Probing Catalyst Function – Electronic Modulation of Chiral Polyborate Anionic Catalysts.

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Supporting Information

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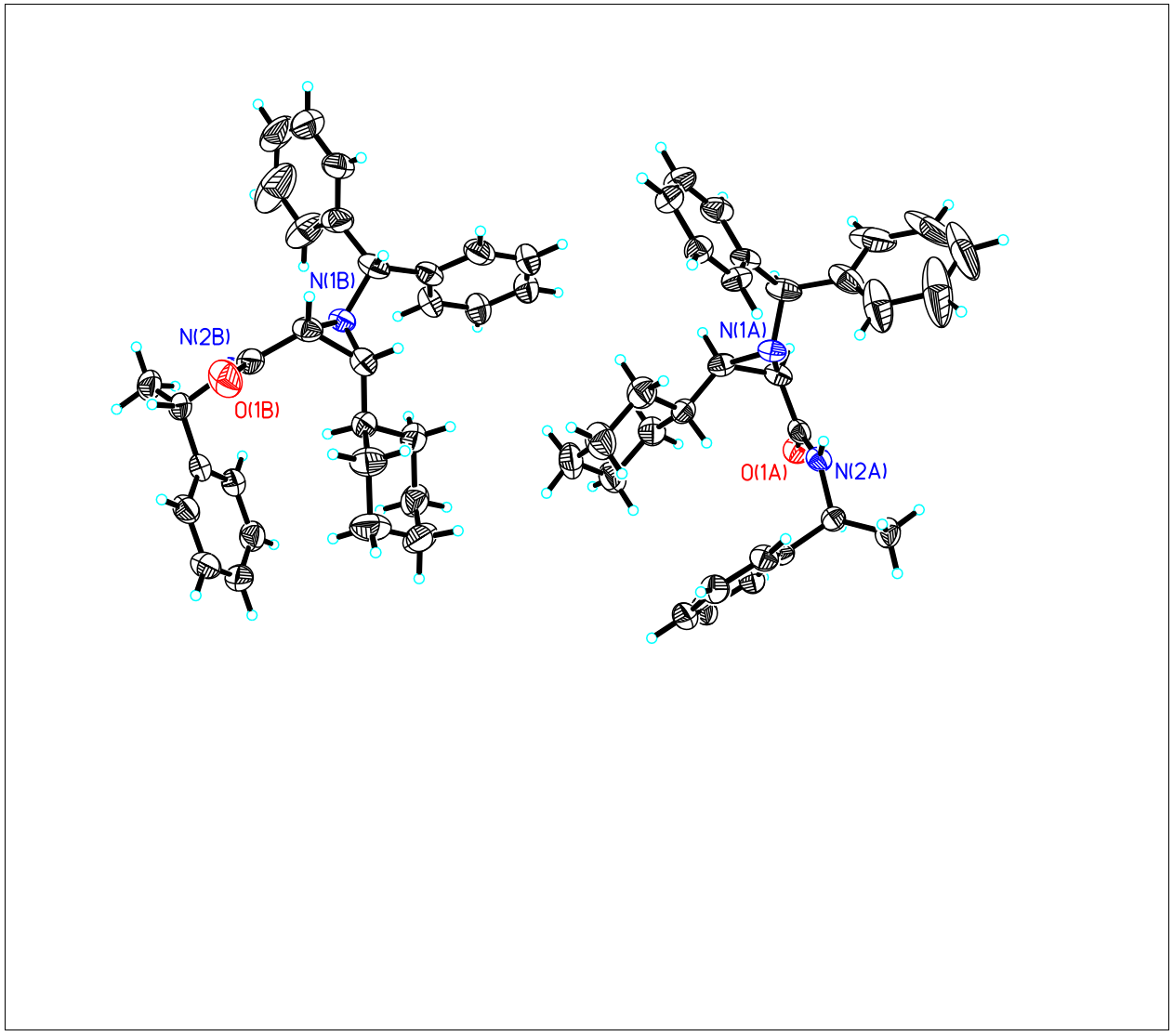
I. Crystal Structure Determination of aziridine 24.



A colorless block crystal with dimensions 0.38 x 0.29 x 0.17 mm was mounted on a Nylon loop using very small amount of paratone oil.

Data were collected using a Bruker CCD (charge coupled device) based diffractometer equipped with an Oxford Cryostream low-temperature apparatus operating at 173 K. Data were measured using omega and phi scans of 1.0° per frame for 20 s. The total number of images was based on results from the program COSMO[1] where redundancy was expected to be 4.0 and completeness to 0.83 Å to 100%. Cell parameters were retrieved using APEX II software[2] and refined using SAINT on all observed reflections. Data reduction was performed using the SAINT software[3] which corrects for Lp. Scaling and absorption corrections were applied using SADABS[4] multi-scan technique, supplied by George Sheldrick. The structures are solved by the direct method using the SHELXS-97 program and refined by least squares method on F^2, SHELXL- 97, which are incorporated in SHELXTL-PC V 6.10.[5]

The structure was solved in the space group $P2_12_12_1$ (# 19). All non-hydrogen atoms are refined anisotropically. Hydrogens were calculated by geometrical methods and refined as a riding model. The Flack[6] parameter is used to determine chirality of the crystal studied, the value should be near zero, a value of one is the other enantiomer and a value of 0.5 is racemic. The Flack parameter was refined to -0.1(3), confirming the absolute stereochemistryAll drawings are done at 50% ellipsoids.

References

1. COSMO V1.61, *Software for the CCD Detector Systems for Determining Data Collection Parameters.* Bruker Analytical X-ray Systems, Madison, WI (2009).

2. APEX2 V2010.11-3. Software *for the CCD Detector System*; Bruker Analytical X-ray Systems, Madison, WI (2010).

3. SAINT V 7.68A Software *for the Integration of CCD Detector System* Bruker Analytical X-ray Systems, Madison, WI (2010).

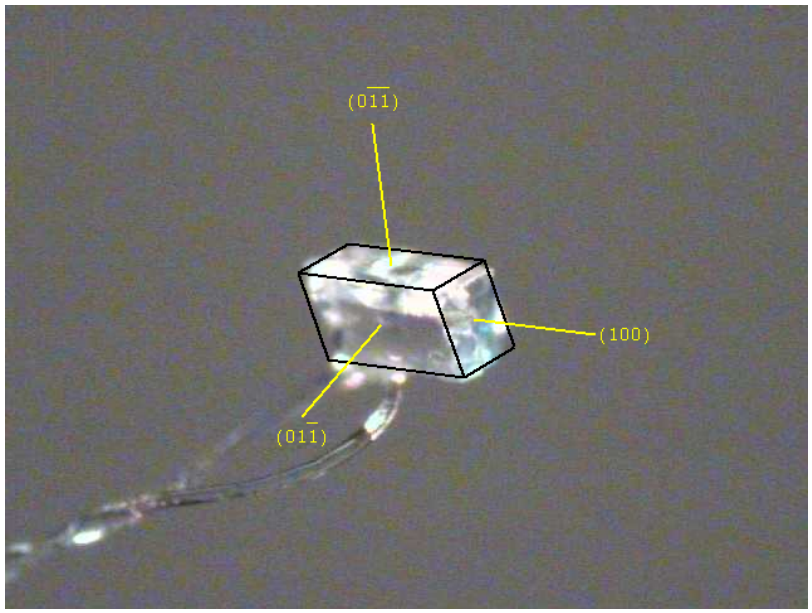
4. SADABS V2008/2 Program for absorption corrections using Bruker-AXS CCD based on the method of Robert Blessing; Blessing, R.H. Acta Cryst. A51, 1995, 33-38.

5. Sheldrick, G.M. "A short history of SHELX". *Acta Cryst*. **A64**, 2008, 112-122.

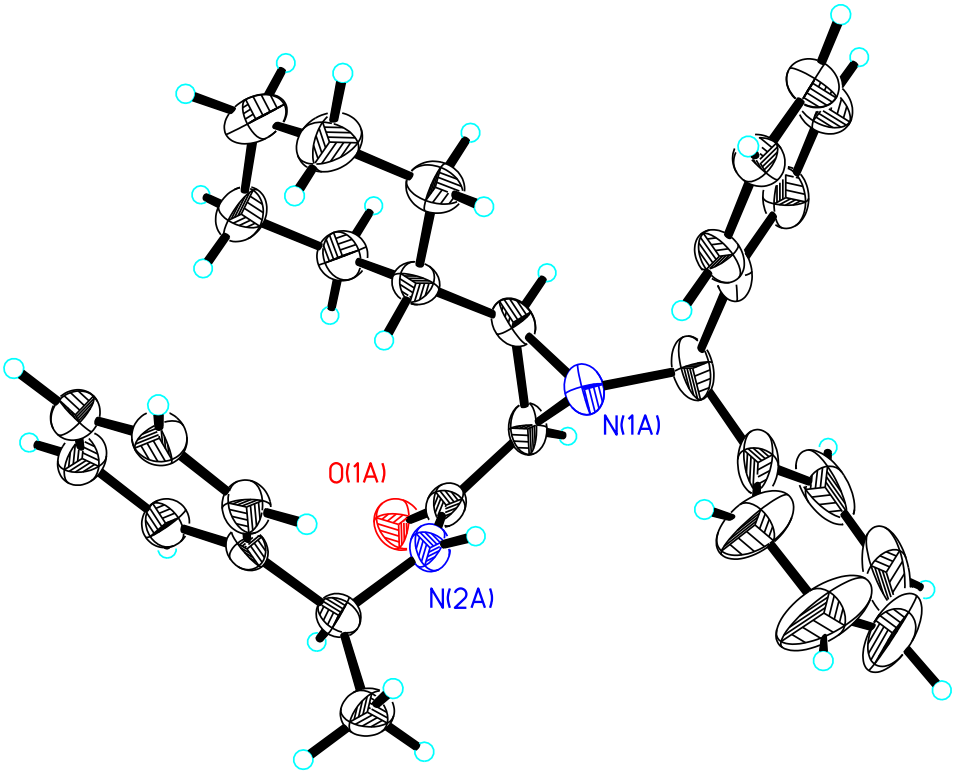
6. Flack, H. D. *Acta Cryst*. **A39**, 1983, 876-881.

[a] Obtained with graphite monochromated Cu Kα (λ = 1.54178Å) radiation.

[b]$R1 = \sum ||F_o| - |F_c| / |F_o|$ [c]$wR_2 = \{|[w(F_o^2 - F_c^2)^2.\{\sum[w(F_o^2)^2]\}^{1/2}$.



The following are 50% thermal ellipsoidal drawings of the molecule in the asymmetric cell with various amount of labeling.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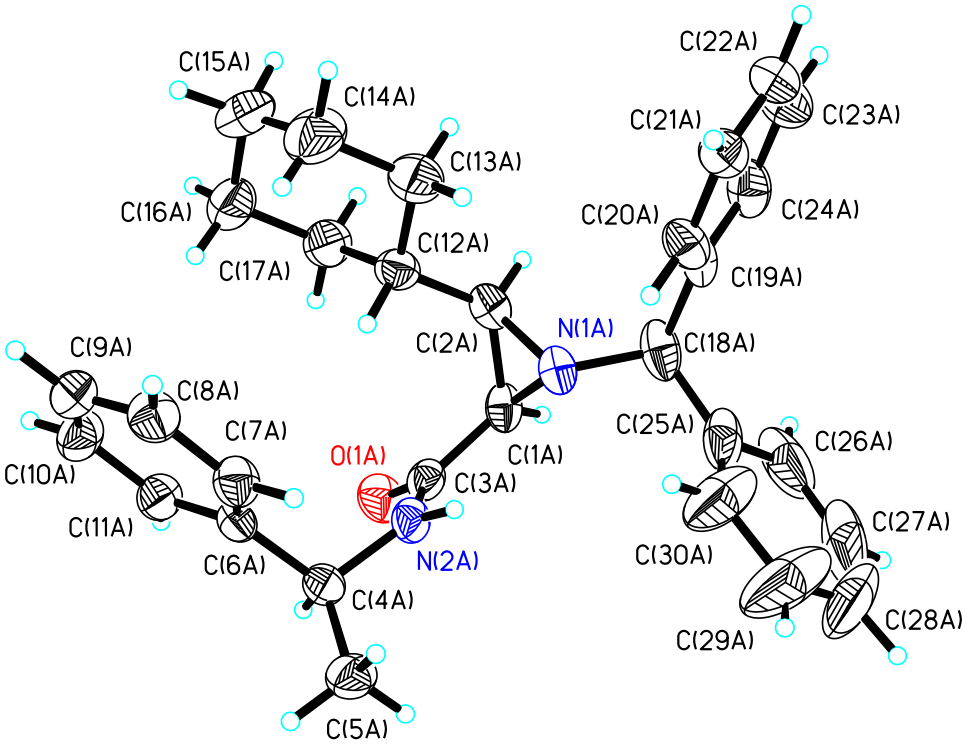
N(1A)
N(2A)


C(15A)
C(14A)
C(13A)
C(16A)
C(17A)
C(12A)
C(2A)
N(1A)
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C(21A)
C(23A)
C(20A)
C(24A)
C(19A)
C(18A)
C(9A)
C(8A)
C(7A)
C(10A)
O(1A)
C(1A)
C(3A)
C(25A)
C(26A)
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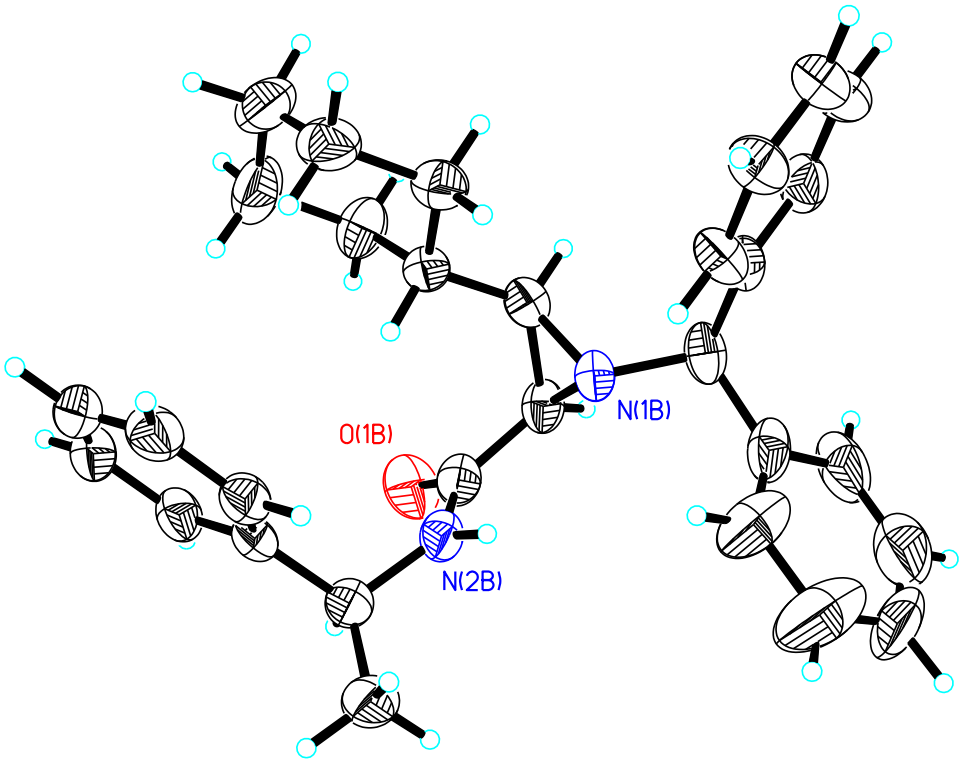
C(4A)
C(28A)
C(29A)
C(5A)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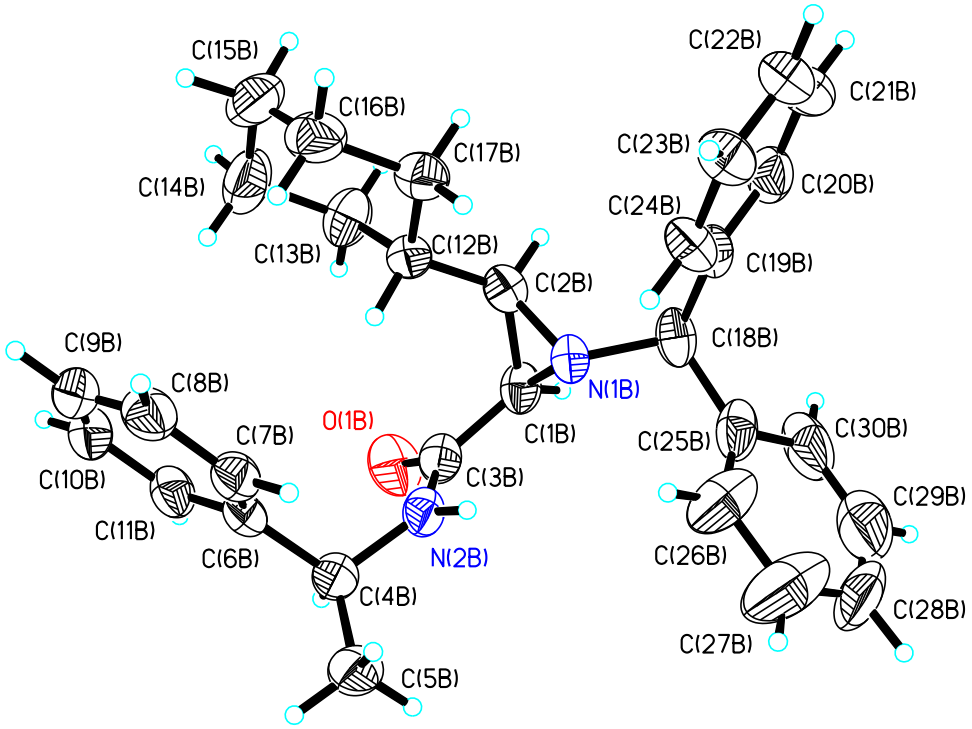
N(1B)
N(2B)


C(15B)
C(16B)
C(17B)
C(14B)
C(13B)
C(12B)
C(2B)
C(22B)
C(21B)
C(23B)
C(20B)
C(24B)
C(19B)
C(18B)
C(9B)
C(8B)
N(1B)
O(1B)
C(7B)
C(1B)
C(25B)
C(30B)
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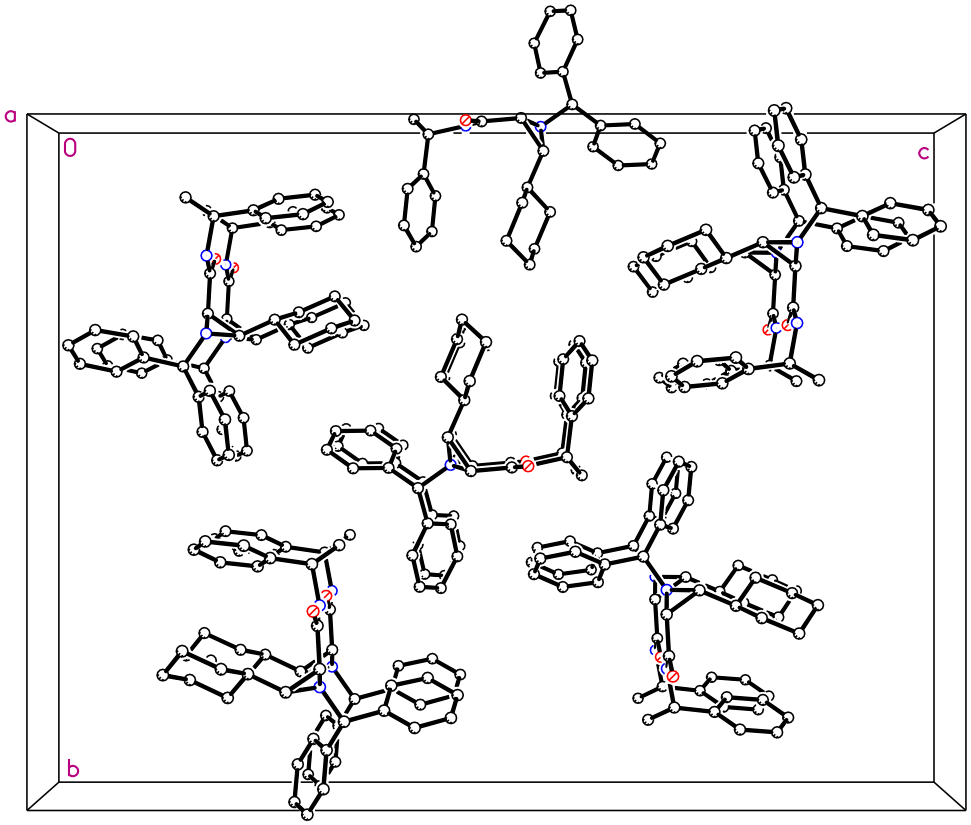


This is a drawing of the packing along the a-axis.

Table SI-1. Crystal data and structure refinement for 24.

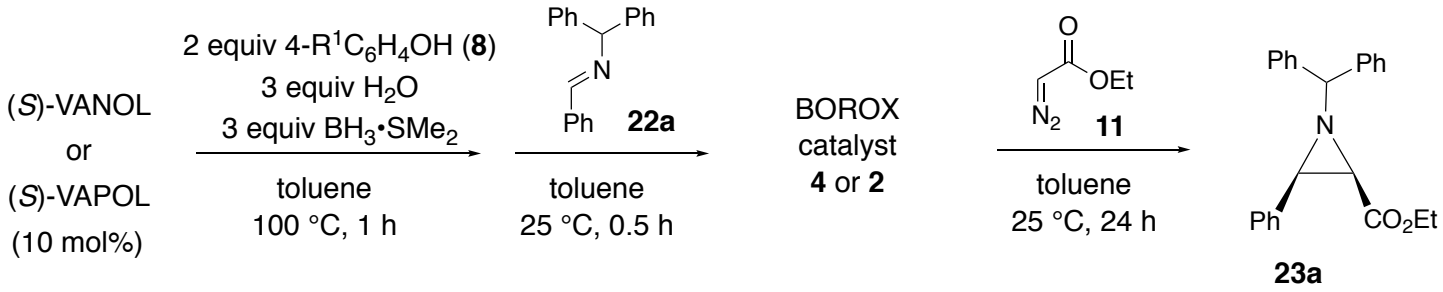
Identification code	24	
Empirical formula	C30 H34 N2 O	
Formula weight	438.59	
Temperature	172(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 6.09190(10) Å	α= 90°.
	b = 24.9451(2) Å	β= 90°.
	c = 33.6623(3) Å	γ = 90°.
Volume	5115.43(10) $Å^3$	
Z	8	
Density (calculated)	1.139 Mg/m^3	
Absorption coefficient	0.527 mm^{-1}	
F(000)	1888	
Crystal size	0.38 x 0.29 x 0.17 mm^3	
Theta range for data collection	2.20 to 67.88°.	
Index ranges	-7<=h<=7, -29<=k<=29, -39<=l<=40	
Reflections collected	33702	
Independent reflections	9133 [R(int) = 0.0235]	
Completeness to theta = 67.88°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9167 and 0.8241	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	9133 / 0 / 598
Goodness-of-fit on F^2	0.983
Final R indices [I>2sigma(I)]	R1 = 0.0527, wR2 = 0.1427
R indices (all data)	R1 = 0.0544, wR2 = 0.1448
Absolute structure parameter	-0.1(3)
Largest diff. peak and hole	0.430 and -0.353 e.$Å^{-3}$

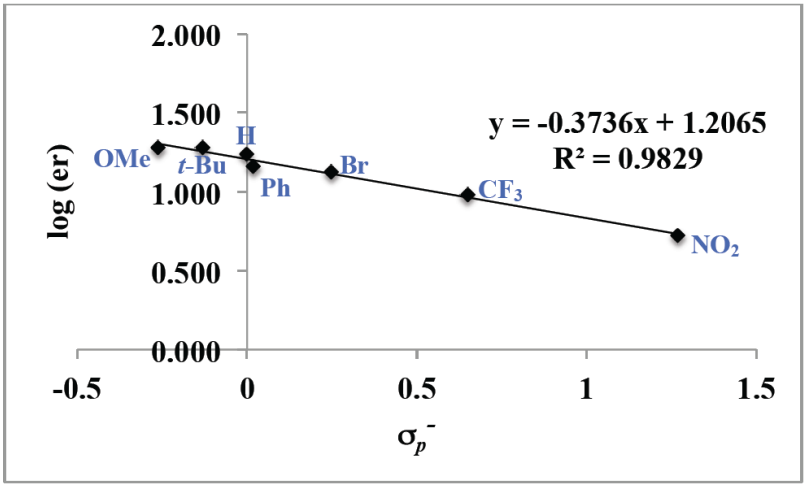
II. **Hammett Analysis.**

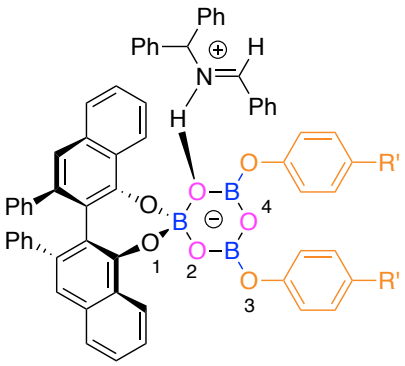
All of the data points collected for the Hammett analysis represent reactions that went to >95% completion. While some data points represent the average for reactions run more than once, most of the data points are from reactions with a single run.

A. *Various BOROX Catalysts in the Aziridination of the Phenyl Substituted Imine* ***22a****.*



With the VANOL Ligand

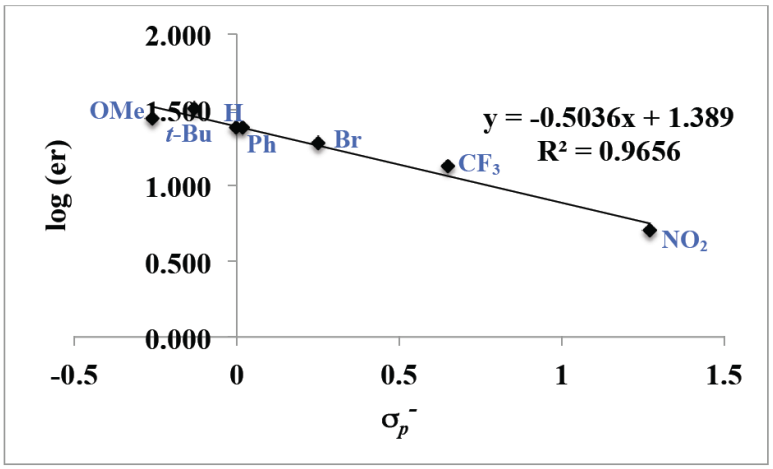


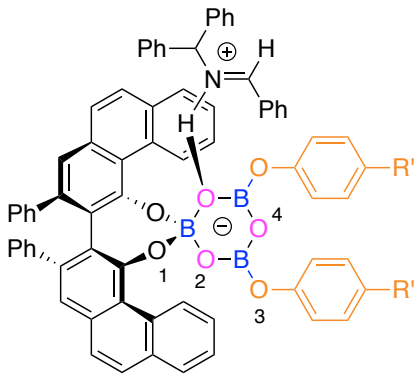


VANOL BOROX catalyst **4**

R^1	% ee	er	log er	σ_p^-
MeO	90	95 : 5	1.279	–0.26
Me_3C	90	95 : 5	1.279	–0.13
H	89	94.5 : 5.5	1.235	0
C_6H_5	87	93.5 : 6.5	1.158	0.02
Br	86	93 : 7	1.123	0.25
CF_3	81	90.5 : 9.5	0.979	0.65
NO_2	68	84 : 16	0.720	1.27

With the VAPOL Ligand

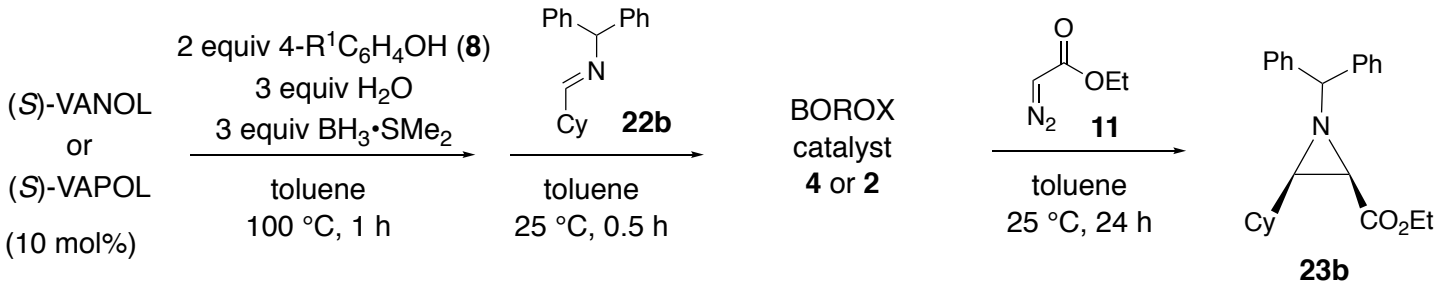




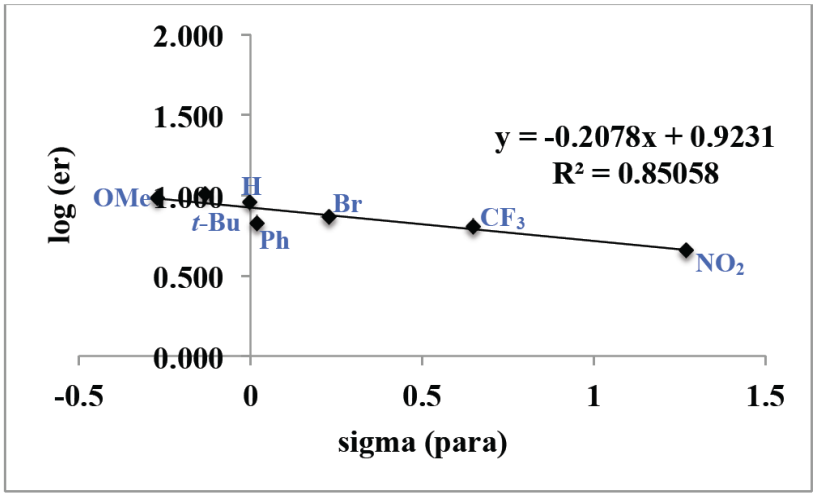
VAPOL BOROX catalyst **2**

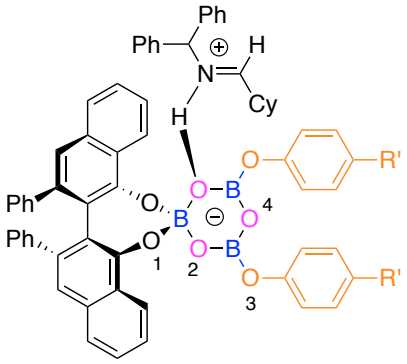
R^3	% ee	er	log er	σ_p^-
MeO	93	96.5 : 3.5	1.440	–0.26
Me_3C	94	97 : 3	1.510	–0.13
H	92	96 : 4	1.380	0
C_6H_5	92	96 : 4	1.380	0.02
Br	90	95 : 5	1.279	0.25
CF_3	86	93 : 7	1.123	0.65
NO_2	67	83.5 : 16.5	0.704	1.27

B. *Various BOROX Catalysts in the Aziridination of the Cyclohexyl Substituted Imine* ***22b****.*



With the VANOL Ligand

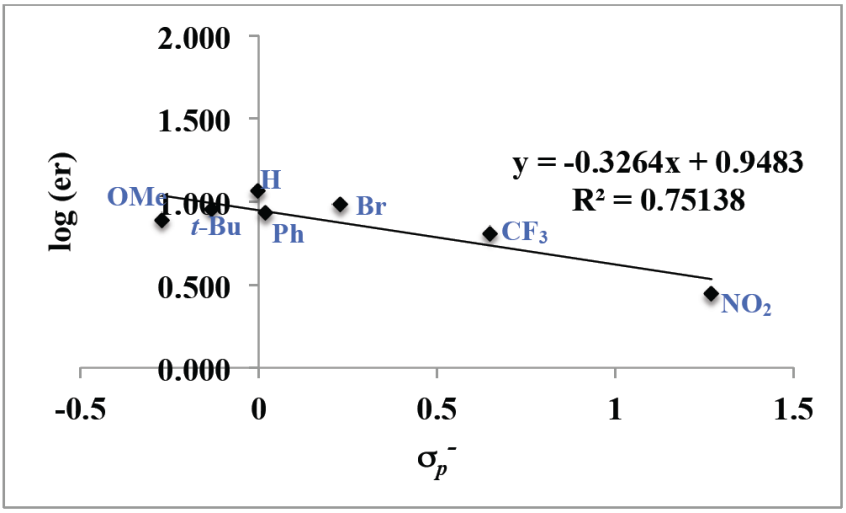


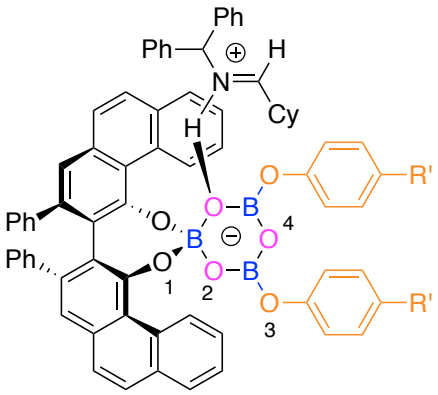


VANOL BOROX catalyst **4**

R^1	% ee	er	log er	σ_p^-
MeO	81	90.5 : 9.5	0.979	–0.26
Me_3C	82	91 : 9	1.005	–0.13
H	79	89.5 : 10.5	0.931	0
C_6H_5	74	87 : 13	0.826	0.02
Br	80	90 : 10	0.954	0.25
CF_3	73	86.5 : 13.5	0.807	0.65
NO_2	64	82 : 18	0.659	1.27

With the VAPOL Ligand





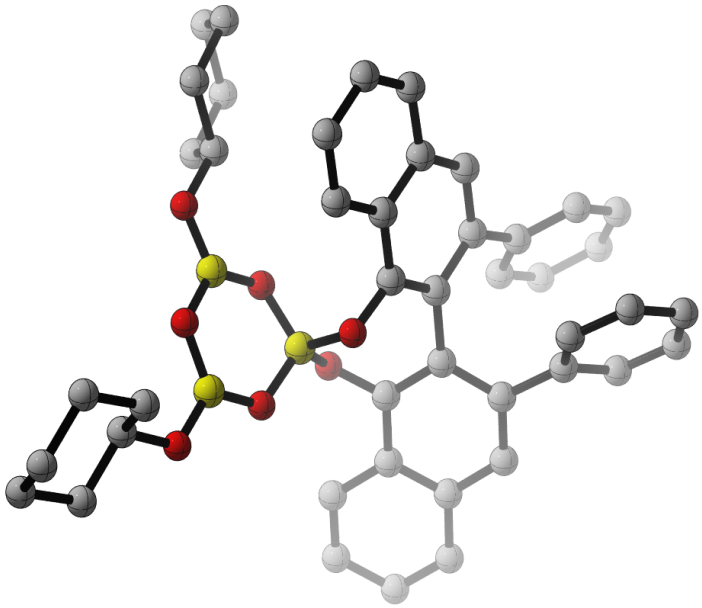
VAPOL BOROX catalyst **2**

R^3	% ee	er	log er	σ_p^-
MeO	77	88.5 : 11.5	0.886	–0.26
Me_3C	80	90 : 10	0.954	–0.13
H	74	87 : 13	0.826	0
C_6H_5	79	89.5 : 10.5	0.931	0.02
Br	76	88 : 12	0.865	0.25
CF_3	73	86.5 : 13.5	0.807	0.65
NO_2	67	83.5 : 16.5	0.704	1.27

III. DFT Calculations

Catalyst Structures Used for ADCH Charge Analysis:

Optimizations of catalyst-borox complexes were carried out at the M06-2X/6-31G* level of theory as implemented by the Gaussian 16 software package with bulk solvent effects accounted for by the self-consistent reaction field polarizable continuum model (PCM) as implemented for toluene.



Entry **1**

Filename: cat1

RRHO Thermochemistry (T = 298)
Zero-point correction (RRHO)= 0.794775 (Hartree/Particle)
Thermal correction to Energy (RRHO)= 0.837485
Thermal correction to Enthalpy (RRHO)= 0.838429
Thermal correction to Gibbs Free Energy (RRHO)= 0.718671
Sum of electronic and zero-point Energies (RRHO)= -2302.086172
Sum of electronic and thermal Energies (RRHO)= -2302.043462
Sum of electronic and thermal Enthalpies (RRHO)= -2302.042518
Sum of electronic and thermal Free Energies (RRHO)= -2302.162276

Quasi-RRHO Thermochemistry (T = 298, v0 = 100 cm-1)
Zero-point correction (QRRHO)= 0.794775 (Hartree/Particle)

Thermal correction to Energy (QRRHO)= 0.837485
Thermal correction to Enthalpy (QRRHO)= 0.838429
Thermal correction to Gibbs Free Energy (QRRHO)= 0.727905
Sum of electronic and zero-point Energies (QRRHO)= -2302.086172
Sum of electronic and thermal Energies (QRRHO)= -2302.043462
Sum of electronic and thermal Enthalpies (QRRHO)= -2302.042518
Sum of electronic and thermal Free Energies (QRRHO)= -2302.153042

Quasi-harmonic Thermochemistry (T = 298, cutoff = 100 cm-1)
Zero-point correction (QHO)= 0.794775 (Hartree/Particle)
Thermal correction to Energy (QHO)= 0.837673
Thermal correction to Enthalpy (QHO)= 0.838429
Thermal correction to Gibbs Free Energy (QHO)= 0.729412
Sum of electronic and zero-point Energies (QHO)= -2302.086172
Sum of electronic and thermal Energies (QHO)= -2302.043274
Sum of electronic and thermal Enthalpies (QHO)= -2302.042518
Sum of electronic and thermal Free Energies (QHO)= -2302.151535

C	4.2345540	0.4294230	-1.4977680	C	5.4584960	-1.5469740	1.2280170
C	4.0414770	1.1147040	-0.2918330	O	-2.0573240	-1.7520770	-0.3733550
C	5.1570700	1.6623690	0.3521640	B	-3.3381750	-1.4025860	-0.1434480
C	6.4322490	1.5243470	-0.1860390	O	-3.7773970	-0.0855470	-0.2435990
C	6.6146640	0.8333340	-1.3814020	B	-2.8871420	0.8558490	-0.7466630
C	5.5101840	0.2892690	-2.0355200	O	-3.3749540	2.1303430	-0.8997160
C	2.6848510	1.2977990	0.2918090	O	-4.2493350	-2.3783220	0.1865560
C	1.7239110	0.2335620	0.3514290	O	-1.6197930	0.5259120	-1.0647090
C	0.4491890	0.5090440	0.8274830	H	-0.0498490	-5.4562710	-3.4767570
C	0.0959380	1.8076230	1.3065830	H	-1.9193960	1.2622710	1.8429910
C	1.0605310	2.8452850	1.2580860	H	-0.8602160	5.3869970	2.4883730
C	2.3470490	2.5568680	0.7400270	H	1.4179570	4.9453220	1.6404150
C	0.6835190	4.1448530	1.6916230	H	3.0677350	3.3661270	0.6522730
C	-0.5834460	4.3880950	2.1627390	H	5.0209590	2.1624080	1.3072800
C	-1.5354670	3.3405520	2.2298800	H	7.2866500	1.9415920	0.3395300
C	-1.2031860	2.0774480	1.8058700	H	7.6098190	0.7177490	-1.8010230
C	1.9975870	-1.1687090	-0.0724380	H	5.6406250	-0.2448270	-2.9722530
C	1.0999560	-1.7723810	-0.9494080	H	3.3773170	0.0060870	-2.0124790
C	1.3295110	-3.0985480	-1.4387000	H	5.8231490	-2.0010060	0.3105730
C	2.4897250	-3.8012230	-1.0267020	H	7.4262260	-1.1988600	2.0149510
C	3.3686140	-3.1856410	-0.1028980	H	6.5951930	-0.0741800	4.0713190
C	3.1349290	-1.9177270	0.3818020	H	4.1491090	0.1982530	4.4160330
C	0.4160180	-3.7170720	-2.3285630	H	2.5543150	-0.6372170	2.7233850
C	0.6556430	-4.9847770	-2.7990880	H	4.2189420	-3.7524650	0.2677440
C	1.8174870	-5.6881380	-2.3977660	H	3.5993470	-5.6489630	-1.2096140
C	2.7099470	-5.1110730	-1.5294420	H	1.9964270	-6.6909260	-2.7753290
O	0.0297430	-1.1234590	-1.4290570	H	-0.4715880	-3.1637180	-2.6133110
B	-1.0550540	-0.7095790	-0.5223630	H	-2.5327880	3.5430240	2.6091360
O	-0.4955310	-0.4456540	0.8345540	C	-5.5902720	-2.0347100	0.4899680
C	4.0788190	-1.3882150	1.4039560	C	-6.4499480	-3.2795090	0.2973010
C	3.6221220	-0.7580360	2.5682040	C	-5.6997630	-1.5147490	1.9223430
C	4.5223640	-0.2881580	3.5194640	H	-5.9363210	-1.2463080	-0.1946460
C	5.8944030	-0.4455080	3.3291220	C	-7.9095280	-3.0077820	0.6701420
C	6.3588970	-1.0815940	2.1805080	H	-6.0422620	-4.0759360	0.9350270

H	-6.3631810	-3.6214490	-0.7398750	H	-1.5010710	2.9922610	-0.7928080
C	-7.1570420	-1.2376190	2.3005740	C	-1.3157600	4.2774950	-3.2247700
H	-5.2751880	-2.2760740	2.5914150	H	-3.2181460	3.2361450	-3.2969160
H	-5.0900380	-0.6106130	2.0221280	H	-1.8216780	2.1640150	-3.0823280
C	-8.0236170	-2.4846090	2.1048320	C	-2.1111010	5.6392670	-1.2542570
H	-8.5070720	-3.9175520	0.5444990	H	-4.0274810	4.6218870	-1.3049810
H	-8.3258630	-2.2583870	-0.0177090	H	-3.1830010	4.4762080	0.2429200
H	-7.2187030	-0.8859230	3.3363400	C	-1.8633400	5.6320000	-2.7658170
H	-7.5460780	-0.4272720	1.6683250	H	-1.1752400	4.2688110	-4.3114760
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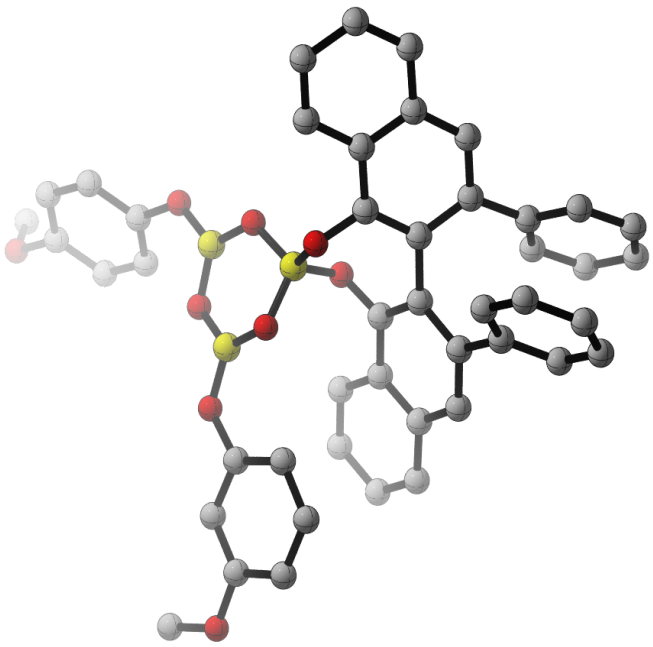
H	-7.6888950	-3.2673320	2.7999350	H	-2.5323970	6.6009110	-0.9393910
C	-2.4679950	3.1539420	-1.2914660	H	-1.1518690	5.5239830	-0.7296910
C	-2.2420830	3.1343380	-2.8008260	H	-1.1732320	6.4372140	-3.0435020
C	-3.0382910	4.4932740	-0.8428320	H	-2.8118370	5.8306820	-3.2850600



Entry **2**

File Name: cat2

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Thermal correction to Energy (RRHO)= 0.763649
Thermal correction to Enthalpy (RRHO)= 0.764593
Thermal correction to Gibbs Free Energy (RRHO)= 0.635302
Sum of electronic and zero-point Energies (RRHO)= -2523.887478

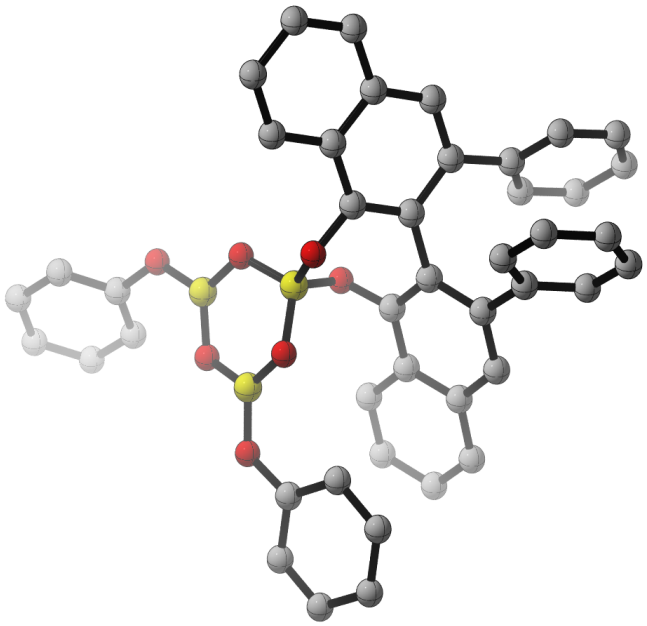
Sum of electronic and thermal Energies (RRHO)= -2523.841795
Sum of electronic and thermal Enthalpies (RRHO)= -2523.840851
Sum of electronic and thermal Free Energies (RRHO)= -2523.970142

Quasi-RRHO Thermochemistry (T = 298, v0 = 100 cm-1)
Zero-point correction (QRRHO)= 0.717966 (Hartree/Particle)
Thermal correction to Energy (QRRHO)= 0.763649
Thermal correction to Enthalpy (QRRHO)= 0.764593
Thermal correction to Gibbs Free Energy (QRRHO)= 0.646839
Sum of electronic and zero-point Energies (QRRHO)= -2523.887478
Sum of electronic and thermal Energies (QRRHO)= -2523.841795
Sum of electronic and thermal Enthalpies (QRRHO)= -2523.840851
Sum of electronic and thermal Free Energies (QRRHO)= -2523.958605

Quasi-harmonic Thermochemistry (T = 298, cutoff = 100 cm-1)
Zero-point correction (QHO)= 0.717966 (Hartree/Particle)
Thermal correction to Energy (QHO)= 0.763859
Thermal correction to Enthalpy (QHO)= 0.764593
Thermal correction to Gibbs Free Energy (QHO)= 0.649624
Sum of electronic and zero-point Energies (QHO)= -2523.887478
Sum of electronic and thermal Energies (QHO)= -2523.841585
Sum of electronic and thermal Enthalpies (QHO)= -2523.840851
Sum of electronic and thermal Free Energies (QHO)= -2523.955820

C	4.6530830	0.5025010	-1.4921550	C	1.5754310	-5.2509060	-2.6624920
C	4.3815870	1.1998340	-0.3084300	C	2.7810450	-5.8380820	-2.2064980
C	5.4376280	1.8457750	0.3445780	C	3.5998640	-5.1551850	-1.3425310
C	6.7316740	1.7898370	-0.1621060	O	0.6062550	-1.3997990	-1.4800050
C	6.9933690	1.0835210	-1.3335630	B	-0.5235250	-1.0131840	-0.6325020
C	5.9481760	0.4428140	-1.9974980	O	-0.0540950	-0.6795540	0.7347770
C	3.0031500	1.2901550	0.2439920	C	4.5722300	-1.2280010	1.4786510
C	2.1253900	0.1554020	0.3055750	C	4.0296900	-0.5999000	2.6065530
C	0.8218900	0.3439310	0.7420110	C	4.8591350	-0.0309720	3.5681460
C	0.3564440	1.6184050	1.1868850	C	6.2448190	-0.0831800	3.4235200
C	1.2426030	2.7236940	1.1494550	C	6.7948660	-0.7140470	2.3102990
C	2.5593280	2.5252060	0.6641940	C	5.9649070	-1.2793200	1.3478750
C	0.7589520	3.9979190	1.5471000	O	-1.4953260	-2.0937890	-0.4987300
C	-0.5403210	4.1581980	1.9596890	B	-2.7855230	-1.7782470	-0.3173520
C	-1.4178600	3.0481610	2.0040410	O	-3.2717590	-0.4872370	-0.4438860
C	-0.9772200	1.8029290	1.6293310	B	-2.4014120	0.4764220	-0.9387550
C	2.5249430	-1.2331050	-0.0628050	O	-2.9816160	1.7236160	-1.0945020
C	1.7094630	-1.9416960	-0.9395830	C	-2.3583760	2.9168410	-1.3188760
C	2.0571560	-3.2624670	-1.3681360	C	-0.9966720	3.0725410	-1.5735500
C	3.2587330	-3.8500200	-0.8989160	C	-0.4999070	4.3652280	-1.7461090
C	4.0578040	-3.1282010	0.0201660	C	-1.3205260	5.4816010	-1.6877070
C	3.7064940	-1.8679380	0.4503620	C	-2.6862090	5.3069470	-1.4430900
C	1.2199810	-3.9899650	-2.2506900	C	-3.2071800	4.0299390	-1.2589360

O	-3.6683550	-2.8052080	-0.0111990	H	8.0041530	1.0318560	-1.7277920
C	-4.9898900	-2.6417130	0.2796460	H	6.1400630	-0.1028400	-2.9167610
C	-5.8873530	-3.5663340	-0.2556450	H	3.8416950	0.0058320	-2.0155900
C	-7.2402050	-3.4922270	0.0585230	H	6.3935880	-1.7298980	0.4568930
C	-7.6999060	-2.4878220	0.9052390	H	7.8727650	-0.7496550	2.1793460
C	-6.8065550	-1.5653090	1.4439300	H	6.8898050	0.3656490	4.1733730
C	-5.4524260	-1.6398140	1.1363250	H	4.4199270	0.4516400	4.4364280
O	-1.1308900	0.1823800	-1.2405250	H	2.9511450	-0.5595230	2.7257450
H	0.9281690	-5.8070640	-3.3340760	H	4.9417020	-3.6079610	0.4328610
H	-1.6347450	0.9391240	1.6597860	H	4.5218190	-5.6036680	-0.9801360
H	-5.5045970	-4.3384420	-0.9150030	H	3.0521330	-6.8361770	-2.5386610
H	-7.9507820	-4.2017640	-0.3548820	H	0.2939410	-3.5260630	-2.5722620
H	-7.1843580	-0.7857970	2.0991090	H	-2.4458220	3.1880600	2.3249690
H	-4.7517390	-0.9199730	1.5429140	O	-3.4361750	6.4470440	-1.3986830
H	-4.2565340	3.8517370	-1.0583930	O	-9.0457550	-2.4006770	1.2003910
H	-0.9367990	6.4870200	-1.8235370	C	-4.8195800	6.3002310	-1.1671590
H	0.5637970	4.4960310	-1.9252000	H	-5.0152400	5.8317870	-0.1950740
H	-0.3447270	2.2107750	-1.6131940	H	-5.2386590	7.3068430	-1.1748090
H	-0.9033460	5.1414910	2.2440530	H	-5.2948460	5.7012260	-1.9531680
H	1.4345330	4.8490990	1.5037780	C	-9.3917090	-3.0927280	2.3876130
H	3.2177260	3.3862680	0.5776330	H	-10.4657550	-2.9622590	2.5316430
H	5.2424080	2.3560370	1.2838360	H	-9.1607130	-4.1619380	2.3009450
H	7.5400960	2.2826980	0.3705970	H	-8.8544040	-2.6853940	3.2532100



Entry **3**

File Name: cat3

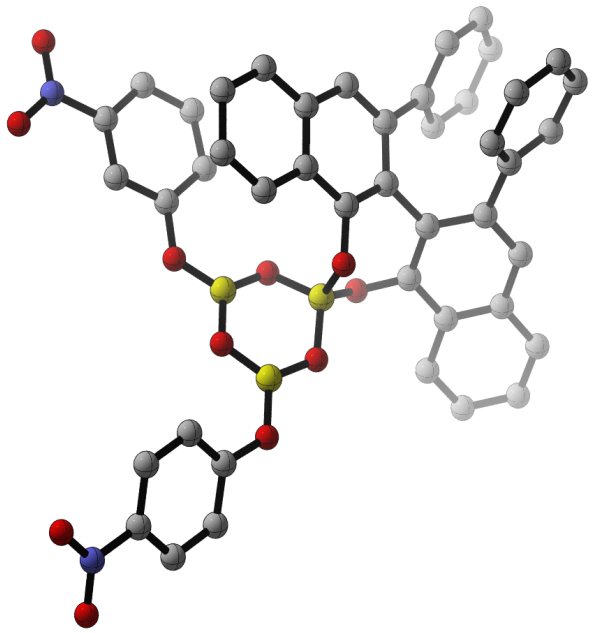
RRHO Thermochemistry (T = 298)
Zero-point correction (RRHO)= 0.652350 (Hartree/Particle)
Thermal correction to Energy (RRHO)= 0.692509
Thermal correction to Enthalpy (RRHO)= 0.693452
Thermal correction to Gibbs Free Energy (RRHO)= 0.578328
Sum of electronic and zero-point Energies (RRHO)= -2295.001058
Sum of electronic and thermal Energies (RRHO)= -2294.960899
Sum of electronic and thermal Enthalpies (RRHO)= -2294.959956
Sum of electronic and thermal Free Energies (RRHO)= -2295.075080

Quasi-RRHO Thermochemistry (T = 298, v0 = 100 cm-1)
Zero-point correction (QRRHO)= 0.652350 (Hartree/Particle)
Thermal correction to Energy (QRRHO)= 0.692509
Thermal correction to Enthalpy (QRRHO)= 0.693452
Thermal correction to Gibbs Free Energy (QRRHO)= 0.587252
Sum of electronic and zero-point Energies (QRRHO)= -2295.001058
Sum of electronic and thermal Energies (QRRHO)= -2294.960899
Sum of electronic and thermal Enthalpies (QRRHO)= -2294.959956
Sum of electronic and thermal Free Energies (QRRHO)= -2295.066156

Quasi-harmonic Thermochemistry (T = 298, cutoff = 100 cm-1)
Zero-point correction (QHO)= 0.652350 (Hartree/Particle)
Thermal correction to Energy (QHO)= 0.692679
Thermal correction to Enthalpy (QHO)= 0.693452
Thermal correction to Gibbs Free Energy (QHO)= 0.588896
Sum of electronic and zero-point Energies (QHO)= -2295.001058
Sum of electronic and thermal Energies (QHO)= -2294.960729
Sum of electronic and thermal Enthalpies (QHO)= -2294.959956
Sum of electronic and thermal Free Energies (QHO)= -2295.064512

C	3.9963290	0.3586370	-1.7026090	C	-1.7976560	3.5046830	1.7650370
C	3.8120770	1.1937600	-0.5936640	C	-1.4157540	2.2082060	1.5225260
C	4.9207860	1.8749630	-0.0777470	C	1.8982280	-1.1282000	0.0160400
C	6.1812990	1.7215890	-0.6456960	C	1.0160760	-1.8952430	-0.7386660
C	6.3557820	0.8801050	-1.7417130	C	1.3108500	-3.2593540	-1.0583290
C	5.2575440	0.2020990	-2.2689880	C	2.5204200	-3.8353950	-0.5958330
C	2.4696260	1.3930720	0.0162200	C	3.3843330	-3.0533460	0.2081940
C	1.5622950	0.3051650	0.2527030	C	3.0894680	-1.7464630	0.5270070
C	0.2909770	0.5883710	0.7315310	C	0.4138510	-4.0396090	-1.8298940
C	-0.1123250	1.9224650	1.0448350	C	0.7166520	-5.3428720	-2.1389840
C	0.8045660	2.9830360	0.8355810	C	1.9274760	-5.9213610	-1.6858530
C	2.0867470	2.6829860	0.3128190	C	2.8054210	-5.1859290	-0.9297150
C	0.3830830	4.3124010	1.1018720	O	-0.1056500	-1.3798080	-1.2647510
C	-0.8886540	4.5685510	1.5497030	B	-1.1721420	-0.8697010	-0.3984240

O	-0.6115150	-0.3993680	0.8911390	H	-6.2142570	-4.0529420	-0.2412880
C	4.0283460	-1.0334110	1.4355370	H	-8.6348780	-3.8021000	0.3030960
C	3.5680690	-0.2775130	2.5205880	H	-9.4010640	-1.8762530	1.6781400
C	4.4659900	0.3614910	3.3700150	H	-7.7384670	-0.2235470	2.5010680
C	5.8389280	0.2537050	3.1539770	H	-5.3347930	-0.4864030	1.9458030
C	6.3073820	-0.5043130	2.0836410	H	-4.8086750	4.0475380	-1.2445000
C	5.4092370	-1.1403780	1.2334590	H	-3.8476340	6.2458530	-1.9164940
O	-2.1575980	-1.8997760	-0.0882440	H	-1.4275420	6.4153030	-2.4826410
B	-3.4353110	-1.5399940	0.0972110	H	-0.0082830	4.3745860	-2.3765350
O	-3.9016850	-0.2590060	-0.1483370	H	-0.9782210	2.1987930	-1.7336780
B	-3.0363650	0.6237820	-0.7812420	H	-1.2063400	5.5909870	1.7321600
O	-3.5953750	1.8609490	-1.0477250	H	1.0840290	5.1255720	0.9278190
C	-2.9586000	2.9989220	-1.4519480	H	2.7650890	3.5042910	0.0952400
C	-1.6020450	3.0818090	-1.7805990	H	4.7937990	2.4945390	0.8060620
C	-1.0679820	4.3161550	-2.1427780	H	7.0317800	2.2453520	-0.2184490
C	-1.8593950	5.4607410	-2.1980150	H	7.3399940	0.7520790	-2.1829320
C	-3.2127130	5.3650030	-1.8798570	H	5.3813120	-0.4497310	-3.1289290
C	-3.7596170	4.1426670	-1.5069220	H	3.1429340	-0.1672310	-2.1201560
O	-4.3281400	-2.5106830	0.5312450	H	5.7739020	-1.6914720	0.3708720
C	-5.6420840	-2.2858340	0.8153460	H	7.3746290	-0.5854730	1.8974070
C	-6.5708450	-3.2199390	0.3559180	H	6.5373730	0.7576040	3.8158290
C	-7.9187090	-3.0709190	0.6666890	H	4.0903770	0.9434640	4.2066280
C	-8.3491430	-1.9930100	1.4372710	H	2.4997380	-0.1928090	2.6955390
C	-7.4152210	-1.0666950	1.8975670	H	4.2766480	-3.5170070	0.6211220
C	-6.0643480	-1.2074880	1.5953930	H	3.7326340	-5.6263840	-0.5709150
O	-1.7863900	0.2670320	-1.1034930	H	2.1562090	-6.9537490	-1.9346620
H	0.0247670	-5.9382440	-2.7271560	H	-0.5127840	-3.5776010	-2.1527500
H	-2.0993470	1.3802300	1.6850210	H	-2.8035050	3.7197330	2.1129390



Entry **4**

File Name: cat4

RRHO Thermochemistry (T = 298)
Zero-point correction (RRHO)= 0.657709 (Hartree/Particle)
Thermal correction to Energy (RRHO)= 0.703162
Thermal correction to Enthalpy (RRHO)= 0.704106
Thermal correction to Gibbs Free Energy (RRHO)= 0.575303
Sum of electronic and zero-point Energies (RRHO)= -2703.865917
Sum of electronic and thermal Energies (RRHO)= -2703.820464
Sum of electronic and thermal Enthalpies (RRHO)= -2703.819520
Sum of electronic and thermal Free Energies (RRHO)= -2703.948323

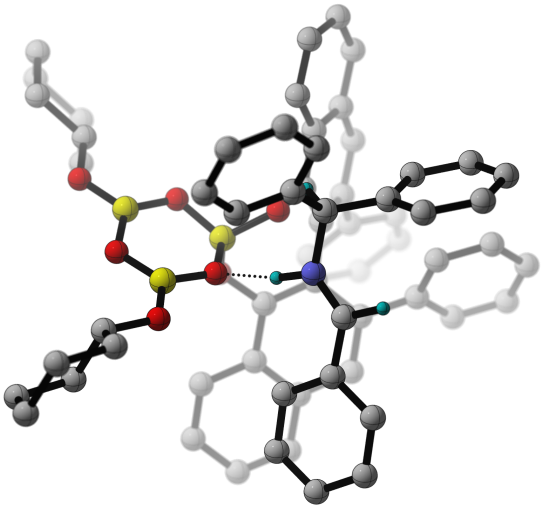
Quasi-RRHO Thermochemistry (T = 298, v0 = 100 cm-1)
Zero-point correction (QRRHO)= 0.657709 (Hartree/Particle)
Thermal correction to Energy (QRRHO)= 0.703162
Thermal correction to Enthalpy (QRRHO)= 0.704106
Thermal correction to Gibbs Free Energy (QRRHO)= 0.586792
Sum of electronic and zero-point Energies (QRRHO)= -2703.865917
Sum of electronic and thermal Energies (QRRHO)= -2703.820464
Sum of electronic and thermal Enthalpies (QRRHO)= -2703.819520
Sum of electronic and thermal Free Energies (QRRHO)= -2703.936834

Quasi-harmonic Thermochemistry (T = 298, cutoff = 100 cm-1)
Zero-point correction (QHO)= 0.657709 (Hartree/Particle)
Thermal correction to Energy (QHO)= 0.703377
Thermal correction to Enthalpy (QHO)= 0.704106

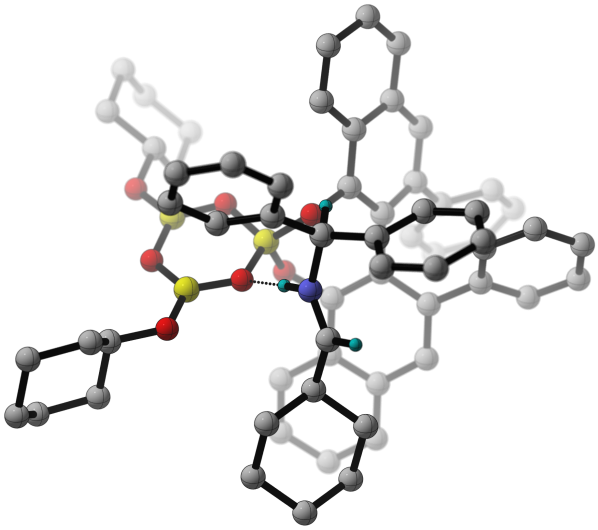
Thermal correction to Gibbs Free Energy (QHO)= 0.589272
Sum of electronic and zero-point Energies (QHO)= -2703.865917
Sum of electronic and thermal Energies (QHO)= -2703.820249
Sum of electronic and thermal Enthalpies (QHO)= -2703.819520
Sum of electronic and thermal Free Energies (QHO)= -2703.934354

C	4.7525880	0.3110220	-1.5033490	C	-2.0941580	5.2223670	-1.3058310
C	4.4993260	1.0320530	-0.3298820	C	-2.7452740	4.0109420	-1.1318900
C	5.5639880	1.6940860	0.2920510	O	-3.6335060	-2.8172700	-0.0349050
C	6.8494230	1.6310440	-0.2352750	C	-4.9384420	-2.6264700	0.2483140
C	7.0933930	0.9009630	-1.3959110	C	-5.8332570	-3.6032370	-0.2078500
C	6.0392860	0.2436520	-2.0286650	C	-7.1822710	-3.5086660	0.0874410
C	3.1298890	1.1308020	0.2428040	C	-7.6254480	-2.4295330	0.8459860
C	2.2531000	-0.0036740	0.3336620	C	-6.7536200	-1.4524560	1.3152690
C	0.9552580	0.1935140	0.7802620	C	-5.4037020	-1.5519640	1.0189290
C	0.4954810	1.4734200	1.2143690	O	-0.9505340	0.0518250	-1.2128610
C	1.3819490	2.5775120	1.1518910	H	1.0722310	-6.0210560	-3.2261970
C	2.6913720	2.3721560	0.6505230	H	-1.4907010	0.8024930	1.7234800
C	0.9007550	3.8592560	1.5285360	H	-5.4429140	-4.4282420	-0.7930750
C	-0.3975010	4.0289280	1.9411680	H	-7.8906880	-4.2513720	-0.2579010
C	-1.2734610	2.9186370	2.0180980	H	-7.1375460	-0.6311060	1.9075750
C	-0.8341800	1.6658400	1.6670790	H	-4.7070380	-0.8016900	1.3698540
C	2.6507670	-1.3983970	-0.0146000	H	-3.7984030	3.9722570	-0.8844530
C	1.8334150	-2.1254490	-0.8733940	H	-0.2779240	6.2889000	-1.7333570
C	2.1865980	-3.4494000	-1.2872300	H	1.0263080	4.1629390	-1.9744090
C	3.3915320	-4.0251330	-0.8126290	H	-0.0789740	1.9773580	-1.6795700
C	4.1910240	-3.2861490	0.0924470	H	-0.7588110	5.0174710	2.2091660
C	3.8389650	-2.0196010	0.5015720	H	1.5758870	4.7094330	1.4641060
C	1.3540420	-4.1908650	-2.1625680	H	3.3482060	3.2318530	0.5419330
C	1.7153030	-5.4550590	-2.5589150	H	5.3837430	2.2221150	1.2244720
C	2.9221070	-6.0321170	-2.0937230	H	7.6652110	2.1368600	0.2733620
C	3.7376850	-5.3348030	-1.2383190	H	8.0975640	0.8435990	-1.8057420
O	0.7209400	-1.6018320	-1.4165410	H	6.2173830	-0.3208200	-2.9392480
B	-0.3906890	-1.1612320	-0.5803800	H	3.9343110	-0.1982810	-2.0035120
O	0.0721360	-0.8266270	0.7834590	H	6.5240800	-1.8652560	0.4713800
C	4.7126470	-1.3557450	1.5076740	H	8.0184350	-0.8411580	2.1547890
C	4.1804820	-0.7090480	2.6297840	H	7.0537850	0.3088280	4.1376920
C	5.0182820	-0.1142570	3.5682550	H	4.5871910	0.3827320	4.4324120
C	6.4021970	-0.1598780	3.4060070	H	3.1033390	-0.6742760	2.7631460
C	6.9421510	-0.8101170	2.2990120	H	5.0793250	-3.7551150	0.5078710
C	6.1038310	-1.4006780	1.3592980	H	4.6615420	-5.7745060	-0.8703710
O	-1.4174460	-2.1953730	-0.4451250	H	3.1973150	-7.0331760	-2.4130310
B	-2.6913420	-1.8218620	-0.3014260	H	0.4286530	-3.7338760	-2.4955130
O	-3.1257590	-0.5146650	-0.4336460	H	-2.2979530	3.0645410	2.3474800
B	-2.2039700	0.4052960	-0.9161910	N	-2.8717210	6.4570050	-1.1488760
O	-2.7158310	1.6865350	-1.0682690	N	-9.0451110	-2.3235890	1.1633110
C	-2.0129370	2.8313290	-1.2697710	O	-9.7924540	-3.1946160	0.7462620
C	-0.6495140	2.8922790	-1.5850590	O	-2.2896070	7.5199120	-1.2906020
C	-0.0346490	4.1317950	-1.7474290	O	-9.4150990	-1.3708100	1.8305860
C	-0.7428080	5.3193850	-1.6117370	O	-4.0577650	6.3596580	-0.8835890

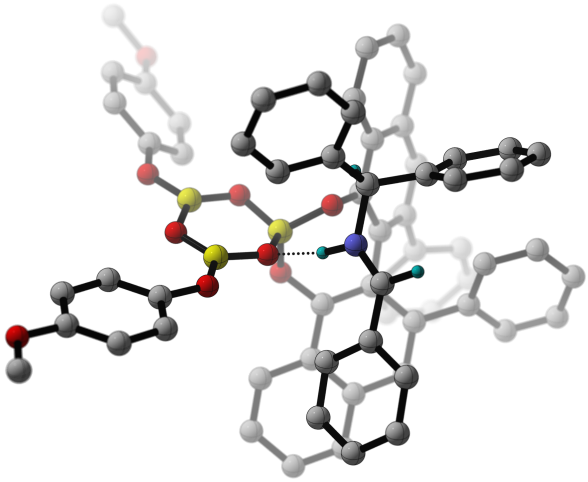
Figure SI-1 Catalyst-imine structures used to determine the H-bond distances seen in Table 4.



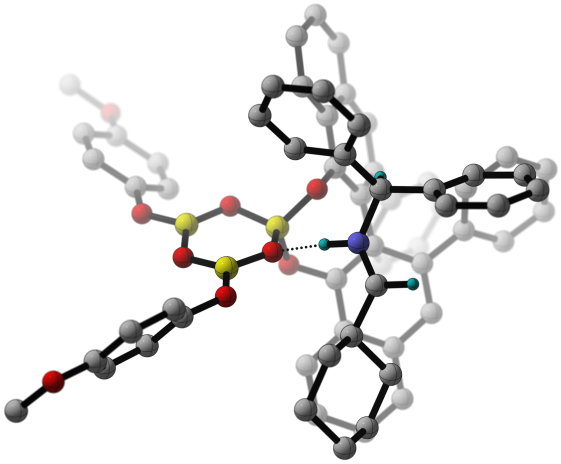
Boroxinate-H-Imine Complex **4a**



Boroxinate-H-Imine Complex **4e**

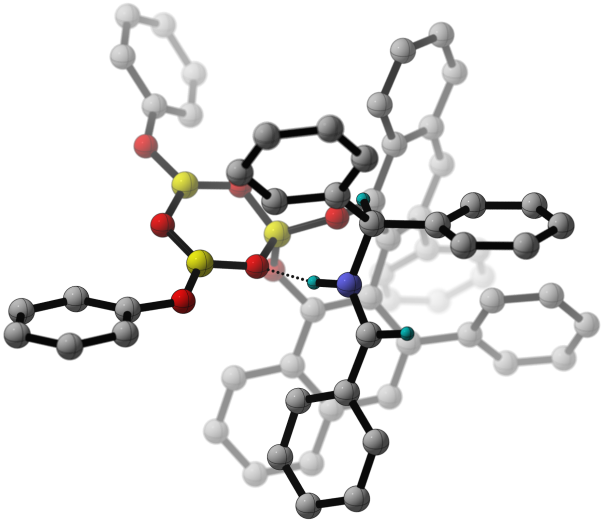


Boroxinate-H-Imine Complex **4b**

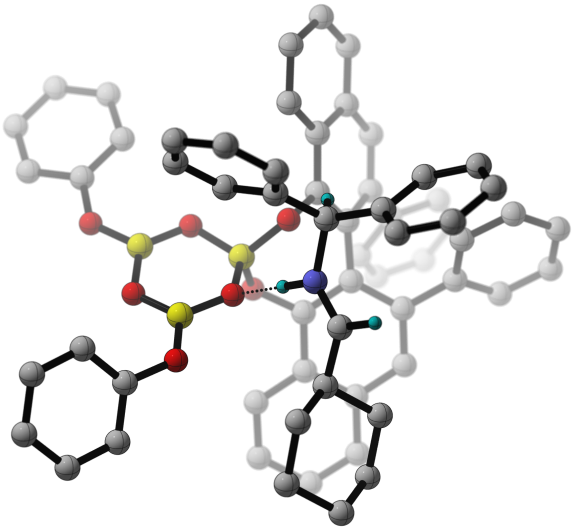


Boroxinate-H-Imine Complex **4f**

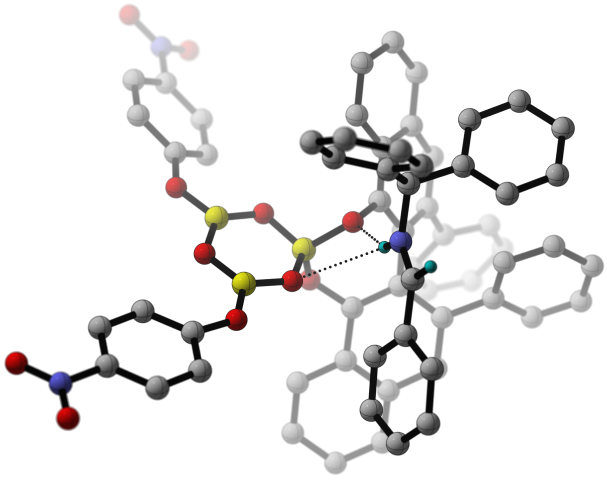
Figure SI-1 (Cont'd)



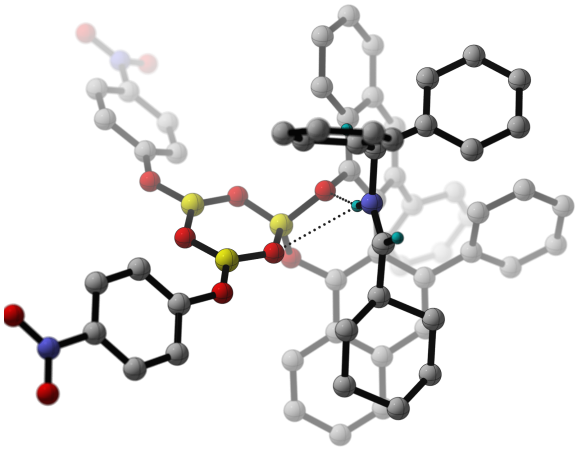
Boroxinate-H-Imine Complex **4c**



Boroxinate-H-Imine Complex **4g**



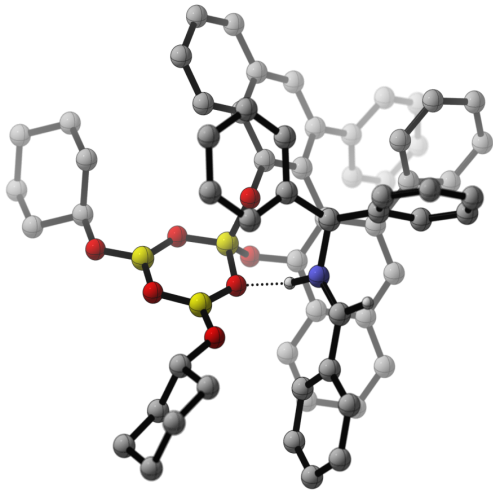
Boroxinate-H-Imine Complex **4d**



Boroxinate-H-Imine Complex **4h**

Coordinates Used for Hydrogen Bonding Interactions in the Catalyst-Iminium Complex:

Optimizations of catalyst-borox-iminium complexes were carried out at the M06-2X/6-31G* level of theory as implemented by the Gaussian 16 software package with bulk solvent effects accounted for with the self-consistent reaction field polarizable continuum model (PCM) as implemented for toluene.



Boroxinate-H-Iminium Complex **4a**

File Name: catim4a

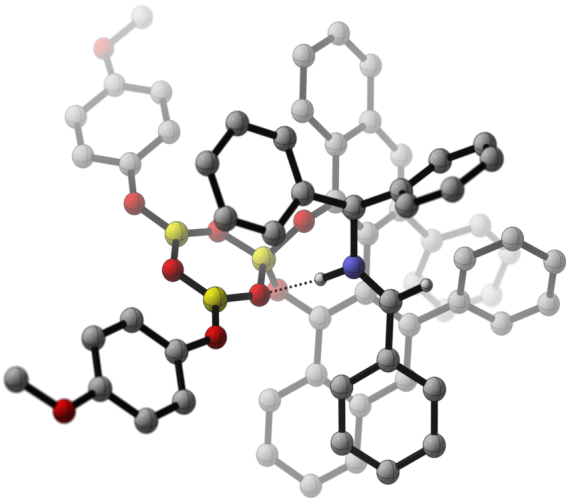
RRHO Thermochemistry (T = 298)
Zero-point correction (RRHO)= 1.126118 (Hartree/Particle)
Thermal correction to Energy (RRHO)= 1.187473
Thermal correction to Enthalpy (RRHO)= 1.188417
Thermal correction to Gibbs Free Energy (RRHO)= 1.026235
Sum of electronic and zero-point Energies (RRHO)= -3129.018780
Sum of electronic and thermal Energies (RRHO)= -3128.957425
Sum of electronic and thermal Enthalpies (RRHO)= -3128.956481
Sum of electronic and thermal Free Energies (RRHO)= -3129.118663

Quasi-RRHO Thermochemistry (T = 298, v0 = 100 cm-1)
Zero-point correction (QRRHO)= 1.126118 (Hartree/Particle)
Thermal correction to Energy (QRRHO)= 1.187473
Thermal correction to Enthalpy (QRRHO)= 1.188417
Thermal correction to Gibbs Free Energy (QRRHO)= 1.042350
Sum of electronic and zero-point Energies (QRRHO)= -3129.018780
Sum of electronic and thermal Energies (QRRHO)= -3128.957425
Sum of electronic and thermal Enthalpies (QRRHO)= -3128.956481
Sum of electronic and thermal Free Energies (QRRHO)= -3129.102548

Quasi-harmonic Thermochemistry (T = 298, cutoff = 100 cm-1)
Zero-point correction (QHO)= 1.126118 (Hartree/Particle)
Thermal correction to Energy (QHO)= 1.187795
Thermal correction to Enthalpy (QHO)= 1.188417
Thermal correction to Gibbs Free Energy (QHO)= 1.045486
Sum of electronic and zero-point Energies (QHO)= -3129.018780
Sum of electronic and thermal Energies (QHO)= -3128.957103
Sum of electronic and thermal Enthalpies (QHO)= -3128.956481
Sum of electronic and thermal Free Energies (QHO)= -3129.099412

C	4.0197040	-1.1760430	1.0080360	B	-2.9171400	0.3451040	-0.3057560
C	3.9513690	-1.6441280	-0.3108010	O	-3.4554530	1.6062740	-0.3073170
C	5.0487520	-2.3444640	-0.8256590	B	-2.6289780	2.6725890	-0.6705980
C	6.1809570	-2.5703500	-0.0496200	O	-3.2337330	3.8943360	-0.7231350
C	6.2356680	-2.1015340	1.2604060	O	-3.6459560	-0.7537730	0.0664490
C	5.1491640	-1.4052030	1.7866280	O	-1.3236740	2.4914180	-0.9633130
C	2.7406680	-1.4573590	-1.1594990	N	-0.7293460	-2.0423670	0.7753840
C	2.0246670	-0.2135690	-1.2260590	C	-1.2798160	-3.2042220	0.7687090
C	0.8783850	-0.1406100	-2.0084090	C	-2.2555000	-3.6838230	-0.1891120
C	0.4408190	-1.2464700	-2.7994460	C	-2.9315050	-4.8708500	0.1317590
C	1.1517490	-2.4704580	-2.7207520	C	-3.9061660	-5.3675140	-0.7226820
C	2.2888990	-2.5458930	-1.8780940	C	-4.1860660	-4.6929080	-1.9113920
C	0.6911760	-3.5752260	-3.4864850	C	-3.4921100	-3.5291100	-2.2478750
C	-0.3953120	-3.4488050	-4.3154080	C	-2.5318440	-3.0147370	-1.3890310
C	-1.0787320	-2.2113750	-4.4175980	C	0.2553600	-1.5801600	1.7831580
C	-0.6776360	-1.1346880	-3.6655690	C	0.8835280	-2.7483000	2.5234760
H	-1.9240050	-2.1198870	-5.0936510	C	0.5133360	-3.0812390	3.8274170
C	2.4274360	1.0134710	-0.4821410	C	1.0995450	-4.1742070	4.4642650
C	1.4565960	1.6297470	0.2961480	C	2.0573110	-4.9385480	3.8036840
C	1.7665910	2.7562110	1.1174410	C	2.4246060	-4.6148650	2.4979960
C	3.0886100	3.2685900	1.1089890	C	1.8359670	-3.5287320	1.8602500
C	4.0529670	2.6620780	0.2656840	C	-0.3700050	-0.5341060	2.6893960
C	3.7488290	1.5738330	-0.5212980	C	0.4895200	0.2537510	3.4587610
C	0.7811850	3.3622680	1.9351140	C	-0.0221910	1.2160740	4.3196110
C	1.1007670	4.4466310	2.7154370	C	-1.4010230	1.4108980	4.4109740
C	2.4184300	4.9665520	2.7089520	C	-2.2584150	0.6315840	3.6420390
C	3.3879510	4.3914940	1.9253100	C	-1.7462670	-0.3474690	2.7886500
H	-0.2191370	2.9406700	1.9290500	H	2.6592670	5.8261080	3.3274850
O	0.2029370	1.1413460	0.3539170	H	4.3995970	4.7892150	1.9148550
B	-0.6560550	1.2171590	-0.8472580	H	5.0469600	3.0986120	0.2117610
O	0.1439580	0.9884680	-2.0531510	H	6.3134150	1.0779820	0.1255360
C	4.8105900	1.0295730	-1.4101210	H	8.1152910	0.2061430	-1.3260660
C	6.1096620	0.8558730	-0.9183730	H	7.6282700	-0.3914040	-3.6895770
C	7.1181950	0.3506960	-1.7318530	H	5.3367420	-0.0622350	-4.5915040
C	6.8441480	0.0095640	-3.0542300	H	3.5499050	0.8434730	-3.1449370
C	5.5569350	0.1887170	-3.5581110	H	5.0256660	-2.6735680	-1.8606510
C	4.5487800	0.6972930	-2.7447570	H	7.0283660	-3.0987690	-0.4763270
O	-1.6265130	0.1048860	-0.6664680	H	7.1196510	-2.2732480	1.8670760

H	5.1788550	-1.0388220	2.8083650	H	-4.1313390	6.3207000	-0.7128950
H	3.1854090	-0.6200630	1.4269190	H	-3.9921570	5.7788700	-2.3879580
H	2.8137190	-3.4948890	-1.7957170	C	-0.8620420	6.7876730	-0.2069300
H	1.2251920	-4.5193650	-3.4143510	H	-2.3037220	5.6729180	0.9674500
H	-0.7317500	-4.2975620	-4.9032740	H	-0.9302540	4.7039070	0.4015060
H	1.0224270	-1.0807770	1.1777230	C	-1.8173680	7.8913280	-0.6683000
H	-1.0266630	-1.2931590	0.0986020	H	-3.3611140	8.2025360	-2.1664350
H	-0.9806000	-3.8839310	1.5653430	H	-1.9939680	7.2380650	-2.7156790
H	-2.6967000	-5.3910610	1.0564880	H	-0.2845310	7.1121350	0.6656190
H	-4.4391990	-6.2777320	-0.4703130	H	-0.1356370	6.5813640	-1.0048100
H	-4.9415410	-5.0834720	-2.5862850	H	-1.2591530	8.7967760	-0.9311520
H	-3.6977890	-3.0194100	-3.1835080	H	-2.4878900	8.1576190	0.1608300
H	-1.9976920	-2.1062250	-1.6511020	C	-5.0425150	-0.6849170	0.3276010
H	-0.2228110	-2.4773620	4.3495400	C	-5.8221520	-0.5353620	-0.9760880
H	2.1152810	-3.2759470	0.8402330	C	-5.4285390	-1.9715130	1.0476040
H	-2.4296970	-0.9395910	2.1868530	H	-5.2498430	0.1816930	0.9729410
H	1.5655190	0.1162790	3.3741180	C	-7.3313260	-0.5934040	-0.7263170
H	0.3414460	4.9102880	3.3388500	H	-5.5205690	-1.3597130	-1.6379060
H	-1.1909790	-0.1805830	-3.7166450	H	-5.5396600	0.4045060	-1.4618310
H	0.6563010	1.8321460	4.9012300	C	-6.9358900	-2.0334450	1.3041270
H	-1.8010780	2.1723200	5.0731500	H	-5.1211230	-2.8141650	0.4107280
H	-3.3325330	0.7804540	3.6997900	H	-4.8637680	-2.0502780	1.9848130
H	3.1757510	-5.2012860	1.9783910	C	-7.7182370	-1.8861810	-0.0036110
H	2.5196100	-5.7829700	4.3053150	H	-7.8714550	-0.5056320	-1.6747480
H	0.8103780	-4.4220040	5.4806780	H	-7.6302000	0.2669850	-0.1120670
C	-2.4591680	5.0399950	-1.0694120	H	-7.1935570	-2.9734100	1.8035270
C	-3.4165690	6.1334550	-1.5259040	H	-7.2226220	-1.2224390	1.9878090
C	-1.6239280	5.5015720	0.1203710	H	-8.7956900	-1.9070620	0.1924240
H	-1.7801470	4.7793340	-1.8935630	H	-7.4929290	-2.7432520	-0.6541210
C	-2.6577960	7.4210120	-1.8592930				



Boronxinate-H-Iminium Complex **4b**

File Name: catim4b

RRHO Thermochemistry (T = 298)
Zero-point correction (RRHO)= 1.050135 (Hartree/Particle)
Thermal correction to Energy (RRHO)= 1.114383
Thermal correction to Enthalpy (RRHO)= 1.115327
Thermal correction to Gibbs Free Energy (RRHO)= 0.943116
Sum of electronic and zero-point Energies (RRHO)= -3350.819070
Sum of electronic and thermal Energies (RRHO)= -3350.754822
Sum of electronic and thermal Enthalpies (RRHO)= -3350.753878
Sum of electronic and thermal Free Energies (RRHO)= -3350.926089

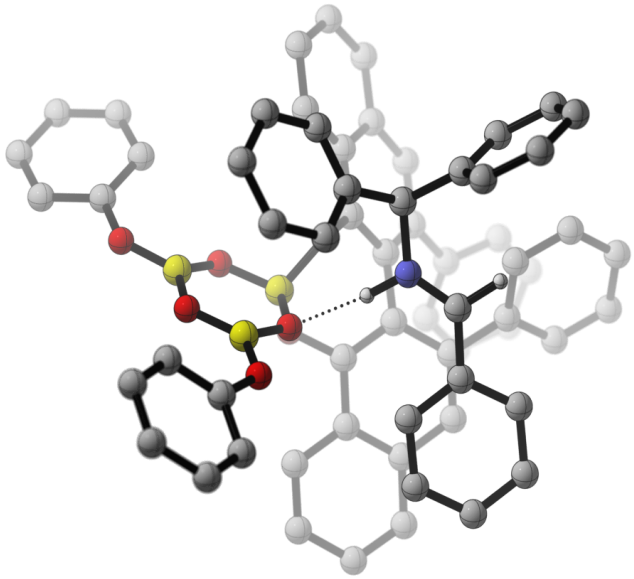
Quasi-RRHO Thermochemistry (T = 298, v0 = 100 cm-1)
Zero-point correction (QRRHO)= 1.050135 (Hartree/Particle)
Thermal correction to Energy (QRRHO)= 1.114383
Thermal correction to Enthalpy (QRRHO)= 1.115327
Thermal correction to Gibbs Free Energy (QRRHO)= 0.962060
Sum of electronic and zero-point Energies (QRRHO)= -3350.819070
Sum of electronic and thermal Energies (QRRHO)= -3350.754822
Sum of electronic and thermal Enthalpies (QRRHO)= -3350.753878
Sum of electronic and thermal Free Energies (QRRHO)= -3350.907145

Quasi-harmonic Thermochemistry (T = 298, cutoff = 100 cm-1)
Zero-point correction (QHO)= 1.050135 (Hartree/Particle)
Thermal correction to Energy (QHO)= 1.114733
Thermal correction to Enthalpy (QHO)= 1.115327
Thermal correction to Gibbs Free Energy (QHO)= 0.967060
Sum of electronic and zero-point Energies (QHO)= -3350.819070

Sum of electronic and thermal Energies (QHO)= -3350.754472
Sum of electronic and thermal Enthalpies (QHO)= -3350.753878
Sum of electronic and thermal Free Energies (QHO)= -3350.902145

C	3.9660350	-0.8420480	1.1401780	C	-2.6808420	4.4157770	-0.6401980
C	4.2695540	-1.1470320	-0.1937790	O	-3.0660230	-2.1524830	-0.5262230
C	5.5690740	-1.5729200	-0.4960670	C	-4.3384260	-2.6614460	-0.4727080
C	6.5304010	-1.7004070	0.5001670	C	-5.4831910	-1.9082330	-0.2297940
C	6.2118560	-1.4074510	1.8247030	C	-6.7299630	-2.5358470	-0.1602320
C	4.9254410	-0.9755040	2.1403100	C	-6.8357780	-3.9149180	-0.3302340
C	3.2327580	-1.0898320	-1.2577650	C	-5.6808290	-4.6677370	-0.5690180
C	2.2223310	-0.0664570	-1.2923510	C	-4.4464840	-4.0455410	-0.6381450
C	1.1469640	-0.2246820	-2.1589730	O	-1.7383870	1.7055380	-1.1917860
C	1.1066110	-1.2976690	-3.1040770	N	0.3379440	-1.4719290	1.4873150
C	2.1933370	-2.2046890	-3.1622890	C	1.1367950	-2.4794970	1.4463350
C	3.2167930	-2.1026860	-2.1892420	C	1.2397460	-3.4157480	0.3464560
C	2.1766400	-3.2325310	-4.1407630	C	2.3284430	-4.2995180	0.3593880
C	1.1143220	-3.3637990	-4.9999070	C	2.4577250	-5.2494320	-0.6446890
C	0.0141900	-2.4747600	-4.9157700	C	1.4917960	-5.3274870	-1.6472970
C	0.0115170	-1.4600940	-3.9894890	C	0.4030690	-4.4537600	-1.6578750
H	-0.8248520	-2.5939790	-5.5943370	C	0.2720720	-3.4907380	-0.6696200
C	2.3249680	1.2026920	-0.5159510	C	0.1436410	-0.5516910	2.6329560
C	1.2111690	1.6601880	0.1712130	C	0.8617280	-1.0205710	3.8789870
C	1.2487920	2.8473420	0.9638790	C	0.3755340	-2.0884730	4.6392510
C	2.4583970	3.5794530	1.0496530	C	1.0635380	-2.5087580	5.7722730
C	3.5782450	3.1265280	0.3101910	C	2.2348020	-1.8578820	6.1614010
C	3.5292030	1.9903060	-0.4671390	C	2.7166150	-0.7869620	5.4145170
C	0.1007640	3.2996380	1.6626340	C	2.0328220	-0.3721350	4.2724280
C	0.1583440	4.4410810	2.4253900	C	-1.3462240	-0.3311560	2.8235900
C	1.3672210	5.1737060	2.5202880	C	-1.7664530	0.8575070	3.4247150
C	2.4878770	4.7540570	1.8470260	C	-3.1210480	1.1075560	3.6125280
H	-0.8155850	2.7246910	1.5687760	C	-4.0689920	0.1687760	3.2050080
O	0.0658890	0.9514250	0.2104940	C	-3.6544340	-1.0238290	2.6209890
B	-0.7268440	0.6873690	-1.0049700	C	-2.2950020	-1.2759990	2.4336540
O	0.1287640	0.6584260	-2.1854220	H	-5.4104490	-0.8361850	-0.0997910
C	4.7447110	1.6495600	-1.2568900	H	-7.6069010	-1.9271100	0.0260780
C	6.0045050	1.7048290	-0.6493560	H	-5.7772970	-5.7407070	-0.6980880
C	7.1585690	1.4186090	-1.3710610	H	-3.5426390	-4.6179620	-0.8221580
C	7.0708280	1.0689480	-2.7163850	H	-5.5942120	4.0571070	-2.3240820
C	5.8219340	1.0166280	-3.3339010	H	-5.3353330	6.5431600	-2.4802380
C	4.6683680	1.3072230	-2.6121530	H	-1.6650980	6.2591990	-0.2685690
O	-1.3221330	-0.6484320	-0.7412220	H	-1.9237320	3.8282070	-0.1365790
B	-2.6628920	-0.8475430	-0.7237910	H	1.4026170	6.0743700	3.1256720
O	-3.5555920	0.1784780	-0.9012140	H	3.4149610	5.3180070	1.9105790
B	-3.0523950	1.4645400	-1.0807050	H	4.4857700	3.7243690	0.3208710
O	-4.0185610	2.4414720	-1.1329310	H	6.0694230	1.9354770	0.4107230
C	-3.7785230	3.7905160	-1.2208600	H	8.1253180	1.4532520	-0.8773920
C	-4.7393560	4.5585820	-1.8820840	H	7.9690730	0.8398020	-3.2819230
C	-4.5982700	5.9340810	-1.9672580	H	5.7443750	0.7542840	-4.3847380
C	-3.4922550	6.5662660	-1.3899360	H	3.6986920	1.2689090	-3.1002720
C	-2.5348840	5.8012110	-0.7255970	H	5.8354880	-1.7583450	-1.5327770

H	7.5362750	-2.0153920	0.2386940	H	-0.7254250	4.7885940	2.9525500
H	6.9618640	-1.5060830	2.6034450	H	-0.8126410	-0.7585780	-3.9210030
H	4.6647170	-0.7443850	3.1692950	H	-3.4383550	2.0397250	4.0691460
H	2.9721230	-0.4785720	1.3899940	H	-5.1268600	0.3691220	3.3413500
H	3.9711070	-2.8839820	-2.1481890	H	-4.3840050	-1.7617780	2.3019390
H	3.0157520	-3.9229520	-4.1850280	H	3.6204160	-0.2692250	5.7206940
H	1.1102380	-4.1534980	-5.7454920	H	2.7652070	-2.1822400	7.0510080
H	0.5808390	0.3992240	2.3157470	H	0.6810490	-3.3375960	6.3592210
H	-0.2192810	-1.2113880	0.6487950	O	-3.4407610	7.9228000	-1.5273800
H	1.7617610	-2.6446780	2.3226350	O	-8.0037590	-4.6149540	-0.2800150
H	3.0732860	-4.2239490	1.1475150	C	-2.3226800	8.5818080	-0.9742730
H	3.3036430	-5.9284780	-0.6443890	H	-2.4532910	9.6412320	-1.1948900
H	1.5894340	-6.0704990	-2.4331370	H	-2.2725550	8.4401620	0.1122810
H	-0.3306230	-4.5047190	-2.4559500	H	-1.3877130	8.2278670	-1.4248830
H	-0.5772810	-2.8133600	-0.6878700	C	-9.1869240	-3.8795990	-0.0519800
H	-0.5491320	-2.5802110	4.3462750	H	-10.0008480	-4.6042620	-0.0540410
H	2.4022350	0.4687480	3.6878740	H	-9.1577210	-3.3678300	0.9175350
H	-1.9903550	-2.2060280	1.9601470	H	-9.3551700	-3.1400700	-0.8439050
H	-1.0256570	1.5919630	3.7325910				



Boroxinate-H-Iminium Complex **4c**

File Name: catim4c

RRHO Thermochemistry (T = 298)
Zero-point correction (RRHO)= 0.983779 (Hartree/Particle)
Thermal correction to Energy (RRHO)= 1.042875
Thermal correction to Enthalpy (RRHO)= 1.043819
Thermal correction to Gibbs Free Energy (RRHO)= 0.883672
Sum of electronic and zero-point Energies (RRHO)= -3121.931149

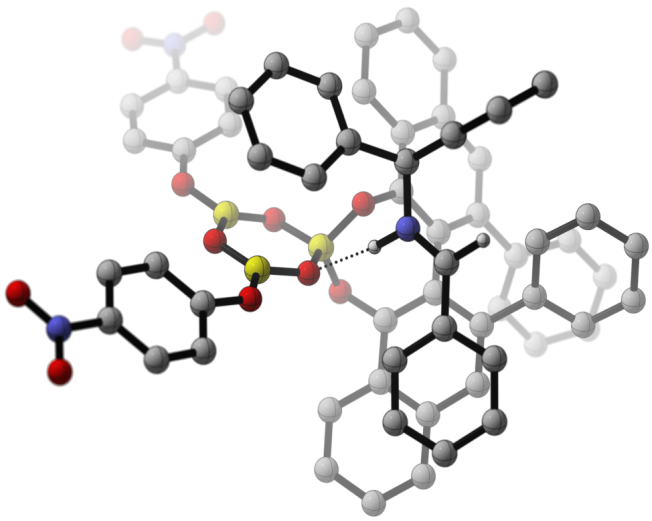
Sum of electronic and thermal Energies (RRHO)= -3121.872053
Sum of electronic and thermal Enthalpies (RRHO)= -3121.871109
Sum of electronic and thermal Free Energies (RRHO)= -3122.031256

Quasi-RRHO Thermochemistry (T = 298, v0 = 100 cm-1)
Zero-point correction (QRRHO)= 0.983779 (Hartree/Particle)
Thermal correction to Energy (QRRHO)= 1.042875
Thermal correction to Enthalpy (QRRHO)= 1.043819
Thermal correction to Gibbs Free Energy (QRRHO)= 0.900819
Sum of electronic and zero-point Energies (QRRHO)= -3121.931149
Sum of electronic and thermal Energies (QRRHO)= -3121.872053
Sum of electronic and thermal Enthalpies (QRRHO)= -3121.871109
Sum of electronic and thermal Free Energies (QRRHO)= -3122.014109

Quasi-harmonic Thermochemistry (T = 298, cutoff = 100 cm-1)
Zero-point correction (QHO)= 0.983779 (Hartree/Particle)
Thermal correction to Energy (QHO)= 1.043201
Thermal correction to Enthalpy (QHO)= 1.043819
Thermal correction to Gibbs Free Energy (QHO)= 0.905115
Sum of electronic and zero-point Energies (QHO)= -3121.931149
Sum of electronic and thermal Energies (QHO)= -3121.871727
Sum of electronic and thermal Enthalpies (QHO)= -3121.871109
Sum of electronic and thermal Free Energies (QHO)= -3122.009813

C	3.6317590	-0.1983350	1.2227850	C	-0.6106570	3.5726990	1.1436300
C	3.9945210	-0.6576970	-0.0508000	C	-0.6760140	4.8072140	1.7431610
C	5.3345370	-0.9979280	-0.2742720	C	0.4555970	5.6594780	1.7437390
C	6.2784920	-0.8932470	0.7410640	C	1.6234580	5.2628830	1.1405150
C	5.9020230	-0.4485920	2.0068720	H	-1.4676360	2.9061830	1.1224230
C	4.5740530	-0.0995520	2.2429280	O	-0.3915030	1.0542080	0.0275130
C	2.9824820	-0.8479800	-1.1231740	B	-1.1315900	0.5538390	-1.1439180
C	1.8797020	0.0574280	-1.3069690	O	-0.2564400	0.4425190	-2.3048800
C	0.8427430	-0.3226000	-2.1512510	C	4.2248720	1.9979500	-1.4950780
C	0.9277550	-1.5109900	-2.9430710	C	5.4623210	2.2567250	-0.8943050
C	2.0982790	-2.3054290	-2.8680370	C	6.6514190	1.9854290	-1.5630920
C	3.0844790	-1.9741280	-1.9074060	C	6.6219370	1.4468590	-2.8472900
C	2.2029950	-3.4519170	-3.6978680	C	5.3952790	1.1905220	-3.4582730
C	1.1787750	-3.8007740	-4.5424690	C	4.2064140	1.4661340	-2.7899820
C	-0.0032070	-3.0209620	-4.5908930	O	-1.6094260	-0.7827570	-0.7010940
C	-0.1253400	-1.8972910	-3.8098350	B	-2.9246390	-1.1061450	-0.6880280
H	-0.8105640	-3.3113200	-5.2560960	O	-3.9023480	-0.2074170	-1.0294810
C	1.8452120	1.4252620	-0.7139060	B	-3.5156680	1.0851530	-1.3722770
C	0.6802360	1.8612050	-0.1024680	O	-4.5688500	1.9440550	-1.5911930
C	0.5883110	3.1427580	0.5200500	C	-4.4679390	3.2841870	-1.8571140
C	1.7208480	3.9937330	0.5111720	C	-5.4887910	3.8437090	-2.6251640
C	2.8927920	3.5558550	-0.1531140	C	-5.4874790	5.2085810	-2.8926220
C	2.9675840	2.3251890	-0.7674240	C	-4.4719710	6.0226450	-2.3946310

C	-3.4584180	5.4553500	-1.6260600	H	-2.6586520	6.0754010	-1.2312340
C	-3.4478980	4.0907120	-1.3503340	H	-2.6487110	3.6529690	-0.7658280
O	-3.2137340	-2.4076770	-0.3235650	H	0.3932710	6.6335030	2.2193600
C	-4.4321320	-3.0262360	-0.2485300	H	2.4910250	5.9176680	1.1307510
C	-5.6450530	-2.3511130	-0.0917550	H	3.7386590	4.2350600	-0.2188670
C	-6.8224510	-3.0898980	0.0114330	H	5.4855670	2.6364810	0.1238050
C	-6.8056750	-4.4811630	-0.0357680	H	7.6013270	2.1803470	-1.0740500
C	-5.5890170	-5.1437720	-0.1873390	H	7.5481910	1.2290630	-3.3705570
C	-4.4062320	-4.4212000	-0.2917930	H	5.3623070	0.7795210	-4.4628020
O	-2.2279700	1.4385460	-1.4782580	H	3.2537190	1.2672870	-3.2725100
N	0.0756300	-1.1142010	1.6463630	H	5.6428640	-1.3019170	-1.2705560
C	0.9721040	-2.0292990	1.7637110	H	7.3151000	-1.1458670	0.5385950
C	1.2060980	-3.0913260	0.8073500	H	6.6385500	-0.3659650	2.8002040
C	2.3737420	-3.8508190	0.9688480	H	4.2674470	0.2485750	3.2253130
C	2.6324080	-4.9096140	0.1090210	H	2.6033700	0.1029340	1.4065360
C	1.7179270	-5.2187440	-0.8971930	H	3.9084480	-2.6656450	-1.7527250
C	0.5516700	-4.4680930	-1.0555010	H	3.1055040	-4.0559150	-3.6396950
C	0.2903900	-3.3991240	-0.2127750	H	1.2682950	-4.6795360	-5.1743520
C	-0.2519280	-0.0698700	2.6461710	H	0.0909270	0.8696120	2.2034580
C	0.4752390	-0.2789850	3.9558540	H	-0.4766200	-1.0319370	0.7701480
C	0.0688030	-1.2604040	4.8646540	H	1.5799590	-2.0064100	2.6669760
C	0.7684970	-1.4440390	6.0525030	H	3.0768300	-3.5947910	1.7572020
C	1.8714420	-0.6416800	6.3463320	H	3.5392810	-5.4935860	0.2239950
C	2.2732390	0.3442400	5.4498890	H	1.9169370	-6.0469110	-1.5707470
C	1.5780720	0.5221480	4.2545930	H	-0.1416480	-4.6984960	-1.8581120
C	-1.7623120	0.0088090	2.7774870	H	-0.6180060	-2.8182100	-0.3475570
C	-2.3277820	1.2164770	3.1930990	H	-0.8041540	-1.8698280	4.6432970
C	-3.7070330	1.3386940	3.3182360	H	1.8837330	1.2966910	3.5531860
C	-4.5346100	0.2525070	3.0331990	H	-2.1726280	-2.0284870	2.1802030
C	-3.9749500	-0.9572150	2.6347700	H	-1.6809200	2.0646490	3.4055180
C	-2.5909150	-1.0806860	2.5098670	H	-1.5988590	5.1367350	2.2115040
H	-5.6629360	-1.2694140	-0.0579820	H	-1.0149300	-1.2781780	-3.8456250
H	-7.7642830	-2.5625390	0.1297750	H	-4.1377490	2.2850570	3.6295500
H	-7.7301980	-5.0434940	0.0447350	H	-5.6118850	0.3512870	3.1201090
H	-5.5581420	-6.2284520	-0.2248560	H	-4.6103000	-1.8090950	2.4127970
H	-3.4474800	-4.9165570	-0.4091710	H	3.1224800	0.9800800	5.6803400
H	-6.2722130	3.1930670	-3.0000080	H	2.4106090	-0.7812010	7.2778790
H	-6.2850750	5.6356810	-3.4931320	H	0.4477890	-2.2062550	6.7553330
H	-4.4705650	7.0874250	-2.6045550				



Boroxinate-H-Iminium Complex **4d**

RRHO Thermochemistry (T = 298.15)
Zero-point correction (RRHO)= 1.147523 (Hartree/Particle)
Thermal correction to Energy (RRHO)= 1.208703
Thermal correction to Enthalpy (RRHO)= 1.209647
Thermal correction to Gibbs Free Energy (RRHO)= 1.046810
Sum of electronic and zero-point Energies (RRHO)= -3530.631429
Sum of electronic and thermal Energies (RRHO)= -3530.570249
Sum of electronic and thermal Enthalpies (RRHO)= -3530.569305
Sum of electronic and thermal Free Energies (RRHO)= -3530.732142

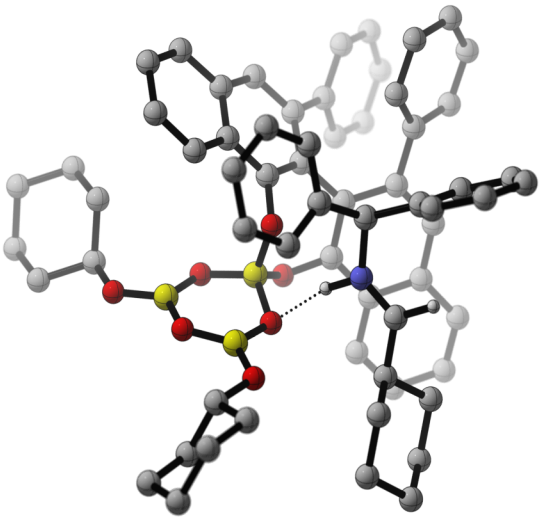
Quasi-RRHO Thermochemistry (T = 298.15, v0 = 100 cm-1)
Zero-point correction (QRRHO)= 1.147523 (Hartree/Particle)
Thermal correction to Energy (QRRHO)= 1.208703
Thermal correction to Enthalpy (QRRHO)= 1.209647
Thermal correction to Gibbs Free Energy (QRRHO)= 1.063021
Sum of electronic and zero-point Energies (QRRHO)= -3530.631429
Sum of electronic and thermal Energies (QRRHO)= -3530.570249
Sum of electronic and thermal Enthalpies (QRRHO)= -3530.569305
Sum of electronic and thermal Free Energies (QRRHO)= -3530.715931

Quasi-harmonic Thermochemistry (T = 298.15, cutoff = 100 cm-1)
Zero-point correction (QHO)= 1.147523 (Hartree/Particle)
Thermal correction to Energy (QHO)= 1.209009
Thermal correction to Enthalpy (QHO)= 1.209647
Thermal correction to Gibbs Free Energy (QHO)= 1.066733

Sum of electronic and zero-point Energies (QHO)= -3530.631429
Sum of electronic and thermal Energies (QHO)= -3530.569943
Sum of electronic and thermal Enthalpies (QHO)= -3530.569305
Sum of electronic and thermal Free Energies (QHO)= -3530.712219

C	4.1431110	-0.8235600	1.1098030	C	-3.5230060	6.4861170	-1.0798970
C	4.4334290	-1.1298860	-0.2268560	C	-2.4483070	5.7383280	-0.6137150
C	5.7337430	-1.5423510	-0.5439050	C	-2.5320490	4.3537370	-0.6194490
C	6.7083330	-1.6571590	0.4408580	O	-2.9383610	-2.2089760	-0.5494180
C	6.4026570	-1.3647500	1.7684090	C	-4.1964440	-2.7094610	-0.4845260
C	5.1159280	-0.9447390	2.0984810	C	-5.3357040	-1.9430890	-0.2046550
C	3.3853950	-1.0874660	-1.2807620	C	-6.5724670	-2.5684440	-0.1239220
C	2.3605330	-0.0776930	-1.3085260	C	-6.6572420	-3.9411910	-0.3188250
C	1.2845830	-0.2482890	-2.1715040	C	-5.5363840	-4.7173490	-0.5938900
C	1.2546530	-1.3158900	-3.1221360	C	-4.3037380	-4.0929720	-0.6740680
C	2.3521560	-2.2093160	-3.1852720	O	-1.6113010	1.6579160	-1.1767700
C	3.3760620	-2.0991640	-2.2136040	N	0.5657500	-1.4834880	1.5127930
C	2.3449710	-3.2358440	-4.1652910	C	1.3760950	-2.4831010	1.4895820
C	1.2828110	-3.3774590	-5.0229510	C	1.5072200	-3.4180560	0.3919590
C	0.1731530	-2.5005840	-4.9356220	C	2.6080530	-4.2862530	0.4155780
C	0.1601970	-1.4885280	-4.0066670	C	2.7608230	-5.2327370	-0.5885720
H	-0.6647420	-2.6269490	-5.6142610	C	1.8069190	-5.3230690	-1.6015040
C	2.4482290	1.1923010	-0.5310330	C	0.7061590	-4.4645140	-1.6227930
C	1.3318250	1.6305730	0.1625890	C	0.5518610	-3.5052350	-0.6346210
C	1.3457560	2.8236460	0.9450170	C	0.3179820	-0.5723500	2.6556760
C	2.5397580	3.5828620	1.0151950	C	1.0388680	-1.0198910	3.9067600
C	3.6653340	3.1462070	0.2745480	C	0.5643410	-2.0939090	4.6648300
C	3.6372880	2.0036390	-0.4942490	C	1.2580360	-2.5090470	5.7964880
C	0.1914340	3.2605680	1.6438570	C	2.4236810	-1.8473120	6.1834470
C	0.2279080	4.4139940	2.3895570	C	2.8945960	-0.7707540	5.4366860
C	1.4208450	5.1741430	2.4679910	C	2.2050630	-0.3603640	4.2966890
C	2.5474020	4.7686700	1.7961670	C	-1.1833870	-0.4221970	2.8227210
H	-0.7140970	2.6667620	1.5616100	C	-1.6736140	0.7537730	3.3950120
O	0.1991040	0.8948580	0.2097470	C	-3.0419940	0.9346590	3.5635710
B	-0.5891530	0.6370060	-1.0026860	C	-3.9337350	-0.0628740	3.1693530
O	0.2504400	0.6200060	-2.1881120	C	-3.4484570	-1.2441780	2.6171700
C	4.8558700	1.6809840	-1.2865690	C	-2.0760020	-1.4244510	2.4433970
C	6.1160240	1.7613780	-0.6827190	H	-5.2496870	-0.8752610	-0.0559050
C	7.2726560	1.4894980	-1.4058260	H	-7.4702740	-2.0018160	0.0904030
C	7.1870280	1.1297170	-2.7486280	H	-5.6417010	-5.7852560	-0.7389800
C	5.9376570	1.0532880	-3.3625830	H	-3.4015980	-4.6568990	-0.8845490
C	4.7813890	1.3292840	-2.6395150	H	-5.6572320	3.9982030	-1.9123970
O	-1.1890380	-0.7019590	-0.7469590	H	-5.5019190	6.5046360	-1.9115860
B	-2.5225110	-0.8941760	-0.7179490	H	-1.5583020	6.2382760	-0.2508020
O	-3.4226780	0.1301870	-0.8685050	H	-1.6977340	3.7572450	-0.2762750
B	-2.9168120	1.4124440	-1.0455380	H	1.4379050	6.0857120	3.0571810
O	-3.8930780	2.3927600	-1.0801330	H	3.4613970	5.3546630	1.8456200
C	-3.6966970	3.7357600	-1.0907580	H	4.5598620	3.7633440	0.2757520
C	-4.7681780	4.5065650	-1.5565940	H	6.1802330	2.0004270	0.3755120
C	-4.6857770	5.8885570	-1.5553300	H	8.2399770	1.5436490	-0.9151850

H	8.0873980	0.9120380	-3.3152280	H	-0.3544070	-2.5955840	4.3676870
H	5.8617640	0.7837910	-4.4117150	H	2.5640150	0.4859580	3.7133920
H	3.8114900	1.2727600	-3.1254470	H	-1.7135450	-2.3487570	1.9996690
H	5.9900970	-1.7262440	-1.5833620	H	-0.9767850	1.5316200	3.6984050
H	7.7144280	-1.9612730	0.1678370	H	-0.6606700	4.7514680	2.9150220
H	7.1630720	-1.4534400	2.5381320	H	-0.6719120	-0.7966500	-3.9365260
H	4.8661300	-0.7123430	3.1298270	H	-3.4136470	1.8567350	3.9989710
H	3.1498810	-0.4672740	1.3714700	H	-5.0020920	0.0802220	3.2959320
H	4.1391750	-2.8720400	-2.1770700	H	-4.1347440	-2.0314920	2.3212570
H	3.1921220	-3.9160320	-4.2130910	H	3.7938080	-0.2451040	5.7427530
H	1.2865820	-4.1652010	-5.7704600	H	2.9590430	-2.1674880	7.0715510
H	0.7168870	0.3974640	2.3442830	H	0.8851540	-3.3424590	6.3830600
H	0.0246490	-1.2264620	0.6680570	N	-3.4325320	7.9442120	-1.0662220
H	1.9841010	-2.6402280	2.3790610	N	-7.9633110	-4.5915390	-0.2268610
H	3.3428650	-4.2023060	1.2120130	O	-8.0107500	-5.7990010	-0.3923870
H	3.6161110	-5.8997850	-0.5802940	O	-8.9305840	-3.8948880	0.0295210
H	1.9234700	-6.0634240	-2.3872090	O	-4.3867050	8.5794170	-1.4845020
H	-0.0169510	-4.5234780	-2.4301040	O	-2.4094170	8.4495580	-0.6352330
H	-0.3053990	-2.8380420	-0.6634330				



Boroxinate-H-Iminium Complex **4e**

File Name: catim4e

RRHO Thermochemistry (T = 298)
Zero-point correction (RRHO)= 1.197594 (Hartree/Particle)
Thermal correction to Energy (RRHO)= 1.260170
Thermal correction to Enthalpy (RRHO)= 1.261114
Thermal correction to Gibbs Free Energy (RRHO)= 1.096845
Sum of electronic and zero-point Energies (RRHO)= -3132.564481

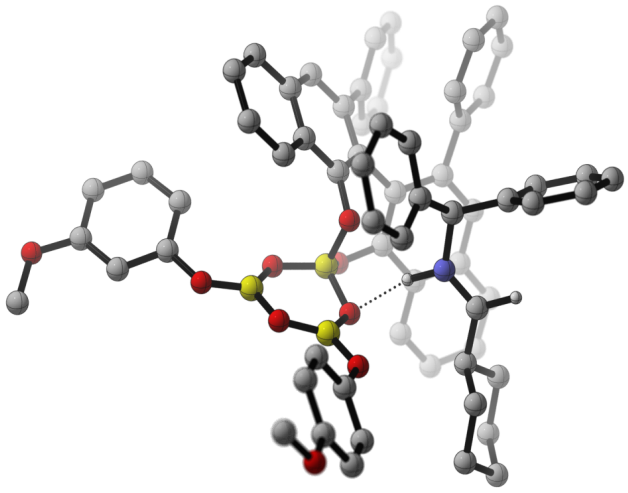
Sum of electronic and thermal Energies (RRHO)= -3132.501905
Sum of electronic and thermal Enthalpies (RRHO)= -3132.500961
Sum of electronic and thermal Free Energies (RRHO)= -3132.665230

Quasi-RRHO Thermochemistry (T = 298, v0 = 100 cm-1)
Zero-point correction (QRRHO)= 1.197594 (Hartree/Particle)
Thermal correction to Energy (QRRHO)= 1.260170
Thermal correction to Enthalpy (QRRHO)= 1.261114
Thermal correction to Gibbs Free Energy (QRRHO)= 1.113037
Sum of electronic and zero-point Energies (QRRHO)= -3132.564481
Sum of electronic and thermal Energies (QRRHO)= -3132.501905
Sum of electronic and thermal Enthalpies (QRRHO)= -3132.500961
Sum of electronic and thermal Free Energies (QRRHO)= -3132.649038

Quasi-harmonic Thermochemistry (T = 298, cutoff = 100 cm-1)
Zero-point correction (QHO)= 1.197594 (Hartree/Particle)
Thermal correction to Energy (QHO)= 1.260497
Thermal correction to Enthalpy (QHO)= 1.261114
Thermal correction to Gibbs Free Energy (QHO)= 1.116060
Sum of electronic and zero-point Energies (QHO)= -3132.564481
Sum of electronic and thermal Energies (QHO)= -3132.501578
Sum of electronic and thermal Enthalpies (QHO)= -3132.500961
Sum of electronic and thermal Free Energies (QHO)= -3132.646015

C	4.0065340	-0.8522870	1.4627390	C	3.4320480	1.8116670	-0.1312470
C	4.2045610	-1.2995620	0.1496420	C	-0.0780500	2.9055670	2.0035290
C	5.4795150	-1.7524910	-0.2116340	C	-0.0628570	4.0023720	2.8287460
C	6.5236790	-1.7602080	0.7068720	C	1.1058560	4.7953790	2.9401700
C	6.3129770	-1.3150470	2.0094150	C	2.2440720	4.4606490	2.2480570
C	5.0494350	-0.8618480	2.3834360	H	-0.9644070	2.2850900	1.9008520
C	3.1040720	-1.3393270	-0.8556830	O	-0.0590830	0.7446250	0.2377450
C	2.1651440	-0.2635630	-1.0238040	B	-0.7067790	0.9060760	-1.0932210
C	1.1304480	-0.4123280	-1.9433880	O	0.2327340	0.5658510	-2.1554960
C	1.0294490	-1.5775520	-2.7682840	C	4.6762360	1.4966230	-0.8823620
C	1.9949760	-2.6067970	-2.6282970	C	5.9172540	1.5766270	-0.2400540
C	2.9996540	-2.4701600	-1.6387080	C	7.0932100	1.2870110	-0.9236710
C	1.9268140	-3.7314170	-3.4942350	C	7.0476090	0.9118620	-2.2643000
C	0.9574780	-3.8113130	-4.4636900	C	5.8181500	0.8397890	-2.9172670
C	-0.0080750	-2.7827720	-4.5950500	C	4.6419090	1.1324160	-2.2338310
C	0.0178760	-1.6944730	-3.7563980	O	-1.8173480	-0.0759620	-1.0261540
H	-0.7717150	-2.8599330	-5.3632330	B	-3.0144400	0.3504700	-0.5324280
C	2.2457340	1.0108520	-0.2522040	O	-3.3161910	1.6863820	-0.4072720
C	1.0953230	1.4257270	0.3995210	B	-2.4009800	2.6275930	-0.8839890
C	1.0843240	2.5496010	1.2753170	O	-2.8344640	3.9191120	-0.9188480
C	2.2690630	3.3165740	1.4071050	O	-3.9223630	-0.6070950	-0.1478290
C	3.4203740	2.9278280	0.6761510	O	-1.1754630	2.2517630	-1.3095180

N	-0.6575860	-2.0517990	0.6050720	H	-2.1316810	-2.4206810	-1.4145170
C	-1.0657520	-3.2027500	0.2272270	C	-2.4991270	-4.6149130	-3.0232570
C	0.2065880	-1.7437630	1.7648370	H	-1.3632960	-5.3954410	-1.3544430
C	0.7143450	-3.0072410	2.4293570	H	-0.5138490	-4.1461010	-2.2780560
C	0.0331640	-3.5900350	3.5003770	C	-4.3801350	-3.9876270	-1.4533360
C	0.4993980	-4.7759480	4.0620690	H	-3.2505370	-4.7637890	0.2237770
C	1.6478530	-5.3839440	3.5589090	H	-3.7216490	-3.0587130	0.3924900
C	2.3286940	-4.8070180	2.4889120	C	-3.8823740	-4.9991980	-2.4903950
C	1.8615040	-3.6238580	1.9237260	H	-2.1326480	-5.3684110	-3.7289170
C	-0.5228900	-0.7966170	2.7028260	H	-2.5687520	-3.6688570	-3.5760220
C	0.2335140	-0.1321700	3.6700780	H	-5.3454910	-4.3048250	-1.0433180
C	-0.3781900	0.7362970	4.5668150	H	-4.5368140	-3.0091240	-1.9271240
C	-1.7541460	0.9524750	4.5034020	H	-4.5978510	-5.0766460	-3.3156210
C	-2.5109660	0.2934430	3.5394470	H	-3.8258630	-5.9921150	-2.0230500
C	-1.8998090	-0.5836860	2.6428090	C	-1.9759780	4.9370310	-1.4329020
H	1.1004500	5.6707250	3.5830000	C	-2.8498280	6.1284930	-1.8058320
H	3.1441620	5.0635850	2.3374140	C	-0.9177840	5.3280040	-0.4062670
H	4.3078880	3.5529650	0.7321050	H	-1.4701020	4.5584320	-2.3327370
H	5.9500450	1.8246870	0.8173290	C	-2.0014590	7.2979100	-2.3118160
H	8.0449730	1.3373170	-0.4027700	H	-3.4072570	6.4327440	-0.9093450
H	7.9638130	0.6787430	-2.7985880	H	-3.5865470	5.8197890	-2.5556270
H	5.7737590	0.5605740	-3.9657640	C	-0.0712340	6.5030220	-0.9015750
H	3.6872720	1.0835780	-2.7494250	H	-1.4310610	5.6013130	0.5265610
H	5.6596380	-2.0564980	-1.2387450	H	-0.2853900	4.4618890	-0.1900170
H	7.5086360	-2.0971610	0.3975820	C	-0.9473250	7.7006510	-1.2767300
H	7.1277140	-1.3151520	2.7270900	H	-2.6448520	8.1494460	-2.5584180
H	4.8730190	-0.5123520	3.3963390	H	-1.4958510	7.0032070	-3.2420000
H	3.0334700	-0.4746040	1.7642530	H	0.6591690	6.7791690	-0.1331130
H	3.7039920	-3.2859940	-1.4960130	H	0.5032510	6.1872480	-1.7833710
H	2.6693070	-4.5181890	-3.3868380	H	-0.3313570	8.5217830	-1.6602250
H	0.9253870	-4.6665400	-5.1322250	H	-1.4538790	8.0737720	-0.3755690
H	1.0508960	-1.2033250	1.3209880	C	-5.2015030	-0.1988680	0.3389750
H	-0.9860160	-1.2229540	0.0625750	C	-6.1287350	0.1522510	-0.8204530
H	-0.7267560	-4.0708330	0.7942630	C	-5.7826610	-1.3311320	1.1756540
H	-0.8539770	-3.1067280	3.9003540	H	-5.0751080	0.6911540	0.9713830
H	2.3861180	-3.1728130	1.0844880	C	-7.5240030	0.5226160	-0.3096000
H	-2.5096480	-1.0802480	1.8916450	H	-6.1910940	-0.7230590	-1.4824720
H	1.3075800	-0.2983630	3.7185750	H	-5.6920330	0.9753130	-1.3952380
H	-0.9520260	4.2713800	3.3913520	C	-7.1721470	-0.9598170	1.7013580
H	-0.7104930	-0.8951170	-3.8405380	H	-5.8556610	-2.2260870	0.5410820
H	0.2222810	1.2573030	5.3056890	H	-5.0994300	-1.5698840	2.0007880
H	-2.2307550	1.6374070	5.1976290	C	-8.1138010	-0.5992920	0.5488620
H	-3.5826530	0.4594260	3.4776890	H	-8.1841750	0.7482420	-1.1534000
H	3.2272330	-5.2727800	2.0970870	H	-7.4549810	1.4393930	0.2915820
H	2.0138060	-6.3041770	4.0033850	H	-7.5834360	-1.7855700	2.2912380
H	-0.0313020	-5.2211140	4.8976530	H	-7.0845010	-0.0987270	2.3783570
C	-2.0086010	-3.3823840	-0.9005290	H	-9.0949590	-0.3065670	0.9377990
C	-1.4914490	-4.4411180	-1.8859500	H	-8.2699980	-1.4884040	-0.0776810
C	-3.3720400	-3.8140980	-0.3166460				



Boroxinate-H-Iminium Complex **4f**

File Name: catim4f

RRHO Thermochemistry (T = 298)
Zero-point correction (RRHO)= 1.121538 (Hartree/Particle)
Thermal correction to Energy (RRHO)= 1.186641
Thermal correction to Enthalpy (RRHO)= 1.187584
Thermal correction to Gibbs Free Energy (RRHO)= 1.017359
Sum of electronic and zero-point Energies (RRHO)= -3354.365852
Sum of electronic and thermal Energies (RRHO)= -3354.300749
Sum of electronic and thermal Enthalpies (RRHO)= -3354.299806
Sum of electronic and thermal Free Energies (RRHO)= -3354.470031

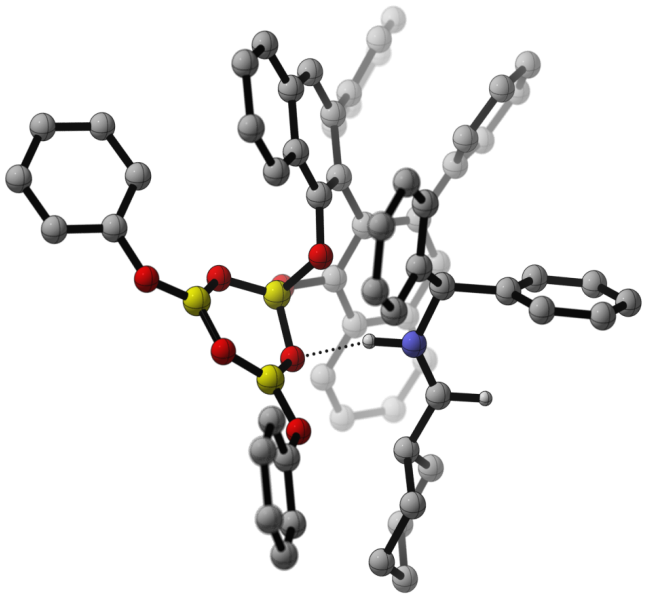
Quasi-RRHO Thermochemistry (T = 298, v0 = 100 cm-1)
Zero-point correction (QRRHO)= 1.121538 (Hartree/Particle)
Thermal correction to Energy (QRRHO)= 1.186641
Thermal correction to Enthalpy (QRRHO)= 1.187584
Thermal correction to Gibbs Free Energy (QRRHO)= 1.034260
Sum of electronic and zero-point Energies (QRRHO)= -3354.365852
Sum of electronic and thermal Energies (QRRHO)= -3354.300749
Sum of electronic and thermal Enthalpies (QRRHO)= -3354.299806
Sum of electronic and thermal Free Energies (QRRHO)= -3354.453130

Quasi-harmonic Thermochemistry (T = 298, cutoff = 100 cm-1)
Zero-point correction (QHO)= 1.121538 (Hartree/Particle)

Thermal correction to Energy (QHO)= 1.186971
Thermal correction to Enthalpy (QHO)= 1.187584
Thermal correction to Gibbs Free Energy (QHO)= 1.037408
Sum of electronic and zero-point Energies (QHO)= -3354.365852
Sum of electronic and thermal Energies (QHO)= -3354.300419
Sum of electronic and thermal Enthalpies (QHO)= -3354.299806
Sum of electronic and thermal Free Energies (QHO)= -3354.449982

C	4.2178940	0.0172990	1.7399500
C	4.6576220	-0.1931010	0.4269190
C	6.0365120	-0.2288300	0.1861800
C	6.9478830	-0.0592830	1.2229610
C	6.4973660	0.1478670	2.5243340
C	5.1278630	0.1844810	2.7786870
C	3.7108480	-0.4126860	-0.7030450
C	2.5231790	0.3766480	-0.8869240
C	1.6651240	0.0626700	-1.9368720
C	1.9653140	-0.9900550	-2.8571520
C	3.1632510	-1.7301460	-2.6893330
C	4.0007380	-1.4317520	-1.5862780
C	3.4805650	-2.7421030	-3.6349910
C	2.6519160	-2.9877050	-4.7020440
C	1.4546280	-2.2471810	-4.8624140
C	1.1108210	-1.2762700	-3.9530650
H	0.8078320	-2.4522460	-5.7102010
C	2.1554390	1.5183880	0.0009240
C	0.8737490	1.5176390	0.5276880
C	0.4321250	2.5029720	1.4564690
C	1.3204150	3.5525640	1.8008980
C	2.6126070	3.5743160	1.2171490
C	3.0366360	2.6008230	0.3394990
C	-0.8691620	2.4599500	2.0181230
C	-1.2773030	3.4442780	2.8829570
C	-0.4044250	4.5100920	3.2143540
C	0.8636670	4.5612730	2.6907300
H	-1.5178800	1.6260000	1.7616820
O	-0.0073220	0.5571560	0.1661560
B	-0.5379930	0.6985590	-1.2167540
O	0.5511060	0.7828290	-2.1724040
C	4.3901840	2.7336340	-0.2617010
C	5.4820680	3.0718750	0.5456320
C	6.7551370	3.2045820	0.0016640
C	6.9568410	3.0018550	-1.3615800
C	5.8742330	2.6758060	-2.1768890
C	4.6001770	2.5449400	-1.6329630
O	-1.3163960	-0.5547610	-1.3853540
B	-2.5949470	-0.5511210	-0.9294420
O	-3.2883270	0.6083160	-0.6949430
B	-2.6579030	1.8226870	-0.9675130
O	-3.4742530	2.9195650	-0.8329010
C	-3.0885490	4.2285550	-0.9687940
C	-4.0682220	5.0934660	-1.4647080
C	-3.7831930	6.4515870	-1.5853540
C	-2.5286820	6.9430150	-1.2078040
C	-1.5756270	6.0642850	-0.7163000
C	-1.8363970	4.6995450	-0.5882460
O	-3.1627740	-1.7915490	-0.7017550
C	-4.4011030	-2.0018820	-0.1399400
C	-4.8910720	-1.2331240	0.9091760
C	-6.1244230	-1.5379330	1.4876660
C	-6.8685880	-2.6195840	1.0165290
C	-6.3707500	-3.3894880	-0.0399860
C	-5.1477570	-3.0820650	-0.6140500
O	-1.3708350	1.8753090	-1.3439990
N	0.1405840	-2.3170320	0.2917840
C	0.0425750	-3.5045090	-0.1718970
C	0.8262870	-1.8963460	1.5342580
C	1.6229260	-3.0342800	2.1413280
C	1.0797010	-3.8613940	3.1268020
C	1.8237600	-4.9236660	3.6345730
C	3.1133330	-5.1620890	3.1642100
C	3.6587700	-4.3389020	2.1809780
C	2.9149260	-3.2800330	1.6688510
C	-0.1661880	-1.2596970	2.4900890
C	0.3460780	-0.4266180	3.4870160
C	-0.4986450	0.1470530	4.4293160
C	-1.8676120	-0.1133660	4.3888630
C	-2.3825750	-0.9431200	3.3980790
C	-1.5369300	-1.5128630	2.4441310
H	-4.3200380	-0.3840620	1.2662040
H	-6.4889160	-0.9178040	2.2982370
H	-6.9646820	-4.2237250	-0.3982210
H	-4.7590720	-3.6698410	-1.4400300
H	-5.0274300	4.6725950	-1.7394780
H	-2.3319820	8.0046220	-1.3101760
H	-0.6015020	6.4420190	-0.4206220
H	-1.0845310	4.0189730	-0.2104760
H	-0.7442640	5.2899900	3.8890130
H	1.5360620	5.3761670	2.9463770
H	3.2694520	4.4115420	1.4390660
H	5.3328350	3.1866560	1.6158220
H	7.5934730	3.4497030	0.6472350
H	7.9508790	3.0994150	-1.7876690
H	6.0199250	2.5290590	-3.2429430

H	3.7576890	2.3006340	-2.2733870
H	6.3914620	-0.3451050	-0.8338320
H	8.0125620	-0.0707170	1.0093580
H	7.2071020	0.2853360	3.3343730
H	4.7644220	0.3441480	3.7895130
H	3.1534210	0.0719210	1.9482510
H	4.8920210	-2.0349220	-1.4312750
H	4.3999840	-3.3074300	-3.5056110
H	2.9112470	-3.7527950	-5.4278200
H	1.5171780	-1.1186070	1.1885280
H	-0.3051080	-1.5475260	-0.2485120
H	0.5067840	-4.3074770	0.4026890
H	0.0800640	-3.6647180	3.5044320
H	3.3351100	-2.6369230	0.8984550
H	-1.9598040	-2.1502090	1.6700680
H	1.4152280	-0.2300530	3.5248660
H	-2.2739470	3.4121170	3.3123740
H	0.1993120	-0.6978220	-4.0569820
H	-0.0899380	0.8063910	5.1883300
H	-2.5291240	0.3325950	5.1248170
H	-3.4460560	-1.1589230	3.3621420
H	4.6658150	-4.5151530	1.8168290
H	3.6945240	-5.9855340	3.5672700
H	1.3977910	-5.5601680	4.4035600
C	-0.6556100	-3.8273030	-1.4378300
C	0.3367150	-4.5183960	-2.3936110
C	-1.8516140	-4.7532120	-1.1380590
H	-1.0195280	-2.8985850	-1.8935020
C	-0.3729440	-4.9039000	-3.6919680
H	0.7343030	-5.4214550	-1.9079460
H	1.1814110	-3.8535720	-2.5998210
C	-2.5506210	-5.1338390	-2.4444530
H	-1.4888490	-5.6616360	-0.6365120
H	-2.5485930	-4.2513030	-0.4592440
C	-1.5808820	-5.8034420	-3.4216360
H	0.3383250	-5.3959210	-4.3643280
H	-0.7045440	-3.9871080	-4.1963210
H	-3.3980910	-5.7936560	-2.2286560
H	-2.9580520	-4.2225480	-2.9037490
H	-2.0939410	-6.0416970	-4.3589720
H	-1.2375510	-6.7553040	-2.9935330
O	-4.6668290	7.3731660	-2.0584020
O	-8.0776120	-3.0007930	1.5126960
C	-5.9382660	6.9079390	-2.4579180
H	-6.4776230	6.4520100	-1.6191490
H	-6.4857240	7.7829090	-2.8080950
H	-5.8574010	6.1780900	-3.2720520
C	-8.6184190	-2.2275380	2.5631300
H	-9.5786740	-2.6796110	2.8099360
H	-7.9693360	-2.2465410	3.4468620
H	-8.7738200	-1.1876650	2.2522990



Boroxinate-H-Iminium Complex **4g**

File Name: catim4g

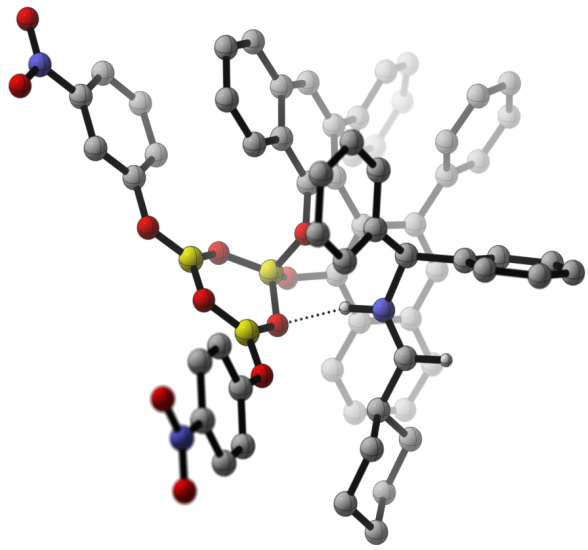
RRHO Thermochemistry (T = 298)
Zero-point correction (RRHO)= 1.055343 (Hartree/Particle)
Thermal correction to Energy (RRHO)= 1.115177
Thermal correction to Enthalpy (RRHO)= 1.116121
Thermal correction to Gibbs Free Energy (RRHO)= 0.958917
Sum of electronic and zero-point Energies (RRHO)= -3125.476145
Sum of electronic and thermal Energies (RRHO)= -3125.416311
Sum of electronic and thermal Enthalpies (RRHO)= -3125.415367
Sum of electronic and thermal Free Energies (RRHO)= -3125.572571

Quasi-RRHO Thermochemistry (T = 298, v0 = 100 cm-1)
Zero-point correction (QRRHO)= 1.055343 (Hartree/Particle)
Thermal correction to Energy (QRRHO)= 1.115177
Thermal correction to Enthalpy (QRRHO)= 1.116121
Thermal correction to Gibbs Free Energy (QRRHO)= 0.973475
Sum of electronic and zero-point Energies (QRRHO)= -3125.476145
Sum of electronic and thermal Energies (QRRHO)= -3125.416311
Sum of electronic and thermal Enthalpies (QRRHO)= -3125.415367
Sum of electronic and thermal Free Energies (QRRHO)= -3125.558013

Quasi-harmonic Thermochemistry (T = 298, cutoff = 100 cm-1)
Zero-point correction (QHO)= 1.055343 (Hartree/Particle)
Thermal correction to Energy (QHO)= 1.115476
Thermal correction to Enthalpy (QHO)= 1.116121
Thermal correction to Gibbs Free Energy (QHO)= 0.975490
Sum of electronic and zero-point Energies (QHO)= -3125.476145
Sum of electronic and thermal Energies (QHO)= -3125.416012
Sum of electronic and thermal Enthalpies (QHO)= -3125.415367
Sum of electronic and thermal Free Energies (QHO)= -3125.555998

C	3.6868120	-0.9045980	1.6846450	O	-3.2516060	1.8847670	-0.7936300
C	3.9695290	-1.4368290	0.4203850	B	-2.2512770	2.7520680	-1.2366310
C	5.2451500	-1.9677410	0.1933800	O	-2.6056360	4.0775000	-1.2011930
C	6.2081850	-1.9678750	1.1967250	C	-1.7987150	5.1480920	-1.4901600
C	5.9134710	-1.4375900	2.4502940	C	-2.4447000	6.2978820	-1.9438170
C	4.6478940	-0.9062400	2.6902870	C	-1.7097540	7.4483750	-2.2090400
C	2.9519180	-1.4854190	-0.6674710	C	-0.3293070	7.4593440	-2.0193420
C	2.0895600	-0.3769130	-0.9746740	C	0.3058430	6.3067170	-1.5634380
C	1.1281500	-0.5303360	-1.9697360	C	-0.4166350	5.1463560	-1.2972850
C	1.0157100	-1.7441370	-2.7178370	O	-3.9945750	-0.3827680	-0.4975100
C	1.9022200	-2.8136170	-2.4323510	C	-5.1902790	-0.0802900	0.1045180
C	2.8427360	-2.6589380	-1.3841560	C	-5.3169780	0.9424890	1.0449140
C	1.8147850	-4.0006440	-3.2086080	C	-6.5445560	1.1438510	1.6706940
C	0.9018570	-4.1041720	-4.2291010	C	-7.6391840	0.3361320	1.3704410
C	0.0182820	-3.0325600	-4.5089380	C	-7.5013470	-0.6805580	0.4282830
C	0.0646330	-1.8804480	-3.7619260	C	-6.2806830	-0.8912810	-0.2058710
H	-0.6988580	-3.1275170	-5.3187540	O	-1.0660790	2.2879350	-1.6663170
C	2.1670560	0.9376210	-0.2720160	N	-1.0026680	-1.8853880	0.5935910
C	0.9845580	1.4440250	0.2424780	C	-1.5213450	-3.0193740	0.3113420
C	0.9362170	2.6491780	0.9990540	C	-0.1546230	-1.5550590	1.7610980
C	2.1350400	3.3854080	1.1717690	C	0.2359670	-2.7983820	2.5352600
C	3.3335780	2.8834410	0.6035320	C	-0.5058010	-3.2373630	3.6340300
C	3.3718450	1.7005790	-0.1020490	C	-0.1414450	-4.4046910	4.3008490
C	-0.2796310	3.1301570	1.5478040	C	0.9659890	-5.1357570	3.8765100
C	-0.3022160	4.3211750	2.2287590	C	1.7085820	-4.7008990	2.7804500
C	0.8863670	5.0769160	2.3843260	C	1.3432660	-3.5373700	2.1099710
C	2.0757940	4.6189380	1.8739790	C	-0.8224740	-0.4862440	2.6067990
H	-1.1773700	2.5281050	1.4303840	C	-0.0070910	0.2612050	3.4592530
O	-0.1816760	0.7940140	0.0240850	C	-0.5582250	1.2190510	4.3014980
B	-0.6944840	0.9207470	-1.3677870	C	-1.9356310	1.4340620	4.3060180
O	0.3092230	0.4810170	-2.3188790	C	-2.7522560	0.6914010	3.4593280
C	4.6653060	1.2785800	-0.7024090	C	-2.1993900	-0.2642480	2.6044670
C	5.8406140	1.3518610	0.0538440	H	-4.4669800	1.5773510	1.2655160
C	7.0615110	0.9660370	-0.4891340	H	-6.6423210	1.9444740	2.3978670
C	7.1268970	0.5000120	-1.8000880	H	-8.5918620	0.5004130	1.8630390
C	5.9642050	0.4340160	-2.5661570	H	-8.3476710	-1.3140280	0.1811150
C	4.7430430	0.8224700	-2.0237760	H	-6.1575620	-1.6744960	-0.9476210
O	-1.8700730	0.0146480	-1.3528300	H	-3.5212230	6.2689160	-2.0780310
B	-3.0331770	0.5349320	-0.8867200	H	-2.2202400	8.3388480	-2.5635580

H	0.2448580	8.3573290	-2.2242330	H	-1.2336080	4.6913360	2.6460160
H	1.3805800	6.3006090	-1.4069070	H	-0.6025500	-1.0486590	-3.9598360
H	0.0832430	4.2511500	-0.9498950	H	0.0885100	1.8054590	4.9462750
H	0.8522100	6.0249660	2.9124050	H	-2.3686310	2.1806260	4.9641850
H	2.9893250	5.1953360	1.9958460	H	-3.8269110	0.8457340	3.4601460
H	4.2396490	3.4773730	0.6927300	H	2.5769720	-5.2621730	2.4508430
H	5.7831210	1.6742450	1.0899430	H	1.2532030	-6.0406460	4.4028130
H	7.9601450	1.0132970	0.1190280	H	-0.7190350	-4.7380770	5.1570960
H	8.0780190	0.1924860	-2.2243190	C	-2.3488260	-3.2564560	-0.8940500
H	6.0079500	0.0848810	-3.5934890	C	-1.7032550	-4.3794030	-1.7292870
H	3.8415300	0.7788910	-2.6278130	C	-3.7754880	-3.6536480	-0.4633820
H	5.4930190	-2.3409150	-0.7961980	H	-2.3910760	-2.3344000	-1.4863690
H	7.1971220	-2.3671270	0.9919900	C	-2.5637390	-4.6756080	-2.9580000
H	6.6653140	-1.4325210	3.2335310	H	-1.6190820	-5.2846710	-1.1106350
H	4.4062890	-0.4905270	3.6640200	H	-0.6917760	-4.0875260	-2.0289360
H	2.7122800	-0.4656930	1.8771470	C	-4.6244840	-3.9500400	-1.7010100
H	3.4871720	-3.4984740	-1.1348820	H	-3.7261120	-4.5492820	0.1721710
H	2.4951790	-4.8193240	-2.9883550	H	-4.2232750	-2.8479090	0.1272640
H	0.8532630	-5.0099740	-4.8261770	C	-3.9936350	-5.0485920	-2.5605410
H	0.7419610	-1.1206000	1.3042700	H	-2.0995180	-5.4762130	-3.5441220
H	-1.1826220	-1.0933870	-0.0550970	H	-2.5821530	-3.7835430	-3.5973240
H	-1.3300090	-3.8432750	1.0004810	H	-5.6362450	-4.2347530	-1.3922330
H	-1.3593020	-2.6575540	3.9744300	H	-4.7135930	-3.0297360	-2.2946540
H	1.9185430	-3.1954780	1.2521050	H	-4.6018080	-5.2249390	-3.4536290
H	-2.8531230	-0.8277940	1.9414540	H	-3.9801500	-5.9884490	-1.9915930
H	1.0666770	0.0876000	3.4632810				



Boroxoinate-H-Iminium Complex **4h**

File Name: catim4h

RRHO Thermochemistry (T = 298)
Zero-point correction (RRHO)= 1.060936 (Hartree/Particle)
Thermal correction to Energy (RRHO)= 1.126019
Thermal correction to Enthalpy (RRHO)= 1.126962
Thermal correction to Gibbs Free Energy (RRHO)= 0.955587
Sum of electronic and zero-point Energies (RRHO)= -3534.333384
Sum of electronic and thermal Energies (RRHO)= -3534.268301
Sum of electronic and thermal Enthalpies (RRHO)= -3534.267358
Sum of electronic and thermal Free Energies (RRHO)= -3534.438733

Quasi-RRHO Thermochemistry (T = 298, v0 = 100 cm-1)
Zero-point correction (QRRHO)= 1.060936 (Hartree/Particle)
Thermal correction to Energy (QRRHO)= 1.126019
Thermal correction to Enthalpy (QRRHO)= 1.126962
Thermal correction to Gibbs Free Energy (QRRHO)= 0.973137
Sum of electronic and zero-point Energies (QRRHO)= -3534.333384
Sum of electronic and thermal Energies (QRRHO)= -3534.268301
Sum of electronic and thermal Enthalpies (QRRHO)= -3534.267358
Sum of electronic and thermal Free Energies (QRRHO)= -3534.421183

Quasi-harmonic Thermochemistry (T = 298, cutoff = 100 cm-1)
Zero-point correction (QHO)= 1.060936 (Hartree/Particle)
Thermal correction to Energy (QHO)= 1.126362
Thermal correction to Enthalpy (QHO)= 1.126962

Thermal correction to Gibbs Free Energy (QHO)= 0.976575
Sum of electronic and zero-point Energies (QHO)= -3534.333384
Sum of electronic and thermal Energies (QHO)= -3534.267958
Sum of electronic and thermal Enthalpies (QHO)= -3534.267358
Sum of electronic and thermal Free Energies (QHO)= -3534.417745

C	4.1170950	-0.1052960	1.9629110	C	-0.9546370	6.8147430	-1.2874870
C	4.6445070	-0.6451520	0.7831670	C	-0.1752700	5.7265480	-1.6633180
C	6.0276810	-0.8489320	0.7053710	C	-0.7220130	4.4530230	-1.7970170
C	6.8588030	-0.5240730	1.7719500	O	-3.2849260	-1.6093270	-0.9901320
C	6.3216010	0.0105530	2.9403680	C	-4.5613250	-1.5687200	-0.5241100
C	4.9467920	0.2179140	3.0318080	C	-5.0404960	-0.5369650	0.2911800
C	3.7830350	-1.0345340	-0.3688960	C	-6.3343030	-0.6045990	0.7880930
C	2.7140650	-0.2050510	-0.8543340	C	-7.1266260	-1.6999690	0.4665010
C	1.9263580	-0.6712290	-1.9024310	C	-6.6676040	-2.7318610	-0.3438800
C	2.1922280	-1.9240720	-2.5380030	C	-5.3756150	-2.6611240	-0.8394370
C	3.2782620	-2.7108580	-2.0762740	O	-0.8658810	1.5684240	-2.0227110
C	4.0361370	-2.2485560	-0.9722030	N	-0.0481190	-2.3249200	0.5670220
C	3.5712440	-3.9311340	-2.7426740	C	-0.2267190	-3.5670090	0.3221420
C	2.8306500	-4.3320600	-3.8271780	C	0.5419910	-1.7229370	1.7839310
C	1.7459160	-3.5425950	-4.2829680	C	1.1238610	-2.7794080	2.7007330
C	1.4233670	-2.3694620	-3.6445310	C	0.3744200	-3.3353450	3.7396430
H	1.1687370	-3.8710380	-5.1420460	C	0.9248740	-4.3328120	4.5406520
C	2.4010520	1.1382230	-0.2836820	C	2.2254270	-4.7761490	4.3101890
C	1.0888900	1.3690480	0.0917080	C	2.9763300	-4.2234400	3.2745530
C	0.6728450	2.5802460	0.7141000	C	2.4265760	-3.2296350	2.4700220
C	1.6341230	3.6059680	0.8986870	C	-0.4737590	-0.8117760	2.4492170
C	2.9671920	3.3792340	0.4694790	C	0.0121590	0.1854460	3.2967850
C	3.3617130	2.1915860	-0.1065320	C	-0.8651100	1.0222870	3.9760910
C	-0.6669120	2.7808880	1.1303210	C	-2.2414180	0.8664240	3.8187930
C	-1.0430270	3.9791070	1.6857380	C	-2.7309900	-0.1267210	2.9761000
C	-0.0961840	5.0200320	1.8458780	C	-1.8512070	-0.9633530	2.2867640
C	1.2119010	4.8351770	1.4701190	H	-4.4072400	0.3107480	0.5196010
H	-1.3758220	1.9631410	1.0209160	H	-6.7335580	0.1797580	1.4195430
O	0.1434740	0.4279640	-0.1530070	H	-7.3181590	-3.5661840	-0.5746580
B	-0.2347880	0.3353240	-1.5848640	H	-4.9785080	-3.4423210	-1.4788050
O	0.9224490	0.0724890	-2.4128740	H	-3.9398220	5.1834640	-0.9630140
C	4.7701310	2.0605490	-0.5651820	H	-0.5449670	7.8102510	-1.1773990
C	5.8143800	2.4888610	0.2622060	H	0.8845400	5.8649310	-1.8501820
C	7.1384850	2.3787400	-0.1489000	H	-0.0996500	3.6142960	-2.0793070
C	7.4400700	1.8381800	-1.3966890	H	-0.4100110	5.9683990	2.2715710
C	6.4071200	1.4188200	-2.2334090	H	1.9419850	5.6303680	1.5981190
C	5.0822710	1.5309900	-1.8231110	H	3.6882340	4.1871850	0.5649100
O	-1.1912520	-0.8016960	-1.5955060	H	5.5821470	2.8704150	1.2527360
B	-2.4800300	-0.5192220	-1.3036360	H	7.9363340	2.7003560	0.5140400
O	-2.9861960	0.7550150	-1.3023240	H	8.4734050	1.7461070	-1.7173720
B	-2.1339980	1.8019180	-1.6544250	H	6.6322310	1.0082330	-3.2131680
O	-2.7159940	3.0480330	-1.5830990	H	4.2806590	1.2112930	-2.4825020
C	-2.0828740	4.2553010	-1.5356200	H	6.4550600	-1.2220690	-0.2209750
C	-2.8870880	5.3308970	-1.1673100	H	7.9308210	-0.6720200	1.6820530
C	-2.3023990	6.5829580	-1.0513410	H	6.9691770	0.2692620	3.7724740

H	4.5167440	0.6332480	3.9382920	C	-2.2111560	-4.7065740	-0.5853440
H	3.0500500	0.0829960	2.0390070	H	-1.0123540	-3.2154300	-1.6060070
H	4.8364500	-2.8775470	-0.5901060	C	-0.5713530	-5.6442940	-2.8587740
H	4.4045790	-4.5321300	-2.3878670	H	0.2721890	-5.9123550	-0.8855940
H	3.0736160	-5.2578580	-4.3400520	H	1.0452050	-4.6266020	-1.8265060
H	1.3545710	-1.1016680	1.3901380	C	-2.8535740	-5.2623660	-1.8578310
H	-0.3528300	-1.6393590	-0.1481930	H	-2.0558800	-5.5209140	0.1359810
H	0.0924700	-4.2793560	1.0842090	H	-2.8652200	-3.9644880	-0.1152930
H	-0.6335320	-2.9769180	3.9295550	C	-1.9344940	-6.2692850	-2.5544340
H	3.0082300	-2.7964030	1.6587560	H	0.0972770	-6.3751880	-3.3260830
H	-2.2521890	-1.7337110	1.6303800	H	-0.6967130	-4.8235390	-3.5767640
H	1.0856930	0.3044000	3.4247020	H	-3.8142460	-5.7270730	-1.6100610
H	-2.0708740	4.1336220	2.0005750	H	-3.0623620	-4.4266180	-2.5401920
H	0.5975670	-1.7505660	-3.9785580	H	-2.4014830	-6.6294970	-3.4766110
H	-0.4740650	1.8037560	4.6195810	H	-1.7974980	-7.1427910	-1.9024460
H	-2.9282010	1.5180210	4.3494080	N	-3.1527650	7.7108950	-0.6482180
H	-3.8015350	-0.2627950	2.8567210	N	-8.4869860	-1.7715390	1.0001000
H	3.9927360	-4.5594740	3.0965420	O	-4.3330080	7.4907200	-0.4391080
H	2.6554200	-5.5478570	4.9408360	O	-2.6301720	8.8070670	-0.5422540
H	0.3397530	-4.7573210	5.3501240	O	-8.8671670	-0.8593430	1.7136180
C	-0.8502810	-4.0622120	-0.9270420	O	-9.1634560	-2.7418010	0.7039770
C	0.0823890	-5.0912980	-1.5921490				

Electrostatic Potential Slice Maps:

Optimizations of catalyst-borox-iminium complexes were carried out at the M06-2X/6-31G* level of theory as implemented by the Gaussian 16 software package with bulk solvent effects accounted for with the self-consistent reaction field polarizable continuum model (PCM) as implemented for toluene. Electrostatic slice maps were generated from NPA charges calculated from these optimized structures using the *cubegen* function provided by Gaussian 16. These were plotted in Jmol to create the colored-in field representing charge such that the outer edges of the map would have a neutral (green) charge using the commands below. The coordinates in brackets following “isosurface plane” represent the plane containing the (im)N—H—O(cat) interaction between the catalyst and the substrate. The coloring gradient was kept consistent between derivatives for accurate qualitative comparison.

```
NO2 derivative:

isosurface plane {0.53651 -1.53177 1.48689}{-0.01663 -1.26501 0.65245}{-1.20492 -0.69855
-0.75211} color absolute -0.16 0.08 map "C:/<full path to cube
file>/M06catnitimphen_ESP_potential.cube" translucent;show isosurface
```

Ph derivative:

```
isosurface plane {-0.71944 -2.04082 0.79600}{-1.62233 0.10086 -0.64239}{-1.02183 -1.29391
0.11814} color absolute -0.16 0.08 map C:/<full path to cube file>/M06cathexSP-
NPA_redo_Pot.cube" translucent;show isosurface
```

Quantitative Electrostatic Potential Data:

Quantitative ESP data was collected by feeding G16 a grid (using the prop=grid keyword) in a fort.52 file that consisted of the coordinates of the substrate, while the catalyst structure was kept in the main input file. The following line was included after the input coordinates to trap the calculated ESP data for the complex in a fort.99 file: “39 2 52 99”, where 39 is the atom count in the fort.52 file, 52 is the designation of the input file (i.e. telling G16 that fort.52 is the input for the grid), and 99 designates the output file for ESP data. An example input file and job file are included below, as well as the quantitative ESP data spreadsheet. Charges on the substrate were calculated with the pop=NPA command in a separate single-point calculation.

Example G16 input file:

```
%chk=M06catnitimphen_ESP.chk
#p M062x/6-311+G** scrf=(pcm,solvent=toluene) nosym prop=grid integral=ultrafine

wulff chemzyme catalyst cyclohexyl substituent with imine phenyl complex gen

-1 1
C                     4.1335   -0.86046   1.10584
C                     4.42999  -1.14799  -0.23359
.
.
.
O                      -4.26489   8.62025  -1.53235
O                      -2.31637   8.46785  -0.62261

39 2 52 99
```

Example job file (note the paths should correspond to your filesystem):

```
#!/bin/bash
#SBATCH --job-name=M06catnitimphen_ESP
#SBATCH --output=M06catnitimphen_ESP.o%j
#SBATCH --error=M06catnitimphen_ESP.e%j
#SBATCH --partition=Standard
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=16
#SBATCH --export=ALL
#SBATCH -t 48:00:00
#SBATCH --mem=32GB
set -x
```

```
module add Gaussian
export OMP_NUM_THREADS=16
export GAUSS_SCRDIR=/data/home/$USER/scratch/$SLURM_JOBID
mkdir -p $GAUSS_SCRDIR
trap "rm -r $GAUSS_SCRDIR" 0 1 2 3 9 13 14 15
df -lh
. /etc/profile.d/modules.sh
find $SLURM_SUBMIT_DIR -maxdepth 1 -name "fort.*" -exec cp {} . \;
cp $SLURM_SUBMIT_DIR/M06catnitimphen_ESP.chk .
/cm/shared/apps/Gaussian/g09/g09 -m="28GB" -p=16
$SLURM_SUBMIT_DIR/M06catnitimphen_ESP.com $SLURM_SUBMIT_DIR/M06catnitimphen_ESP.log
rm -f Gau*      #Clean up any temporary files from crashed job
/cm/shared/apps/Gaussian/g09/formchk M06catnitimphen_ESP.chk
cp M06catnitimphen_ESP.chk $SLURM_SUBMIT_DIR/.
cp M06catnitimphen_ESP.fchk $SLURM_SUBMIT_DIR/.
find . -maxdepth 1 -name "fort.*" -exec cp {} $SLURM_SUBMIT_DIR/. \;
exit
```

Example fort.52 input file (just coordinates—no atom names):

```
 0.53651  -1.53177   1.48689
 1.3468   -2.53002   1.43379
 .
 .
 .
 3.01265  -2.24314   7.02462
 0.94163  -3.42951   6.34637
```

Quantitative ESP data:

fort.99	NPA charge substrate	Stab. Energy R^3=4-NO_2Ph (kcal/mol)		Stab. Energy R^3=Cy
-0.12427	-0.46035	35.9	<-- N -->	36.2
-0.10437	0.28686	-18.8		-23.1
-0.1039	-0.17778	11.6		3.2
-0.08787	-0.13045	7.2		5.5
-0.07694	-0.20313	9.8		9.5
-0.08054	-0.13634	6.9		7.8
-0.09661	-0.19766	12.0		7.4
-0.11344	-0.15214	10.8		8.8
-0.1071	-0.04099	2.8		10.9
-0.08079	-0.09644	4.9		4.4
-0.0706	-0.20613	9.1		11.0
-0.06036	-0.19401	7.3		9.4
-0.05708	-0.18829	6.7		9.0
-0.06063	-0.1961	7.5		9.2
-0.07271	-0.19687	9.0		13.0
-0.09621	-0.06594	4.0		-18.4
-0.08216	-0.19566	10.1	H (Cy) -->	-46.0

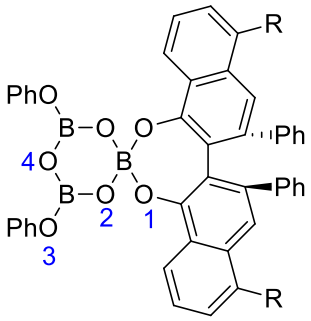
-0.07038	-0.18798	8.3		-14.0
-0.06886	-0.19645	8.5		-10.8
-0.07482	-0.19276	9.0		-13.8
-0.08872	-0.232	12.9		-12.8
-0.11784	0.24579	-18.2		-11.8
-0.1642	0.43916	-45.2	<-- H (NO_2Ph)	-10.8
-0.08987	0.24876	-14.0		-9.5
-0.08386	0.23315	-12.3		-10.1
-0.06626	0.23821	-9.9		-9.8
-0.0703	0.23516	-10.4		-8.0
-0.09513	0.23706	-14.2		-8.4
-0.13933	0.21985	-19.2		20.9
-0.07146	0.23009	-10.3		22.8
-0.07841	0.22359	-11.0		21.1
-0.0968	0.21547	-13.1		-19.0
-0.08374	0.22529	-11.8		19.9
-0.06479	0.22818	-9.3		-10.8
-0.06365	0.22772	-9.1		-14.7
-0.07401	0.22625	-10.5		17.9
-0.05576	0.22936	-8.0		-10.2
-0.05129	0.2285	-7.4		-12.8
-0.05551	0.22901	-8.0		17.0
	Example calculation:	=A2*B2*627.503		-10.0
				-11.0
				-8.5
				-9.7
				-8.4
				-7.9

Scaling factors for Jmol	Scaling factors (kcal/mol)
-0.16	-100.40048
0.08	50.20024
Example calculation:	=L12*627.503

Difference in H-bond Stab. Energy =

$$(-46.0\ kcal/mol) - (-45.2\ kcal/mol)$$
$$= -0.8\ kcal/mol)$$

Catalyst 5,5' substitution analysis:



Calculated ADCH charges on numbered oxygens

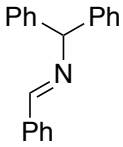
Entry	O1	O2	O3	O4	Substitution
1	-0.22315	-0.27277	-0.18776	-0.24852	H
2	-0.33572	-0.34204	-0.30230	-0.24970	Me
3	-0.33412	-0.34185	-0.30119	-0.24637	OMe
4	-0.32791	-0.34049	-0.30028	-0.34049	Br
5	-0.32980	-0.33779	-0.29442	-0.25586	Cl
6	-0.32538	-0.34079	-0.30106	-0.26235	CF3

Difference in ADCH charge with respect to R=H

Entry	O1	O2	O3	O4	Substitution
1	0.00000	0.00000	0.00000	0.00000	H
2	-0.11257	-0.06927	-0.11455	-0.00118	OMe
3	-0.11097	-0.06908	-0.11343	0.00214	Me
4	-0.10476	-0.06772	-0.11253	-0.09197	Br
5	-0.10666	-0.06502	-0.10667	-0.00734	Cl
6	-0.10224	-0.06802	-0.11330	-0.01383	CF3

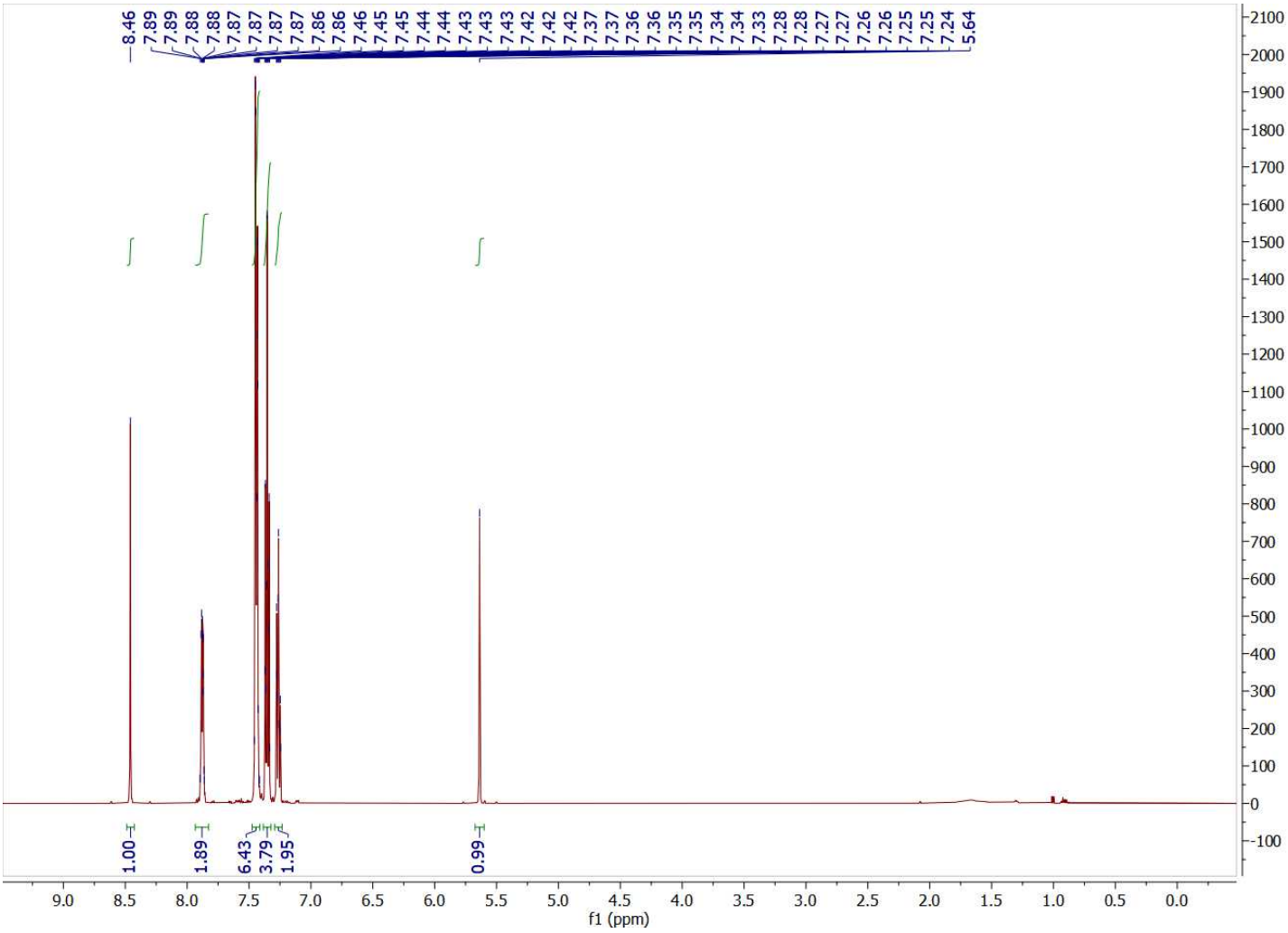
ADCH charges were calculated on the numbered oxygens in the BOROX ring on the catalyst with various functional group substitutions on the 5,5' positions of the hydrocarbon backbone of the catalyst including methoxy (OMe), methyl (Me), bromo (Br), chloro (Cl), and trifluoromethyl (CF_3) substitutions. These were first optimized at the M06-2X/6-31G* level of theory with bulk solvent effects accounted for by the PCM model for toluene included in the Gaussian 16 package. ADCH charges were then calculated using multiwfn from the resulting checkpoint file. A slight decrease in negative charge is observed as the electron withdrawing nature of the substituting group increases for O1, but this trend is not observed for O2, O3, and O4. Since O2 is the oxygen that interacts with the substrate, this suggests that 5,5' substitution should not have a significant effect on the activity of the catalyst.

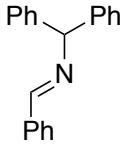
IV. ^{1}Hand ^{13}C spectra for compounds 22a, 22b, 23a, 23b and 41.



22a

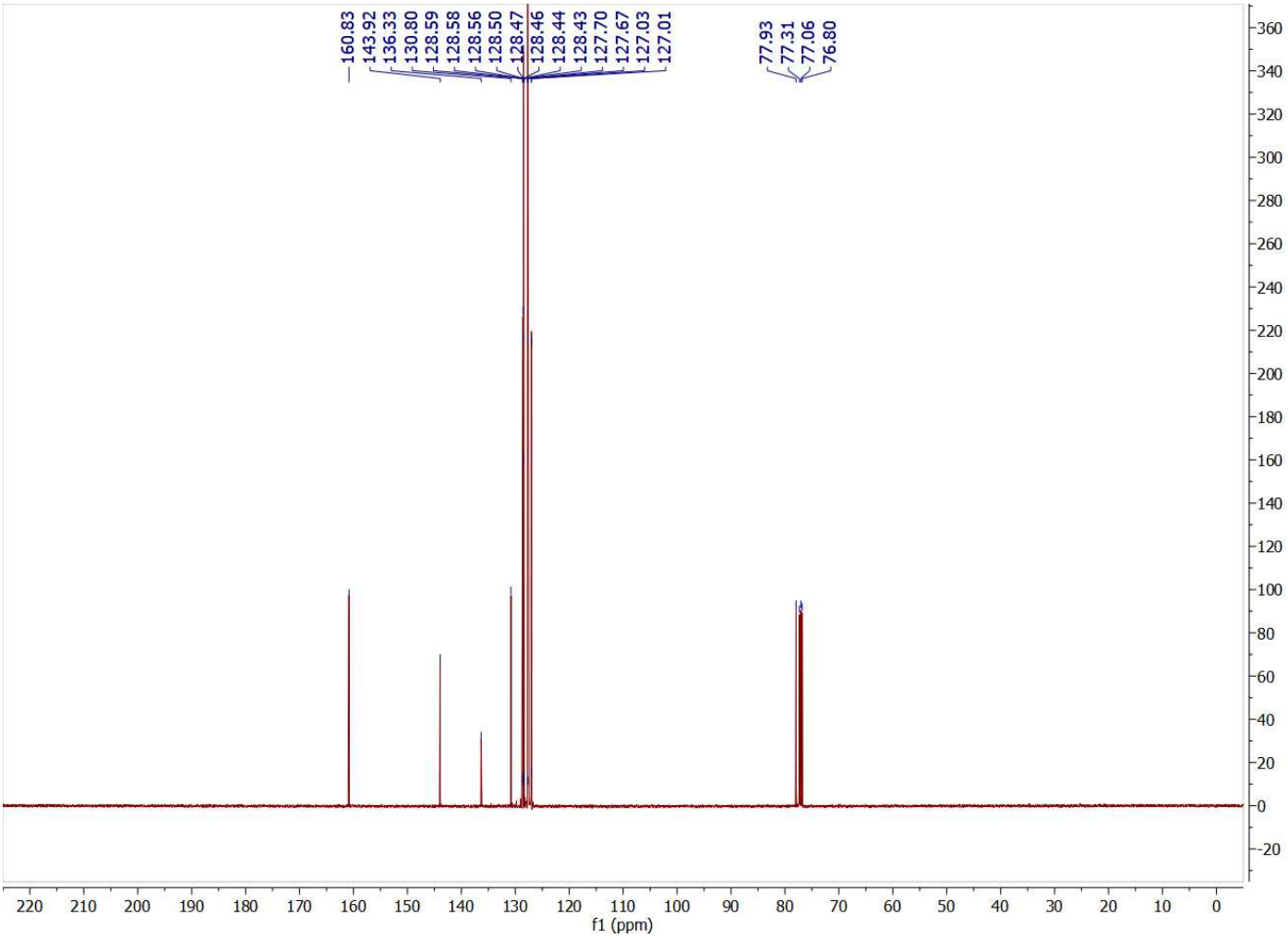
(*E*)-N-benzhydryl-1-phenylmethanimine **22a**-^{1}H NMR (500 MHz, $CDCl_3$)

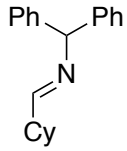




22a

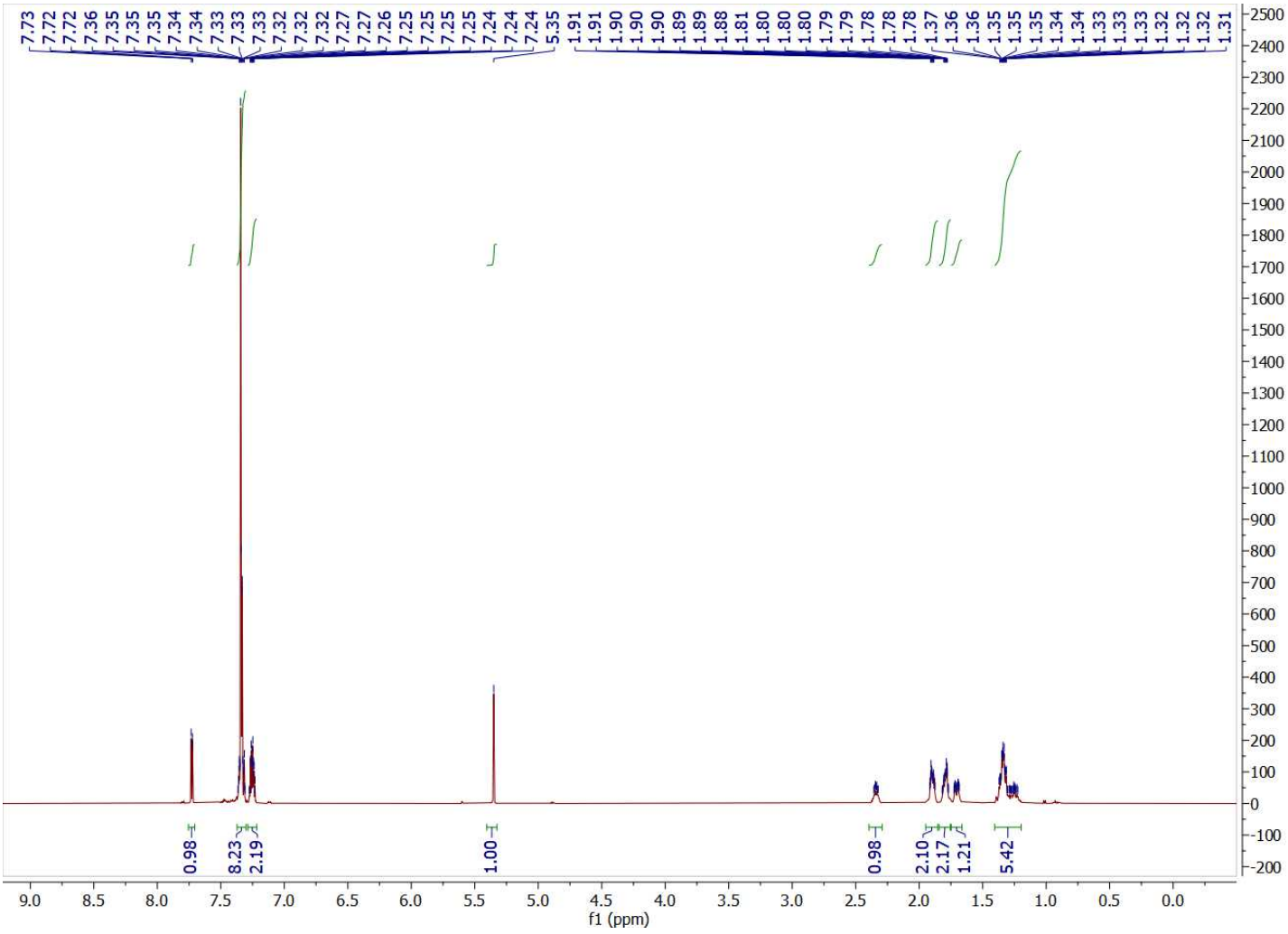
(*E*)-N-benzhydryl-1-phenylmethanimine **22a**-$^{13}C\{^{1}H\}$ (126 MHz, $CDCl_3$)

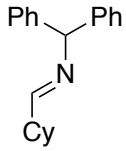




22b

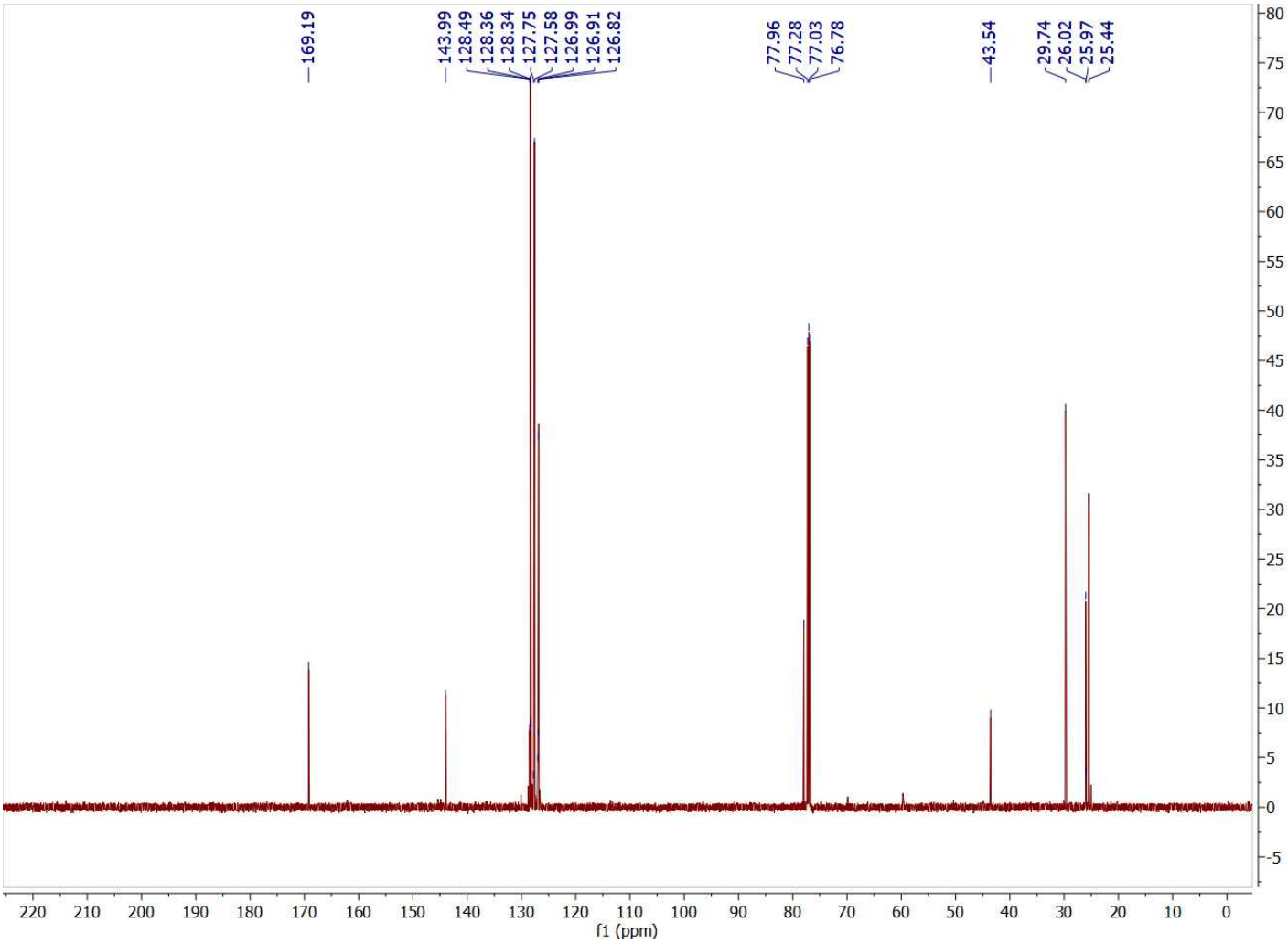
(*E*)-N-benzhydryl-1-cyclohexylmethanimine **22b**-^{1}H NMR (500 MHz, $CDCl_3$)

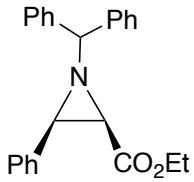




22b

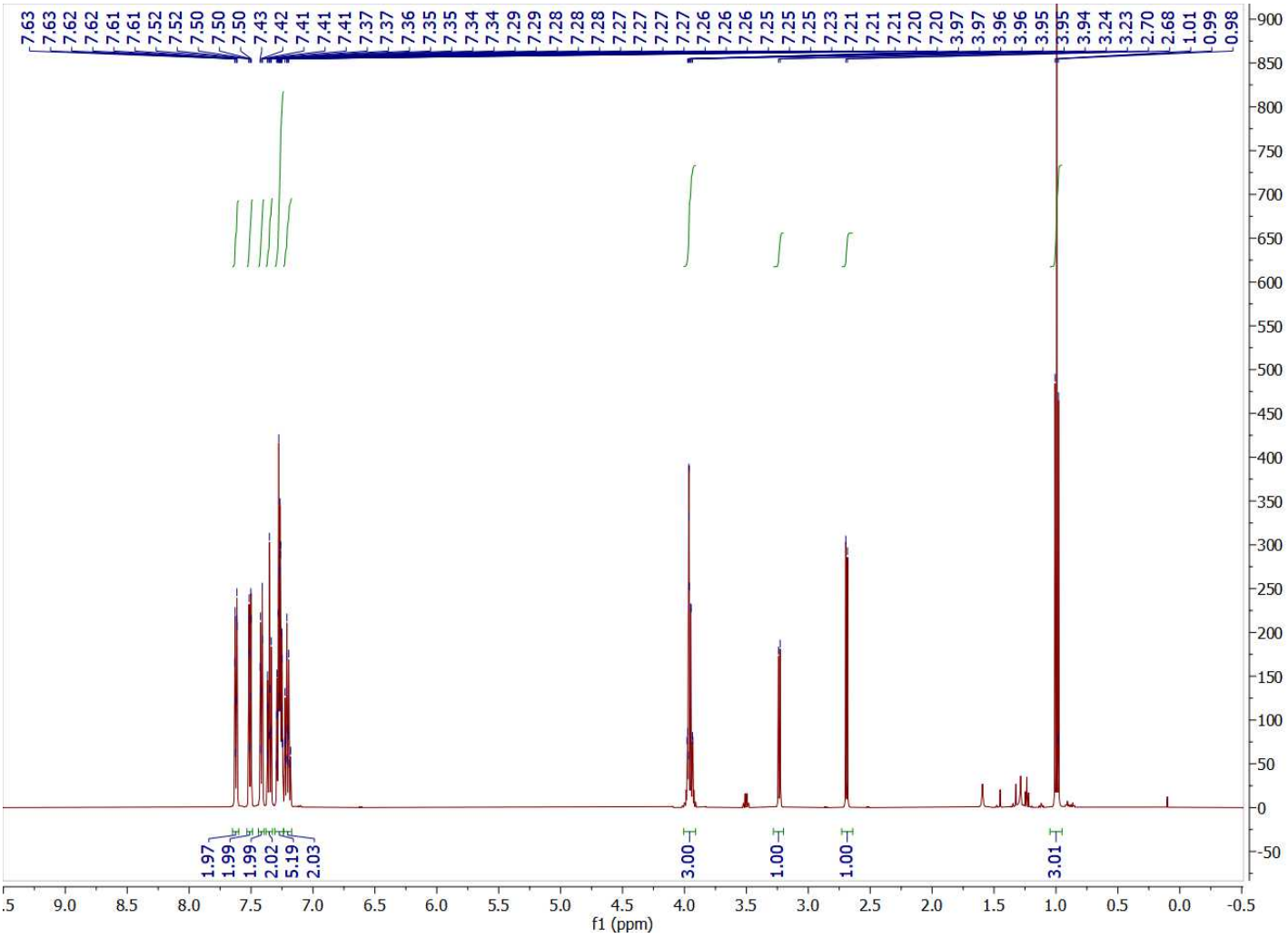
(*E*)-N-benzhydryl-1-cyclohexylmethanimine **22b**-$^{13}C\{^{1}H\}$ (126 MHz, $CDCl_3$)

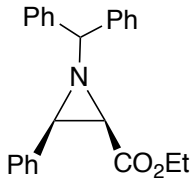




23a

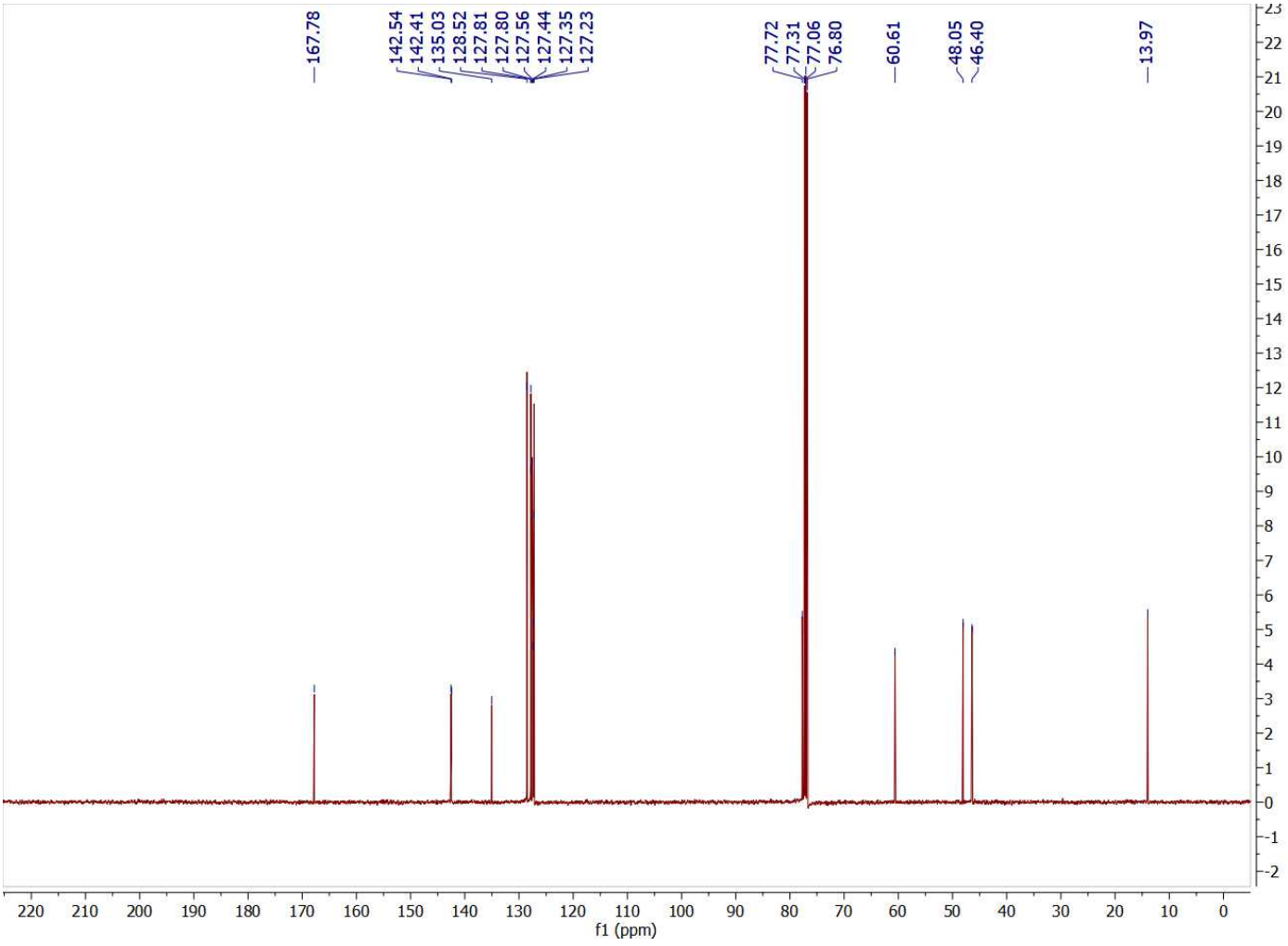
(*2R*,*3R*)-ethyl-1-benzhydryl-3-phenylaziridine-2-carboxylate **23a**-^{1}H NMR (500 MHz, $CDCl_3$)

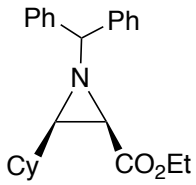




23a

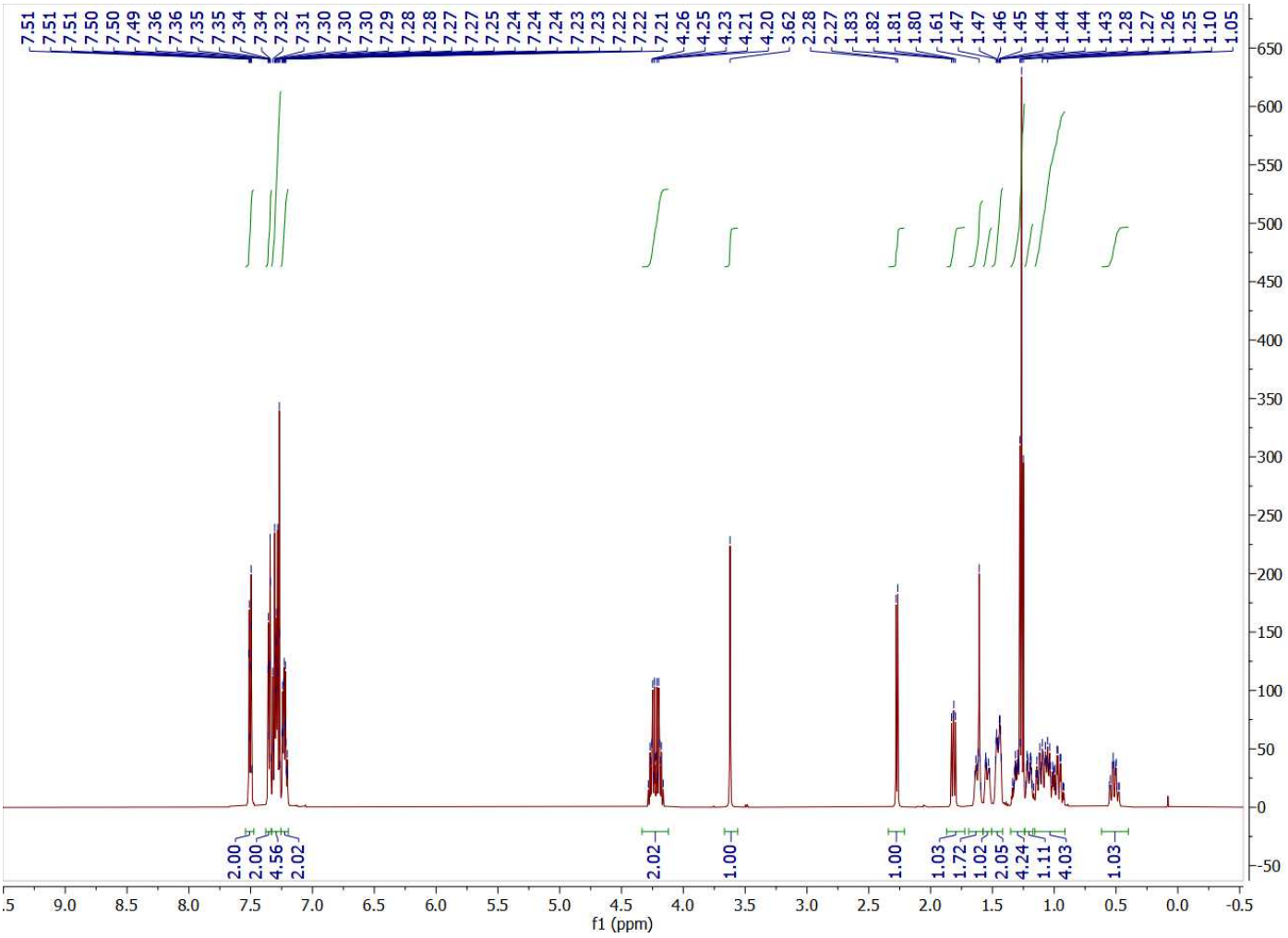
(*2R*,*3R*)-ethyl-1-benzhydryl-3-phenylaziridine-2-carboxylate **23a**-$^{13}C\{^{1}H\}$ (126 MHz, $CDCl_3$)

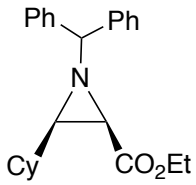




23b

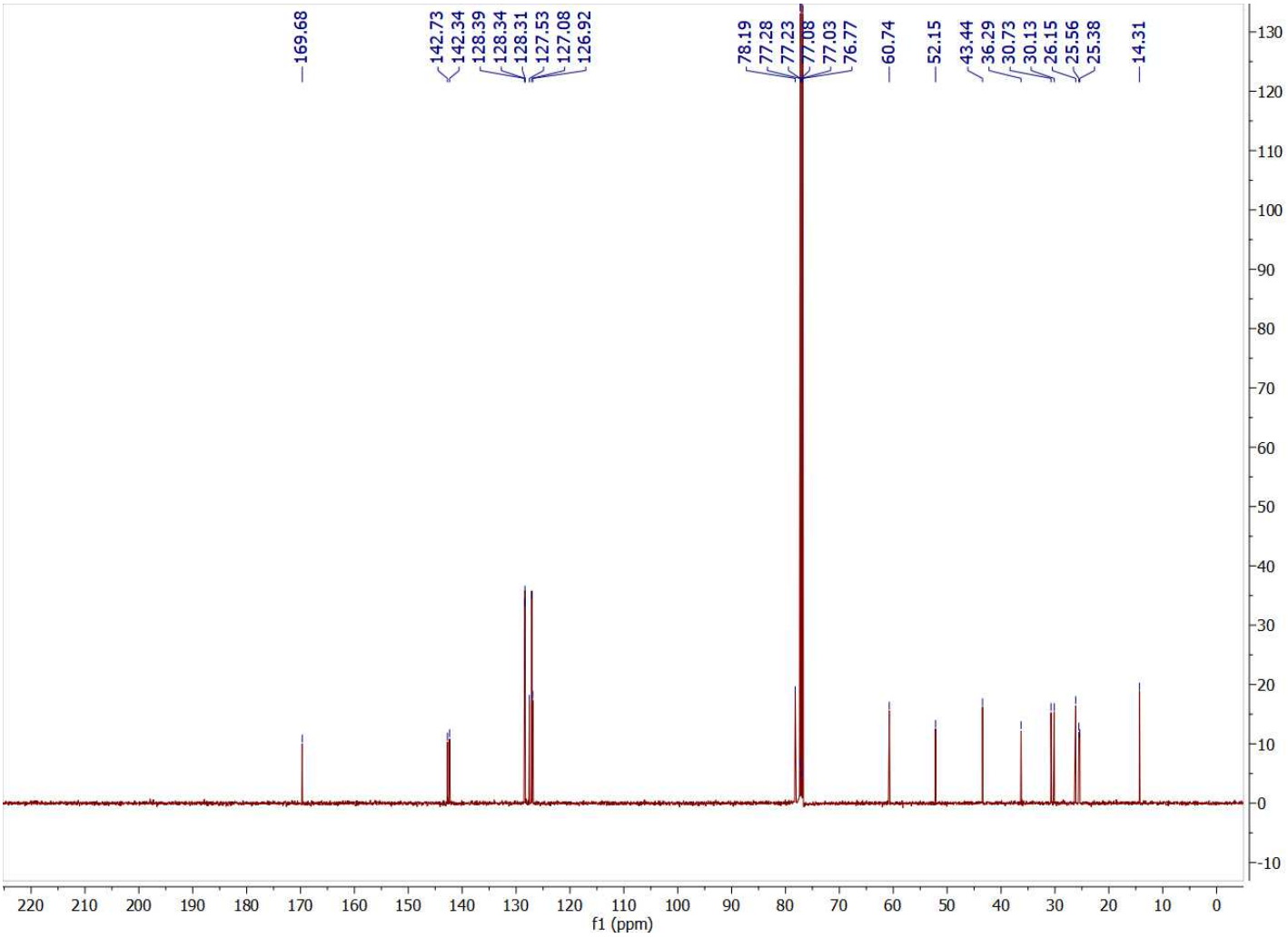
(*2R*,*3R*)-ethyl-1-benzhydryl-3-cyclohexylaziridine-2-carboxylate **23b**-^{1}H NMR (500 MHz, $CDCl_3$)

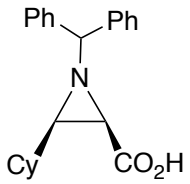




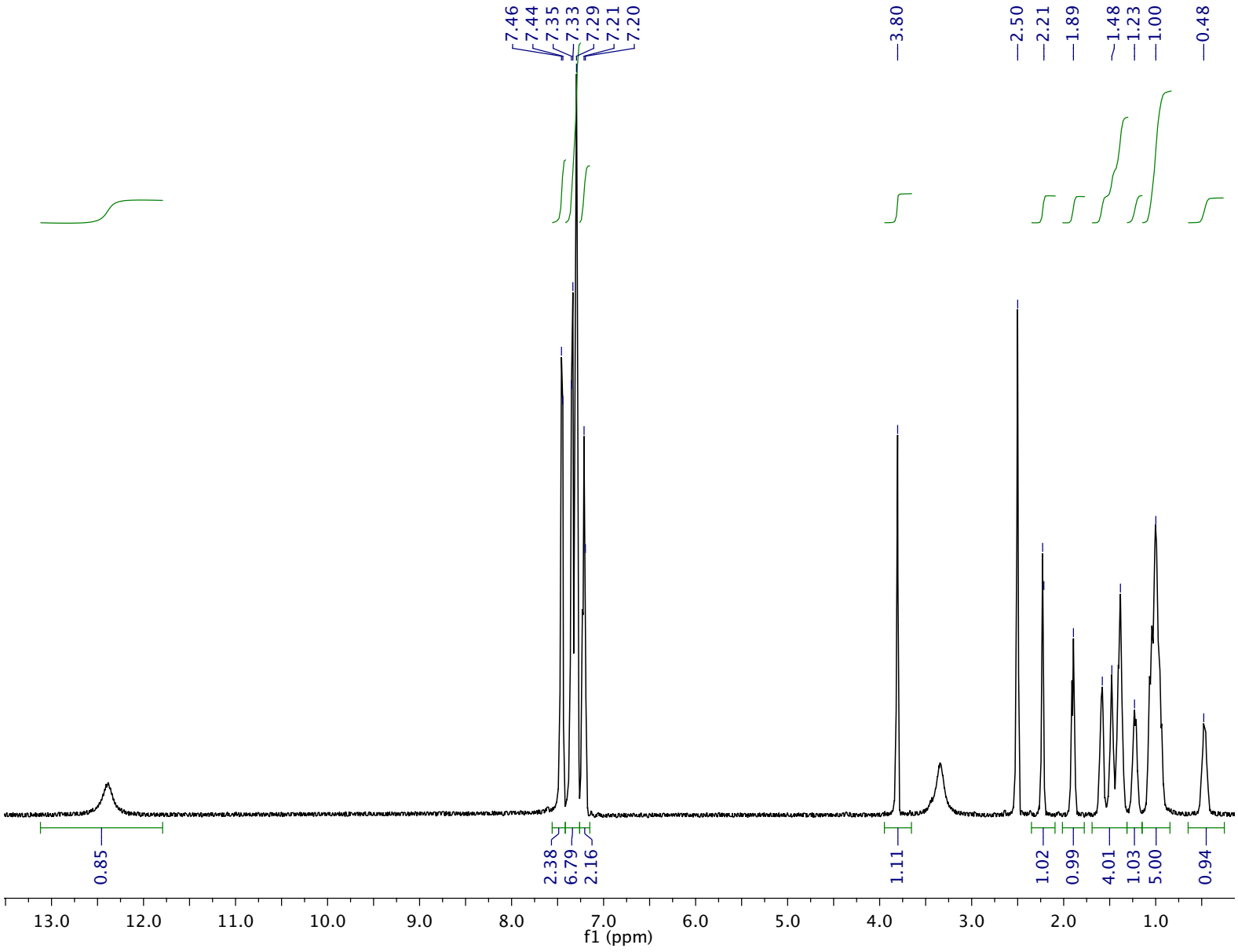
23b

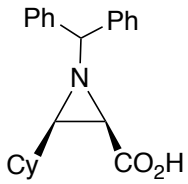
(*2R*,*3R*)-ethyl-1-benzhydryl-3-cyclohexylaziridine-2-carboxylate **23b**-$^{13}C\{^{1}H\}$ (126 MHz, $CDCl_3$)



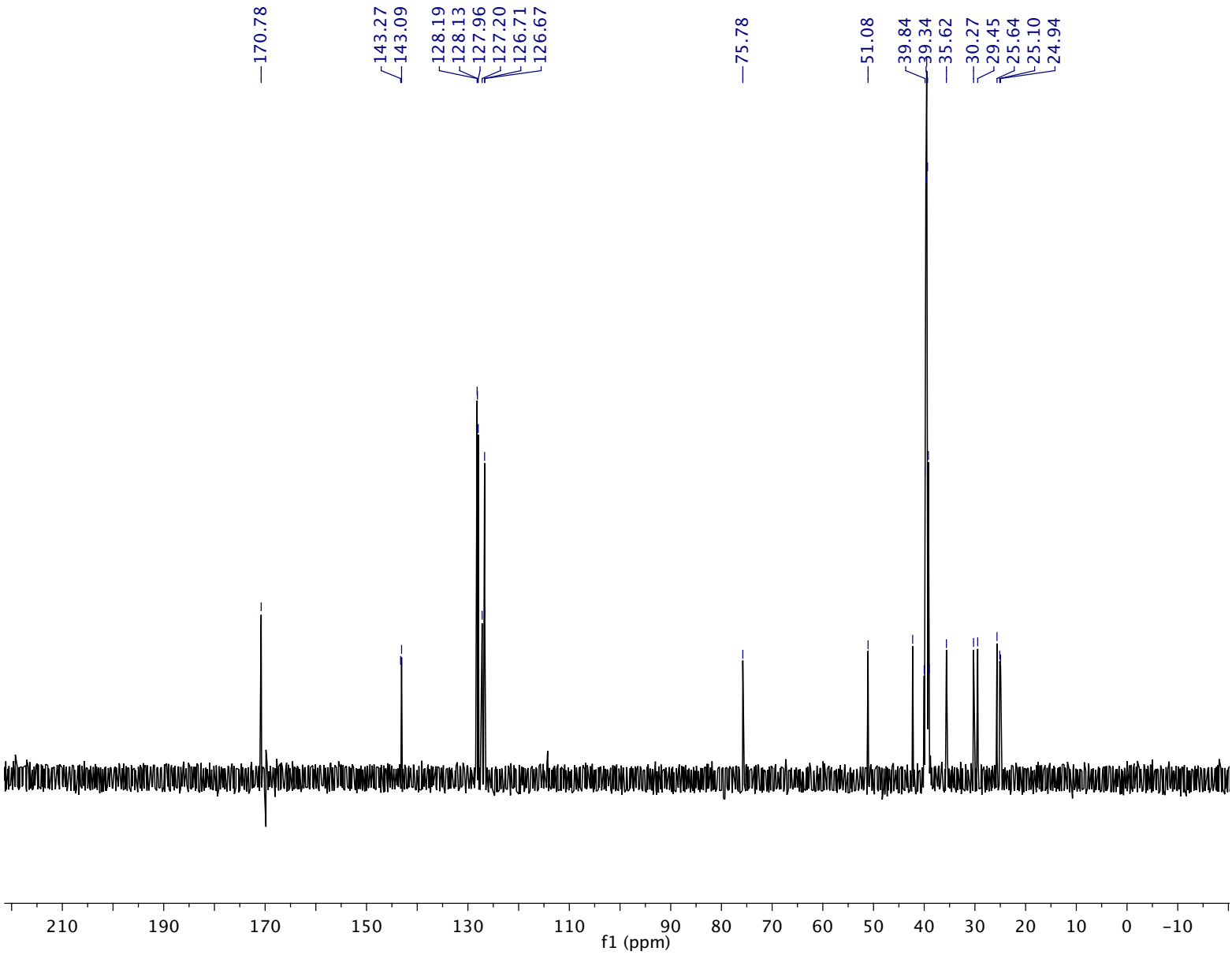

Ph
Ph
N
Cy
CO2H

41


7.46
7.44
7.35
7.33
7.29
7.21
7.20
3.80
2.50
2.21
1.89
1.48
1.23
1.00
0.48
0.85
2.38
6.79
2.16
1.11
1.02
0.99
4.01
1.03
5.00
0.94
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
f1 (ppm)


Ph
Ph
N
Cy
CO2H

41


170.78
143.27
143.09
128.19
128.13
127.96
127.20
126.71
126.67
75.78
51.08
39.84
39.34
35.62
30.27
29.45
25.64
25.10
24.94
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)