.24583000	0.25659900	0.25007000
C	-6.86286400	1.29389800	-0.46535300
C	-8.17580800	1.16838200	-0.91718700
C	-8.89640700	-0.00020400	-0.65908400
C	-8.29626200	-1.03747100	0.05583000
H	-6.52465400	-1.71725900	1.07220400
H	-6.31178900	2.21239100	-0.65834700
H	-8.63994700	1.98492200	-1.46352500
H	-9.92071300	-0.09798200	-1.00717400
H	-8.85260600	-1.94603300	0.26902900
C	-4.81249000	0.40388500	0.72170100
C	-3.78698600	0.15336600	-0.41422100
H	-4.62597800	-0.30126300	1.54146400
H	-4.66861000	1.41216900	1.12579100
C	-3.72635500	-1.32788500	-0.80898600
H	-3.06987100	-1.49861600	-1.66829200
H	-3.37018100	-1.95178600	0.01924200
H	-4.72655400	-1.67668600	-1.08091900
H	-4.11724300	0.72355500	-1.29006200



3E

C	-2.50281000	3.89716900	-0.54473900
C	-2.42031000	3.84109200	0.85458800
C	-2.92508900	4.85587300	1.64737400
C	-3.52343700	5.95017500	0.99661000
C	-3.60448300	6.00609300	-0.39438400
C	-3.08954900	4.96865400	-1.19351900
H	-2.85258300	4.80475000	2.72925000
H	-3.92666700	6.76449500	1.59232000
H	-4.07062700	6.86277800	-0.87327200
H	-3.14654700	5.00084200	-2.27738600
O	-1.93409700	2.77902400	-1.10306100
O	-1.80317500	2.68492500	1.25275800
B	-1.52986400	1.96253600	0.02820300
C	-2.82395300	-0.04421700	1.17607900
C	-3.61543000	-1.17881600	1.21679600
C	-4.23709300	-1.64857700	0.04572700
C	-4.01522000	-0.90693200	-1.12665400
C	-3.21216400	0.22197200	-1.09451700
H	-3.77249100	-1.67933600	2.16584400
H	-4.44951000	-1.21856200	-2.07020200
H	-3.02484500	0.83174700	-1.97058900
N	-2.61784900	0.64241200	0.03653300
C	-5.08677200	-2.86027500	0.05088700
C	-6.22358900	-2.94406500	-0.77105000
C	-4.77216900	-3.95208700	0.87786900
C	-7.02377000	-4.08449800	-0.76232300
H	-6.50005900	-2.09997700	-1.39643900
C	-5.56927700	-5.09474100	0.87971700
H	-3.88058200	-3.91874400	1.49742000
C	-6.69845100	-5.16400800	0.06138100
H	-7.90574300	-4.12744100	-1.39511000
H	-5.30402200	-5.93429800	1.51599900
H	-7.32117000	-6.05413600	0.06523700
C	0.56432200	1.00553200	1.06863600
C	1.62855400	0.18509900	1.06008500
C	2.19772600	-0.46393200	-0.18983100

C	1.38948400	0.03995700	-1.37757700
C	0.31698300	0.84397100	-1.27363200
H	0.22100300	1.48714100	1.97765000
H	2.13580500	0.00891800	2.00390300
H	1.69795600	-0.28313900	-2.36856200
N	-0.15566500	1.35588000	-0.06964000
C	2.06702500	-2.01226900	-0.15440700
C	1.37539900	-2.66930700	0.87124600
C	2.60007600	-2.80359800	-1.18700500
C	1.24020400	-4.05965900	0.88342300
H	0.92900900	-2.07970500	1.66622300
C	2.46156400	-4.19138400	-1.18420500
H	3.12695100	-2.33482800	-2.01380000
C	1.78396900	-4.82982500	-0.14347400
H	0.70542100	-4.53971300	1.69995000
H	2.88480100	-4.77499200	-1.99827800
H	1.67920700	-5.91166800	-0.13724600
C	6.94056400	0.40486300	1.03525300
C	6.07244600	-0.57768300	0.54114000
C	6.61683700	-1.60520600	-0.24469000
C	7.98082900	-1.64611900	-0.53174600
C	8.83295400	-0.65651700	-0.03535700
C	8.30754600	0.36917900	0.75069400
H	6.54019800	1.20531400	1.65362400
H	5.96086300	-2.38459900	-0.62745500
H	8.38087800	-2.45449600	-1.13903000
H	9.89668200	-0.68814100	-0.25641300
H	8.96107800	1.14258600	1.14669400
C	4.58689600	-0.54348800	0.83609300
C	3.72278700	-0.06795800	-0.36377000
H	4.40567400	0.11581200	1.69356400
H	4.26231800	-1.54787600	1.13413100
C	3.90464900	1.43412800	-0.61807700
H	3.44817600	1.73100800	-1.56755700
H	3.43360700	2.03342600	0.16941400
H	4.96927900	1.68809300	-0.66278100
H	4.08869000	-0.59925500	-1.25237100
H	-2.34637300	0.36225400	2.05983000
H	-0.23154400	1.17164400	-2.15143800
O	0.97083700	3.88116900	0.06641700
C	1.15722100	4.26506800	-1.23682000
H	1.53814800	3.42832400	-1.85037800
H	0.26728500	4.70678800	-1.71417800
H	1.96831100	5.02133900	-1.24167200



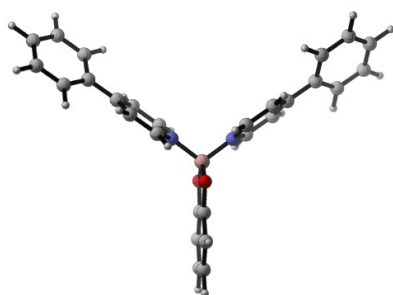
3E-TS

Imaginary frequency: -121.81

C	-2.63703600	-3.83470400	0.53521300
C	-2.55924900	-3.78237900	-0.86250300
C	-3.29828500	-4.63552400	-1.66190100
C	-4.13312700	-5.56022700	-1.01150300
C	-4.21067600	-5.61161600	0.38163800
C	-3.45557000	-4.74011800	1.18535600
H	-3.22747300	-4.58953300	-2.74388000
H	-4.72700500	-6.24734700	-1.60762300
H	-4.86427100	-6.33769800	0.85681400
H	-3.50565900	-4.77259600	2.26922800
O	-1.79950300	-2.89133300	1.08736100
O	-1.67595400	-2.80265000	-1.24764400
B	-1.27483900	-2.19958400	-0.03401200
C	-2.86235700	0.09618400	-1.16502100
C	-3.66132000	1.23187600	-1.21108800
C	-4.27221800	1.70140000	-0.03646400
C	-4.03239100	0.96872500	1.13716800
C	-3.21954100	-0.15781900	1.09170400
H	-3.82940500	1.73122400	-2.15970400
H	-4.45596400	1.28633600	2.08439100
H	-3.01710100	-0.74912000	1.98033000
N	-2.63872900	-0.58848300	-0.03556300
C	-5.13083600	2.90985000	-0.03695400
C	-6.27149900	2.98127500	0.78001500
C	-4.82150400	4.00956800	-0.85460300
C	-7.07956700	4.11665800	0.77658300
H	-6.54267600	2.13099100	1.39943600
C	-5.62700700	5.14678200	-0.85325900
H	-3.92810600	3.98444100	-1.47210200
C	-6.75956500	5.20384600	-0.03883300
H	-7.96389600	4.14932800	1.40701100
H	-5.36549500	5.99184000	-1.48411600
H	-7.38855800	6.08970400	-0.03938800
C	0.70129900	-1.11017700	-1.08711500
C	1.74595600	-0.26898900	-1.07269900

C	2.30441300	0.38298900	0.17985900
C	1.50470500	-0.13465400	1.36707300
C	0.44922000	-0.95811600	1.26731900
H	0.35785400	-1.58625500	-1.99831000
H	2.24013000	-0.06583500	-2.01785600
H	1.79747600	0.20773200	2.35609500
N	-0.00917700	-1.47961300	0.05702900
C	2.14590500	1.92832400	0.15017600
C	1.42262200	2.57396100	-0.86074900
C	2.68342100	2.72640000	1.17505000
C	1.26221400	3.96157400	-0.86676000
H	0.96974400	1.97956700	-1.64820400
C	2.52015300	4.11146000	1.17771400
H	3.23311600	2.26592500	1.99156100
C	1.81183800	4.73923500	0.15119300
H	0.70169100	4.43296900	-1.67070600
H	2.94753100	4.70091500	1.98527600
H	1.68692000	5.81887700	0.14963700
C	7.05919000	-0.39913700	-1.05425900
C	6.17708900	0.56409500	-0.54721900
C	6.70611600	1.58898800	0.25231300
C	8.06937100	1.64586600	0.54015500
C	8.93573900	0.67543900	0.03075100
C	8.42549200	-0.34730400	-0.76900000
H	6.67057800	-1.19681600	-1.68361700
H	6.03895300	2.35390600	0.64480500
H	8.45766100	2.45190700	1.15800400
H	9.99888400	0.71976500	0.25225800
H	9.09030400	-1.10556200	-1.17529400
C	4.69216800	0.51232400	-0.84340000
C	3.83498000	0.00916800	0.35014000
H	4.52091000	-0.13890600	-1.70912900
H	4.35307700	1.51530000	-1.12918000
C	4.04251700	-1.49223300	0.58707700
H	3.57245000	-1.81292300	1.52206700
H	3.60300000	-2.08868400	-0.22071800
H	5.11096700	-1.72465400	0.65013300
H	4.19108800	0.53512100	1.24559200
H	-2.38989700	-0.30103400	-2.05906300
H	-0.10536600	-1.28486200	2.14050900
O	0.99799300	-4.02545400	-0.02811900
C	1.26181800	-4.36929000	1.27325000
H	1.70375000	-3.51559600	1.82021900
H	0.39298200	-4.75644200	1.83036100

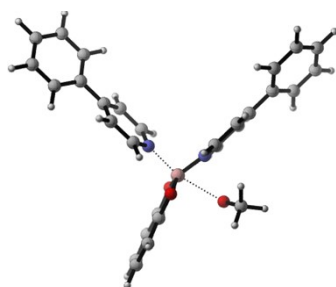
H	2.05417900	-5.14406300	1.26368500
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4E

C	-0.00254000	3.64027100	-0.69862800
C	0.00253900	3.64027100	0.69862700
C	0.00316200	4.81414900	1.42774000
C	0.00134500	6.01527300	0.69791100
C	-0.00134900	6.01527300	-0.69791300
C	-0.00316500	4.81414800	-1.42774100
H	0.00495700	4.80356100	2.51268700
H	0.00217400	6.95899200	1.23449300
H	-0.00218000	6.95899100	-1.23449500
H	-0.00495900	4.80356100	-2.51268800
O	-0.00632200	2.33772200	-1.17618000
O	0.00632200	2.33772200	1.17618000
B	0.00000000	1.51771000	0.00000000
C	-1.71312700	-0.02117800	1.15279900
C	-2.83779400	-0.81888100	1.20175600
C	-3.59651400	-1.05791500	0.03636400
C	-3.14058800	-0.43626200	-1.14328500
C	-2.00833600	0.35515200	-1.12800600
H	-3.14860300	-1.22414100	2.15757200
H	-3.66143100	-0.58046200	-2.08266500
H	-1.64447100	0.87190900	-2.00783200
N	-1.29176300	0.55191600	0.00180200
C	-4.80518500	-1.89987300	0.05623700
C	-5.87422400	-1.64091700	-0.82187800
C	-4.91328900	-2.97748100	0.95518900
C	-7.01824600	-2.43331400	-0.79648400
H	-5.82951100	-0.79315900	-1.49911900
C	-6.05339300	-3.77569800	0.96886900
H	-4.08875700	-3.21634200	1.62062500
C	-7.10963200	-3.50411300	0.09592400
H	-7.84160900	-2.21122300	-1.46845000
H	-6.11647200	-4.61263300	1.65767400
H	-8.00110100	-4.12398600	0.11188700
C	2.00833800	0.35515500	1.12800600
C	3.14059100	-0.43625800	1.14328400

C	3.59651500	-1.05791500	-0.03636300
C	2.83779300	-0.81888300	-1.20175500
C	1.71312600	-0.02118000	-1.15279800
H	1.64447500	0.87191500	2.00783000
H	3.66143500	-0.58045500	2.08266400
H	3.14860000	-1.22414600	-2.15757100
N	1.29176400	0.55191600	-0.00180200
C	4.80518600	-1.89987200	-0.05623700
C	5.87422600	-1.64091400	0.82187600
C	4.91328900	-2.97748200	-0.95518600
C	7.01824800	-2.43331000	0.79648200
H	5.82951400	-0.79315400	1.49911400
C	6.05339300	-3.77569900	-0.96886600
H	4.08875500	-3.21634500	-1.62062000
C	7.10963300	-3.50411100	-0.09592400
H	7.84161200	-2.21121700	1.46844600
H	6.11647000	-4.61263600	-1.65766900
H	8.00110200	-4.12398400	-0.11188600
H	1.13517200	0.21271000	-2.03887400
H	-1.13517600	0.21271400	2.03887600

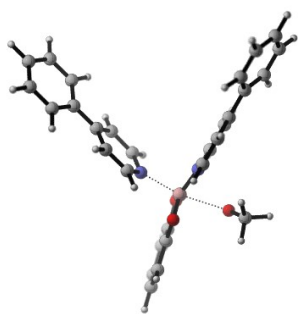


4E-TS

Imaginary frequency: -190.15

C	0.89055800	-3.66954200	-0.58223000
C	0.86217700	-3.62438300	0.81859200
C	1.39123300	-4.64548800	1.58531500
C	1.95556200	-5.73729200	0.90237300
C	1.98186000	-5.78244400	-0.49183700
C	1.44476000	-4.73653100	-1.26327500
H	1.35997800	-4.60269800	2.66936300
H	2.37425400	-6.56044200	1.47477700
H	2.42022200	-6.64022300	-0.99433100
H	1.45395300	-4.76272200	-2.34842800
O	0.32455600	-2.52883500	-1.10858000
O	0.27953000	-2.45567400	1.24796000
B	-0.06650100	-1.79481600	0.04298700
C	1.50909200	0.29325900	1.13497200
C	2.46869000	1.29372000	1.17750200
C	3.21108100	1.60079900	0.02398300

C	2.92811100	0.84837000	-1.12750100
C	1.95109500	-0.13752200	-1.08844400
H	2.65958000	1.80923400	2.11263500
H	3.45191200	1.04109400	-2.05772300
H	1.71321600	-0.75163200	-1.95060600
N	1.24478400	-0.40555700	0.02001400
C	4.24537000	2.66127000	0.02611200
C	5.42580800	2.51458400	-0.72171800
C	4.06600100	3.83573500	0.77626800
C	6.39903100	3.51178400	-0.71621900
H	5.59585300	1.60164300	-1.28530500
C	5.03670800	4.83535700	0.77483400
H	3.14835600	3.97945000	1.33965500
C	6.20702800	4.67602000	0.03022500
H	7.31103900	3.37612400	-1.29068900
H	4.87607100	5.74185600	1.35161500
H	6.96503100	5.45420400	0.03199400
H	0.93878400	0.01394000	2.01478700
O	-2.13945700	-3.08505800	0.13882000
C	-2.85220900	-3.20442200	-0.99434800
H	-2.83071000	-2.25012000	-1.62220400
H	-2.49878000	-3.99360400	-1.69951700
H	-3.94257600	-3.37498000	-0.83210800
C	-1.95895500	-0.58226100	1.16459700
C	-2.97613400	0.33207800	1.17979500
C	-3.42069800	0.95323500	-0.02183700
C	-2.77025400	0.56391900	-1.19160000
C	-1.73721300	-0.37125300	-1.16285600
H	-3.42955900	0.58552700	2.13140600
H	-3.07556100	0.95747700	-2.15516100
H	-1.18610700	-0.65405100	-2.04951600
N	-1.31839100	-0.92817000	0.00381600
C	-4.51448200	1.94585100	-0.02208900
C	-4.53903600	3.00112000	-0.95294300
C	-5.56507300	1.86328600	0.91045000
C	-5.57387900	3.93342200	-0.95350700
H	-3.72428600	3.10652600	-1.66386500
C	-6.59951000	2.79675700	0.90955800
H	-5.58890700	1.04113100	1.61968100
C	-6.60980000	3.83686600	-0.02170900
H	-5.56626400	4.74356000	-1.67803500
H	-7.40529100	2.70491300	1.63303000
H	-7.41642400	4.56477900	-0.02176400
H	-1.61459700	-1.10206100	2.04817500

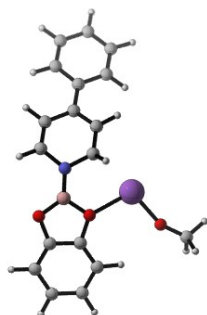


5E-TS

Imaginary frequency: -466.99

C	-4.07712400	-0.04535600	-0.62172500
C	-4.04741500	-0.04118500	0.78508600
C	-5.16104800	-0.39007600	1.52801400
C	-6.32852600	-0.74499400	0.82675300
C	-6.35787100	-0.74770700	-0.56739900
C	-5.21999600	-0.39542600	-1.31743000
H	-5.12670700	-0.38154300	2.61338400
H	-7.22037400	-1.01948500	1.38545900
H	-7.27220900	-1.02386800	-1.08749400
H	-5.22991600	-0.39144500	-2.40337000
O	-2.86030900	0.31418400	-1.12690300
O	-2.81115600	0.31363700	1.23742400
B	-2.07671100	0.54784900	0.04054900
C	-0.49027700	-1.66344700	1.18261300
C	0.51293200	-2.60935800	1.22473200
C	1.03636900	-3.17015600	0.02683100
C	0.44535900	-2.67493400	-1.16633100
C	-0.55258500	-1.72247900	-1.11836700
H	0.86096200	-2.95322400	2.19385200
H	0.78418200	-3.02174300	-2.13771200
H	-1.01645500	-1.34834800	-2.02725500
N	-1.03868600	-1.20036000	0.03353700
C	2.09127200	-4.18157800	0.02558700
C	2.31046700	-5.03140700	-1.08817700
C	2.94794000	-4.36543500	1.14061100
C	3.31254900	-5.99427400	-1.08471300
H	1.66048300	-4.95356400	-1.95470000
C	3.94808500	-5.33069700	1.14023600
H	2.84592000	-3.71510900	2.00417500
C	4.14529000	-6.15860000	0.02888600
H	3.44039300	-6.63228900	-1.95712300
H	4.59027100	-5.43141400	2.01307600
H	4.92892000	-6.91179700	0.02970200
H	-0.91402600	-1.25038400	2.09423600
O	-2.87454000	2.76997700	0.19838600

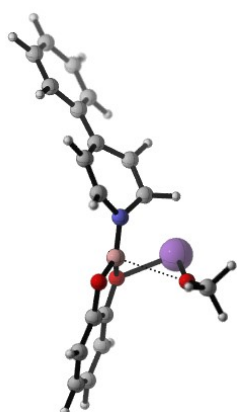
C	-2.80569000	3.53975000	-0.90436800
H	-1.86017100	3.38399700	-1.51122300
H	-3.62843500	3.38596800	-1.65322200
H	-2.79661800	4.64209800	-0.69382600
C	-0.30078900	1.87994100	1.17429500
C	0.89342200	2.54335500	1.19224800
C	1.63818000	2.78113000	-0.00299400
C	1.02588700	2.30867000	-1.18555100
C	-0.18506800	1.64961800	-1.16180200
H	1.27422600	2.87028500	2.15375800
H	1.47644000	2.49509100	-2.15470500
H	-0.66502300	1.28328100	-2.05892900
N	-0.84532600	1.39196100	0.00967500
C	2.92512800	3.47216000	-0.00352500
C	3.84830400	3.32516300	-1.06859000
C	3.31560200	4.32273900	1.06009600
C	5.07161600	3.98568900	-1.06985100
H	3.61176400	2.65428000	-1.88920000
C	4.54158800	4.97897500	1.05650400
H	2.62931500	4.49655600	1.88348600
C	5.43574400	4.82059300	-0.00773000
H	5.75531200	3.83745500	-1.90350300
H	4.79819700	5.63109400	1.88916000
H	6.39365600	5.33436400	-0.00903200
H	-0.89648700	1.71285800	2.06090600



1D'

C	0.60196300	0.20029800	-1.33583700
C	1.92205300	0.45750200	-1.03073900
C	2.77150700	-0.48370400	-0.39463500
C	2.27177000	-1.84856400	-0.49020300
C	0.98816500	-2.13466300	-0.79311200
H	0.13299500	0.65206000	-2.21574100
H	2.34031300	1.39096900	-1.41171200
H	2.96580100	-2.68400500	-0.42958300
H	0.61960300	-3.13605000	-0.99462900
N	0.03423700	-1.06661600	-0.87839700
C	4.09931400	-0.15440300	0.07585700

C	4.55235300	1.19255800	0.18260600
C	5.04617500	-1.14252100	0.47027100
C	5.83931000	1.51312300	0.59630100
H	3.86323400	2.00165400	-0.04380300
C	6.32968600	-0.81389600	0.89133300
H	4.76413700	-2.19119500	0.44869700
C	6.75577800	0.51733300	0.95488900
H	6.12787400	2.56217800	0.65569600
H	7.01104900	-1.61481800	1.17763500
H	7.75861000	0.77098500	1.28996300
C	-3.33130700	-0.40460900	0.03297100
C	-3.29435900	-1.79181800	0.20686500
C	-4.40538500	-2.47903100	0.66688800
C	-5.55197700	-1.71561900	0.95278700
C	-5.56722200	-0.32646800	0.79115700
C	-4.43813300	0.36875200	0.32416100
H	-4.38316600	-3.55553200	0.80543200
H	-6.44270600	-2.22162200	1.31715900
H	-6.46746500	0.23051100	1.03755200
H	-4.37987400	1.45039300	0.21367300
O	-2.11046500	0.02083600	-0.43476400
O	-2.05045800	-2.27845700	-0.12411500
B	-1.29555100	-1.14228800	-0.49946300
C	-3.19533900	4.57392200	0.16530600
H	-3.75568700	4.68840800	1.12963900
H	-2.49579600	5.45067500	0.15092100
H	-3.95461900	4.81771700	-0.62332400
O	-2.59616800	3.36261500	0.00732200
Na	-1.07050800	2.05057500	-0.27729200

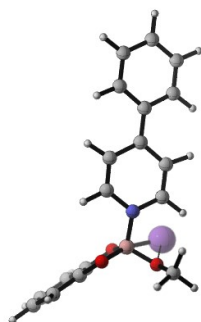


1-TS'

Imaginary frequency: -96.18

C	-0.64160500	1.44495400	-0.12022100
C	-1.99403700	1.18745700	-0.31965300
C	-2.68449800	0.16039400	0.35596600

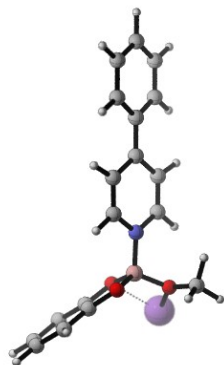
C	-2.00163400	-0.28795300	1.57171600
C	-0.68685100	-0.06282500	1.77260900
H	-0.34726100	2.49648700	0.02442800
H	-2.55642400	1.90696300	-0.92003900
H	-2.57871300	-0.70019400	2.39627800
H	-0.17057100	-0.27751800	2.70482200
N	0.08566600	0.48003300	0.70104700
C	-4.04347900	-0.21490400	0.02642800
C	-4.65327300	0.17510500	-1.20071900
C	-4.86398900	-0.99513800	0.88937400
C	-5.97126700	-0.13982600	-1.50785800
H	-4.05953700	0.71608200	-1.93242000
C	-6.17870700	-1.31660100	0.57084900
H	-4.45764300	-1.35405100	1.83040100
C	-6.76159900	-0.88851900	-0.62731300
H	-6.38481800	0.18858100	-2.46126400
H	-6.76057000	-1.91363700	1.27284500
H	-7.78861800	-1.14623500	-0.87542600
C	3.08073800	-0.74951600	-0.81230200
C	3.27248500	-1.09765400	0.53286100
C	4.38992400	-1.80421200	0.94146900
C	5.32942200	-2.15645100	-0.04456100
C	5.13662300	-1.81059200	-1.38243600
C	3.99520700	-1.09573600	-1.79006000
H	4.52828500	-2.06873400	1.98526500
H	6.22050600	-2.70807600	0.24515200
H	5.87679100	-2.09724800	-2.12546900
H	3.83059400	-0.82997400	-2.83066400
O	1.88719500	-0.09890800	-0.95193700
O	2.22335500	-0.65965700	1.28504100
B	1.37770700	0.04222900	0.39294900
C	3.15967800	2.92305300	1.27429000
H	4.23059800	3.22927900	1.17289500
H	2.62143300	3.86654600	1.54713600
H	3.12959400	2.29896300	2.19725200
O	2.65780100	2.28054500	0.17670300
Na	1.43022800	2.09266700	-1.45130500



2D'

C	0.68723200	1.52478900	-0.15574400
C	2.02127500	1.24502300	0.03064400
C	2.57190300	-0.04813300	-0.17116000
C	1.57044200	-1.05500200	-0.48079700
C	0.26076800	-0.74322000	-0.65288600
H	0.32905700	2.54553900	-0.14953200
H	2.65795800	2.08310300	0.29752900
H	1.84836800	-2.10184300	-0.54639600
H	-0.48439800	-1.50084300	-0.86740200
N	-0.23391800	0.55906300	-0.58996800
C	3.97565100	-0.34417400	-0.04366100
C	4.91275500	0.58856900	0.49711200
C	4.52581800	-1.60095000	-0.44057400
C	6.26168100	0.28984900	0.62274400
H	4.56425100	1.55653400	0.84522600
C	5.87742900	-1.88934300	-0.31037600
H	3.87675800	-2.35015200	-0.88403700
C	6.77342400	-0.95275800	0.22209700
H	6.92933300	1.03779000	1.04920500
H	6.24267200	-2.86257500	-0.63700000
H	7.83137700	-1.18201100	0.32183000
C	-3.24473900	-0.56441000	0.73277800
C	-3.46627600	-0.69799300	-0.65403400
C	-4.49989700	-1.48484400	-1.13733300
C	-5.32268200	-2.14508300	-0.20410200
C	-5.10127700	-2.01322600	1.16528700
C	-4.04861100	-1.21527200	1.65454100
H	-4.66035800	-1.58327300	-2.20742500
H	-6.14076500	-2.76598500	-0.56241600
H	-5.74654500	-2.53201600	1.87054500
H	-3.86209700	-1.11160300	2.72011000
O	-2.17638900	0.23447700	0.96554600
O	-2.55067600	0.00238800	-1.36746900
B	-1.73781800	0.77733800	-0.40077200
C	-2.04483300	2.94658300	-1.52503700

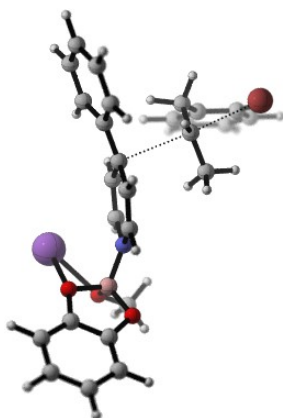
H	-2.38325600	3.96501200	-1.29879800
H	-1.04157100	3.00537300	-1.97533300
H	-2.72392900	2.50385600	-2.26531000
O	-2.04839300	2.20075000	-0.32623100
Na	-1.17882400	2.08632900	1.94100700



³2D**

C	0.70755000	1.41454700	0.18346500
C	2.04727000	1.20838100	0.33321200
C	2.67971200	-0.02776700	-0.04105900
C	1.75680700	-1.00044200	-0.56426000
C	0.42215600	-0.74755800	-0.68561500
H	0.24005600	2.35511600	0.45193900
H	2.63315100	2.03224500	0.72650200
H	2.10180300	-1.98564900	-0.85940100
H	-0.26940900	-1.48216000	-1.07791000
N	-0.15189700	0.46024200	-0.33408100
C	4.09706900	-0.26743500	0.09289900
C	4.96018500	0.63590100	0.78111600
C	4.72814400	-1.42271000	-0.45632300
C	6.32241100	0.40192600	0.90552200
H	4.54523700	1.52578400	1.24432700
C	6.09138200	-1.64878400	-0.32690600
H	4.13629900	-2.14257000	-1.01322400
C	6.91475100	-0.74287200	0.35510400
H	6.93471600	1.12147500	1.44701400
H	6.52294100	-2.54486000	-0.77057900
H	7.98202800	-0.92301200	0.45479600
C	-3.26457900	-0.52461100	0.75987100
C	-3.24425500	-0.95841500	-0.57940200
C	-4.09242200	-1.96376200	-1.01717600
C	-4.97384400	-2.53735100	-0.08128200
C	-4.99156000	-2.10744800	1.24439000
C	-4.12852700	-1.08596300	1.68577900
H	-4.06867600	-2.29122800	-2.05280100
H	-5.64895600	-3.32727600	-0.40228300

H	-5.68030000	-2.56275400	1.95190200
H	-4.13111200	-0.74452700	2.71702600
O	-2.35340800	0.46911100	0.95509200
O	-2.31237400	-0.28365000	-1.29777500
B	-1.68515100	0.70498700	-0.38411000
C	-1.62541200	2.58685800	-1.97637200
H	-0.53527400	2.59610100	-2.11889500
H	-2.07485900	1.97671200	-2.77079300
H	-1.99922700	3.61322600	-2.06310500
O	-1.97832800	2.09604100	-0.69742700
Na	-3.13523100	2.77361400	1.18524600

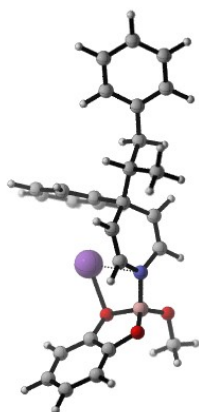


2D-TS'

Imaginary frequency: -245.34

C	-1.02406900	-0.61515900	-1.16613300
C	0.02057400	0.25144000	-1.35844900
C	0.32107200	1.32698700	-0.45556900
C	-0.64811600	1.42281700	0.63754500
C	-1.68899100	0.56820200	0.76799500
H	-1.11747200	-1.51076200	-1.77015500
H	0.69731800	0.02184000	-2.17594200
H	-0.54352700	2.19644700	1.39094400
H	-2.39603400	0.65176100	1.58585700
N	-1.94795800	-0.49267500	-0.11610100
C	1.15140000	2.45061600	-0.85033100
C	1.71014100	2.55637800	-2.15381700
C	1.45659700	3.51534200	0.04258700
C	2.52849600	3.62457300	-2.51963800
H	1.47285100	1.80733100	-2.90363500
C	2.26960600	4.57579200	-0.33047900
H	1.06612200	3.49315100	1.05549400
C	2.82251100	4.64642500	-1.61708200
H	2.93130000	3.65888400	-3.53069500
H	2.48303500	5.35875000	0.39463600
H	3.46265300	5.47696800	-1.90295300

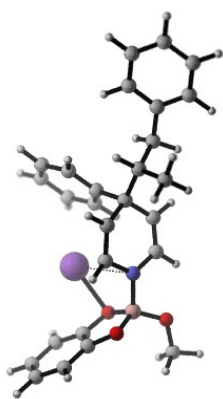
C	-5.34285300	0.25160800	0.08627600
C	-5.19873600	-0.71598700	1.10064700
C	-6.16930100	-0.87314200	2.07720800
C	-7.30194000	-0.03915300	2.02452000
C	-7.44215600	0.91843200	1.02173600
C	-6.45328900	1.07751500	0.03207700
H	-6.04710900	-1.61906900	2.85714200
H	-8.07568400	-0.14627900	2.78093000
H	-8.32359400	1.55462300	0.99958100
H	-6.54857300	1.82693900	-0.74943800
O	-4.26629900	0.23178600	-0.73992500
O	-4.02933700	-1.39398000	0.97638200
B	-3.39688200	-0.96519300	-0.27987000
C	-3.15290300	-3.25561000	-1.16835600
H	-2.07366600	-3.38291700	-0.99152600
H	-3.68839300	-3.65310500	-0.29787400
H	-3.43081300	-3.84035300	-2.05311500
O	-3.50201100	-1.90380700	-1.39797300
Na	-3.03574600	0.13281100	-2.59865800
C	3.55690900	-1.75123400	-2.03660700
C	3.86353800	-1.30519700	-0.74444300
C	4.58555000	-2.16333200	0.10232900
C	4.97834000	-3.42714600	-0.33786800
C	4.66336100	-3.86161700	-1.62867700
C	3.95042600	-3.01686500	-2.47927900
H	3.00929400	-1.09304600	-2.70873400
H	4.82314700	-1.81957600	1.10741300
H	5.53631300	-4.07726800	0.33281000
H	4.97223300	-4.84831100	-1.96762400
H	3.70039000	-3.33956100	-3.48802000
C	3.45569400	0.08425700	-0.28707300
C	2.43379600	0.16704200	0.81779600
H	3.08941800	0.65301200	-1.15788000
H	4.34134900	0.62768000	0.06148200
C	1.60127600	-0.99098900	1.25102400
H	0.84382000	-0.67562700	1.97153900
H	1.09610500	-1.45520400	0.39012900
H	2.21713200	-1.76443300	1.72074200
Br	4.19707700	0.10233200	2.93938900
H	2.31760500	1.12630500	1.29208100



6A'

C	0.55142800	-1.53005400	1.27255700
C	-0.74656100	-1.19097700	1.12370300
C	-1.22528800	-0.30152500	-0.01533300
C	-0.21377100	-0.47362300	-1.14916300
C	1.06234900	-0.85507100	-0.92186000
H	0.91719200	-2.08968300	2.12585000
H	-1.46132900	-1.53542200	1.86491000
H	-0.53112600	-0.27319500	-2.16927200
H	1.79376000	-0.92597000	-1.72155200
N	1.53222600	-1.22551900	0.33272800
C	-1.20672900	1.20757700	0.38865300
C	-0.91490900	1.63033500	1.69791200
C	-1.39633300	2.20810900	-0.58531500
C	-0.79597000	2.99135000	2.01857100
H	-0.77713600	0.87997900	2.47217200
C	-1.28573500	3.56245100	-0.26997300
H	-1.61800200	1.92296900	-1.60986500
C	-0.97554000	3.96390000	1.03434100
H	-0.57471300	3.28330800	3.04243000
H	-1.43784800	4.30843500	-1.04578100
H	-0.88555000	5.01860300	1.27838500
C	4.47668000	0.43437300	-0.25567800
C	4.66057800	-0.76794700	-0.96272700
C	5.58465700	-0.85062000	-1.99363900
C	6.32870200	0.30087800	-2.30826400
C	6.14619100	1.49094600	-1.60579400
C	5.20846500	1.57128200	-0.55860100
H	5.72304100	-1.78257500	-2.53342800
H	7.05897100	0.25663500	-3.11183500
H	6.73600500	2.36720200	-1.86066000
H	5.07646300	2.48879700	0.01096100
O	3.51360200	0.27876400	0.70170300
O	3.84070500	-1.74459800	-0.50491000

B	3.05565800	-1.23926400	0.64312800
C	4.55142100	-2.08620100	2.35294700
H	5.15567100	-2.66118800	1.63848500
H	5.05874100	-1.12944100	2.54565100
H	4.49798700	-2.64440400	3.29409100
O	3.23464500	-1.89342900	1.88154700
Na	1.55534500	1.29000400	0.63334200
C	-6.01201000	-1.58215000	0.22435400
C	-5.16940400	-0.47915200	0.03492700
C	-5.66910500	0.62021400	-0.67934300
C	-6.96526100	0.61557400	-1.19369300
C	-7.79207000	-0.49358300	-1.00054200
C	-7.31106500	-1.59246400	-0.28827000
H	-5.64744900	-2.44122100	0.78330900
H	-5.03483800	1.49255800	-0.82577300
H	-7.33281300	1.48028800	-1.74055300
H	-8.80340200	-0.49831300	-1.39823400
H	-7.94713400	-2.45916800	-0.12747800
C	-3.75401000	-0.45947200	0.57682600
C	-2.66801300	-0.69299800	-0.50725900
H	-3.65619400	-1.22397600	1.35737100
H	-3.57716300	0.50793600	1.06244200
C	-2.71458400	-2.13337300	-1.03390800
H	-1.99465000	-2.28968800	-1.84303500
H	-2.47070400	-2.84816100	-0.23932000
H	-3.71340500	-2.37060900	-1.41404300
H	-2.90334200	-0.02134800	-1.34601500

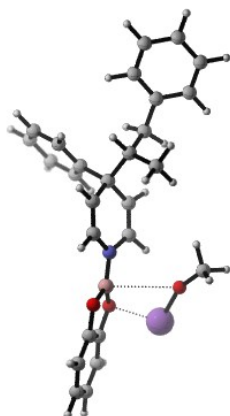


³6A**

C	0.53246300	-1.58658400	1.02115000
C	-0.74656300	-1.10094600	1.03189500
C	-1.27491600	-0.21232100	-0.06455600
C	-0.32386500	-0.23970900	-1.23288800
C	1.10294400	-0.43287700	-0.99880900
H	0.91673800	-2.22650800	1.80529300
H	-1.38908500	-1.34372500	1.87188500

H	-0.64471600	0.20111600	-2.17191300
H	1.78701600	-0.47153000	-1.83874000
N	1.45627900	-1.26177400	0.06132200
C	-1.20536200	1.28897700	0.34759000
C	-0.45699800	1.72175400	1.46723900
C	-1.77091100	2.29385300	-0.46694000
C	-0.28343400	3.08704000	1.74882400
H	-0.07514300	0.98284100	2.16713800
C	-1.60270600	3.64578200	-0.18345000
H	-2.34307900	2.01543800	-1.34669500
C	-0.85157000	4.05845600	0.92746000
H	0.26497000	3.38019300	2.64250000
H	-2.06195600	4.38701400	-0.83236600
H	-0.73079400	5.11423100	1.15154900
C	4.50229000	0.24492700	0.14165800
C	4.61108000	-0.57930500	-0.99506300
C	5.50733600	-0.27195300	-2.00719200
C	6.29235200	0.88787500	-1.86529700
C	6.18069000	1.70575400	-0.74251600
C	5.27306100	1.38985100	0.28872200
H	5.59298600	-0.91209500	-2.87991400
H	7.00071200	1.14485200	-2.64809400
H	6.80543700	2.58959400	-0.64993200
H	5.20854200	1.99514100	1.19098800
O	3.53938300	-0.23051400	0.98692500
O	3.75324000	-1.62195900	-0.92598800
B	2.99346700	-1.53936700	0.34426900
C	4.34050200	-3.12502500	1.58298600
H	4.95687500	-3.38624100	0.71229000
H	4.88079200	-2.37785800	2.18202300
H	4.20033100	-4.02330400	2.19355700
O	3.06530500	-2.65793100	1.19345900
Na	2.06598300	1.45069000	0.43447000
C	-6.00072200	-1.61693000	0.31430900
C	-5.19601300	-0.47924000	0.16876400
C	-5.75502600	0.65229800	-0.44413300
C	-7.07205200	0.64584000	-0.90267900
C	-7.86039600	-0.49757700	-0.75455600
C	-7.32009600	-1.62922200	-0.14303600
H	-5.59023400	-2.50180600	0.79575000
H	-5.15091300	1.55099900	-0.55342000
H	-7.48570700	1.53584900	-1.37029500
H	-8.88780700	-0.50380700	-1.10865200
H	-7.92577500	-2.52313500	-0.01766800

C	-3.75859700	-0.45865100	0.64810600
C	-2.72259700	-0.64237000	-0.49232800
H	-3.61761700	-1.24781900	1.39696900
H	-3.56594100	0.49472700	1.15519800
C	-2.74478100	-2.07266700	-1.05008000
H	-2.03090700	-2.18452800	-1.87230900
H	-2.47907600	-2.80290800	-0.27709600
H	-3.74248000	-2.32256800	-1.42484000
H	-3.02038100	0.02854900	-1.30921500

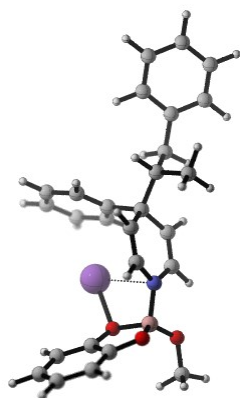


6A-TS'

Imaginary frequency: -43.51

C	0.79087400	-0.39822500	0.73136500
C	-0.53020500	-0.20041100	0.81637200
C	-1.36798100	0.51829800	-0.22638000
C	-0.49598900	0.71802700	-1.45776300
C	0.82443000	0.51299500	-1.48836700
H	1.35180400	-1.02600200	1.41971600
H	-1.04020100	-0.62340500	1.67682700
H	-0.97782100	1.07651800	-2.36360900
H	1.42050000	0.70265900	-2.37353900
N	1.55157600	0.04357700	-0.37316300
C	-1.83476200	1.91831100	0.25449000
C	-1.44137800	2.44296400	1.49181400
C	-2.64588300	2.72134400	-0.56599400
C	-1.85506000	3.71159900	1.90587800
H	-0.79618500	1.85391200	2.13624100
C	-3.05699700	3.99030100	-0.15941000
H	-2.95855500	2.35955600	-1.54199700
C	-2.66634400	4.49196600	1.08387900
H	-1.53668900	4.08920400	2.87465100
H	-3.68269700	4.58874800	-0.81715300
H	-2.98734200	5.47987500	1.40359400
C	5.09747300	0.23767700	0.20111300
C	5.01691700	0.25260200	-1.19318200

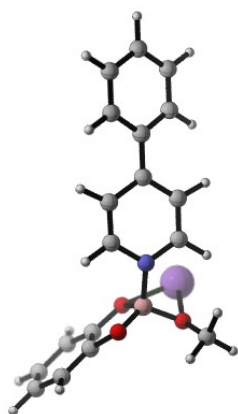
C	6.14767100	0.36973400	-1.98056800
C	7.37997100	0.47171600	-1.31287900
C	7.45944400	0.46260100	0.08132400
C	6.30294500	0.34698600	0.87371900
H	6.07898800	0.37990800	-3.06303000
H	8.28978500	0.56525800	-1.89794300
H	8.42593800	0.56027600	0.56606400
H	6.35296800	0.39143500	1.95965400
O	3.82910200	0.08447900	0.73418000
O	3.70628700	0.13335200	-1.57649100
B	2.96250200	0.02156000	-0.39396600
C	1.84092700	-3.73068900	0.75277500
H	0.81073700	-3.36313200	0.54561400
H	2.16165700	-4.24750200	-0.17812700
H	1.71865200	-4.53574800	1.51108200
O	2.69375100	-2.72321500	1.14236100
C	-5.39854800	-2.33770700	0.31639100
C	-4.98408700	-1.00647600	0.17825700
C	-5.89472400	-0.08261200	-0.35713600
C	-7.17445900	-0.47670100	-0.74649700
C	-7.57181000	-1.80864100	-0.60628000
C	-6.67895700	-2.73808000	-0.07229600
H	-4.71110100	-3.06785700	0.73788200
H	-5.59530500	0.95857700	-0.46002900
H	-7.86500300	0.25749300	-1.15433800
H	-8.56973500	-2.11703900	-0.90692400
H	-6.97829800	-3.77654300	0.04599700
C	-3.59537400	-0.56032100	0.58843100
C	-2.62751000	-0.35914100	-0.60935200
H	-3.16930100	-1.29974100	1.27788100
H	-3.67707000	0.38050300	1.14480400
C	-2.23197200	-1.70511900	-1.23081900
H	-1.62331000	-1.56819000	-2.12994700
H	-1.64535200	-2.30890000	-0.52852600
H	-3.12589100	-2.27349600	-1.50841200
H	-3.17695200	0.20741300	-1.37326900
Na	4.28613300	-1.87195700	1.96046400



7A'

C	0.57913600	-1.53430200	1.20496500
C	-0.69451400	-1.07728100	1.11681800
C	-1.18235500	-0.22970600	-0.03830800
C	-0.20732800	-0.40446100	-1.18910800
C	1.04767600	-0.89050900	-1.02501500
H	0.95361100	-2.09091200	2.05589000
H	-1.37985300	-1.30819800	1.92582300
H	-0.52045500	-0.10235500	-2.18376700
H	1.75787000	-0.96261100	-1.84120400
N	1.50787600	-1.35332300	0.19260700
C	-1.14099900	1.28465200	0.35373400
C	-0.93380700	1.71091100	1.68146300
C	-1.26887900	2.27562700	-0.63722300
C	-0.83401600	3.07422100	1.99955500
H	-0.88431400	0.97987100	2.48440500
C	-1.17376400	3.63191300	-0.32049400
H	-1.44766400	1.99212400	-1.66975700
C	-0.94417300	4.03966100	0.99690500
H	-0.70054400	3.37335700	3.03599400
H	-1.28105600	4.37273900	-1.10753000
H	-0.87429900	5.09530400	1.24075000
C	4.37292300	0.40595500	-0.13443100
C	4.60351200	-0.67544000	-1.02289500
C	5.52687900	-0.56899700	-2.05825200
C	6.20429600	0.64532400	-2.19006700
C	5.96958400	1.72309500	-1.31239100
C	5.04351000	1.61949400	-0.27245600
H	5.70356600	-1.40189100	-2.73011000
H	6.93201300	0.76242400	-2.98693600
H	6.52922400	2.64424700	-1.43922800
H	4.88705700	2.43504900	0.42885800
O	3.44755600	0.06217400	0.79031100
O	3.81792800	-1.72370500	-0.73073900
B	3.04536700	-1.45065900	0.49722700

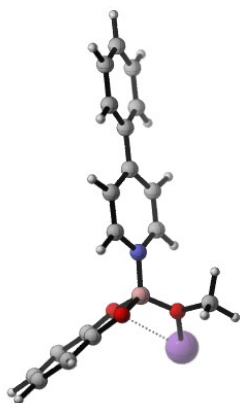
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H	5.06788400	-3.14454200	1.18946000
H	5.09687700	-1.80404100	2.37170600
H	4.41053700	-3.38146300	2.82868600
O	3.21550000	-2.27877200	1.59696200
Na	1.62221100	1.34488100	1.06374000
C	-5.93128400	-1.58896900	0.28114500
C	-5.12702200	-0.46434800	0.05674400
C	-5.65848200	0.60096500	-0.68488000
C	-6.95502400	0.54166700	-1.19435400
C	-7.74497700	-0.58779500	-0.96748800
C	-7.23041300	-1.65216700	-0.22644000
H	-5.54145600	-2.41985000	0.86509000
H	-5.05487100	1.49093700	-0.85488000
H	-7.35211800	1.37902800	-1.76154400
H	-8.75646300	-0.63423900	-1.36054000
H	-7.84054800	-2.53113500	-0.03828900
C	-3.70985300	-0.38938400	0.59237300
C	-2.63894400	-0.63810100	-0.50069300
H	-3.59011000	-1.12620900	1.39676000
H	-3.55179000	0.59875300	1.04121200
C	-2.67480800	-2.08683800	-1.00746900
H	-1.97048600	-2.25240500	-1.82947500
H	-2.42584100	-2.79458200	-0.20750100
H	-3.67652200	-2.33184900	-1.37052200
H	-2.87590200	0.02550300	-1.34414800



2C'

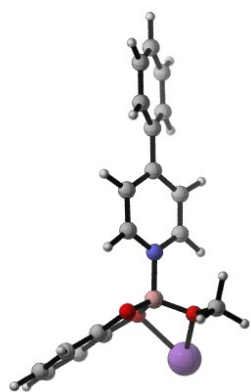
C	0.68925400	1.57100000	-0.21193500
C	2.02403300	1.28358900	-0.03734100
C	2.54865400	-0.01805900	-0.24101300
C	1.56848000	-0.99456400	-0.64349900
C	0.25378600	-0.67284700	-0.79744800
H	0.33013000	2.59381700	-0.20667500
H	2.68581400	2.11037300	0.20168800

H	1.85796000	-2.02704800	-0.80419600
H	-0.48818300	-1.40902200	-1.08273600
N	-0.23993000	0.60829900	-0.60951500
C	3.95973200	-0.33821400	-0.06259700
C	4.81742100	0.48402700	0.70823700
C	4.53847700	-1.48900000	-0.65026900
C	6.16373800	0.17818900	0.87325700
H	4.41539300	1.35994100	1.20951300
C	5.88517800	-1.79248800	-0.48054200
H	3.93086400	-2.13606200	-1.27547800
C	6.71326100	-0.96319800	0.28133700
H	6.78851100	0.83087700	1.47858600
H	6.29470400	-2.68080100	-0.95562400
H	7.76493400	-1.20186700	0.41252100
C	-3.18081200	-0.62546100	0.75284100
C	-3.45647100	-0.68140700	-0.62315600
C	-4.48644600	-1.46664500	-1.11378400
C	-5.24529500	-2.20449800	-0.18795800
C	-4.96819100	-2.14943600	1.17742300
C	-3.91942400	-1.35166100	1.67030500
H	-4.69234100	-1.50430500	-2.17902900
H	-6.05983800	-2.82732000	-0.54732500
H	-5.56655300	-2.72961800	1.87433200
H	-3.69037800	-1.30907000	2.73169800
O	-2.11631700	0.20241300	0.98688200
O	-2.58717900	0.09392900	-1.33511200
B	-1.76188100	0.81166400	-0.37421900
C	-2.19101000	3.03352400	-1.38020300
H	-1.23308800	3.17129800	-1.90336700
H	-2.89903700	2.56620200	-2.07247900
H	-2.57481800	4.01542500	-1.08522000
O	-2.04215500	2.24134600	-0.21021000
Na	-1.15419600	1.97656000	1.87337000



$^{13}\text{C}^*$

C	0.66172300	1.37595800	0.26717500
C	1.99597200	1.17163100	0.42709100
C	2.66227300	0.00187000	-0.07670000
C	1.78704500	-0.91474200	-0.75676900
C	0.45285700	-0.68865400	-0.89037700
H	0.16596600	2.26667900	0.63464500
H	2.55823800	1.95130000	0.92870500
H	2.17407700	-1.84038400	-1.16812600
H	-0.19742800	-1.38485600	-1.40336800
N	-0.16768200	0.46348600	-0.39898200
C	4.08325500	-0.23049800	0.08262100
C	4.86863300	0.52826500	0.99255200
C	4.76876400	-1.22936700	-0.66081700
C	6.23030500	0.30335200	1.14421000
H	4.39620500	1.28518000	1.61056900
C	6.13098300	-1.44911200	-0.50405700
H	4.22925800	-1.82128800	-1.39344600
C	6.88060400	-0.68721700	0.39928700
H	6.79164300	0.90201600	1.85774900
H	6.61732600	-2.21842200	-1.09935600
H	7.94607900	-0.86086500	0.51966500
C	-3.13370300	-0.62787000	0.81252400
C	-3.18089800	-1.03647600	-0.57458700
C	-4.04652300	-2.05740200	-0.99924500
C	-4.83474600	-2.65176900	-0.02927800
C	-4.78227700	-2.25439400	1.34339100
C	-3.94078100	-1.25034000	1.78346700
H	-4.07870700	-2.35643400	-2.04088600
H	-5.51788400	-3.44720500	-0.31124500
H	-5.43053600	-2.75866900	2.05329800
H	-3.89334600	-0.93703500	2.82014600
O	-2.29095800	0.35274500	0.98200900
O	-2.33967100	-0.34431100	-1.29955700
B	-1.64979600	0.69776300	-0.40313800
C	-1.69326900	2.63691500	-1.89326500
H	-0.60240200	2.69226700	-1.97618700
H	-2.09363200	2.07767500	-2.74636100
H	-2.10834500	3.64870000	-1.90511700
O	-2.08283700	2.02743800	-0.65839800
Na	-3.38975700	3.10365900	1.00291800



5C'

C	0.68938900	1.35925700	0.47292100
C	2.04428000	1.13380100	0.60166400
C	2.64808700	0.02958300	-0.03658800
C	1.79407800	-0.79636200	-0.79232600
C	0.44292000	-0.51849300	-0.88041000
H	0.20131200	2.21025400	0.93226700
H	2.63941500	1.83563900	1.17428500
H	2.17652100	-1.67797300	-1.29329700
H	-0.24488800	-1.13190500	-1.44806100
N	-0.10957100	0.54579600	-0.25586300
C	4.09197300	-0.24092600	0.07947200
C	4.79380500	0.10232800	1.24994600
C	4.79434100	-0.84922900	-0.97749400
C	6.15598000	-0.16173000	1.36113100
H	4.26612500	0.54116300	2.09175700
C	6.15919900	-1.09976500	-0.86800300
H	4.28071100	-1.09327200	-1.90274900
C	6.84261200	-0.76001400	0.30195800
H	6.68100100	0.09390800	2.27650500
H	6.69089500	-1.55580600	-1.69757800
H	7.90627600	-0.96107600	0.38807800
C	-3.17742000	-0.61458800	0.74233300
C	-3.16857200	-0.90190400	-0.62719400
C	-3.97588400	-1.89543600	-1.15504800
C	-4.79903400	-2.60030600	-0.26055300
C	-4.80274100	-2.31336500	1.10558300
C	-3.97983200	-1.30356800	1.63527200
H	-3.96833200	-2.11530600	-2.21767100
H	-5.44182400	-3.38664600	-0.64394300
H	-5.44264000	-2.88059200	1.77408100
H	-3.95478600	-1.09081200	2.70049500
O	-2.30895900	0.43719300	1.01357100
O	-2.28513300	-0.08759900	-1.29246400
B	-1.70579500	0.80169200	-0.30187500

C	-1.63641900	2.82046600	-1.73802800
H	-0.55120300	2.83476900	-1.89460800
H	-2.11039100	2.27166700	-2.55793100
H	-2.00084200	3.85052500	-1.73076700
O	-1.96117200	2.22210600	-0.47695200
Na	-3.53544000	2.31948500	1.10077300