SUPPORTING INFORMATION

Copper-Catalyzed Ring-Opening Reactions of Alkyl Aziridines with B_2pin_2: Experimental and Computational Studies

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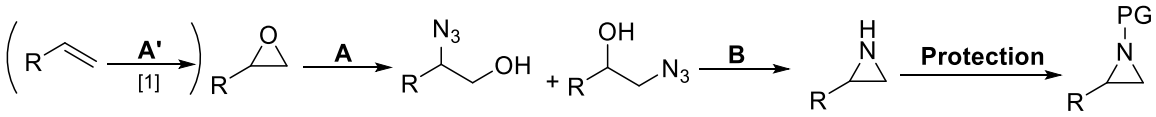
Contents

General synthetic pathway for substrates formation

Aziridines were synthesized following the synthetic pathway shown in **Scheme S1**. Only aziridine **5c** was formed starting from the corresponding alkene following a literature procedure **A′**.[1]



Scheme S1*. Synthetic pathway for the synthesis of aziridines.*

A. A round-bottomed flask was charged with the corresponding epoxide, NaN_3, NH_4Cl and solvent, and the mixture was left to stir overnight at reflux. After workup, the crude containing a regioisomeric mixture was used without any further purification. Complete procedures and spectra are described in the literature for each compound.[2–7]

B. A round-bottomed flask was charged with the corresponding azido alcohol regioisomeric mixture (1.0 equiv.) in CH_3CN or MTBE, and PPh_3 (1.0 equiv.) was portionwise added. When no evolution of nitrogen was noticed, the mixture was warmed up to reflux overnight. Then, the solvent was evaporated, and the solid residue was suspended in a 1:1 mixture of hexane/AcOEt. The residue solid (triphenylphosphine oxide) was filtered away. Complete procedures and spectra are described in the literature for each compounds.[1,3–5,8–11]

Aziridines protection

2-(phenoxymethyl)-1-tosylaziridine (1a)

According to literature procedure,[12] a three-neck round-bottomed flask was charged with corresponding unprotected aziridine (300 mg, 2.0 mmol), dry Et_2O (7 mL), Et_3N (0.38 mL) and 2-(trifluoromethyl)benzenesolfonyl chloride (434 mg, 2.3 mmol, portionwise) under argon. The reaction was left to react until no aziridine was detected by TLC, and cooled at 0°C. Then, 10 mL of water and 10 mL of saturated solution of $NaHCO_3$ were slowly added. The organic layer was separated and the aqueous layer was extracted three times with Et_2O (20 mL). Collected organic layers were washed with brine (15 mg) and dried with $MgSO_4$. The crude was purified by flash chromatography (hexane/AcOEt 8:2) affording the title compound (321.6 mg, 60%) as white solid. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.92 – 7.76 (m, 2H), 7.38 – 7.27 (m, 2H), 7.26 – 7.16 (m, 2H), 7.01 – 6.87 (m, 1H), 6.80 – 6.68 (m, 2H), 4.05 (dd, J = 10.8, 4.4 Hz, 1H), 3.92 (dd, J = 10.8, 6.0 Hz, 1H), 3.21 – 3.10 (m, 1H), 2.80 (d, J = 7.1 Hz, 1H), 2.45 (s, 3H), 2.35 (d, J = 4.4 Hz, 1H). ^{13}C NMR (63 MHz, $CDCl_3$) δ ppm: 158.1, 144.8, 129.8, 129.6, 128.2, 121.4, 114.6, 67.1, 38.3, 31.2, 21.8. $[M + Na]^+$ found = 326.0825, $C_{16}H_{17}NO_3SNa^+$ requires 326.0821.

2-(phenoxymethyl)-1-((2-(trifluoromethyl)phenyl)sulfonyl)aziridine (1b)

According to literature procedure,[12] a three-neck round-bottomed flask was charged with corresponding unprotected aziridine (300 mg, 2.0 mmol), dry Et_2O (7 mL), Et_3N (0.38 mL) and 2-(trifluoromethyl)benzenesolfonyl chloride (580 mg, 2.3 mmol, portionwise) under argon. The reaction was left to react until no aziridine was detected by TLC, and cooled at 0°C. Then, 10 mL of water and 10 mL of saturated solution of $NaHCO_3$ were slowly added. The organic layer was separated and the aqueous layer was extracted three times with Et_2O (20 mL). Collected organic layers were washed with brine (15 mg) and dried with $MgSO_4$. The crude was purified by flash chromatography (hexane/AcOEt 8:2) affording the title compound (321.6 mg, 45%) as white solid. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.42 – 8.30 (m, 1H), 8.01 – 7.93 (m, 1H), 7.87 – 7.75 (m, 2H), 7.35 – 7.25 (m, 2H), 7.05 – 6.96 (m, 1H), 6.87 – 6.77 (m, 2H), 4.26 – 4.01 (m, 2H), 3.47 – 3.36 (m, 1H), 3.05 (d, *J* = 7.2 Hz, 1H), 2.55 (d, *J* = 4.6 Hz, 1H).^{13}C NMR (63 MHz, $CDCl_3$) δ 158.1, 133.7, 132.4, 132.2, 129.6, 128.44 (q, *J* = 6.3 Hz), 124.7,121.5, 120.3, 114.6, 66.9, 39.4, 32.4. $[M + Na]^+$ found = 380.0542, $C_{16}H_{14}F_3NO_3SNa^+$ requires 380.0539.

Picolin-2-yl protection

General procedure C. A round-bottomed flask was charged with 2-picolinic acid (1.05 equiv.), DCC (1.1 equiv.), DMAP (0.2 equiv.) and freshly distilled DCM (8 mL per equivalent of aziridine). Then, a solution of corresponding aziridine (1.0 equiv., DCM 1 M) was slowly added. The reaction mixture was left to vigorously stir until no aziridine was detected by TLC, and the reaction mixture was filtered on celite. After evaporation of the solvent, the crude was purified by flash chromatography.[13]

(2-(phenoxymethyl)aziridin-1-yl)(pyridin-2-yl)methanone (1c)

According to general procedure C, a round-bottomed flask was charged with 2-picolinic acid (264 mg, 2.1 mmol), DCC (454 mg, 2.2 mmol), DMAP (24.4 mg, 0.2 mmol), DCM (8 mL), and corresponding unprotected aziridine (300 mg, 2.0 mmol in 2 mL of DCM). After standard workup, the crude was purified by flash chromatography (hexanes/AcOEt 7:3) affording the title compound (280 mg, 55%) as waxy yellow solid. m.p. = 55-56°C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.67 (d, J = 4.7 Hz, 1H), 8.11 (d, J = 7.9 Hz, 1H), 7.77 (dd, J = 7.7, 1.8 Hz, 1H), 7.41 (ddd, J = 7.6, 4.7, 1.3 Hz, 1H), 7.28 – 7.18 (m, 2H), 6.96 – 6.84 (m, 3H), 4.52 (dd, J = 10.4, 3.8 Hz, 1H), 4.09 (dd, J = 10.5, 5.7 Hz, 1H), 3.17 – 3.09 (m, 1H), 2.66 (d, J = 5.6 Hz, 1H), 2.57 (d, J = 3.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.5, 158.4, 150.4, 149.3, 136.9, 129.5, 126.8, 124.2, 121.2, 114.6, 7.6, 36.8, 29.6. $[M + Na]^+$ found = 277.0954, $C_{15}H_{14}N_2O_2Na^+$ requires 277.0947.

(2-(((tert-butyldimethylsilyl)oxy)methyl)aziridin-1-yl)(pyridin-2-yl)methanone (4c)

According to procedure C, a round-bottomed flask was charged with 2-picolinic acid (643 mg, 5.2 mmol), DCC (1.07 g, 5.2 mmol), DMAP (39.5 mg, 0.32 mmol), DCM (15 mL), and corresponding unprotected aziridine (605 mg, 3.2 mmol in 3.2 mL of DCM). After standard workup, the crude was purified by flash chromatography (petroleum ether/AcOEt 9:1 + 3% Et_3N) affording the title compound (191 mg, 20%) as white solid. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.75 – 8.64 (m, 1H), 8.19 – 8.12 (m, 1H), 7.81 (td, J = 7.7, 1.8 Hz, 1H), 7.43 (ddd, J = 7.6, 4.7,

1.2 Hz, 1H), 4.08 (dd, J = 11.2, 3.0 Hz, 1H), 3.84 (dd, J = 11.2, 4.2 Hz, 1H), 3.02 – 2.93 (m, 1H), 2.54 – 2.46 (m, 2H), 0.82 (s, 9H), -0.01 (s, 3H), -0.10 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.7, 149.3, 148.4, 136.9, 126.5, 124.2, 61.8, 39.9, 27.9, 26.0, 25.9, -5.4, -5.4. $[M + Na]^+$ found = 315.1501, $C_{15}H_{24}N_2O_2SiNa^+$ requires 315.1499.

(7-azabicyclo[4.1.0]hept-3-en-7-yl)(pyridin-2-yl)methanone (5c)

A modified procedure was used because of volatility of NH-free aziridine. In a round-bottomed flask, to a solution of corresponding azido alcohol 6-azidocyclohex-3-en-1-ol (409 mg, 2.294 mmol) in MTBE (4 mL, 0.88 M), PPh_3 was portionwise added. When no formation of N_2 was observed, the reaction mixture was heated up to reflux overnight. Then, the solution was filtered in order to separate triphenylphosphine oxide. Meanwhile, a round-bottomed flask was charged with 2-picolinic acid (380 mg, 3.09 mmol), DCC (667 mg, 2.32 mmol), DMAP (36 mg, 0.29 mmol), DCM (14 mL) and the previously filtered solution was dropwise added. The reaction mixture was left to react overnight, and after standard workup, the crude was purified by flash chromatography (hexanes/Et_2O 5:5 + 2% Et_3N) affording the title compound (325 mg, 55%) as white solid. The spectral data are consistent with literature.[14]

(2-benzylaziridin-1-yl)(pyridin-2-yl)methanone (6c)

According to procedure C, a round-bottomed flask was charged with 2-picolinic acid (606 mg, 5.52 mmol), DCC (1.2 g, 5.79 mmol), DMAP (63.5 mg, 0.53 mmol), DCM (16 mL), and corresponding unprotected aziridine (700 mg, 5.26 mmol in 4 mL of DCM). After standard workup, the crude was purified by flash chromatography (hexanes/AcOEt 7:3; R_f = 0.45) affording the title compound (400 mg, 35%) as yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, J = 4.8 Hz, 0H), 8.14 (d, J = 7.9 Hz, 1H), 7.84 (td, J = 7.7, 1.8 Hz, 1H), 7.48 (ddd, J = 7.6, 4.7, 1.3 Hz, 1H), 7.40 – 7.20 (m, 4H), 3.42 (dd, J = 14.3, 4.5 Hz, 1H), 3.06 – 2.93 (m, 1H), 2.80 (dd, J = 14.4, 7.6 Hz, 1H), 2.62 (d, J = 5.6 Hz, 1H), 2.42 (d, J = 3.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.2, 158.2, 150.2, 149.0, 136.7, 129.3, 126.5, 123.9, 121.0, 114.4, 67.3, 36.6, 29.3. $[M + Na]^+$ found = 261.0989, $C_{15}H_{14}N_2ONa^+$ requires 261.0998

(2-hexylaziridin-1-yl)(pyridin-2-yl)methanone (7c)

According to procedure C, a round-bottomed flask was charged with 2-picolinic acid (264 mg, 2.1 mmol), DCC (454 mg, 2.2 mmol), DMAP (24.4 mg, 0.2 mmol), DCM (8 mL), and corresponding unprotected aziridine (254.5 mg, 2.0 mmol in 2 mL of DCM). After standard workup, the crude was purified by flash chromatography (hexanes/AcOEt 7:3) affording the title compound (209 mg, 45%) as yellow oil. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.69 (dt, *J* = 4.8, 1.4 Hz, 1H), 8.09 (d, *J* = 7.8 Hz, 1H), 7.81 (td, *J* = 7.8, 1.8 Hz, 1H), 7.42 (ddd, *J* = 7.6, 4.8, 1.2 Hz, 1H), 2.74 – 2.63 (m, 1H), 2.53 (d, *J* = 5.7 Hz, 1H), 2.29 (d, *J* = 3.7 Hz, 1H), 1.95 – 1.81 (m, 1H), 1.54 – 1.23 (m, 9H), 0.86 (t, *J* = 6.5 Hz, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 177.4, 150.9, 149.4, 136.9, 126.6, 124.1, 38.9, 32.3, 32.0, 31.8, 29.1, 26.8, 22.7, 14.2. $[M + Na]^+$ found = 255.1471, $C_{14}H_{20}N_2ONa^+$ requires 255.1468

(6-azabicyclo[3.1.0]hexan-6-yl)(pyridin-2-yl)methanone (8c)

According to procedure C, a round-bottomed flask was charged with 2-picolinic acid (946 mg, 7.6 mmol), DCC (1.79 g, 8.69 mmol), DMAP (88.4 mg, 0.724 mmol), DCM (20 mL), and unprotected aziridine (603 mg, 7.24

mmol in 7.2 mL of DCM). After standard workup, the crude was purified by flash chromatography (Petroleum ether/AcOEt 8:2 + 3% Et_3N, R*f* = 0.26) affording the title compound (1.08 g, 79%) as yellowish solid. The spectral data are consistent with literature.[15]

(7-azabicyclo[4.1.0]heptan-7-yl)(pyridin-2-yl)methanone (9c)

According to procedure C, a round-bottomed flask was charged with 2-picolinic acid (1.3 g, 10.5 mmol), DCC (2.27 g, 11.0 mmol), DMAP (122.2 mg, 1.0 mmol), DCM (40 mL), and unprotected aziridine (972 mg, 10.0 mmol in 10 mL of DCM). After standard workup, the crude was purified by flash chromatography (Hexane/AcOEt 7:3, R*f* = 0.25) affording the title compound (1.02 g, 50%) as yellowish solid. The spectral data are consistent with literature.[15]

(2-phenethylaziridin-1-yl)(pyridin-2-yl)methanone (10)

According to procedure C, a round-bottomed flask was charged with 2-picolinic acid (388 mg, 3.15 mmol), DCC (618 mg, 3.3 mmol), DMAP (36.7 mg, 0.3 mmol), DCM (15 mL), and unprotected aziridine (441 mg, 3.0 mmol in 3 mL of DCM). After standard workup, the crude was purified by flash chromatography (hexane/AcOEt 7:3 + 1% Et_3N, R*f* = 0.33) affording the title compound (400 mg, 53%) as yellowish solid. ^1H NMR (250 MHz, $CDCl_3$) δ 8.70 (ddd, J = 4.7, 1.8, 0.9 Hz, 1H), 8.10 (dt, J = 7.9, 1.1 Hz, 1H), 7.81 (td, J = 7.7, 1.8 Hz, 1H), 7.43 (ddd, J = 7.6, 4.8, 1.3 Hz, 1H), 7.33 – 7.13 (m, 5H), 2.93 – 2.70 (m, 3H), 2.53 (d, J = 5.8 Hz, 1H), 2.29 (d, J = 3.7 Hz, 1H), 2.27 – 2.13 (m, 1H), 1.90 – 1.73 (m, 1H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 177.0, 150.5, 149.1, 141.2, 136.7, 128.3, 126.4, 125.8, 123.8, 38.0, 33.9, 32.9, 31.8. $[M + Na]^+$ found = 275.1159, $C_{16}H_{16}N_2ONa^+$ requires 275.1155

References

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COMPUTATIONAL SECTION

Table S1. Two-Copper model, substitution of chloride with alkoxide anion: comparison of activation Free Energies (kJ/mol) corresponding to **TS3** and **TS4** from *N*-(2-picolinoyl)-methyl aziridine.

Anion	ΔG‡ (**TS3**)	ΔG‡ (**TS4**)	ΔΔG* (**TS3-TS4**)
Cl^-	+82.6	+69.0	13.6
MeO^-	+74.4	+58.5	15.9
t-BuO^-	+76.7	+58.4	18.3

[a] (A) see ref. 29, main text, and Thermochemical Data , pag S77-S86.

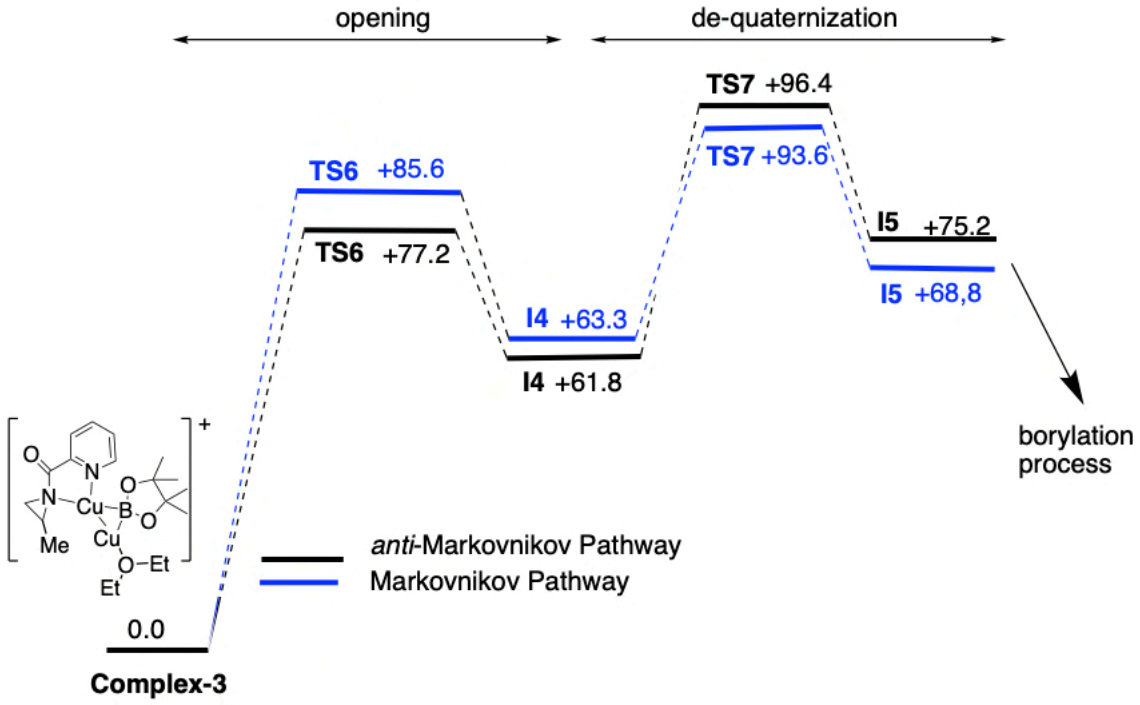


Figure S1. Particular of the reaction energy profile comparison between the *anti*-Markovnikov (blue) and Markovnikov (black) pathways of *N*-(2-picolinoyl)-methyl aziridine (model with the Et_2O molecule). The ΔG values are in kJ/mol.

Table S2. One-Copper model, *N*-(2-picolinoyl)-methyl aziridine: comparison between Free Energies obtained at different theory level.

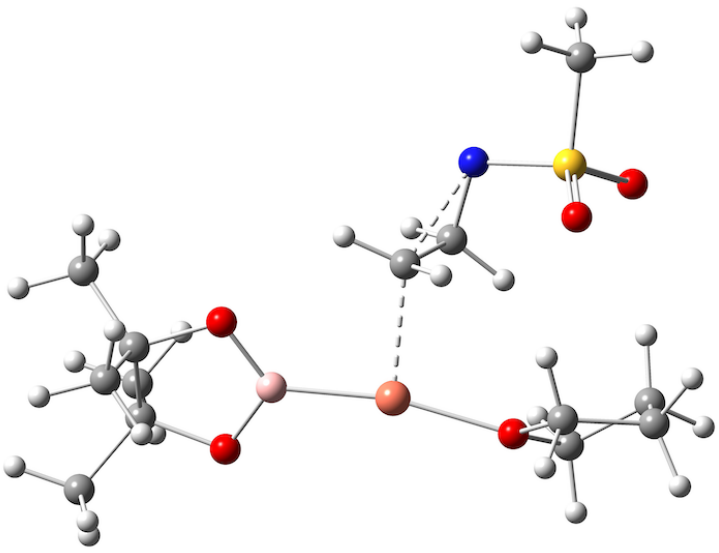
Structure	ΔG (kJ/mol)[a]	G (Hartree) [a]	ΔG (kJ/mol) [b]	G (Hartree) [b]
	Anti-Markovnikov (A)		*Anti*-Markovnikov (B)	
Complex-1	0,0	-1142,35944836	0,0	-1142.36293795
TS1	+78.7	-1142.32948224	+78.8	-1142.33293874
I1	-10.2	-1142.36334256	-9.0	-1142.36637520
TS2	+4.8	-1142.35763571	+5,8	-1142.36073507
P1	-202.0	-1142.43640126	-201.5	-1142.43967762
	Markovnikov (A)		Markovnikov (B)	
TS1	+75.2	-1142.33080044	+75.4	-1142.33420243
I1	-7.2	-1142.36219417	-5.6	-1142.36508446
TS2	+8.3	-1142.35630147	+9.2	-1142.35942931

[a] (A) see Table 3 and Computational Section, main text, and Thermochemical Data, SI.

[b] (B) B3LYP-D3/6-311+G(2D,P)//B3LYP-D3/6-311+G(2D,P) corrected by a solvent-simulation SP at same theory level (PCM calculation)

CARTESIAN COORDINATES and THEMOCHEMICAL DATA

PRELIMINARY RESULTS (ANTIPERIPLANAR RING OPENING, REF 25, MAIN TEXT)



TS (Ref 25) Substrate: mesylaziridine

CARTESIAN COORDINATES

C	-1.214511	1.044693	1.111519
N	-1.974511	2.155272	0.564555
O	-4.251355	1.057294	1.167402
C	-0.515316	0.947208	-0.202602
Cu	0.309145	-1.056888	-0.155875
B	2.134057	-0.331278	-0.106477
O	3.183049	-1.088144	0.376530
O	2.551876	0.922031	-0.509785
C	4.350244	-0.215069	0.507539
C	4.012935	0.939724	-0.501981
O	-1.379057	-2.156960	-0.195956
C	-2.053010	-2.645184	1.000157
C	-2.323451	-2.113699	-1.322463
C	-3.528990	-2.361437	0.748275
H	-1.839691	-3.717683	1.096574
H	-1.623950	-2.115552	1.854617
C	-3.654358	-2.626467	-0.763526
H	-2.400098	-1.074283	-1.643231
H	-1.905675	-2.734477	-2.120138
H	-3.769098	-1.317655	0.974502
H	-4.179005	-3.007328	1.347199
H	-4.497546	-2.090616	-1.207281
H	-3.774398	-3.698618	-0.960870
H	-1.103806	0.643324	-1.065341
H	0.273111	1.663075	-0.400617
H	-1.790659	0.166537	1.418377
C	4.480293	2.328638	-0.076980
H	5.572093	2.353498	0.024163
H	4.190370	3.063124	-0.835700
H	4.033267	2.631527	0.872730
C	4.463562	0.644438	-1.938293
H	4.019606	1.387591	-2.608342
H	5.553707	0.695762	-2.035348
H	4.128404	-0.346237	-2.261641
C	5.601844	-1.021460	0.174760
H	6.488508	-0.375751	0.179968
H	5.745160	-1.805530	0.925617
H	5.523633	-1.502006	-0.803170
C	4.389310	0.246729	1.969841
H	4.424291	-0.634430	2.618410
H	5.271936	0.863530	2.172648
H	3.493572	0.821214	2.226856
S	-3.490197	1.691519	0.059727
C	-4.205734	3.306491	-0.282501
H	-3.595750	3.797393	-1.042869
H	-5.218608	3.126753	-0.650358
H	-4.220826	3.884116	0.642982
O	-3.482421	0.924046	-1.218888
H	-0.562954	1.363892	1.928597

Electronic Energy = -1562.96129548 (Hartree/Particle)
Dipole Moment (Debye): 3.6448
index 0
Harmonic frequencies
Number of imaginary frequencies= 1
Negatives Eigenvalues: -182.255

THERMOCHEMICAL DATA

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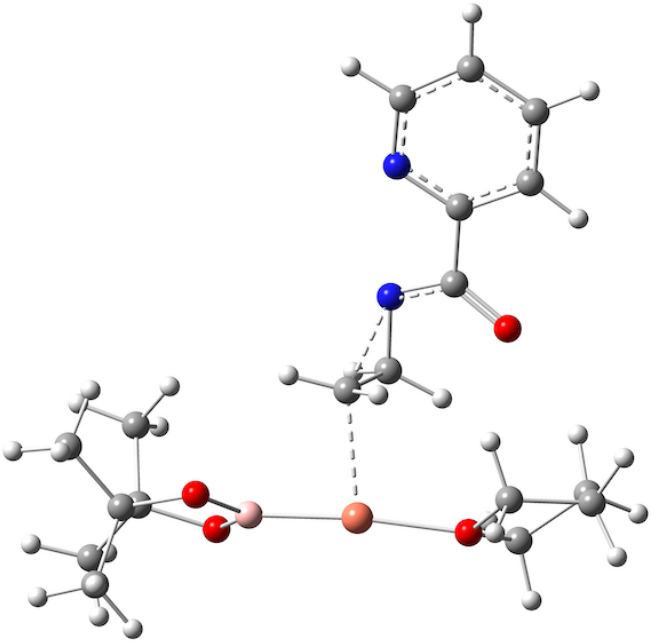
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.409514
(Hartree/Particle)
 Thermal correction to Energy=                    0.435819
 Thermal correction to Enthalpy=                  0.436763
 Thermal correction to Gibbs Free Energy=         0.349837
 Sum of electronic and zero-point Energies=          -1562.551781
 Sum of electronic and thermal Energies=             -1562.525477
 Sum of electronic and thermal Enthalpies=           -1562.524533
 Sum of electronic and thermal Free Energies=        -1562.611458
 PCM-SP (solvent=THF;6-311+g(2d,p)) = -1563.31552956
 Corrected Free Energy =  -1562.96569208
 Corrected Free Energy =  -1533.52220177
```



TS (Ref 25) Substrate: N-(2picolinoyl)-aziridine

CARTESIAN COORDINATES

C	0.679183	-0.020737	1.429902
N	1.673513	-1.015347	1.084563
C	2.814244	-0.481574	0.541481
O	3.039292	0.733514	0.352355
C	0.168996	-0.312002	0.069698
C	3.885059	-1.483858	0.172043
C	5.189901	-1.012577	-0.044352
C	6.187407	-1.924605	-0.385231
C	5.846317	-3.272460	-0.514334
C	4.514373	-3.640683	-0.291999
N	3.551416	-2.779291	0.049630
Cu	-1.152326	1.511397	-0.301088
H	0.018884	-0.356390	2.230585
H	5.391249	0.048171	0.057719
H	7.209061	-1.590847	-0.549363
H	4.207475	-4.680967	-0.391907
H	6.586457	-4.022036	-0.781035
B	-2.614208	0.214806	-0.214424

```
 O              -3.455072    0.099943    0.877218
 O              -2.894594   -0.739084   -1.175497
 C              -4.204268   -1.147901    0.742295
 C              -4.139800   -1.406850   -0.805104
 O               0.203027    2.996973   -0.370751
 C               0.539217    3.761412    0.827362
 C               1.345859    2.968876   -1.288296
 C               2.055714    3.925880    0.777606
 H               0.008324    4.719116    0.767259
 H               0.173534    3.200759    1.691568
 C               2.322138    4.004354   -0.735674
 H               1.781201    1.967374   -1.250718
 H               0.960696    3.190260   -2.286837
 H               2.548176    3.039830    1.189318
 H               2.390075    4.815368    1.320823
 H               3.355349    3.755143   -0.992652
 H               2.093485    5.005193   -1.122606
 H               0.717052    0.059287   -0.790464
 H              -0.416710   -1.206072   -0.093020
 H               1.043791    0.996471    1.590392
 C              -4.043615   -2.874649   -1.211470
 H              -4.926354   -3.428478   -0.869034
 H              -3.992835   -2.952188   -2.302652
 H              -3.150403   -3.349712   -0.798942
 C              -5.263178   -0.712656   -1.585895
 H              -5.036545   -0.768176   -2.655494
 H              -6.232006   -1.193509   -1.409877
 H              -5.339883    0.344084   -1.310577
 C              -5.606646   -0.940774    1.306366
 H              -6.223332   -1.833247    1.143707
 H              -5.547030   -0.758060    2.384518
 H              -6.102841   -0.082913    0.846549
 C              -3.451208   -2.200060    1.567117
 H              -3.367931   -1.846867    2.599930
 H              -3.975884   -3.161925    1.569398
 H              -2.438452   -2.357355    1.182041

 Electronic Energy =  -1335.50039192 (Hartree/Particle)
 Dipole Moment (Debye):      3.1329
 index           1
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -322.373

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.450274
(Hartree/Particle)
 Thermal correction to Energy=                    0.478160
 Thermal correction to Enthalpy=                  0.479105
 Thermal correction to Gibbs Free Energy=         0.386814
 Sum of electronic and zero-point Energies=          -1335.050118
 Sum of electronic and thermal Energies=             -1335.022231
 Sum of electronic and thermal Enthalpies=           -1335.021287
 Sum of electronic and thermal Free Energies=        -1335.113582
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1335.83942948
 Corrected Free Energy =  -1335.45261956
```

MODEL: Az-Cu-Bpin

SUBSTRATE: N-MESYL-AZIRIDINE

N-mesyl-aziridine

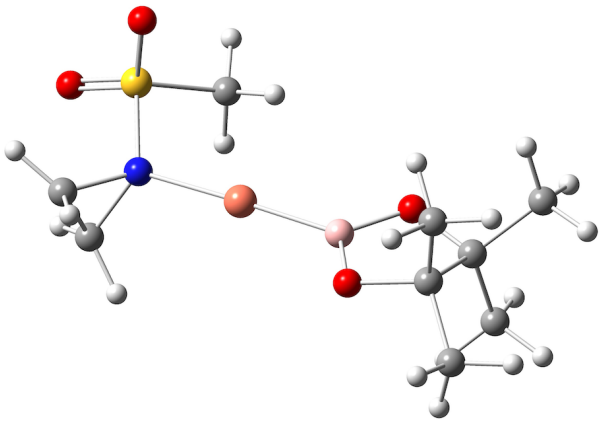
CARTESIAN COORDINATES

C	2.019232	-0.608194	-0.197541
C	1.912543	0.834411	0.143586
H	1.841746	-1.321369	0.605557
H	2.490274	1.576843	-0.400705
N	0.867954	0.183199	-0.679551
H	2.675838	-0.950295	-0.992513
H	1.656183	1.079936	1.172243
S	-0.632935	-0.175458	0.087113
O	-0.516997	-0.056953	1.552431
O	-1.124224	-1.421630	-0.507619
C	-1.611208	1.205657	-0.525850
H	-2.613207	1.085760	-0.106944
H	-1.159879	2.137448	-0.178901
H	-1.633305	1.154043	-1.615359

Electronic Energy = -721.839183223 (Hartree/Particle)
Dipole Moment (Debye): 4.0306
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.108343
(Hartree/Particle)
Thermal correction to Energy= 0.115923
Thermal correction to Enthalpy= 0.116867
Thermal correction to Gibbs Free Energy= 0.076193
Sum of electronic and zero-point Energies= -721.730840
Sum of electronic and thermal Energies= -721.723260
Sum of electronic and thermal Enthalpies= -721.722316
Sum of electronic and thermal Free Energies= -721.762990
PCM-SP (solvent=THF;6-311+g(2d,p)) = -721.994189343
Corrected Free Energy = -721.917996120



Complex-1 Substrate: N-mesyl-aziridine

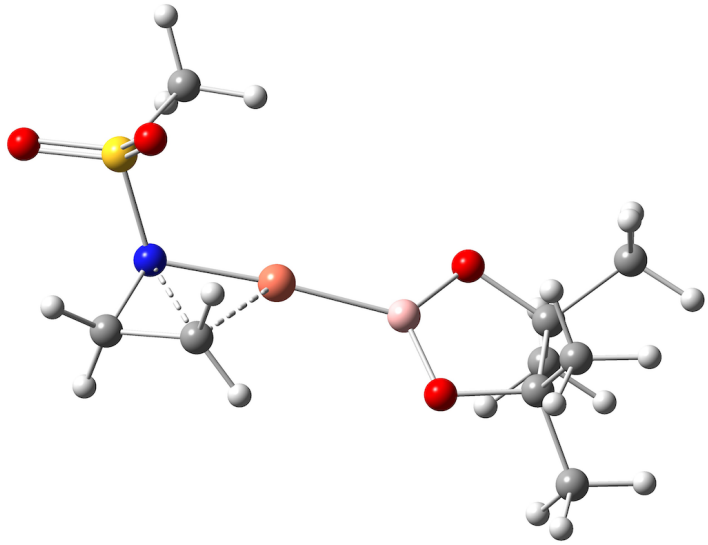
CARTESIAN COORDINATES

C	-3.100354	-1.568728	-1 .265188
C	-3.178320	-2.019169	0.144267
H	-4.025511	-1.253842	-1.740983
H	-2.452342	-2.718786	0.546056
N	-2.591149	-0.686416	-0.175152
Cu	-0.556083	-0.450515	-0.032506
B	1.385038	-0.194298	-0.014723
O	2.332615	-1.200985	0.123822
O	2.005551	1.045201	-0.138632
C	3.637505	-0.587854	0.328979
C	3.437797	0.835758	-0.300255
C	4.698647	-1.452060	-0.348108
H	5.684615	-0.974700	-0.286373
H	4.757010	-2.423809	0.153952
H	4.460869	-1.631219	-1.399420
C	3.877354	-0.552881	1.845055
H	3.803662	-1.572437	2.237310
H	4.869997	-0.156758	2.088478
H	3.120972	0.057707	2.348328
C	3.724557	0.878773	-1.808060
H	3.372439	1.835821	-2.207054
H	4.796255	0.787138	-2.019052
H	3.192837	0.077670	-2.331431
C	4.182961	1.966174	0.405550
H	5.266108	1.793554	0.377232
H	3.974860	2.916050	-0.098864
H	3.870605	2.064133	1.447910
H	-2.311039	-1.932680	-1.916104
H	-4.155348	-2.014541	0.621821
S	-3.609941	0.679444	0.291328
O	-3.440866	0.834826	1.734529
O	-4.945908	0.483484	-0.290023
C	-2.762778	2.006827	-0.579610
H	-3.330463	2.916954	-0.368970
H	-1.741757	2.076447	-0.197031
H	-2.770813	1.782280	-1.648044

Electronic Energy = -1330.51255415 (Hartree/Particle)
Dipole Moment (Debye): 3.2042
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.291959
(Hartree/Particle)
Thermal correction to Energy= 0.312198
Thermal correction to Enthalpy= 0.313143
Thermal correction to Gibbs Free Energy= 0.240581
Sum of electronic and zero-point Energies= -1330.220595
Sum of electronic and thermal Energies= -1330.200356
Sum of electronic and thermal Enthalpies= -1330.199412
Sum of electronic and thermal Free Energies= -1330.271973
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1330.79867657
Corrected Free Energy = -1330.55809542



TS1 Substrate: N-mesyl-aziridine

CARTESIAN COORDINATES

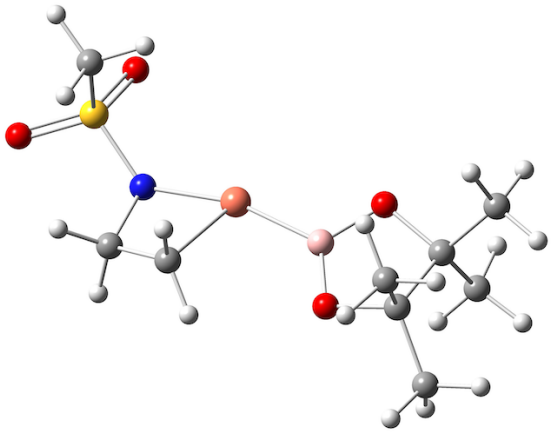
Cu	-0.660995	-0.149623	-0.420382
B	1.299961	0.010456	-0.191299
O	2.033328	1.184527	-0.116695
C	3.452580	0.849631	-0.155559
C	4.211526	1.827197	0.738111
N	-2.563877	-0.442353	-0.687457
C	-1.787653	-1.953704	0.260251
C	-2.932729	-1.881900	-0.663351
O	2.127825	-1.097967	-0.060054
C	3.455758	-0.641393	0.335780
C	3.531971	-0.778077	1.862646
C	4.500518	-1.538058	-0.323416
C	3.903688	1.010113	-1.613899
H	-3.922623	-2.094645	-0.254542
H	-1.976254	-1.775610	1.314097
H	-0.855332	-2.439626	-0.020197
H	5.512803	-1.170383	-0.114819
H	4.417767	-2.554953	0.075146
H	4.362388	-1.588856	-1.406018
H	3.328405	-1.818874	2.135154

H	4.523301	-0.507101	2.243222
H	2.783073	-0.147298	2.352129
H	3.683298	2.031338	-1.941247
H	4.979548	0.833509	-1.725502
H	3.363911	0.320829	-2.271069
H	5.271849	1.552443	0.799171
H	4.143645	2.837088	0.319736
H	3.797433	1.853742	1.748816
H	-2.801217	-2.334724	-1.646042
S	-3.666953	0.492911	0.271291
O	-3.604330	0.093053	1.688146
O	-4.960063	0.449174	-0.425343
C	-2.943080	2.131224	0.084598
H	-1.951841	2.132795	0.545568
H	-2.887920	2.367472	-0.979050
H	-3.614362	2.819040	0.605163

Electronic Energy = -1330.47537013 (Hartree/Particle)
Dipole Moment (Debye): 2.6389
index 1
Number of imaginary frequencies= 1
Negatives Eigenvalues: -276.427

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.289830
(Hartree/Particle)
Thermal correction to Energy= 0.309650
Thermal correction to Enthalpy= 0.310595
Thermal correction to Gibbs Free Energy= 0.239583
Sum of electronic and zero-point Energies= -1330.185540
Sum of electronic and thermal Energies= -1330.165720
Sum of electronic and thermal Enthalpies= -1330.164775
Sum of electronic and thermal Free Energies= -1330.235787
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1330.761392330
Corrected Free Energy = -1330.521809200



I1 Substrate: N-mesyl-aziridine

CARTESIAN COORDINATES

Cu	0.642652	-0.143437	-0.284199
B	-1.318963	-0.028205	-0.098457

```
 O              -2.123989    1.071973   -0.216555
 C              -3.479553    0.665147    0.178271
 C              -4.481727    1.407347   -0.698874
 N               2.479654    0.228452   -0.604136
 C               2.260502    1.700584   -0.512522
 C               0.863760    1.780693    0.078729
 O              -2.004528   -1.187310    0.154002
 C              -3.435599   -0.893374   -0.034850
 C              -3.780877   -1.326350   -1.463385
 C              -4.231299   -1.708325    0.978177
 C              -3.643476    1.076525    1.645567
 H               2.997709    2.202185    0.130747
 H              -5.501667    1.064341   -0.488664
 H              -4.432183    2.480641   -0.488478
 H              -4.274878    1.261397   -1.761381
 H              -3.467192    2.153160    1.734384
 H              -4.653196    0.859487    2.010040
 H              -2.922141    0.559254    2.286405
 H              -3.531360   -2.385054   -1.583535
 H              -4.848189   -1.195102   -1.671485
 H              -3.207821   -0.756894   -2.202082
 H              -5.295452   -1.449111    0.924706
 H              -4.127488   -2.775078    0.755831
 H              -3.880232   -1.540237    1.998739
 H               0.801645    1.838354    1.166847
 H               0.086395    2.354877   -0.422539
 H               2.320795    2.153528   -1.507103
 S               3.882980   -0.385196   -0.002809
 C               3.741918   -0.322673    1.810577
 H               2.906476   -0.957016    2.115934
 H               4.680153   -0.698202    2.227139
 H               3.583609    0.713549    2.121326
 O               3.920429   -1.810572   -0.367094
 O               5.002559    0.513802   -0.348982

 Electronic Energy =  -1330.48570273 (Hartree/Particle)
 Dipole Moment (Debye):     10.8658
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.290784
(Hartree/Particle)
 Thermal correction to Energy=                    0.310947
 Thermal correction to Enthalpy=                  0.311891
 Thermal correction to Gibbs Free Energy=         0.240029
 Sum of electronic and zero-point Energies=          -1330.194918
 Sum of electronic and thermal Energies=             -1330.174756
 Sum of electronic and thermal Enthalpies=           -1330.173812
 Sum of electronic and thermal Free Energies=        -1330.245674
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1330.78025244
 Corrected Free Energy =  -1330.54022371

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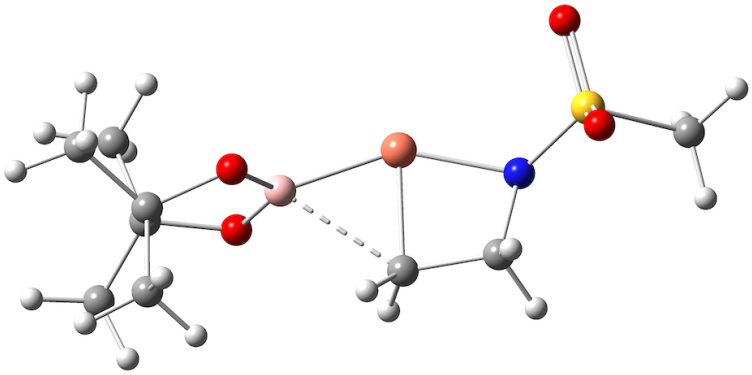


TS2 Substrate: N-mesyl-aziridine

CARTESIAN COORDINATES

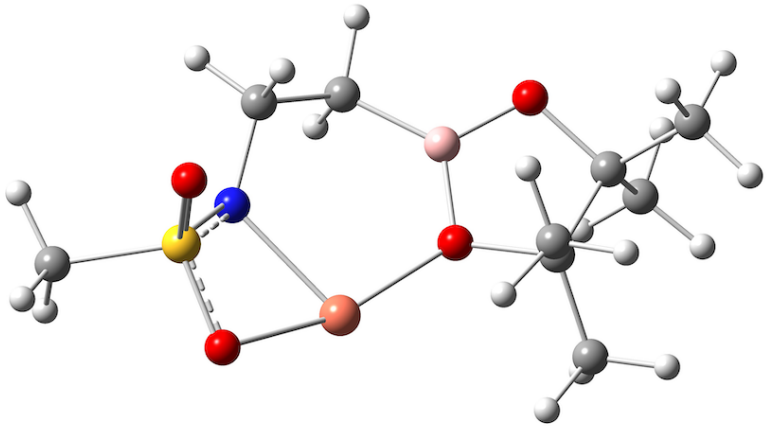
Cu	-0.648959	-0.378699	0.061505
B	1.311276	-0.149153	-0.008806
O	1.968780	0.981073	-0.414033
C	3.384473	0.621264	-0.579362
C	4.236664	1.814397	-0.161214
N	-2.467881	-0.226409	0.601905
C	-2.165880	0.959099	1.453407
C	-0.754910	1.336549	1.028064
O	2.142278	-1.180890	0.329633
C	3.514514	-0.646238	0.344294
C	3.826337	-0.309163	1.806092
C	4.459173	-1.726827	-0.168451
C	3.583757	0.315881	-2.067892
H	-2.861526	1.794319	1.284704
H	5.301006	1.552846	-0.190205
H	4.070415	2.646673	-0.852734
H	3.987913	2.156606	0.845907
H	3.283850	1.190726	-2.653167
H	4.632098	0.091357	-2.291418
H	2.969395	-0.532495	-2.386048
H	3.699572	-1.210549	2.413424
H	4.855864	0.046441	1.921473
H	3.147123	0.458178	2.191697
H	5.479782	-1.334308	-0.250050
H	4.471006	-2.568322	0.531493
H	4.149670	-2.104738	-1.145331
H	-0.659489	2.066483	0.222988
H	0.011396	1.457678	1.792705
H	-2.221700	0.687234	2.512417
S	-3.901763	-0.259643	-0.197900
C	-3.766099	0.937889	-1.562391
H	-2.967244	0.611812	-2.232578
H	-4.724875	0.950453	-2.087157
H	-3.553130	1.927994	-1.150385
O	-4.016529	-1.587210	-0.823634
O	-4.971093	0.257242	0.680590

Electronic Energy = -1330.48452246 (Hartree/Particle)
Dipole Moment (Debye): 11.2461
index 0
Harmonic frequencies
Number of imaginary frequencies= 1

Negatives Eigenvalues: -16.336

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.290658
(Hartree/Particle)
Thermal correction to Energy= 0.309967
Thermal correction to Enthalpy= 0.310911
Thermal correction to Gibbs Free Energy= 0.242113
Sum of electronic and zero-point Energies= -1330.193864
Sum of electronic and thermal Energies= -1330.174555
Sum of electronic and thermal Enthalpies= -1330.173611
Sum of electronic and thermal Free Energies= -1330.242409
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1330.78049149
Corrected Free Energy = -1330.53837803



P1 Substrate: N-mesyl-aziridine

CARTESIAN COORDINATES

C	-1.353679	2.049226	0.012723
Cu	-0.739178	-0.987884	-0.562338
B	1.168639	1.227236	-0.290043
O	1.082040	-0.171239	-0.459895
C	2.255803	-0.784976	0.204661
C	2.634011	-2.035222	-0.576005
C	0.039774	2.268621	-0.627333
N	-1.903204	0.794614	-0.505440
O	2.407379	1.569987	0.172353
C	3.278929	0.399432	0.140476
C	4.052670	0.461760	-1.181483
C	4.236591	0.474666	1.325270
C	1.811399	-1.141164	1.625236
H	-1.991735	2.907352	-0.251024
H	-0.097478	2.271688	-1.720312
H	0.409859	3.266655	-0.358244
H	4.846206	-0.434516	1.384539
H	4.907927	1.329916	1.199169
H	3.701094	0.601908	2.268663
H	4.590671	1.413308	-1.231154
H	4.780070	-0.353497	-1.256333
H	3.376737	0.408229	-2.041205
H	0.945891	-1.811251	1.574082

H	2.611248	-1.651308	2.171292
H	1.513226	-0.250583	2.186633
H	3.543009	-2.483596	-0.159816
H	1.825147	-2.770827	-0.500054
H	2.799057	-1.819522	-1.633817
H	-1.268499	2.037713	1.108990
S	-3.005568	-0.008979	0.330010
C	-4.639454	0.218086	-0.413979
H	-4.566249	-0.034446	-1.473236
H	-5.341973	-0.442124	0.100173
H	-4.927480	1.263587	-0.278981
O	-2.670392	-1.472169	0.009188
O	-3.137591	0.346241	1.761999

Electronic Energy = -1330.56983965 (Hartree/Particle)
Dipole Moment (Debye): 6.4223
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.292852
(Hartree/Particle)
Thermal correction to Energy= 0.312324
Thermal correction to Enthalpy= 0.313268
Thermal correction to Gibbs Free Energy= 0.245148
Sum of electronic and zero-point Energies= -1330.276988
Sum of electronic and thermal Energies= -1330.257516
Sum of electronic and thermal Enthalpies= -1330.256572
Sum of electronic and thermal Free Energies= -1330.324692
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1330.85610185
Corrected Free Energy = -1330.61095420

SUBSTRATE: N-TOSYL-AZIRIDINE

N-tosyl-aziridine

CARTESIAN COORDINATES

C	-3.081264	-0.437755	-0.877590
C	-2.067213	-1.522640	-0.958585
H	-3.581488	-0.301747	0.079509
H	-1.867585	-2.031399	-1.897930
N	-1.641945	-0.107525	-0.954165
H	-3.644443	-0.129452	-1.753980
H	-1.896401	-2.100761	-0.052647
S	-0.947445	0.498482	0.502044
O	-1.372423	-0.315244	1.656589
O	-1.183403	1.944701	0.487712
C	0.783745	0.168579	0.178296
C	1.490678	1.044498	-0.649247
C	1.384016	-0.953505	0.752218
C	2.834768	0.778364	-0.913606
H	0.994720	1.915176	-1.066026
C	2.731073	-1.206576	0.480574

H	0.808925	-1.598341	1.408821
C	3.452242	-0.345059	-0.351653
H	3.400998	1.449837	-1.553076
H	3.216134	-2.072025	0.923554
H	4.500211	-0.545415	-0.558632

Electronic Energy = -913.586590503 (Hartree/Particle)
Dipole Moment (Debye): 4.6379
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.161572
(Hartree/Particle)
Thermal correction to Energy= 0.172181
Thermal correction to Enthalpy= 0.173125
Thermal correction to Gibbs Free Energy= 0.123997
Sum of electronic and zero-point Energies= -913.425019
Sum of electronic and thermal Energies= -913.414409
Sum of electronic and thermal Enthalpies= -913.413465
Sum of electronic and thermal Free Energies= -913.462594
PCM-SP (solvent=THF;6-311+g(2d,p)) = -913.784535565
Corrected Free Energy = -913.660539062

Complex-1 Substrate: N-tosyl-aziridine

CARTESIAN COORDINATES

C	-2.852053	-1.808241	-1.619934
C	-2.826559	-2.803543	-0.520288
H	-3.801741	-1.322090	-1.827468
H	-2.102167	-3.611929	-0.517046
N	-2.208606	-1.463488	-0.323723
Cu	-0.172070	-1.225181	-0.267445
B	1.708918	-0.697944	-0.149375
O	2.840373	-1.348321	-0.621995
O	2.068563	0.502132	0.473050
C	4.022534	-0.675170	-0.105207
C	3.476038	0.761399	0.210114
C	5.122282	-0.731153	-1.163029
H	6.000665	-0.158159	-0.840451
H	5.430190	-1.770688	-1.318491
H	4.778187	-0.336543	-2.122113
C	4.459759	-1.445136	1.149143
H	4.631846	-2.491728	0.877702
H	5.385531	-1.038057	1.572083
H	3.679881	-1.419868	1.916834
C	3.533714	1.710715	-0.995651
H	2.959181	2.613835	-0.762788
H	4.562697	2.006133	-1.230870
H	3.088236	1.246757	-1.881276
C	4.090855	1.434491	1.434991
H	5.172419	1.564849	1.304979
H	3.643564	2.424817	1.576388
H	3.914362	0.853837	2.343464

H	-2.145809	-1.872460	-2.442165
H	-3.758110	-2.988981	0.009102
S	-3.113249	-0.382635	0.757483
O	-2.673871	-0.746714	2.103055
O	-4.531426	-0.449363	0.373658
C	-2.428935	1.192434	0.272627
C	-3.141032	1.991903	-0.626132
C	-1.168817	1.553033	0.761082
C	-2.563987	3.191451	-1.047850
H	-4.122413	1.683450	-0.971340
C	-0.600466	2.746997	0.315251
H	-0.633789	0.914358	1.454892
C	-1.295957	3.561909	-0.583246
H	-3.102297	3.832796	-1.739970
H	0.391833	3.017193	0.661107
H	-0.847979	4.490613	-0.926837

Electronic Energy = -1522.26036101 (Hartree/Particle)
Dipole Moment (Debye): 4.0242
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.345112
(Hartree/Particle)
Thermal correction to Energy= 0.368409
Thermal correction to Enthalpy= 0.369353
Thermal correction to Gibbs Free Energy= 0.289816
Sum of electronic and zero-point Energies= -1521.915249
Sum of electronic and thermal Energies= -1521.891952
Sum of electronic and thermal Enthalpies= -1521.891008
Sum of electronic and thermal Free Energies= -1521.970545
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1522.590872550
Corrected Free Energy = -1522.301056540

TS1 Substrate: N-tosyl-aziridine

CARTESIAN COORDINATES

Cu	-0.332187	-0.913672	-0.480565
B	1.590291	-0.479914	-0.263171
O	2.045575	0.728972	0.256381
C	3.492711	0.788054	0.098553
C	4.086825	1.528040	1.294529
N	-2.215322	-1.373741	-0.655081
C	-1.271629	-2.769831	0.316371
C	-2.491312	-2.825039	-0.509216
O	2.659761	-1.319073	-0.547398
C	3.876498	-0.730221	-0.003191
C	4.114009	-1.388816	1.363062
C	5.037713	-1.042713	-0.943675
C	3.765304	1.571559	-1.193129
H	-3.425512	-3.069313	0.000327
H	-1.392651	-2.558949	1.373861
H	-0.340272	-3.221803	-0.016503

H	5.953868	-0.540971	-0.608161
H	5.223284	-2.122113	-0.953989
H	4.821103	-0.729727	-1.967756
H	4.174743	-2.473507	1.226446
H	5.047707	-1.043810	1.821760
H	3.287006	-1.179709	2.049338
H	3.291124	2.555558	-1.116088
H	4.838946	1.714771	-1.360511
H	3.338819	1.058751	-2.061000
H	5.182977	1.516698	1.252677
H	3.756586	2.572573	1.282570
H	3.768235	1.084919	2.241186
H	-2.413365	-3.333595	-1.470329
S	-3.286090	-0.425381	0.337747
O	-3.225145	-0.891615	1.734652
O	-4.575537	-0.407860	-0.365845
C	-2.501524	1.177580	0.201512
C	-2.925215	2.054418	-0.798743
C	-1.434356	1.477460	1.053542
C	-2.250382	3.268210	-0.947621
H	-3.758893	1.784722	-1.438700
C	-0.760412	2.687151	0.881711
H	-1.131499	0.774477	1.822032
C	-1.168646	3.578322	-0.115458
H	-2.564474	3.966409	-1.718421
H	0.092252	2.917216	1.512113
H	-0.638069	4.517298	-0.248814

Electronic Energy = -1522.22116686 (Hartree/Particle)
Dipole Moment (Debye): 3.2788
index 1
Number of imaginary frequencies= 1
Negatives Eigenvalues: -277.345

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342780
(Hartree/Particle)
Thermal correction to Energy= 0.365792
Thermal correction to Enthalpy= 0.366736
Thermal correction to Gibbs Free Energy= 0.287514
Sum of electronic and zero-point Energies= -1521.878387
Sum of electronic and thermal Energies= -1521.855375
Sum of electronic and thermal Enthalpies= -1521.854431
Sum of electronic and thermal Free Energies= -1521.933653
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1522.55292705
Corrected Free Energy = -1522.26541319

I1 Substrate: N-tosyl-aziridine

CARTESIAN COORDINATES

Cu	-0.146098	-1.138052	-0.149097
B	1.729532	-0.540415	-0.013173
O	2.523558	-0.491431	1.101594
C	3.739188	0.247920	0.739655

C	4.919588	-0.364760	1.485274
N	-1.948906	-1.722963	0.167552
C	-1.757361	-1.604615	1.650124
C	-0.499336	-0.768556	1.756013
O	2.354084	-0.092061	-1.148970
C	3.779221	0.078279	-0.823831
C	4.485209	-1.201821	-1.282825
C	4.306729	1.284466	-1.592591
C	3.512551	1.695524	1.190476
H	-2.614919	-1.133541	2.148363
H	5.857480	0.110598	1.174372
H	4.797457	-0.207459	2.561877
H	4.995783	-1.439812	1.307493
H	3.300054	1.703521	2.264217
H	4.397722	2.314115	1.007489
H	2.658685	2.143468	0.671908
H	4.294105	-1.349447	-2.350243
H	5.567787	-1.136083	-1.129488
H	4.108368	-2.078407	-0.746238
H	5.344417	1.495341	-1.307523
H	4.282827	1.075903	-2.666979
H	3.704176	2.176675	-1.408066
H	-0.643031	0.313260	1.755771
H	0.339531	-1.099805	2.365551
H	-1.629207	-2.606899	2.068298
S	-3.254256	-0.931266	-0.468436
O	-3.251974	-1.218746	-1.910731
O	-4.450196	-1.179695	0.359206
C	-2.860913	0.828764	-0.279550
C	-3.341227	1.535719	0.824854
C	-1.984315	1.424356	-1.194172
C	-2.918984	2.854529	1.026168
H	-4.044066	1.058293	1.500572
C	-1.566380	2.739755	-0.983828
H	-1.651734	0.862194	-2.062510
C	-2.028323	3.453394	0.129241
H	-3.291079	3.414418	1.880352
H	-0.888893	3.209798	-1.691969
H	-1.703505	4.478183	0.289697

Electronic Energy = -1522.23482096 (Hartree/Particle)
Dipole Moment (Debye): 10.8657
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.344144
(Hartree/Particle)
Thermal correction to Energy= 0.367282
Thermal correction to Enthalpy= 0.368227
Thermal correction to Gibbs Free Energy= 0.288094
Sum of electronic and zero-point Energies= -1521.890677
Sum of electronic and thermal Energies= -1521.867539
Sum of electronic and thermal Enthalpies= -1521.866594
Sum of electronic and thermal Free Energies= -1521.946726
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1522.57473379
Corrected Free Energy = -1522.28663883

SUBSTRATE: N-(2-PICOLINOYL)-AZIRIDINE

N-(2-picolinoyl)-aziridine

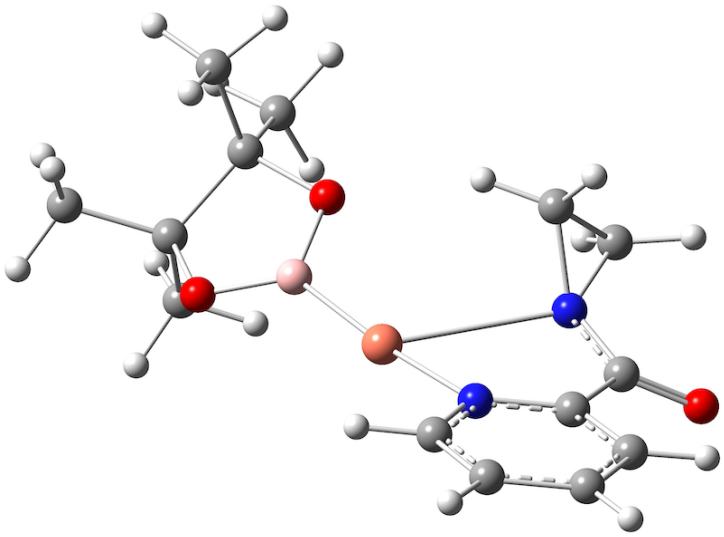
CARTESIAN COORDINATES

C	-3.256706	-0.213857	0.114189
C	-2.299273	-1.355547	0.337341
H	-3.453074	0.470213	0.938665
H	-1.850832	-1.460163	1.323339
H	-2.405086	-2.282572	-0.220964
N	-1.922587	-0.193835	-0.443387
C	-0.969823	0.757536	-0.137435
C	0.459104	0.271375	-0.075166
C	1.476976	1.222972	0.071304
C	2.797611	0.780803	0.131453
H	1.214297	2.273506	0.131456
C	1.963234	-1.459467	-0.088757
C	3.050316	-0.589668	0.049367
H	3.613065	1.491068	0.239930
H	2.120886	-2.534648	-0.152690
H	4.062585	-0.981700	0.091817
O	-1.244142	1.945106	0.001024
N	0.692381	-1.049127	-0.152119
H	-4.065895	-0.320708	-0.604978

Electronic Energy = -494.386797421 (Hartree/Particle)
Dipole Moment (Debye): 3.1534
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.149540
(Hartree/Particle)
Thermal correction to Energy= 0.158597
Thermal correction to Enthalpy= 0.159541
Thermal correction to Gibbs Free Energy= 0.114419
Sum of electronic and zero-point Energies= -494.237257
Sum of electronic and thermal Energies= -494.228201
Sum of electronic and thermal Enthalpies= -494.227257
Sum of electronic and thermal Free Energies= -494.272378
PCM-SP (solvent=THF;6-311+g(2d,p)) = -494.520574019
Corrected Free Energy = -494.406154598



Complex-1 Substrate: N-(2-picolinoyl)-aziridine

CARTESIAN COORDINATES

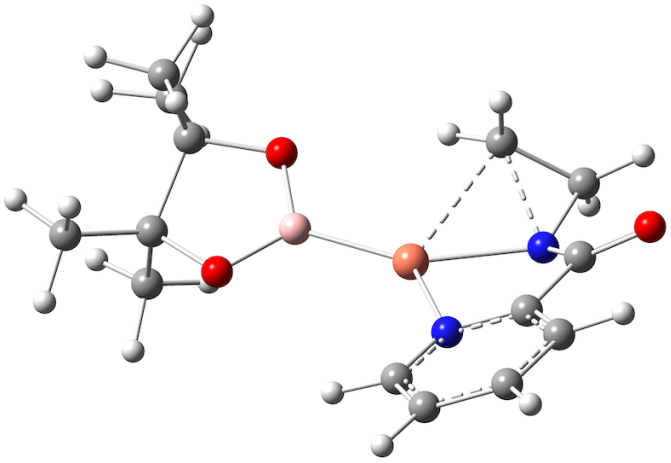
C	1.073592	3.121071	0.030476
C	0.967944	2.077211	1.102678
H	1.829370	3.899325	0.122055
H	1.661810	2.137183	1.939928
H	0.010477	1.599264	1.294885
N	1.554787	1.777761	-0.212130
C	2.881065	1.498872	-0.469347
C	3.342295	0.097202	-0.134153
C	4.718755	-0.127709	-0.034222
C	5.181525	-1.408430	0.261987
H	5.393238	0.705256	-0.197985
C	2.895256	-2.132689	0.310473
C	4.250197	-2.432713	0.438812
H	6.246723	-1.603245	0.349268
H	2.134557	-2.898672	0.426923
H	4.558342	-3.448364	0.666356
O	3.652619	2.287585	-1.003560
N	2.438565	-0.896008	0.032862
Cu	0.426010	-0.740512	-0.126889
B	-1.525247	-0.541938	-0.091173
O	-2.101551	0.650941	0.372091
O	-2.526913	-1.425604	-0.476901
C	-3.538711	0.464444	0.497597
C	-3.801388	-0.726596	-0.488856
C	-4.239570	1.772412	0.136910
H	-5.329148	1.642933	0.137015
H	-3.987760	2.541770	0.875437
H	-3.930534	2.135752	-0.846195
C	-3.815293	0.109003	1.965746
H	-3.421544	0.908090	2.603066
H	-4.888589	0.005237	2.163271
H	-3.313825	-0.823455	2.243546
C	-4.046492	-0.271783	-1.935179
H	-4.017364	-1.149100	-2.589566
H	-5.022358	0.215026	-2.047620
H	-3.265901	0.420759	-2.265844

C	-4.898876	-1.695907	-0.054680
H	-5.863384	-1.179249	0.028889
H	-5.000870	-2.492741	-0.799299
H	-4.665995	-2.162585	0.905510
H	0.176202	3.389377	-0.521609

Electronic Energy = -1103.06390231 (Hartree/Particle)
Dipole Moment (Debye): 4.5991
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.333410
(Hartree/Particle)
Thermal correction to Energy= 0.355091
Thermal correction to Enthalpy= 0.356035
Thermal correction to Gibbs Free Energy= 0.280581
Sum of electronic and zero-point Energies= -1102.730493
Sum of electronic and thermal Energies= -1102.708811
Sum of electronic and thermal Enthalpies= -1102.707867
Sum of electronic and thermal Free Energies= -1102.783322
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1103.33107889
Corrected Free Energy = -1103.050498580



TS1 Substrate: N-(2-picolinoyl)-aziridine

CARTESIAN COORDINATES

N	-2.157884	1.000066	-0.271207
C	-3.282602	0.341837	0.061414
C	-4.442247	1.000531	0.478829
C	-4.432869	2.394943	0.519740
C	-3.266031	3.078186	0.163773
C	-2.143022	2.337054	-0.211243
C	-3.233571	-1.160401	-0.000298
O	-4.166339	-1.846490	0.413908
Cu	-0.480548	-0.345464	-0.446033
B	1.450238	0.003426	-0.197391
O	2.159526	1.179032	-0.428992
C	3.583943	0.903599	-0.315392

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 C                 4.276348    2.126322    0.282442
 N                -2.069422   -1.661372   -0.590599
 C                -0.856338   -2.519069    0.461252
 C                -1.861239   -3.098972   -0.451267
 O                 2.315644   -0.984333    0.284941
 C                 3.603993   -0.379215    0.588232
 C                 3.603978   -0.062970    2.090852
 C                 4.709767   -1.381527    0.265845
 C                 4.103321    0.650330   -1.738112
 H                -2.698245   -3.642021   -0.012823
 H                -1.143856   -2.341834    1.492116
 H                 0.205212   -2.533565    0.239113
 H                -5.310271    0.414869    0.761745
 H                -5.319565    2.941489    0.829176
 H                -1.199610    2.809268   -0.471470
 H                -3.220386    4.162887    0.179675
 H                 5.698638   -0.925452    0.400264
 H                 4.636289   -2.241709    0.940425
 H                 4.630923   -1.750805   -0.759493
 H                 3.413284   -0.987348    2.646325
 H                 4.566177    0.347031    2.419107
 H                 2.812910    0.651217    2.340744
 H                 3.871665    1.522393   -2.358364
 H                 5.187921    0.491397   -1.751616
 H                 3.613454   -0.220675   -2.184886
 H                 5.339399    1.921968    0.461889
 H                 4.203250    2.968190   -0.414632
 H                 3.813704    2.429522    1.224826
 H                -1.476275   -3.555922   -1.362811

 Electronic Energy =  -1103.03395879 (Hartree/Particle)
 Dipole Moment (Debye):      2.2937
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -360.238

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.331157
(Hartree/Particle)
 Thermal correction to Energy=                    0.352398
 Thermal correction to Enthalpy=                  0.353342
 Thermal correction to Gibbs Free Energy=         0.278812
 Sum of electronic and zero-point Energies=          -1102.702801
 Sum of electronic and thermal Energies=             -1102.681561
 Sum of electronic and thermal Enthalpies=           -1102.680617
 Sum of electronic and thermal Free Energies=        -1102.755147
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1103.29923250
 Corrected Free Energy =  -1103.020420710

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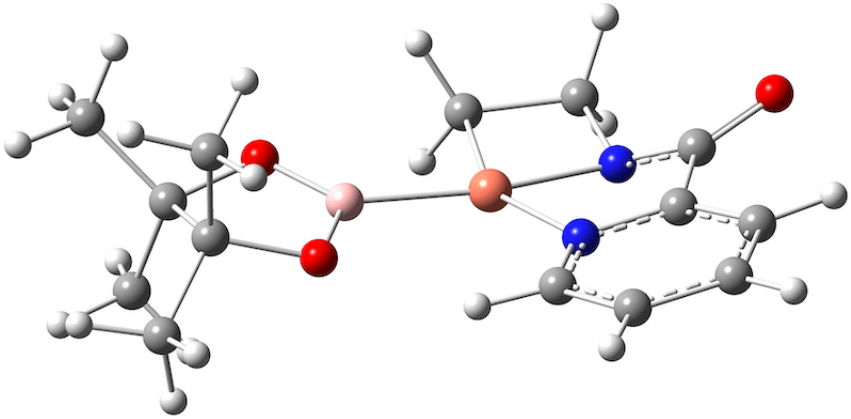


I1 Substrate: N-(2-picolinoyl)-aziridine

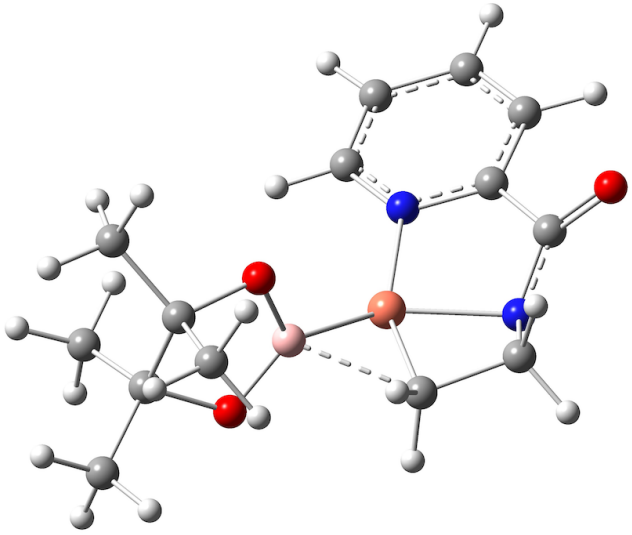
CARTESIAN COORDINATES

C	1.909592	-3.004087	0.020938
C	0.386511	-2.758070	0.011979
H	2.233571	-3.753591	-0.713782
H	-0.165147	-3.152630	-0.842693
H	-0.151938	-2.922717	0.945758
N	2.328969	-1.650163	-0.341823
C	3.349825	-0.939388	0.157533
C	3.046163	0.556562	0.008636
C	4.028876	1.532833	0.149306
C	3.663801	2.875918	0.037545
H	5.046787	1.214574	0.349414
C	1.388163	2.175133	-0.292605
C	2.324066	3.204833	-0.189247
H	4.412508	3.658083	0.132132
H	0.327480	2.353424	-0.440114
H	2.002539	4.238067	-0.275959
O	4.399111	-1.318212	0.692253
N	1.749757	0.887021	-0.202915
Cu	0.640164	-0.823538	-0.244799
B	-1.267967	-0.342678	-0.078820
O	-2.323634	-1.167325	0.225614
O	-1.668631	0.969134	-0.261215
C	-3.560325	-0.413073	0.030472
C	-3.067488	1.073846	0.161875
C	-4.571263	-0.853267	1.084827
H	-5.482805	-0.246656	1.021760
H	-4.844824	-1.900149	0.917338
H	-4.162992	-0.769703	2.094673
C	-4.069217	-0.763217	-1.373460
H	-4.200696	-1.847745	-1.441333
H	-5.031044	-0.282456	-1.583535
H	-3.350131	-0.461003	-2.141598
C	-3.048448	1.584130	1.607828
H	-2.512997	2.538573	1.641240
H	-4.062754	1.742659	1.990324
H	-2.530268	0.881695	2.268301
C	-3.777644	2.074056	-0.744592
H	-4.849050	2.109268	-0.513147
H	-3.362666	3.075429	-0.587505
H	-3.655424	1.819348	-1.799858
H	2.293408	-3.302519	1.005583

Electronic Energy = -1103.07323400 (Hartree/Particle)
Dipole Moment (Debye): 7.2003
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.333209
(Hartree/Particle)
Thermal correction to Energy= 0.354210
Thermal correction to Enthalpy= 0.355154
Thermal correction to Gibbs Free Energy= 0.282281
Sum of electronic and zero-point Energies= -1102.740025
Sum of electronic and thermal Energies= -1102.719024
Sum of electronic and thermal Enthalpies= -1102.718080
Sum of electronic and thermal Free Energies= -1102.790953
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1103.340038680
Corrected Free Energy = -1103.057757680



TS2 Substrate: N-(2-picolinoyl)-aziridine

CARTESIAN COORDINATES

C	0.962623	-2.788739	-0.216965
Cu	0.594820	-0.375960	-0.588670
B	-1.323467	-0.250497	-0.211515
O	-2.284309	-0.032510	-1.173965
C	-3.401320	0.644253	-0.515072
C	-4.699844	0.189254	-1.173154
C	-0.391142	-2.103047	-0.589507
N	1.958578	-1.772640	-0.577250
C	2.925178	-1.397048	0.266941
O	3.527766	-2.025945	1.152619
C	3.199275	0.108823	0.121152
C	4.427952	0.679749	0.451481
C	4.582234	2.062188	0.361629
C	3.490379	2.847039	-0.025081
C	2.281458	2.214791	-0.304201
N	2.139804	0.880091	-0.239955

```
 O              -1.773573   -0.012249    1.066433
 C              -3.220565    0.197219    0.982384
 C              -3.878460   -1.151757    1.295503
 C              -3.621766    1.238534    2.021296
 C              -3.193434    2.148891   -0.727391
 H               1.074002   -3.727796   -0.779275
 H              -0.666301   -2.268078   -1.635351
 H              -1.214738   -2.419579    0.055693
 H               5.227081    0.022723    0.778178
 H               5.536497    2.526619    0.596065
 H               1.394117    2.774855   -0.582911
 H               3.566156    3.927445   -0.097953
 H              -4.685142    1.488307    1.924099
 H              -3.453875    0.839532    3.026935
 H              -3.034862    2.154320    1.920198
 H              -3.535957   -1.493973    2.277128
 H              -4.970482   -1.068497    1.317318
 H              -3.605301   -1.910864    0.555258
 H              -3.127550    2.348883   -1.801573
 H              -4.025060    2.730352   -0.314995
 H              -2.263263    2.488171   -0.259971
 H              -5.564788    0.606948   -0.644065
 H              -4.730501    0.539784   -2.209985
 H              -4.786730   -0.899634   -1.182883
 H               1.011118   -3.031597    0.852738

 Electronic Energy =  -1103.06636388 (Hartree/Particle)
 Dipole Moment (Debye):      7.3715
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -116.042

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.332836
(Hartree/Particle)
 Thermal correction to Energy=                    0.353061
 Thermal correction to Enthalpy=                  0.354005
 Thermal correction to Gibbs Free Energy=         0.284125
 Sum of electronic and zero-point Energies=          -1102.733528
 Sum of electronic and thermal Energies=             -1102.713303
 Sum of electronic and thermal Enthalpies=           -1102.712359
 Sum of electronic and thermal Free Energies=        -1102.782239
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1103.338300330
 Corrected Free Energy =  -1103.054175450

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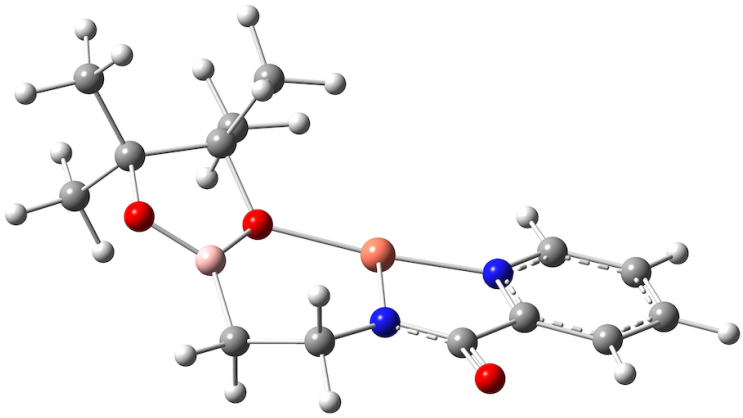

P1 Substrate: N-(2-picolinoyl)-aziridine

CARTESIAN COORDINATES

C	-0.233591	2.661788	0.058186
Cu	-0.503801	-0.444046	-0.302499
B	1.945344	1.187104	-0.328031
O	1.483527	-0.146111	-0.348564
C	2.508505	-0.999375	0.286224
C	2.487553	-2.354599	-0.406261
C	1.086935	2.440110	-0.722403
N	-1.070188	1.482986	-0.030576
C	-2.369706	1.595940	0.220838
O	-3.038189	2.607135	0.527906
C	-3.116820	0.258172	0.100111
C	-4.505312	0.229460	0.253871
C	-5.185741	-0.981407	0.140357
C	-4.459348	-2.146821	-0.120693
C	-3.076534	-2.048854	-0.254973
N	-2.417599	-0.880634	-0.147709
O	3.264356	1.223203	0.031669
C	3.796114	-0.134402	0.060383
C	4.457745	-0.376640	-1.301519
C	4.828725	-0.229093	1.179374
C	2.105773	-1.134897	1.756994
H	-0.754038	3.545227	-0.338039
H	0.824792	2.330819	-1.787373
H	1.717888	3.335213	-0.646035
H	-5.005901	1.169488	0.458662
H	-6.266147	-1.019043	0.253938
H	-2.463378	-2.922346	-0.453227
H	-4.946130	-3.112541	-0.216483
H	5.186149	-1.259949	1.286770
H	5.686176	0.407955	0.940458
H	4.418175	0.103034	2.135536
H	5.218991	0.392156	-1.465429
H	4.940408	-1.358965	-1.342313
H	3.728028	-0.310248	-2.115134
H	1.094895	-1.554914	1.809956
H	2.787862	-1.801131	2.294913
H	2.092665	-0.162230	2.258013
H	3.276726	-3.000824	-0.005821
H	1.520888	-2.838056	-0.225238
H	2.621137	-2.260820	-1.486118
H	-0.004512	2.892409	1.112568

```
 Electronic Energy =  -1103.14609975 (Hartree/Particle)
 Dipole Moment (Debye):      8.8804
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.334744
(Hartree/Particle)
 Thermal correction to Energy=                    0.355453
 Thermal correction to Enthalpy=                  0.356397
 Thermal correction to Gibbs Free Energy=         0.285303
 Sum of electronic and zero-point Energies=          -1102.811355
 Sum of electronic and thermal Energies=             -1102.790647
 Sum of electronic and thermal Enthalpies=           -1102.789702
 Sum of electronic and thermal Free Energies=        -1102.860796
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1103.41620638
 Corrected Free Energy =   -1103.13090263

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SUBSTRATE: N-(2-PICOLINOYL)-METHYL AZIRIDINE

N-(2-picolinoyl)-methyl aziridine

 CARTESIAN COORDINATES

  N               0.739112    0.955005   -0.079436
  C               0.776532   -0.387910   -0.072773
  C               1.967630   -1.120861    0.008367
  C               3.174191   -0.425834    0.075142
  C               3.145540    0.969825    0.065820
  C               1.903300    1.608771   -0.009241
  C              -0.528476   -1.147080   -0.140626
  O              -0.556011   -2.370787   -0.055804
  N              -1.655332   -0.388689   -0.382427
  C              -2.238070    0.636589    0.469511
  C              -2.633731    1.941152   -0.174604
  C              -2.954307   -0.662022    0.196876
  H              -1.786307    0.724153    1.458422
  H               1.921745   -2.204427    0.015446
  H               4.117646   -0.962213    0.133503
  H               1.841136    2.695632   -0.014609
  H               4.059521    1.554850    0.116273
  H              -2.993625   -1.420789    0.977345
  H              -3.351531    2.479435    0.456363
  H              -1.745589    2.566318   -0.314562
  H              -3.090604    1.765469   -1.154598
  H              -3.786413   -0.672113   -0.504951

 Electronic Energy =  -533.711901220 (Hartree/Particle)
 Dipole Moment (Debye):      3.3143
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA
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```
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.177547
(Hartree/Particle)
 Thermal correction to Energy=                    0.188078
 Thermal correction to Enthalpy=                  0.189022
 Thermal correction to Gibbs Free Energy=         0.140571
 Sum of electronic and zero-point Energies=          -533.534355
 Sum of electronic and thermal Energies=             -533.523824
 Sum of electronic and thermal Enthalpies=           -533.522879
 Sum of electronic and thermal Free Energies=        -533.571331
 PCM-SP (solvent=THF;6-311+g(2d,p)) =    -533.855563883
 Corrected Free Energy =  -533.714993663
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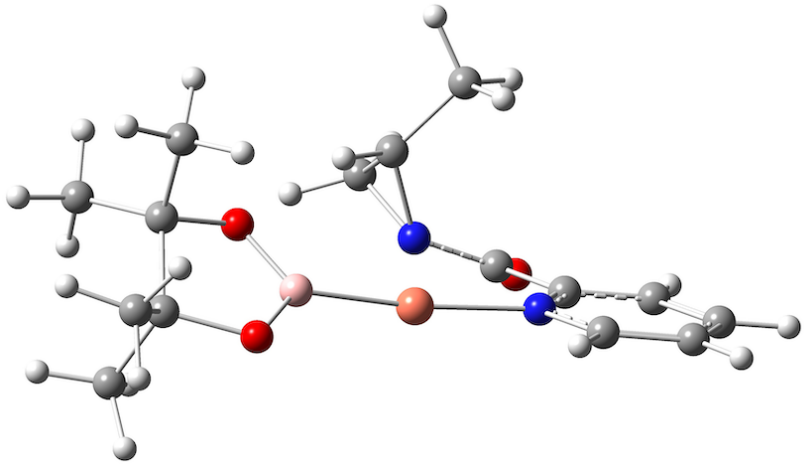

Complex-1 Substrate: N-(2-picolinoyl)-methyl aziridine

CARTESIAN COORDINATES

N	2.310494	-1.036268	0.010075
C	3.262244	-0.127749	-0.305403
C	4.626386	-0.418974	-0.198799
C	5.025672	-1.673261	0.257416
C	4.044335	-2.609506	0.586416
C	2.706040	-2.250223	0.443192
C	2.883953	1.251159	-0.804598
O	3.709505	1.920604	-1.419434
Cu	0.304735	-0.832843	-0.135828
B	-1.640870	-0.585303	-0.090424
O	-2.662583	-1.496993	-0.331330
C	-3.927240	-0.784768	-0.414428
C	-5.028670	-1.666306	0.170436
N	1.586293	1.651535	-0.591680
C	0.960401	2.082498	0.674070
C	1.788387	2.110464	1.936381
C	1.211784	3.044612	-0.450602
O	-2.189882	0.668535	0.216275
C	-3.626402	0.525714	0.393716
C	-3.876200	0.379592	1.901905
C	-4.316164	1.783470	-0.129922
C	-4.196769	-0.528514	-1.904510
H	-0.057390	1.711631	0.783576
H	5.340987	0.345318	-0.482345
H	6.080548	-1.915537	0.351402

```
 H                1.908241   -2.949205    0.675767
 H                4.301056   -3.602262    0.942516
 H               -5.407198    1.673193   -0.092095
 H               -4.038637    2.642411    0.491287
 H               -4.021996    2.003621   -1.158963
 H               -3.457981    1.251935    2.415550
 H               -4.946310    0.321467    2.132494
 H               -3.381556   -0.514088    2.295391
 H               -4.193722   -1.487620   -2.432588
 H               -5.168024   -0.045659   -2.064037
 H               -3.413939    0.099174   -2.342030
 H               -5.983245   -1.125996    0.202097
 H               -5.159265   -2.555385   -0.455893
 H               -4.781123   -2.001528    1.180556
 H                0.377495    3.364651   -1.070886
 H                1.309549    2.758553    2.679661
 H                1.866738    1.105151    2.366697
 H                2.799788    2.490447    1.748244
 H                2.032654    3.755389   -0.359733

 Electronic Energy =  -1142.38831055 (Hartree/Particle)
 Dipole Moment (Debye):      4.6135
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.361536
(Hartree/Particle)
 Thermal correction to Energy=                    0.384669
 Thermal correction to Enthalpy=                  0.385614
 Thermal correction to Gibbs Free Energy=         0.306949
 Sum of electronic and zero-point Energies=          -1142.026774
 Sum of electronic and thermal Energies=             -1142.003641
 Sum of electronic and thermal Enthalpies=           -1142.002697
 Sum of electronic and thermal Free Energies=        -1142.081362
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1142.66700664
 Corrected Free Energy =   -1142.36293795

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PATH: ANTI_MARKOVNIKOV
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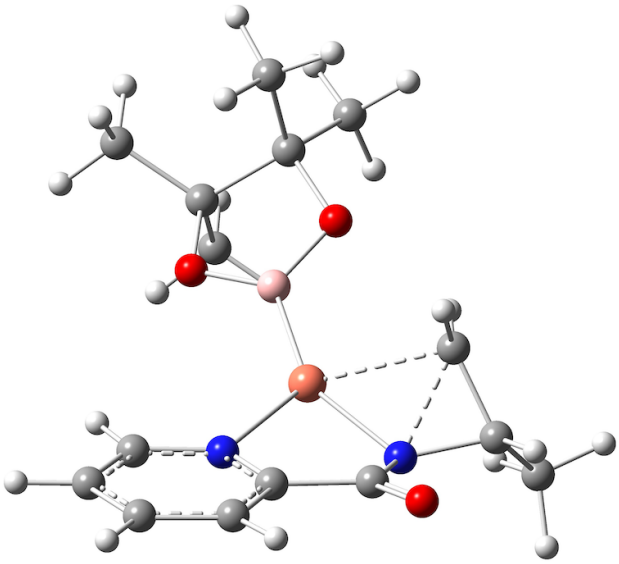


TS1 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: anti-Markovnikov

CARTESIAN COORDINATES

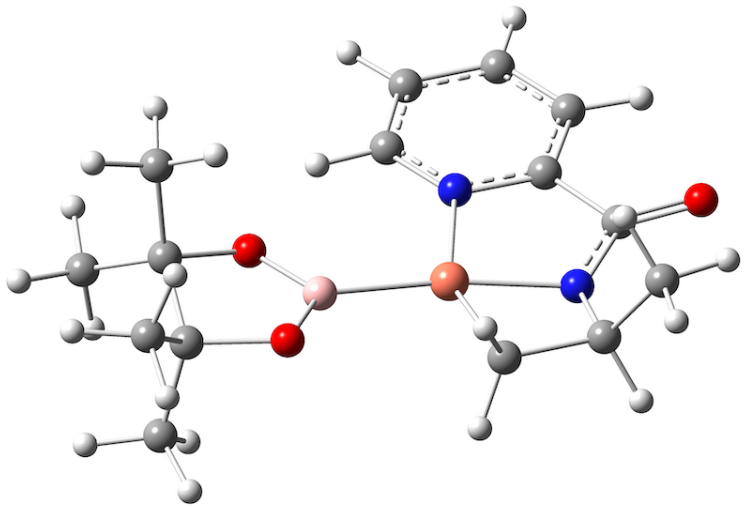
N	2.057018	-1.213949	-0.293452
C	3.209598	-0.643956	0.100543
C	4.343246	-1.392129	0.428787
C	4.276012	-2.780849	0.312625
C	3.079822	-3.371362	-0.105903
C	1.986722	-2.547088	-0.384306
C	3.221174	0.857104	0.211014
O	4.188470	1.453991	0.681304
Cu	0.435591	0.228720	-0.323142
B	-1.508174	-0.091876	-0.147358
O	-2.244819	-1.213992	-0.518856
C	-3.663120	-0.913037	-0.395126
C	-4.397529	-2.174613	0.053320
N	2.069033	1.464836	-0.292666
C	0.895790	2.238601	0.870009
C	1.901326	2.887832	0.001663
O	-2.355983	0.860152	0.429432
C	-3.664612	0.261728	0.645159
C	-3.698938	-0.219037	2.103140
C	-4.737825	1.324505	0.420944
C	-4.151586	-0.489503	-1.787999
H	2.764029	3.320390	0.510918
H	-0.168345	2.315457	0.667226
H	5.236467	-0.877943	0.766940
H	5.140930	-3.394545	0.549349
H	1.023343	-2.947967	-0.687820
H	2.989082	-4.448192	-0.211605
H	-5.740765	0.884820	0.490109
H	-4.652681	2.102194	1.187967
H	-4.631799	1.802836	-0.555729
H	-3.493398	0.632388	2.760586
H	-4.677151	-0.635567	2.370185
H	-2.931390	-0.978476	2.283217
H	-3.930772	-1.293068	-2.498224
H	-5.231568	-0.301619	-1.799482
H	-3.632813	0.412551	-2.127718

H	-5.457655	-1.961603	0.239912
H	-4.335125	-2.935687	-0.732114
H	-3.958890	-2.593440	0.962307
H	1.189671	1.931727	1.868194
C	1.399719	3.709539	-1.169951
H	1.070017	4.697261	-0.826731
H	2.197783	3.845043	-1.908044
H	0.557262	3.206102	-1.657275

Electronic Energy = -1142.35837407 (Hartree/Particle)
Dipole Moment (Debye): 2.0990
index 0
Harmonic frequencies
Number of imaginary frequencies= 1
Negatives Eigenvalues: -354.351

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.359037
(Hartree/Particle)
Thermal correction to Energy= 0.381795
Thermal correction to Enthalpy= 0.382739
Thermal correction to Gibbs Free Energy= 0.305011
Sum of electronic and zero-point Energies= -1141.999337
Sum of electronic and thermal Energies= -1141.976579
Sum of electronic and thermal Enthalpies= -1141.975635
Sum of electronic and thermal Free Energies= -1142.053363
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1142.63449331
Corrected Free Energy = -1142.32948224



I1 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: anti-Markovnikov

CARTESIAN COORDINATES

N	1.558320	1.183179	-0.137824
C	2.892995	0.955679	-0.070341
C	3.800082	2.004675	0.049651
C	3.316521	3.314496	0.084419
C	1.938985	3.537163	0.009527

```
 C                 1.086008    2.437365   -0.095070
 C                 3.350771   -0.510453   -0.091974
 O                 4.528727   -0.806044    0.150037
 Cu                0.571913   -0.597708   -0.258717
 N                 2.304409   -1.280140   -0.399751
 C                 2.014522   -2.704292   -0.247622
 C                 0.471312   -2.563756   -0.245167
 C                 2.586320   -3.325828    1.026405
 B                -1.371635   -0.280073   -0.099900
 O                -2.373595   -1.215635    0.002134
 C                -3.655752   -0.526247   -0.122240
 C                -4.670108   -1.214962    0.785734
 O                -1.867142    1.012749   -0.071536
 C                -3.284350    0.944106    0.290936
 C                -3.360874    1.190095    1.802701
 C                -4.034243    2.037849   -0.462851
 C                -4.082116   -0.655937   -1.590002
 H                 2.367570   -3.271856   -1.122082
 H                -0.054371   -2.890488   -1.143845
 H                -0.043749   -2.887974    0.660911
 H                 4.856061    1.763882    0.117117
 H                 4.004299    4.151525    0.172076
 H                 0.005414    2.530999   -0.141131
 H                 1.525581    4.540569    0.036755
 H                 2.282759   -4.377172    1.107892
 H                 3.678731   -3.265251    1.025037
 H                -5.622435   -0.670917    0.782363
 H                -4.855772   -2.231861    0.424701
 H                -4.308788   -1.283996    1.814404
 H                -4.127681   -1.717681   -1.852232
 H                -5.069008   -0.212381   -1.762420
 H                -3.358991   -0.173973   -2.255788
 H                -2.901324    2.157690    2.029270
 H                -4.398478    1.208523    2.153929
 H                -2.816594    0.418707    2.356656
 H                -5.113366    1.957349   -0.284642
 H                -3.704163    3.021685   -0.112399
 H                -3.851982    1.983601   -1.538639
 H                 2.215522   -2.786634    1.907685

 Electronic Energy =  -1142.39531716 (Hartree/Particle)
 Dipole Moment (Debye):      6.9198
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.361253
(Hartree/Particle)
 Thermal correction to Energy=                    0.383694
 Thermal correction to Enthalpy=                  0.384638
 Thermal correction to Gibbs Free Energy=         0.308618
 Sum of electronic and zero-point Energies=          -1142.034064
 Sum of electronic and thermal Energies=             -1142.011624
 Sum of electronic and thermal Enthalpies=           -1142.010679
 Sum of electronic and thermal Free Energies=        -1142.086699
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1142.67196072
 Corrected Free Energy =   -1142.36334256
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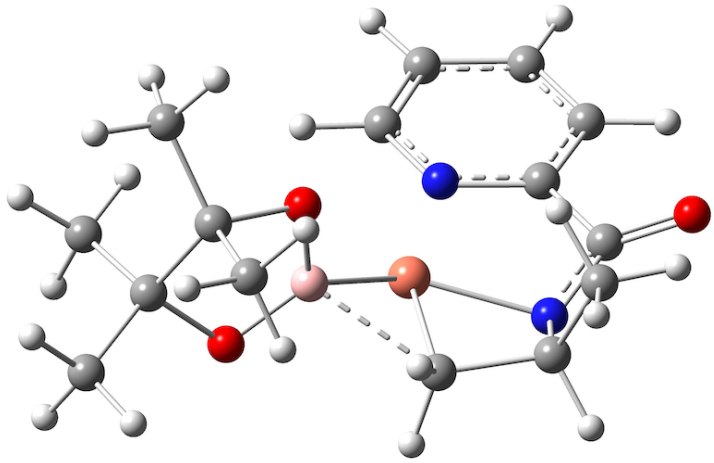

TS2 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: anti-Markovnikov

CARTESIAN COORDINATES

N	-2.099117	-1.086394	-0.150624
C	-3.189198	-0.299227	0.056007
C	-4.424153	-0.854772	0.389819
C	-4.550240	-2.240614	0.474401
C	-3.426625	-3.042189	0.248390
C	-2.216450	-2.421327	-0.051646
C	-2.977765	1.228833	0.010769
O	-3.753701	1.949791	0.661220
Cu	-0.549437	0.123497	-0.618419
N	-1.904558	1.506996	-0.729222
C	-0.917532	2.577166	-0.519454
C	0.413771	1.841702	-0.907374
C	-0.873951	3.122477	0.911475
B	1.384831	0.111068	-0.281556
O	1.854710	0.070601	1.012327
C	3.303334	-0.128048	0.940417
C	3.733496	-0.998493	2.116039
O	2.339708	-0.233359	-1.213665
C	3.474624	-0.788506	-0.477284
C	3.289744	-2.311008	-0.462182
C	4.758210	-0.416567	-1.212433
C	3.942779	1.261798	1.042289
H	-1.069028	3.415334	-1.219265
H	0.592981	1.849057	-1.987057
H	1.284047	2.264509	-0.397959
H	-5.250292	-0.178248	0.581942
H	-5.507843	-2.693081	0.718626
H	-1.307315	-2.991774	-0.215253
H	-3.478964	-4.124555	0.312549
H	-0.092945	3.887571	1.005567
H	-1.839403	3.554115	1.186436
H	4.799680	-1.244375	2.042528
H	3.570372	-0.457800	3.054020
H	3.160582	-1.927620	2.159061
H	3.606788	1.739863	1.967776
H	5.036226	1.198345	1.059677

```
  H                3.648100    1.899754    0.202682
  H                3.215377   -2.668647   -1.494072
  H                4.135435   -2.812675    0.020473
  H                2.370420   -2.591023    0.062392
  H                5.635892   -0.739280   -0.639623
  H                4.782848   -0.915206   -2.186902
  H                4.827191    0.660194   -1.383218
  H               -0.650888    2.310963    1.616027

 Electronic Energy =  -1142.38693333 (Hartree/Particle)
 Dipole Moment (Debye):      7.2355
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -111.628

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.360854
(Hartree/Particle)
 Thermal correction to Energy=                    0.382440
 Thermal correction to Enthalpy=                  0.383384
 Thermal correction to Gibbs Free Energy=         0.310726
 Sum of electronic and zero-point Energies=          -1142.026079
 Sum of electronic and thermal Energies=             -1142.004493
 Sum of electronic and thermal Enthalpies=           -1142.003549
 Sum of electronic and thermal Free Energies=        -1142.076207
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1142.66836204
 Corrected Free Energy =   -1142.36073507
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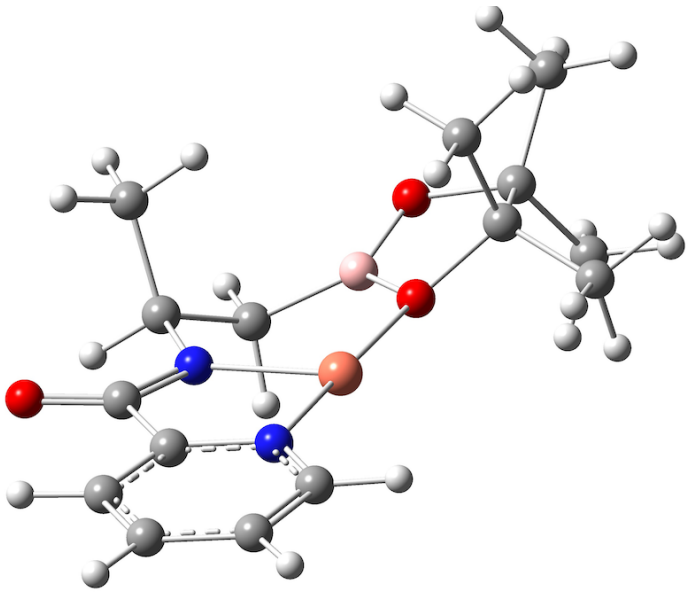

P1 Substrate: N-(2-picolinoyl)-methyl aziridine
    Path: anti-Markovnikov

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 CARTESIAN COORDINATES

  N               -2.430702   -1.023142   -0.088177
  C               -3.131893    0.138097   -0.005961
```

C	-4.523968	0.130434	0.112516
C	-5.206048	-1.084646	0.136912
C	-4.477552	-2.274195	0.046959
C	-3.091251	-2.195014	-0.062312
C	-2.381755	1.479420	-0.032352
O	-3.052990	2.521286	0.137838
Cu	-0.511750	-0.610163	-0.260342
N	-1.077708	1.334187	-0.240736
C	-0.225451	2.511176	-0.246389
C	1.063838	2.192484	-1.052907
B	1.938104	0.995376	-0.536323
O	3.268806	1.068751	-0.230507
C	3.796821	-0.276206	-0.034955
C	4.862674	-0.226162	1.055373
C	0.104355	2.954692	1.189603
O	1.472996	-0.325976	-0.366695
C	2.514240	-1.093757	0.344782
C	2.155532	-1.026673	1.831667
C	2.467758	-2.529635	-0.157792
C	4.415470	-0.705233	-1.370664
H	-0.746393	3.343164	-0.742667
H	0.758121	1.957141	-2.084568
H	1.696093	3.088095	-1.108554
H	-5.025992	1.089198	0.182787
H	-6.289211	-1.106870	0.225514
H	-2.476660	-3.087101	-0.130992
H	-4.965426	-3.243972	0.063215
H	0.768055	3.829355	1.195369
H	-0.819060	3.210379	1.718555
H	5.220498	-1.235474	1.290428
H	5.714138	0.367179	0.707376
H	4.481916	0.234725	1.969535
H	5.174238	0.028396	-1.659600
H	4.892882	-1.687891	-1.292769
H	3.661404	-0.743330	-2.163621
H	1.144210	-1.425890	1.969325
H	2.849635	-1.620878	2.434656
H	2.162118	0.004583	2.197190
H	3.267255	-3.121558	0.301759
H	1.505799	-2.977505	0.116094
H	2.567744	-2.582921	-1.244035
H	0.600620	2.140521	1.736950

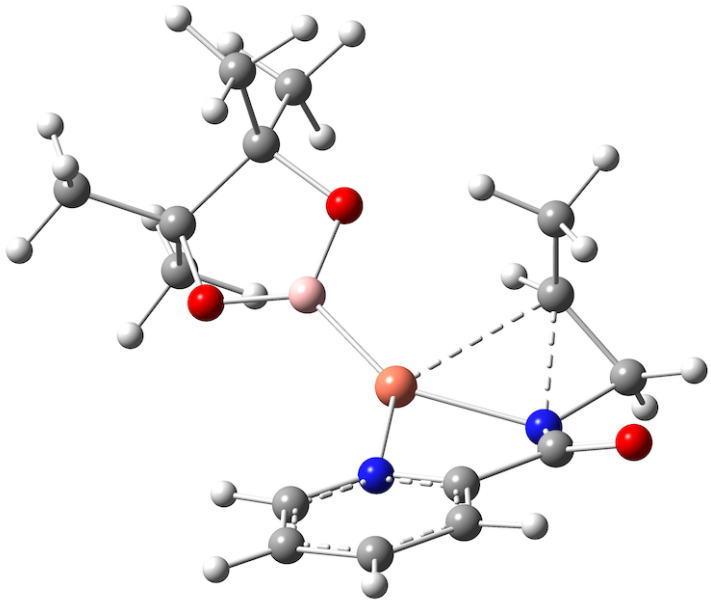
Electronic Energy = -1142.46838562 (Hartree/Particle)
Dipole Moment (Debye): 8.6974
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.362904
(Hartree/Particle)
Thermal correction to Energy= 0.384972
Thermal correction to Enthalpy= 0.385916
Thermal correction to Gibbs Free Energy= 0.312272
Sum of electronic and zero-point Energies= -1142.105482
Sum of electronic and thermal Energies= -1142.083414
Sum of electronic and thermal Enthalpies= -1142.082470

Sum of electronic and thermal Free Energies= -1142.156113
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1142.74867388
Corrected Free Energy = -1142.43640126

PATH: MARKOVNIKOV



TS1 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: Markovnikov

CARTESIAN COORDINATES

N	-2.155983	1.164611	-0.261196
C	-3.255037	0.437938	0.010750
C	-4.431410	1.013409	0.498589
C	-4.469085	2.396173	0.678069
C	-3.329482	3.151195	0.384191
C	-2.186756	2.489596	-0.069926
C	-3.158712	-1.050446	-0.200301
O	-4.062352	-1.799143	0.179462
Cu	-0.443061	-0.074003	-0.605668
B	1.491177	0.187544	-0.292179
O	2.274575	1.328513	-0.442721
C	3.675534	0.970522	-0.285141
C	4.406916	2.127327	0.392339
N	-2.007052	-1.444339	-0.865368
C	-0.690391	-2.442545	0.018735
C	-1.757598	-2.883471	-0.901216
O	2.285781	-0.867668	0.180181
C	3.589403	-0.347455	0.561679
C	3.540891	-0.093772	2.075484
C	4.653685	-1.394646	0.242090
C	4.240456	0.747627	-1.695597
H	-2.559515	-3.491203	-0.478258
H	0.320958	-2.342076	-0.361461
H	-5.276327	0.372593	0.726269

```
 H              -5.370782    2.878399    1.045772
 H              -1.262994    3.018037   -0.288909
 H              -3.319561    4.229887    0.507728
 H               5.658695   -0.999972    0.437346
 H               4.505219   -2.276966    0.874601
 H               4.600584   -1.715858   -0.800973
 H               3.278119   -1.028643    2.582139
 H               4.507909    0.249334    2.461226
 H               2.778525    0.651827    2.322975
 H               4.080776    1.655441   -2.286493
 H               5.314914    0.531068   -1.672799
 H               3.724733   -0.076581   -2.198568
 H               5.449052    1.857292    0.604780
 H               4.408148    2.999951   -0.269800
 H               3.921886    2.416824    1.327773
 H              -1.436499   -3.227891   -1.885476
 C              -0.851407   -2.493092    1.503824
 H              -0.523145   -3.489000    1.842080
 H              -0.219737   -1.745465    1.990818
 H              -1.892912   -2.364325    1.813650

 Electronic Energy =  -1142.35990393 (Hartree/Particle)
 Dipole Moment (Debye):      2.0494
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -305.921

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.359211
(Hartree/Particle)
 Thermal correction to Energy=                    0.381992
 Thermal correction to Enthalpy=                  0.382936
 Thermal correction to Gibbs Free Energy=         0.305466
 Sum of electronic and zero-point Energies=          -1142.000693
 Sum of electronic and thermal Energies=             -1141.977912
 Sum of electronic and thermal Enthalpies=           -1141.976968
 Sum of electronic and thermal Free Energies=        -1142.054438
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1142.63626637
 Corrected Free Energy =  -1142.33080044

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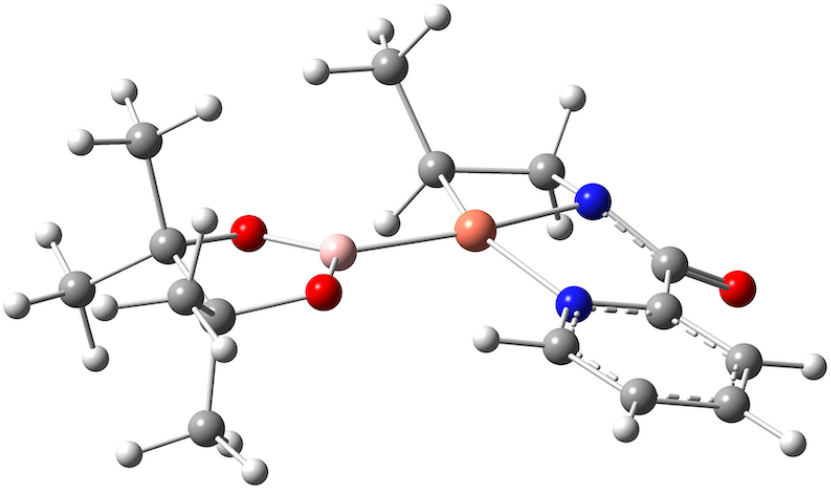


I1 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: Markovnikov

CARTESIAN COORDINATES

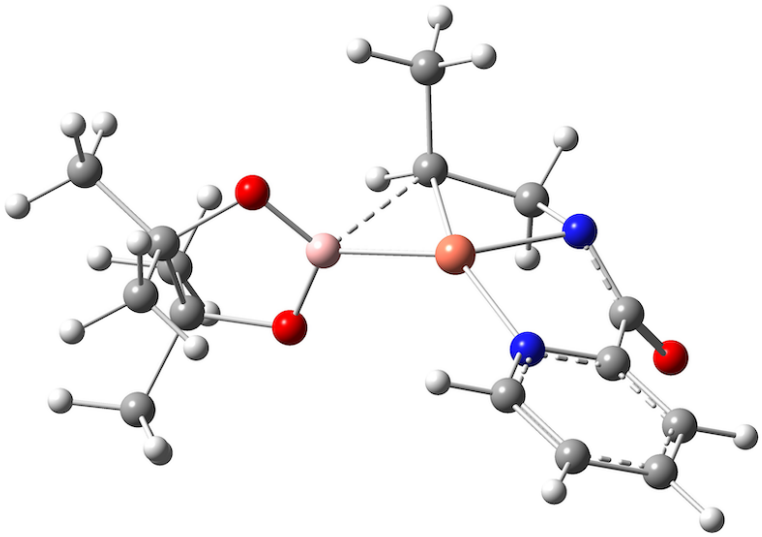
N	1.781262	1.010488	-0.223980
C	3.074491	0.684617	0.007474
C	4.067995	1.658077	0.074952
C	3.715615	2.993253	-0.131877
C	2.378209	3.318020	-0.377542
C	1.432343	2.292247	-0.404530
C	3.363220	-0.797960	0.264021
O	4.412765	-1.150064	0.816567
Cu	0.644335	-0.702321	-0.143585
N	2.331275	-1.535701	-0.169947
C	1.922238	-2.856130	0.296693
C	0.392902	-2.642335	0.228956
B	-1.256414	-0.176246	-0.004991
O	-1.638556	1.134630	-0.237266
C	-3.037486	1.277722	0.169624
C	-3.724191	2.255943	-0.778259
O	-2.332561	-0.969884	0.322414
C	-3.554197	-0.204072	0.088043
C	-4.055762	-0.597311	-1.307324
C	-4.582386	-0.588821	1.147437
C	-3.022051	1.839956	1.596427
H	2.265220	-3.664990	-0.365371
H	-0.123451	-2.699374	1.189599
H	5.083474	1.344933	0.294580
H	4.472152	3.772793	-0.095722
H	0.372725	2.470379	-0.560366
H	2.066250	4.345593	-0.536809
H	-4.796823	2.316801	-0.557901
H	-3.294189	3.255545	-0.653551
H	-3.597246	1.961565	-1.822634
H	-2.469392	2.785103	1.599884
H	-4.036459	2.030516	1.963909
H	-2.521972	1.152962	2.286418
H	-4.206349	-1.681214	-1.336671
H	-5.006949	-0.108577	-1.545598
H	-3.323806	-0.336337	-2.078435
H	-5.483231	0.029652	1.053148

H	-4.871792	-1.636651	1.015852
H	-4.182286	-0.474716	2.157564
C	-0.338336	-3.355341	-0.887260
H	-0.309807	-4.443298	-0.708704
H	-1.383670	-3.041012	-0.941695
H	0.139304	-3.172187	-1.856684
H	2.288072	-3.067114	1.310852

Electronic Energy = -1142.39413538 (Hartree/Particle)
Dipole Moment (Debye): 6.9373
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.361533
(Hartree/Particle)
Thermal correction to Energy= 0.383998
Thermal correction to Enthalpy= 0.384942
Thermal correction to Gibbs Free Energy= 0.309154
Sum of electronic and zero-point Energies= -1142.032603
Sum of electronic and thermal Energies= -1142.010138
Sum of electronic and thermal Enthalpies= -1142.009193
Sum of electronic and thermal Free Energies= -1142.084981
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1142.67134855
Corrected Free Energy = -1142.36219417



TS2 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: Markovnikov

CARTESIAN COORDINATES

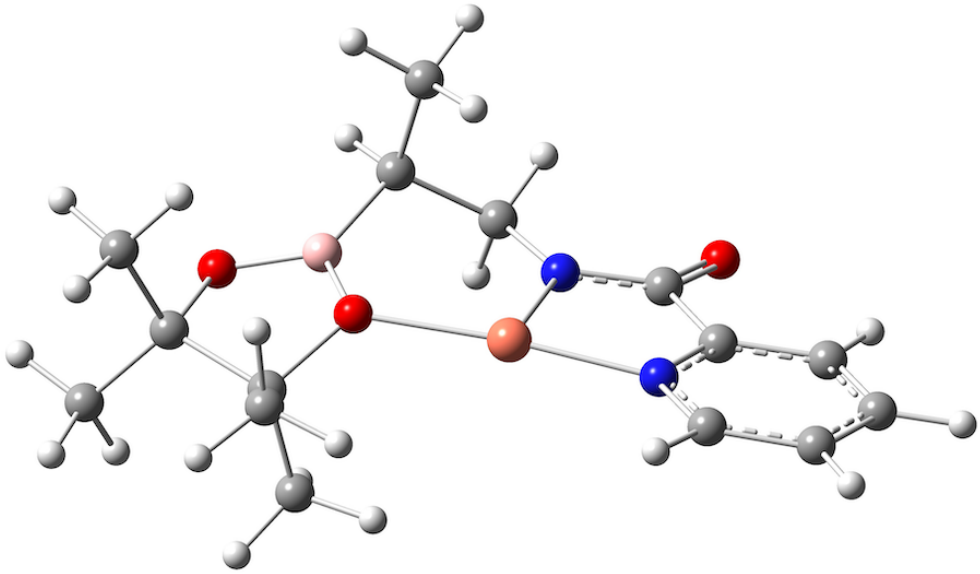
N	2.197798	0.892005	-0.362836
C	3.198238	0.175305	0.214581
C	4.433076	0.758932	0.497797
C	4.658491	2.085599	0.135169
C	3.627854	2.811491	-0.472361
C	2.407034	2.178577	-0.690584

C	2.842468	-1.254275	0.652846
O	3.347361	-1.691370	1.701168
Cu	0.618250	-0.356492	-0.554583
N	1.921203	-1.774863	-0.163616
C	0.850871	-2.639019	0.346213
C	-0.434056	-2.056761	-0.327910
B	-1.295602	-0.162580	-0.151490
O	-1.667236	0.237534	1.112623
C	-3.106181	0.502939	1.078066
C	-3.408221	1.667716	2.014421
O	-2.299057	-0.002935	-1.082742
C	-3.349354	0.793173	-0.448676
C	-3.090904	2.254397	-0.835925
C	-4.699138	0.330852	-0.987729
C	-3.800493	-0.772542	1.569988
H	0.963405	-3.697714	0.062203
H	-1.310565	-2.235578	0.303881
H	5.180750	0.156677	1.003055
H	5.620031	2.554086	0.328265
H	1.563835	2.700184	-1.133124
H	3.759211	3.849744	-0.760751
H	-4.464339	1.954474	1.943393
H	-3.201834	1.372307	3.048245
H	-2.790870	2.538956	1.783920
H	-3.419221	-1.022602	2.564968
H	-4.885481	-0.637026	1.636313
H	-3.599374	-1.619112	0.905280
H	-3.076260	2.334172	-1.927581
H	-3.873570	2.915688	-0.448770
H	-2.122979	2.597224	-0.456071
H	-5.516437	0.844327	-0.467287
H	-4.770880	0.566686	-2.054572
H	-4.831798	-0.747216	-0.871076
C	-0.662941	-2.600597	-1.738514
H	-0.907737	-3.671065	-1.676595
H	-1.482815	-2.085735	-2.246187
H	0.243127	-2.505330	-2.346411
H	0.790558	-2.592550	1.441737

Electronic Energy = -1142.38486250 (Hartree/Particle)
Dipole Moment (Debye): 7.2577
index 0
Harmonic frequencies
Number of imaginary frequencies= 1
Negatives Eigenvalues: -112.199

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.361217
(Hartree/Particle)
Thermal correction to Energy= 0.382847
Thermal correction to Enthalpy= 0.383792
Thermal correction to Gibbs Free Energy= 0.311286
Sum of electronic and zero-point Energies= -1142.023646
Sum of electronic and thermal Energies= -1142.002015
Sum of electronic and thermal Enthalpies= -1142.001071
Sum of electronic and thermal Free Energies= -1142.073576
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1142.66758797
Corrected Free Energy = -1142.35630147



P1 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: Markovnikov

CARTESIAN COORDINATES

N	-2.462138	-0.933162	-0.196503
C	-3.147293	0.170975	0.202296
C	-4.538010	0.143763	0.335079
C	-5.234626	-1.028245	0.046757
C	-4.522368	-2.157349	-0.367803
C	-3.136845	-2.063903	-0.473685
C	-2.383088	1.468221	0.513537
O	-3.046923	2.447482	0.918982
Cu	-0.540834	-0.512883	-0.265586
N	-1.078407	1.359916	0.293391
C	-0.221475	2.501601	0.534061
C	1.087881	2.388316	-0.291952
B	1.921755	1.078373	-0.042335
O	3.235444	1.049060	0.336795
C	3.757429	-0.301797	0.164849
C	4.778845	-0.573257	1.264823
O	1.449923	-0.232407	-0.264015
C	2.461582	-1.180086	0.245879
C	2.042322	-1.530670	1.675855
C	2.438598	-2.415554	-0.642611
C	4.429007	-0.340404	-1.213073
H	-0.734548	3.440300	0.273603
H	1.732240	3.232266	-0.007167
H	-5.027223	1.054586	0.662571
H	-6.316780	-1.063835	0.143078
H	-2.534248	-2.910350	-0.787750
H	-5.022140	-3.092008	-0.603130
H	5.128124	-1.611418	1.217970
H	5.642863	0.085515	1.132087
H	4.361621	-0.386186	2.256823
H	5.198038	0.437073	-1.252523
H	4.903597	-1.309731	-1.399416

H	3.706742	-0.143908	-2.012232
H	1.028291	-1.946010	1.656138
H	2.714420	-2.275183	2.114572
H	2.030168	-0.643613	2.316331
H	3.219173	-3.121225	-0.336810
H	1.466793	-2.912657	-0.545439
H	2.583985	-2.161273	-1.694706
C	0.781780	2.504452	-1.806533
H	0.275973	3.454969	-2.019160
H	1.692756	2.463956	-2.418099
H	0.114164	1.696643	-2.127165
H	0.025221	2.577079	1.606895

Electronic Energy = -1142.46291962 (Hartree/Particle)
Dipole Moment (Debye): 8.8624
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.363179
(Hartree/Particle)
Thermal correction to Energy= 0.385327
Thermal correction to Enthalpy= 0.386271
Thermal correction to Gibbs Free Energy= 0.312250
Sum of electronic and zero-point Energies= -1142.099741
Sum of electronic and thermal Energies= -1142.077593
Sum of electronic and thermal Enthalpies= -1142.076649
Sum of electronic and thermal Free Energies= -1142.150669
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1142.74378919
Corrected Free Energy = -1142.43153857

SUBSTRATE: 1c

1c

CARTESIAN COORDINATES

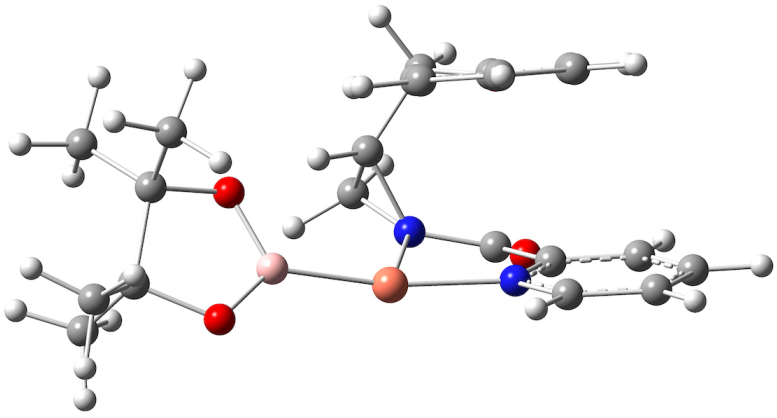
C	-2.972280	-1.942506	0.233467
C	-2.302083	-1.440191	-1.017106
H	-2.352174	-2.428390	0.984127
N	-2.730748	-0.529033	0.026683
C	-1.957973	0.237868	0.883219
C	-1.100412	1.301607	0.244185
C	-0.292353	2.086294	1.076206
C	0.531914	3.046001	0.492930
H	-0.322380	1.922697	2.147550
C	-0.327695	2.358978	-1.639032
C	0.516080	3.189400	-0.895436
H	1.178301	3.666001	1.108385
H	-0.367072	2.440565	-2.723955
H	1.143062	3.921775	-1.395971
O	-2.018738	0.119198	2.101652
N	-1.120283	1.430622	-1.092205
H	-4.012749	-2.259073	0.197053
C	-0.830943	-1.676609	-1.284332

H	-0.456285	-0.868044	-1.921453
H	-0.695841	-2.638422	-1.800997
O	-0.146524	-1.683352	-0.037266
C	1.177907	-1.335288	0.017545
C	1.653409	-0.974033	1.285618
C	2.036614	-1.337186	-1.087131
C	2.988695	-0.610995	1.443111
H	0.957478	-0.972752	2.119244
C	3.375229	-0.964405	-0.913156
H	1.680722	-1.632430	-2.068607
C	3.858135	-0.599642	0.344279
H	3.351367	-0.327660	2.428085
H	4.040561	-0.967506	-1.773069
H	4.898500	-0.312901	0.470340
H	-2.889643	-1.377512	-1.933366

Electronic Energy = -839.994211918 (Hartree/Particle)
Dipole Moment (Debye): 4.1141
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.263916
(Hartree/Particle)
Thermal correction to Energy= 0.279548
Thermal correction to Enthalpy= 0.280492
Thermal correction to Gibbs Free Energy= 0.218680
Sum of electronic and zero-point Energies= -839.730296
Sum of electronic and thermal Energies= -839.714664
Sum of electronic and thermal Enthalpies= -839.713720
Sum of electronic and thermal Free Energies= -839.775531
PCM-SP (solvent=THF;6-311+g(2d,p)) = -840.217420194
Corrected Free Energy = -839.998739276



Complex-1 Substrate: 1c

CARTESIAN COORDINATES

C	-0.672592	-3.165588	1.478305
N	-1.143900	-2.297956	0.424495
C	-2.469124	-2.226866	0.029465

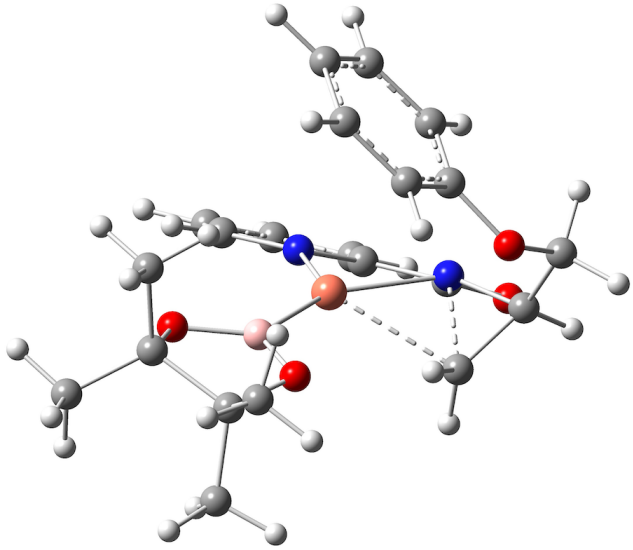
O	-3.269567	-3.138254	0.203813
C	-0.501938	-1.674776	1.589485
C	-2.870600	-1.001196	-0.757603
C	-4.237654	-0.740706	-0.888412
C	-4.654967	0.366248	-1.623295
C	-3.688323	1.181386	-2.212985
C	-2.346179	0.854060	-2.041343
N	-1.932588	-0.214787	-1.332239
Cu	0.078993	-0.345234	-1.180681
B	1.997858	-0.207229	-0.800263
O	3.093561	-0.042219	-1.638881
C	4.317688	-0.187355	-0.869200
C	5.373945	0.756605	-1.439837
O	2.438802	-0.234464	0.538472
C	3.839771	0.152993	0.584550
C	3.874958	1.656292	0.896989
C	4.533661	-0.628195	1.697645
C	4.775527	-1.644573	-1.028569
H	-1.432200	-3.649361	2.091544
H	0.478120	-1.261896	1.366426
H	-4.941067	-1.414037	-0.412120
H	-5.712935	0.588340	-1.732078
H	-1.560012	1.463154	-2.476261
H	-3.958805	2.058558	-2.792145
H	5.612044	-0.426248	1.701054
H	4.128020	-0.326443	2.669960
H	4.380211	-1.704519	1.587702
H	3.335525	1.836776	1.833283
H	4.900913	2.024113	1.012651
H	3.384045	2.230029	0.104455
H	4.893566	-1.861508	-2.095105
H	5.733454	-1.826362	-0.527283
H	4.028677	-2.336006	-0.625412
H	6.284673	0.737078	-0.827989
H	5.637170	0.442335	-2.455471
H	5.007786	1.784802	-1.492324
C	-1.362998	-0.908948	2.583265
H	-0.716531	-0.462692	3.351429
H	-2.070561	-1.583829	3.071975
O	-2.202121	0.084734	1.996002
C	-1.689944	1.286384	1.569541
C	-2.653474	2.233413	1.193897
C	-0.327697	1.584194	1.458116
C	-2.254429	3.472932	0.700389
H	-3.702935	1.970745	1.287391
C	0.057345	2.836218	0.962580
H	0.442715	0.861533	1.694704
C	-0.892599	3.783515	0.581019
H	-3.008632	4.200043	0.409169
H	1.117487	3.047703	0.857533
H	-0.580822	4.749153	0.192674
H	0.187766	-3.778956	1.220263

Electronic Energy = -1448.67011541 (Hartree/Particle)
Dipole Moment (Debye): 3.2139
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

```
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.448049
(Hartree/Particle)
 Thermal correction to Energy=                    0.476249
 Thermal correction to Enthalpy=                  0.477193
 Thermal correction to Gibbs Free Energy=         0.387698
 Sum of electronic and zero-point Energies=          -1448.222067
 Sum of electronic and thermal Energies=             -1448.193867
 Sum of electronic and thermal Enthalpies=           -1448.192923
 Sum of electronic and thermal Free Energies=        -1448.282417
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1449.030321190
 Corrected Free Energy =   -1448.64262276
```

PATH: ANTI_MARKOVNIKOV



TS1 Substrate: 1c
Path: anti-Markovnikov

CARTESIAN COORDINATES

N	-2.291319	-1.371703	0.591008
C	-3.420292	-0.994961	-0.038151
C	-4.620853	-1.699748	0.089542
C	-4.648641	-2.814577	0.926908
C	-3.477999	-3.196635	1.590303
C	-2.314632	-2.454045	1.379031
C	-3.334711	0.218586	-0.919769
O	-4.291466	0.583987	-1.603280
Cu	-0.573845	-0.386797	-0.214258
B	1.332467	-0.899835	-0.298911
O	2.013409	-1.871554	0.428860
C	3.444536	-1.679443	0.251446
C	4.128218	-3.044964	0.244074
N	-2.108786	0.881323	-0.839832
C	-0.950318	0.848894	-2.226872
C	-1.880145	1.925827	-1.828150
O	2.221136	-0.227586	-1.141621

```
 C                3.512239   -0.894752   -1.107781
 C                3.571957   -1.811323   -2.337729
 C                4.610527    0.163400   -1.189244
 C                3.930595   -0.855233    1.452162
 H               -2.741282    2.100018   -2.477413
 H               -1.292925    0.106626   -2.938957
 H                0.118269    0.957076   -2.074576
 H               -5.490972   -1.365310   -0.465090
 H               -5.566674   -3.380995    1.057614
 H               -1.367452   -2.719468    1.840383
 H               -3.460451   -4.056049    2.253601
 H                5.602310   -0.293138   -1.080508
 H                4.568870    0.663041   -2.163402
 H                4.488593    0.925424   -0.415606
 H                3.418420   -1.205663   -3.237277
 H                4.540852   -2.317378   -2.421220
 H                2.781388   -2.567587   -2.300239
 H                3.676417   -1.390926    2.372847
 H                5.015868   -0.701245    1.426935
 H                3.432096    0.117568    1.483327
 H                5.200081   -2.942027    0.032770
 H                4.017613   -3.516365    1.226701
 H                3.686694   -3.712460   -0.499954
 C               -1.295320    3.236941   -1.311053
 H               -1.219290    3.929981   -2.155482
 H               -1.964965    3.682646   -0.564707
 O                0.035029    3.122091   -0.822346
 C                0.307225    2.813165    0.489757
 C                1.670169    2.802602    0.816973
 C               -0.651002    2.517411    1.465828
 C                2.070053    2.503358    2.116379
 H                2.392205    3.011631    0.034066
 C               -0.232871    2.217298    2.768154
 H               -1.703489    2.472201    1.218121
 C                1.121186    2.207811    3.103691
 H                3.129637    2.495391    2.359385
 H               -0.982751    1.976708    3.517718
 H                1.436442    1.966051    4.114850

 Electronic Energy =  -1448.63550863 (Hartree/Particle)
 Dipole Moment (Debye):      2.7296
 index           1
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -354.111

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.445180
(Hartree/Particle)
 Thermal correction to Energy=                    0.473169
 Thermal correction to Enthalpy=                  0.474114
 Thermal correction to Gibbs Free Energy=         0.383444
 Sum of electronic and zero-point Energies=          -1448.190329
 Sum of electronic and thermal Energies=             -1448.162339
 Sum of electronic and thermal Enthalpies=           -1448.161395
 Sum of electronic and thermal Free Energies=        -1448.252065
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1448.996090760
 Corrected Free Energy =  -1448.612647130
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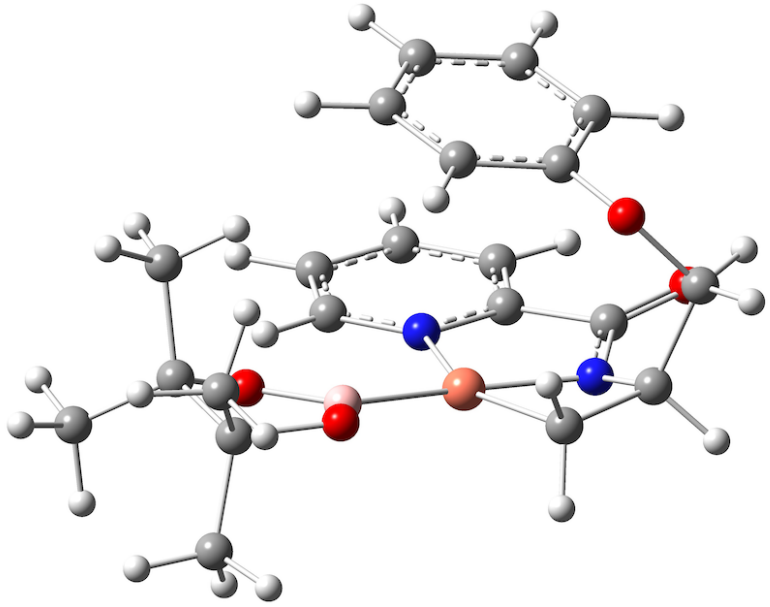

I1 Substrate: 1c
Path: anti-Markovnikov

CARTESIAN COORDINATES

C	1.553884	-2.534828	-1.172968
C	0.009315	-2.423661	-1.166077
H	1.942091	-3.164843	-1.989855
H	-0.476346	-2.669574	-2.111688
H	-0.515222	-2.841373	-0.309064
N	1.820199	-1.117939	-1.396185
C	2.885483	-0.346167	-1.179434
C	2.425700	1.108616	-1.038206
C	3.333243	2.160164	-0.951939
C	2.849432	3.453459	-0.748682
H	4.391312	1.932614	-1.030752
C	0.621358	2.553164	-0.712092
C	1.472479	3.654996	-0.621783
H	3.536488	4.292909	-0.680066
H	-0.456204	2.630446	-0.607374
H	1.058692	4.644113	-0.451594
O	4.080480	-0.650435	-1.050325
N	1.091870	1.316676	-0.925094
Cu	0.103567	-0.459240	-1.039093
B	-1.790402	-0.193976	-0.569722
O	-2.730077	-1.160691	-0.300658
O	-2.294007	1.082088	-0.385624
C	-4.021524	-0.502314	-0.118761
C	-3.595257	0.957893	0.274234
C	2.137712	-3.095697	0.136568
H	2.018348	-4.183030	0.148252
H	3.204507	-2.856105	0.195210
O	1.430815	-2.658768	1.309841
C	1.575510	-1.368479	1.762204
C	0.402041	-0.708271	2.155124
C	2.814301	-0.729339	1.889635
C	0.466386	0.596486	2.647368
H	-0.545266	-1.226760	2.043493

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 C                 2.863859    0.581376    2.371156
 H                 3.725546   -1.224749    1.575551
 C                 1.696940    1.252772    2.750359
 H                -0.450290    1.106664    2.931011
 H                 3.827445    1.079326    2.443138
 H                 1.746518    2.273733    3.119082
 C                -4.805560   -1.256292    0.951013
 H                -5.745220   -0.738155    1.177851
 H                -5.047484   -2.261160    0.589715
 H                -4.230651   -1.360768    1.874118
 C                -4.749014   -0.580476   -1.466669
 H                -4.829902   -1.630683   -1.764314
 H                -5.757983   -0.158038   -1.403340
 H                -4.194081   -0.049438   -2.246731
 C                -3.341633    1.131511    1.776703
 H                -2.850282    2.095294    1.945370
 H                -4.277160    1.113926    2.346325
 H                -2.684681    0.344679    2.159585
 C                -4.511559    2.062710   -0.240908
 H                -5.523819    1.943140    0.163753
 H                -4.130492    3.038667    0.078529
 H                -4.568039    2.062566   -1.331882

 Electronic Energy =  -1448.67962787 (Hartree/Particle)
 Dipole Moment (Debye):      6.3387
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.447803
(Hartree/Particle)
 Thermal correction to Energy=                    0.475187
 Thermal correction to Enthalpy=                  0.476132
 Thermal correction to Gibbs Free Energy=         0.390052
 Sum of electronic and zero-point Energies=          -1448.231825
 Sum of electronic and thermal Energies=             -1448.204440
 Sum of electronic and thermal Enthalpies=           -1448.203496
 Sum of electronic and thermal Free Energies=        -1448.289576
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1449.039370430
 Corrected Free Energy = -1448.649318560

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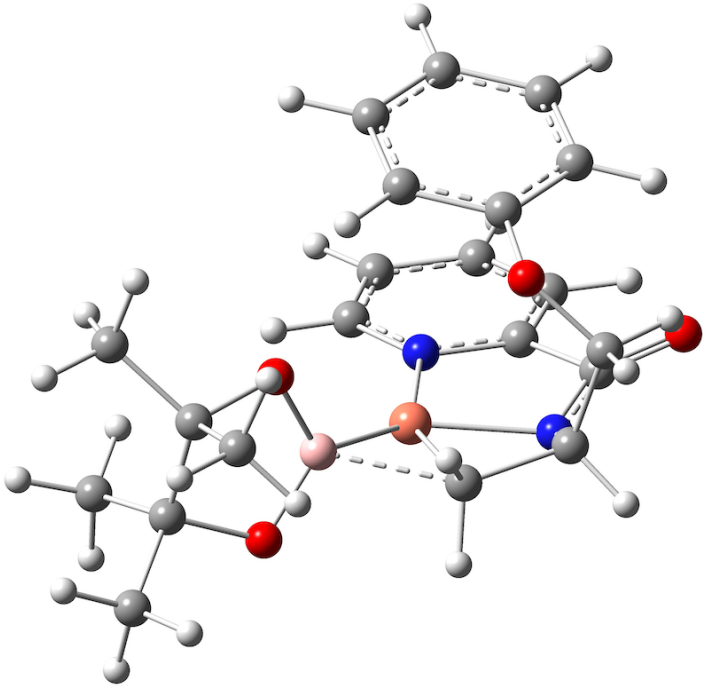

TS2 Substrate: 1c
Path: anti-Markovnikov

CARTESIAN COORDINATES

C	2.762474	0.203021	2.914445
C	1.364116	0.254095	2.913464
C	0.622846	-0.659388	2.162962
C	1.281865	-1.638297	1.404807
C	2.678892	-1.718394	1.423078
C	3.408043	-0.786970	2.167868
O	0.468845	-2.511869	0.716488
C	0.837770	-3.004873	-0.578263
C	0.453823	-2.041783	-1.718578
Cu	-0.023885	0.279332	-0.962088
B	-1.923049	-0.003698	-0.479176
O	-2.930854	0.539543	-1.250978
C	-4.016420	0.905911	-0.344373
C	-5.342697	0.717489	-1.073390
C	-0.983825	-1.419310	-1.520474
N	1.283116	-0.851868	-1.831821
C	2.554956	-0.650012	-1.516776
O	3.539030	-1.411866	-1.511544
C	2.723823	0.796778	-1.007630
C	3.989987	1.362848	-0.867131
C	4.113496	2.640591	-0.324022
C	2.962263	3.316377	0.088845
C	1.729823	2.685299	-0.065759
N	1.607188	1.462488	-0.605382
O	-2.327149	-0.265396	0.811448
C	-3.775658	-0.071425	0.863268
C	-4.408556	-1.453188	0.661278
C	-4.141013	0.488751	2.233333
C	-3.810708	2.381383	0.020685
H	0.450650	-2.647390	-2.642119
H	-1.444425	-1.223976	-2.491923
H	-1.625993	-2.080136	-0.931644

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 H                4.846072    0.772291   -1.175911
 H                5.092002    3.100684   -0.213011
 H                0.806110    3.157531    0.254090
 H                3.011707    4.307024    0.530068
 H                0.267845   -3.933384   -0.685454
 H                1.904621   -3.236182   -0.645005
 H               -0.459858   -0.619245    2.126356
 H                3.203342   -2.456619    0.829675
 H                0.844078    1.016349    3.489522
 H                4.493757   -0.839567    2.153626
 H                3.340443    0.923017    3.487891
 H               -5.208791    0.734679    2.275695
 H               -3.930744   -0.258458    3.005525
 H               -3.564265    1.386774    2.466776
 H               -4.023251   -2.134442    1.426315
 H               -5.499671   -1.410592    0.748839
 H               -4.156166   -1.866304   -0.320903
 H               -3.785988    2.973436   -0.899643
 H               -4.623118    2.754442    0.653634
 H               -2.861142    2.528309    0.545576
 H               -6.183236    0.894694   -0.391753
 H               -5.414834    1.432494   -1.899442
 H               -5.434155   -0.288610   -1.489069

 Electronic Energy =  -1448.67004685 (Hartree/Particle)
 Dipole Moment (Debye):      6.6134
 index           1
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -152.728

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.446976
(Hartree/Particle)
 Thermal correction to Energy=                    0.473918
 Thermal correction to Enthalpy=                  0.474862
 Thermal correction to Gibbs Free Energy=         0.389903
 Sum of electronic and zero-point Energies=          -1448.223071
 Sum of electronic and thermal Energies=             -1448.196129
 Sum of electronic and thermal Enthalpies=           -1448.195185
 Sum of electronic and thermal Free Energies=        -1448.280147
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1449.033067670
 Corrected Free Energy =  -1448.643167820

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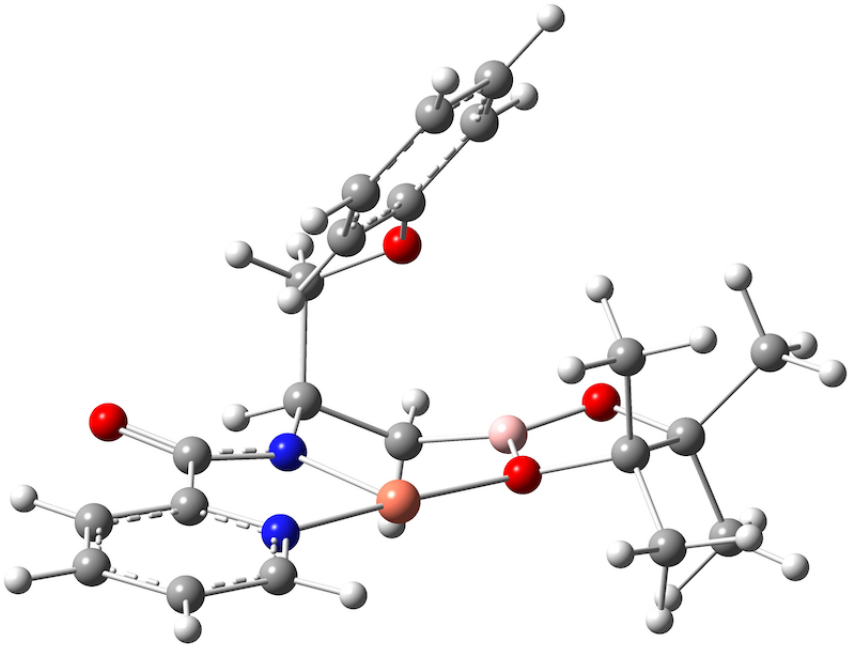

P1 Substrate: 1c
Path: anti-Markovnikov

CARTESIAN COORDINATES

C	-0.048315	3.941478	-1.977978
C	-1.275774	4.092846	-1.321442
C	-1.535260	3.397449	-0.139798
C	-0.570479	2.528255	0.390055
C	0.662516	2.375247	-0.257551
C	0.915054	3.086564	-1.434558
O	-0.943003	1.821903	1.501215
C	0.022460	1.487811	2.523713
C	0.322704	-0.019112	2.564250
Cu	0.622526	-1.103700	-0.374093
B	-1.837331	-0.854811	1.217260
O	-1.335445	-1.202334	-0.054352
C	-2.426712	-1.107145	-1.045006
C	-2.243319	-2.243596	-2.042816
C	-0.990346	-0.838031	2.543007
N	1.176959	-0.440140	1.471535
C	2.481753	-0.204201	1.556445
O	3.135468	0.325407	2.483359
C	3.245182	-0.630804	0.295081
C	4.637935	-0.531845	0.264226
C	5.327654	-0.902012	-0.889204
C	4.604579	-1.357061	-1.995236
C	3.216422	-1.423544	-1.898727
N	2.548489	-1.071690	-0.785220
O	-3.197341	-0.728103	1.167590
C	-3.689053	-1.213739	-0.113796
C	-4.153407	-2.656864	0.119098
C	-4.864634	-0.340729	-0.543835
C	-2.273144	0.245195	-1.737629
H	0.834678	-0.184640	3.525315
H	-0.722412	-1.885854	2.751504
H	-1.643854	-0.517584	3.364903
H	5.135295	-0.161025	1.153812

```
  H                6.411774   -0.834764   -0.928559
  H                2.606261   -1.764431   -2.729041
  H                5.098091   -1.652746   -2.915926
  H               -0.445647    1.795508    3.466458
  H                0.946269    2.057290    2.387077
  H               -2.479400    3.505866    0.386670
  H                1.397055    1.687458    0.139889
  H               -2.031745    4.762008   -1.725436
  H                1.873654    2.958351   -1.931773
  H                0.155188    4.487105   -2.895435
  H               -5.217393   -0.631612   -1.540290
  H               -5.690388   -0.467346    0.163582
  H               -4.593193    0.716975   -0.560936
  H               -4.914014   -2.659474    0.905880
  H               -4.588373   -3.090555   -0.787788
  H               -3.324729   -3.292029    0.449040
  H               -1.265199    0.317021   -2.161415
  H               -3.001359    0.357275   -2.547624
  H               -2.392356    1.072699   -1.037673
  H               -3.065923   -2.253556   -2.766597
  H               -1.305624   -2.092739   -2.589840
  H               -2.193716   -3.216986   -1.549916

 Electronic Energy =  -1448.75568260 (Hartree/Particle)
 Dipole Moment (Debye):      7.6320
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.449187
(Hartree/Particle)
 Thermal correction to Energy=                    0.476571
 Thermal correction to Enthalpy=                  0.477515
 Thermal correction to Gibbs Free Energy=         0.390519
 Sum of electronic and zero-point Energies=          -1448.306495
 Sum of electronic and thermal Energies=             -1448.279111
 Sum of electronic and thermal Enthalpies=           -1448.278167
 Sum of electronic and thermal Free Energies=        -1448.365164
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1449.11747741
 Corrected Free Energy =  -1448.72695881

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PATH: MARKOVNIKOV
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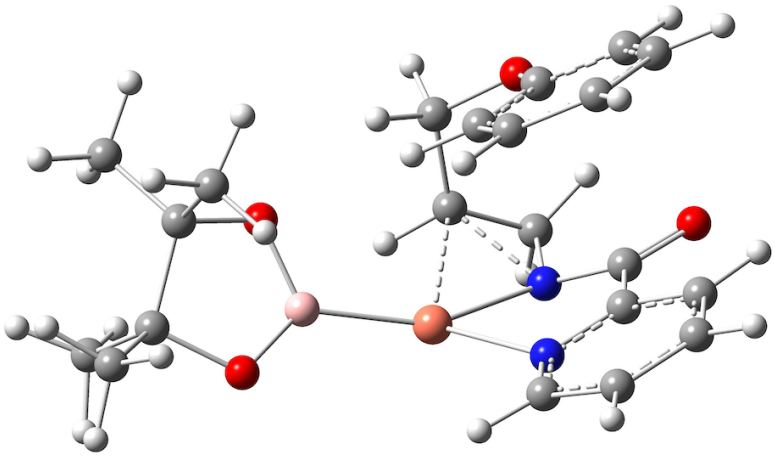

TS1 Substrate: 1c
Path: Markovnikov

CARTESIAN COORDINATES

C	-1.539071	-3.219791	-0.940023
N	-1.497699	-1.820718	-1.343657
C	-2.643205	-1.070986	-1.052892
O	-3.728369	-1.557097	-0.748347
C	-0.358641	-2.671925	-0.247513
C	-2.482551	0.408716	-1.251461
C	-3.551502	1.273344	-1.006355
C	-3.361162	2.638075	-1.213195
C	-2.112495	3.092770	-1.647103
C	-1.091884	2.161698	-1.842005
N	-1.277590	0.848614	-1.655983
Cu	0.219586	-0.594883	-1.334917
B	2.044159	-0.193478	-0.688605
O	3.056997	0.571332	-1.257198
C	4.232022	0.530664	-0.399565
C	4.936621	1.883685	-0.466210
O	2.425076	-0.575314	0.611436
C	3.612040	0.174370	0.995135
C	3.123362	1.404304	1.774884
C	4.484804	-0.700501	1.890914
C	5.151497	-0.568230	-0.951006
H	-2.401069	-3.475072	-0.323064
H	0.618844	-2.874188	-0.676276
H	-4.488927	0.862177	-0.650254
H	-4.170449	3.339208	-1.028985
H	-0.092138	2.455976	-2.149126
H	-1.925890	4.147756	-1.823884
H	5.431023	-0.196129	2.123239
H	3.964521	-0.899333	2.834474
H	4.707370	-1.660972	1.419706
H	2.519943	1.069481	2.625353
H	3.958706	2.002199	2.156759
H	2.494888	2.042049	1.144456
H	5.375429	-0.346917	-1.999551
H	6.095795	-0.622856	-0.396842
H	4.661550	-1.546332	-0.910108
H	5.778350	1.918542	0.236852
H	5.327772	2.045694	-1.476361

```
 H                 4.253136    2.704572   -0.235553
 C                -0.328779   -2.388779    1.232940
 H                 0.512281   -1.737232    1.476755
 H                -0.153527   -3.360476    1.720537
 O                -1.566105   -1.927303    1.750422
 C                -1.787810   -0.580650    1.934959
 C                -3.089133   -0.252092    2.339597
 C                -0.832024    0.424850    1.747645
 C                -3.430656    1.079487    2.562689
 H                -3.814496   -1.051577    2.451452
 C                -1.193824    1.758589    1.972720
 H                 0.172714    0.199970    1.411299
 C                -2.484160    2.096708    2.380634
 H                -4.443381    1.324569    2.873234
 H                -0.448283    2.534027    1.814762
 H                -2.753684    3.135854    2.548710
 H                -1.363748   -3.926068   -1.753743

 Electronic Energy =  -1448.64018835 (Hartree/Particle)
 Dipole Moment (Debye):      2.2655
 index           1
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -319.822

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.445787
(Hartree/Particle)
 Thermal correction to Energy=                    0.473495
 Thermal correction to Enthalpy=                  0.474439
 Thermal correction to Gibbs Free Energy=         0.386458
 Sum of electronic and zero-point Energies=          -1448.194401
 Sum of electronic and thermal Energies=             -1448.166693
 Sum of electronic and thermal Enthalpies=           -1448.165749
 Sum of electronic and thermal Free Energies=        -1448.253731
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1448.999723900
 Corrected Free Energy =  -1448.613266550
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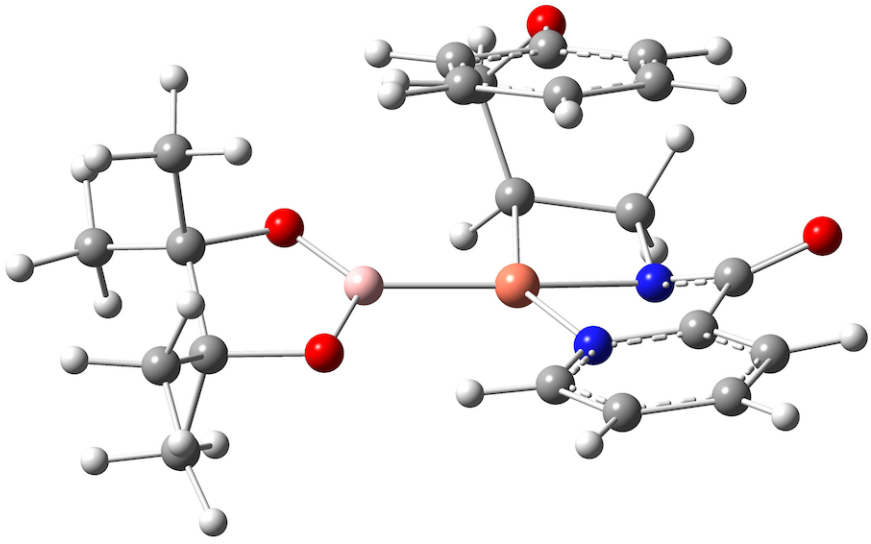

I1 Substrate: 1c
Path: Markovnikov

CARTESIAN COORDINATES

C	-1.428552	0.783966	2.961970
C	-2.522516	0.070286	2.460296
C	-2.336254	-1.158196	1.824283
C	-1.045633	-1.681231	1.686717
C	0.054373	-0.984665	2.206116
C	-0.143821	0.247562	2.834591
O	-0.929703	-2.906657	1.072728
C	0.074298	-3.079084	0.057429
C	-0.237905	-2.350303	-1.237568
Cu	-0.316172	-0.373191	-1.043184
B	1.567790	-0.056663	-0.549372
O	2.550517	-0.974385	-0.250103
C	3.735295	-0.248111	0.205227
C	4.974873	-0.983010	-0.295277
C	-1.705885	-2.402463	-1.719998
N	-1.975892	-0.967064	-1.700351
C	-3.050389	-0.340789	-1.203542
C	-2.671726	1.090734	-0.813390
C	-3.630083	2.054738	-0.514170
C	-3.206076	3.319273	-0.101847
C	-1.837552	3.575858	0.017611
C	-0.934395	2.555484	-0.282527
N	-1.348703	1.351188	-0.697627
O	-4.198363	-0.763311	-1.013179
O	2.050144	1.239434	-0.513102
C	3.508851	1.177622	-0.416674
C	4.048082	1.311782	-1.845954
C	3.988762	2.343470	0.442310
C	3.700053	-0.252360	1.738027
H	-2.357260	-2.958892	-1.035282
H	0.514108	-2.580888	-1.996299
H	-4.677430	1.783524	-0.597787
H	-3.932613	4.093188	0.132008
H	0.140648	2.675944	-0.196265
H	-1.469832	4.543855	0.343695
H	5.882989	-0.419477	-0.049385
H	5.040938	-1.964134	0.186605
H	4.941137	-1.140068	-1.375788
H	3.654899	-1.287681	2.091323
H	4.595587	0.216878	2.159573
H	2.819750	0.275648	2.115282
H	3.678548	2.247169	-2.278117
H	5.143424	1.330253	-1.861730
H	3.701853	0.487831	-2.477920
H	5.070531	2.279381	0.610530
H	3.779495	3.288761	-0.069580
H	3.484675	2.364933	1.411449
H	1.070257	-2.811523	0.421846
H	0.057554	-4.161394	-0.130454
H	-3.172334	-1.699819	1.394246
H	1.051241	-1.398076	2.108580
H	-3.526622	0.477785	2.541706
H	0.713230	0.790321	3.226593
H	-1.575649	1.746117	3.445054
H	-1.810454	-2.826653	-2.727383

Electronic Energy = -1448.68016741 (Hartree/Particle)

```
 Dipole Moment (Debye):      7.7856
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.448298
(Hartree/Particle)
 Thermal correction to Energy=                    0.475662
 Thermal correction to Enthalpy=                  0.476606
 Thermal correction to Gibbs Free Energy=         0.390666
 Sum of electronic and zero-point Energies=          -1448.231870
 Sum of electronic and thermal Energies=             -1448.204505
 Sum of electronic and thermal Enthalpies=           -1448.203561
 Sum of electronic and thermal Free Energies=        -1448.289502
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1449.04101926
 Corrected Free Energy =   -1448.650353850

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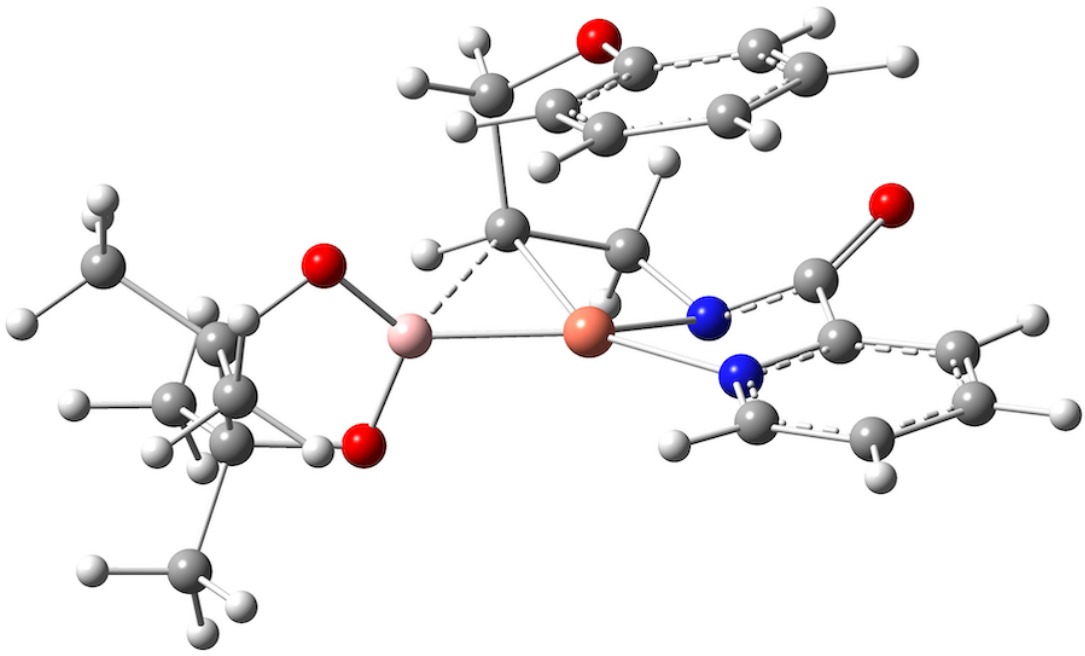


TS2 Substrate: 1c
Path: Markovnikov

CARTESIAN COORDINATES

C	-2.608680	1.650478	2.384837
C	-3.340835	0.479817	2.145806
C	-2.692444	-0.740353	1.969959
C	-1.293223	-0.799684	2.031609
C	-0.547674	0.364487	2.269157
C	-1.216409	1.582334	2.444999
O	-0.748238	-2.049051	1.867634
C	0.600296	-2.189937	1.424443
C	0.795546	-1.920119	-0.075970
Cu	-0.090813	-0.177955	-0.674358
B	1.836120	-0.155208	-0.271237

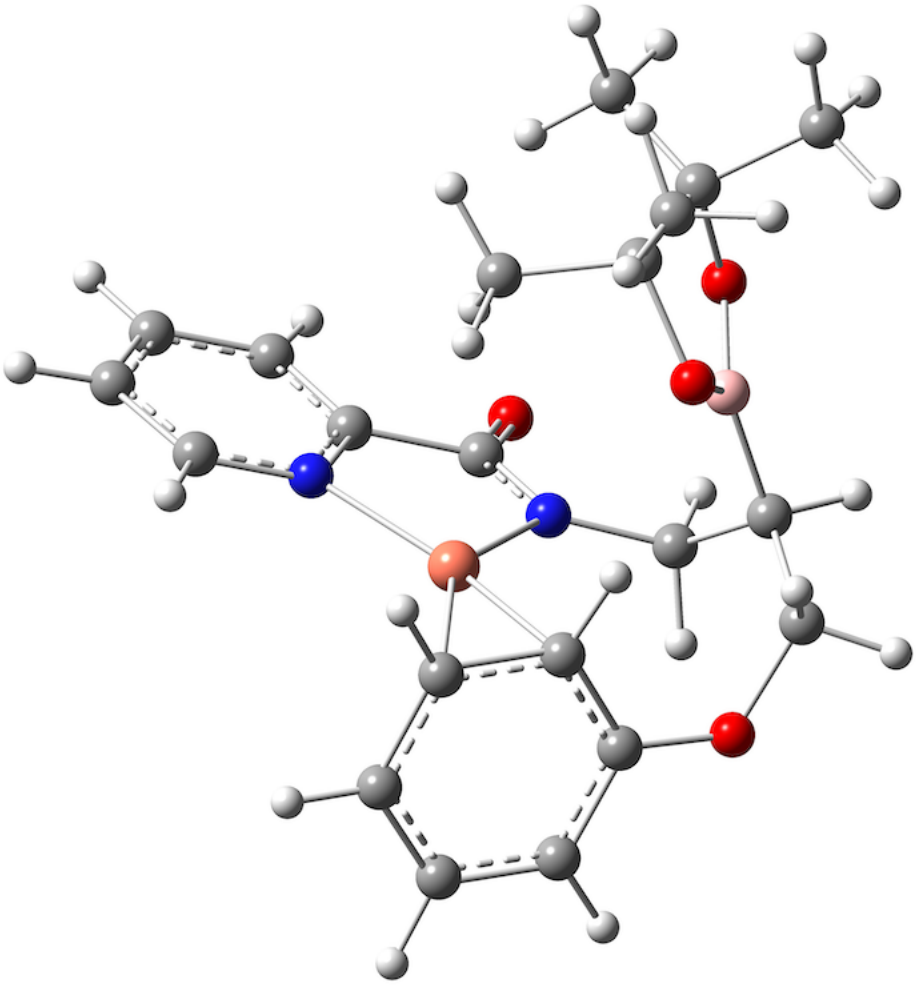
```
 O                2.480294    0.145262    0.910408
 C                3.723072    0.832320    0.560205
 C                4.784582    0.469676    1.593118
 C               -0.279437   -2.664462   -0.963874
 N               -1.142497   -1.613390   -1.476431
 C               -2.437747   -1.456807   -1.218338
 C               -2.789568    0.042555   -1.301000
 C               -4.097329    0.470648   -1.525369
 C               -4.377127    1.836461   -1.530372
 C               -3.343972    2.742735   -1.276370
 C               -2.067171    2.241976   -1.029920
 N               -1.790428    0.930019   -1.055350
 O               -3.326132   -2.264353   -0.893941
 O                2.639468    0.017869   -1.375105
 C                3.994843    0.295515   -0.892990
 C                4.745399   -1.040909   -0.914418
 C                4.653519    1.293702   -1.838100
 C                3.420797    2.335051    0.606063
 H               -0.813081   -3.407453   -0.354496
 H                1.801424   -2.267939   -0.339942
 H               -4.862166   -0.283695   -1.677350
 H               -5.387065    2.191859   -1.718705
 H               -1.234857    2.899121   -0.797390
 H               -3.519747    3.813845   -1.255112
 H                5.754996    0.894716    1.310590
 H                4.504262    0.877290    2.569916
 H                4.893147   -0.612377    1.697183
 H                3.043905    2.590207    1.601602
 H                4.319326    2.930198    0.411362
 H                2.654213    2.605794   -0.127059
 H                4.713155   -1.449816   -1.929033
 H                5.793617   -0.915436   -0.622279
 H                4.283890   -1.768805   -0.238769
 H                5.637159    1.592489   -1.456365
 H                4.792667    0.833486   -2.821613
 H                4.040382    2.188271   -1.968638
 H                1.288870   -1.602456    2.038225
 H                0.816471   -3.250586    1.597924
 H               -3.240057   -1.646104    1.732211
 H                0.534094    0.338444    2.306448
 H               -4.424698    0.518702    2.075704
 H               -0.631747    2.481865    2.624151
 H               -3.119351    2.601004    2.513161
 H                0.222888   -3.183021   -1.789506

 Electronic Energy =  -1448.66478263 (Hartree/Particle)
 Dipole Moment (Debye):      8.3356
 index           1
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -140.390

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.447377
(Hartree/Particle)
 Thermal correction to Energy=                    0.474279
 Thermal correction to Enthalpy=                  0.475223
 Thermal correction to Gibbs Free Energy=         0.390899
 Sum of electronic and zero-point Energies=          -1448.217405
```

Sum of electronic and thermal Energies= -1448.190504
Sum of electronic and thermal Enthalpies= -1448.189560
Sum of electronic and thermal Free Energies= -1448.273884
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1449.030306880
Corrected Free Energy = -1448.639408250



P1 Substrate: 1c
Path: Markovnikov

CARTESIAN COORDINATES

C	-3.720677	-1.064927	1.660248
C	-4.284119	-1.700216	0.560295
C	-3.488324	-2.399862	-0.365100
C	-2.107940	-2.476668	-0.190124
C	-1.501859	-1.863195	0.947081
C	-2.319055	-1.136806	1.858339
O	-1.405655	-3.124084	-1.149974
C	0.032711	-3.210205	-1.095218
C	0.819114	-1.982362	-1.658552
Cu	-1.308521	0.082452	0.332527
B	1.787618	-1.296943	-0.618496
O	1.757550	-1.514107	0.745628
C	2.631471	-0.523752	1.365677
C	3.309506	-1.161446	2.574277
C	-0.018159	-0.857133	-2.340479
N	-0.391429	0.211415	-1.414576

C	-0.218931	1.470287	-1.838132
C	-0.650742	2.522177	-0.813862
C	-0.426116	3.877891	-1.066747
C	-0.830351	4.821917	-0.123856
C	-1.458318	4.389248	1.048440
C	-1.652634	3.021304	1.228367
N	-1.256477	2.112115	0.323621
O	0.232672	1.883079	-2.924705
O	2.785216	-0.434841	-0.991642
C	3.596475	-0.141586	0.178001
C	4.836422	-1.040188	0.091122
C	4.002208	1.329282	0.128757
C	1.734994	0.638155	1.810102
H	-0.921983	-1.291901	-2.787570
H	1.458117	-2.385122	-2.457609
H	0.056522	4.146310	-2.000064
H	-0.662531	5.881443	-0.299261
H	-2.139129	2.626925	2.116223
H	-1.794176	5.090724	1.806028
H	4.038755	-0.471161	3.014539
H	2.559013	-1.396509	3.336826
H	3.821755	-2.088822	2.307420
H	0.956136	0.252570	2.477304
H	2.305422	1.403029	2.347768
H	1.240333	1.102460	0.953912
H	5.349439	-0.842064	-0.855210
H	5.533980	-0.845477	0.913199
H	4.559288	-2.099459	0.110048
H	4.541329	1.613663	1.040578
H	4.662181	1.497647	-0.728241
H	3.132873	1.980056	0.011561
H	0.342457	-3.455145	-0.073602
H	0.235958	-4.088247	-1.712121
H	-3.926800	-2.872796	-1.238224
H	-0.467345	-2.074201	1.200710
H	-5.358218	-1.654111	0.400151
H	-1.887740	-0.795549	2.797124
H	-4.341485	-0.527748	2.370935
H	0.577893	-0.429498	-3.152805

Electronic Energy = -1448.75207130 (Hartree/Particle)
Dipole Moment (Debye): 6.8666
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.449885
(Hartree/Particle)
Thermal correction to Energy= 0.476964
Thermal correction to Enthalpy= 0.477908
Thermal correction to Gibbs Free Energy= 0.392388
Sum of electronic and zero-point Energies= -1448.302186
Sum of electronic and thermal Energies= -1448.275108
Sum of electronic and thermal Enthalpies= -1448.274163
Sum of electronic and thermal Free Energies= -1448.359683
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1449.11552297
Corrected Free Energy = -1448.72313467

MODEL: Az-(Cu2Cl)-Bpin

THF-(Cu2Cl)-Bpin complex

CARTESIAN COORDINATES

Cu	-0.833728	1.102582	0.105023
Cu	-0.540900	-1.170849	-0.063251
B	1.036585	0.290464	0.036155
O	1.818024	0.099455	1.160279
O	1.801216	0.468626	-1.100956
C	3.188111	-0.142964	0.708316
C	3.202355	0.566217	-0.692600
C	3.530706	2.062475	-0.615138
H	4.586187	2.228223	-0.372808
H	3.320842	2.522278	-1.586165
H	2.914847	2.563176	0.138972
C	4.064802	-0.113883	-1.751291
H	4.005551	0.445233	-2.690900
H	5.113885	-0.139841	-1.432666
H	3.731101	-1.135648	-1.945322
C	3.348567	-1.666244	0.621561
H	4.369566	-1.946238	0.340268
H	3.123927	-2.102024	1.599941
H	2.651255	-2.096990	-0.104297
C	4.152848	0.437275	1.737312
H	4.062131	-0.113976	2.678896
H	5.187665	0.347092	1.385561
H	3.942047	1.489886	1.940494
Cl	-1.653706	-2.988961	-0.225159
O	-2.689389	1.853829	0.145814
C	-3.487459	1.316948	1.246945
C	-3.451626	1.528327	-1.058133
C	-4.029126	-0.025217	0.733120
H	-2.828643	1.244069	2.114528
H	-4.283184	2.043923	1.453239
C	-3.989603	0.111485	-0.816752
H	-4.250477	2.275568	-1.147483
H	-2.769346	1.622981	-1.905289
H	-5.036689	-0.215267	1.114808
H	-3.382203	-0.852155	1.040718
H	-4.971966	-0.023291	-1.279068
H	-3.308470	-0.639028	-1.229035

Electronic Energy = -1498.79415092 (Hartree/Particle)
Dipole Moment (Debye): 6.7869
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.303731
(Hartree/Particle)
Thermal correction to Energy= 0.325086

```
 Thermal correction to Enthalpy=                  0.326030
 Thermal correction to Gibbs Free Energy=         0.249514
 Sum of electronic and zero-point Energies=          -1498.490420
 Sum of electronic and thermal Energies=             -1498.469065
 Sum of electronic and thermal Enthalpies=           -1498.468121
 Sum of electronic and thermal Free Energies=        -1498.544637
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1499.03284364
 Corrected Free Energy =  -1498.78332972

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Cl-Cu-THF

 CARTESIAN COORDINATES

  Cu              1.062744    0.000000    0.000000
  Cl              3.157013    0.000000    0.000000
  O              -0.862046    0.000000    0.000000
  C              -1.657972    1.213414    0.000000
  C              -1.657973   -1.213414    0.000000
  C              -3.132607    0.776735    0.000000
  H              -1.377069    1.783257    0.890423
  H              -1.377069    1.783257   -0.890423
  C              -3.132606   -0.776734    0.000000
  H              -1.377070   -1.783257   -0.890423
  H              -1.377069   -1.783258    0.890422
  H              -3.649301    1.167712   -0.880917
  H              -3.649301    1.167713    0.880917
  H              -3.649302   -1.167712   -0.880916
  H              -3.649301   -1.167712    0.880917

 Electronic Energy =  -890.093411832 (Hartree/Particle)
 Dipole Moment (Debye):     10.0129
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            2
 Negatives Eigenvalues:           -196.601
                                  -193.939

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.120025
(Hartree/Particle)
 Thermal correction to Energy=                    0.127414
 Thermal correction to Enthalpy=                  0.128359
 Thermal correction to Gibbs Free Energy=         0.084918
 Sum of electronic and zero-point Energies=           -889.973386
 Sum of electronic and thermal Energies=              -889.965997
 Sum of electronic and thermal Enthalpies=            -889.965053
 Sum of electronic and thermal Free Energies=         -890.008494
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -890.210751525
 Corrected Free Energy = -890.125833693

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THF

 CARTESIAN COORDINATES
```

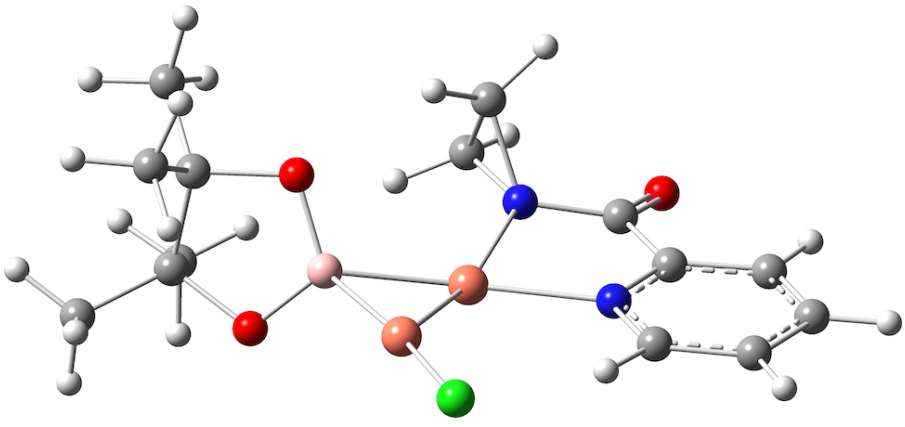
C	1.110010	-0.503453	0.199533
O	-0.032909	-1.209485	-0.279624
C	-1.166880	-0.427611	0.103690
C	-0.725575	1.057410	0.015153
C	0.819692	0.972490	-0.115508
H	1.224249	-0.661468	1.286536
H	1.989161	-0.909054	-0.308634
H	-1.987023	-0.688794	-0.570743
H	-1.462949	-0.688033	1.133022
H	-1.170085	1.558784	-0.850285
H	-1.030421	1.611974	0.909101
H	1.133082	1.202613	-1.139318
H	1.343769	1.656845	0.560099

Electronic Energy = -232.466403941 (Hartree/Particle)
Dipole Moment (Debye): 1.8228
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.117173
(Hartree/Particle)
Thermal correction to Energy= 0.122138
Thermal correction to Enthalpy= 0.123083
Thermal correction to Gibbs Free Energy= 0.087703
Sum of electronic and zero-point Energies= -232.349231
Sum of electronic and thermal Energies= -232.344266
Sum of electronic and thermal Enthalpies= -232.343321
Sum of electronic and thermal Free Energies= -232.378701
PCM-SP (solvent=THF;6-311+g(2d,p)) = -232.534621381
Corrected Free Energy = -232.446918440

SUBSTRATE: N-PICOLINOYL-AZIRIDINE



Complex-2 Substrate: N-(2-picolinoyl)-aziridine

CARTESIAN COORDINATES

C	-0.542709	-2.662926	1.258566

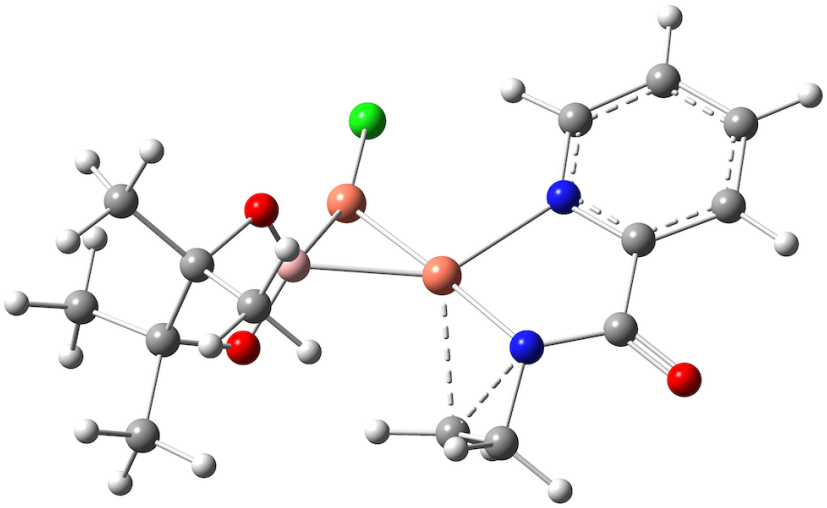
N	-1.155239	-2.128528	-0.015373
C	-2.575430	-2.280262	-0.141559
O	-3.130360	-3.349775	-0.304831
C	-0.349094	-3.362143	-0.030492
C	-3.321888	-0.980578	-0.080847
C	-4.713650	-0.970393	0.008373
C	-5.362897	0.265170	0.073534
C	-4.600361	1.433490	0.047512
C	-3.207985	1.337602	-0.050543
N	-2.587351	0.150731	-0.118283
Cu	0.332869	2.014387	-0.026419
H	-5.253469	-1.911019	0.027108
H	-6.445753	0.312126	0.145970
H	-2.563608	2.214700	-0.071679
H	-5.064816	2.413153	0.099423
H	-0.897284	-4.283501	-0.206653
H	0.592498	-3.246119	-0.557266
H	-1.247745	-3.091259	1.967234
Cu	-0.542970	-0.090629	-0.279139
B	1.482328	0.229692	-0.143114
O	2.030928	-0.410763	0.973650
O	2.413466	0.296315	-1.169298
C	3.472608	-0.511966	0.777380
C	3.597613	-0.459105	-0.787202
Cl	-0.489750	3.994594	0.216554
H	0.242055	-2.027072	1.659324
C	4.094086	0.703814	1.477615
H	3.794457	0.697460	2.530408
H	5.188332	0.682867	1.425846
H	3.737165	1.638169	1.033345
C	4.832163	0.269557	-1.312034
H	5.748881	-0.225236	-0.968435
H	4.826900	0.260972	-2.406991
H	4.850897	1.311521	-0.985191
C	3.966212	-1.803367	1.423900
H	5.034360	-1.951822	1.224752
H	3.826246	-1.749257	2.508856
H	3.419678	-2.675431	1.055369
C	3.475748	-1.835066	-1.455612
H	3.361727	-1.696040	-2.535219
H	4.361610	-2.453682	-1.273513
H	2.594265	-2.370681	-1.089471

Electronic Energy = -1760.73090756 (Hartree/Particle)
Dipole Moment (Debye): 8.8294
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.335852
(Hartree/Particle)
Thermal correction to Energy= 0.361316
Thermal correction to Enthalpy= 0.362260
Thermal correction to Gibbs Free Energy= 0.277426
Sum of electronic and zero-point Energies= -1760.395055
Sum of electronic and thermal Energies= -1760.369592
Sum of electronic and thermal Enthalpies= -1760.368648

Sum of electronic and thermal Free Energies= -1760.453482
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1761.03892194
Corrected Free Energy = -1760.76149638



TS3 Substrate: N-(2-picolinoyl)-aziridine

CARTESIAN COORDINATES

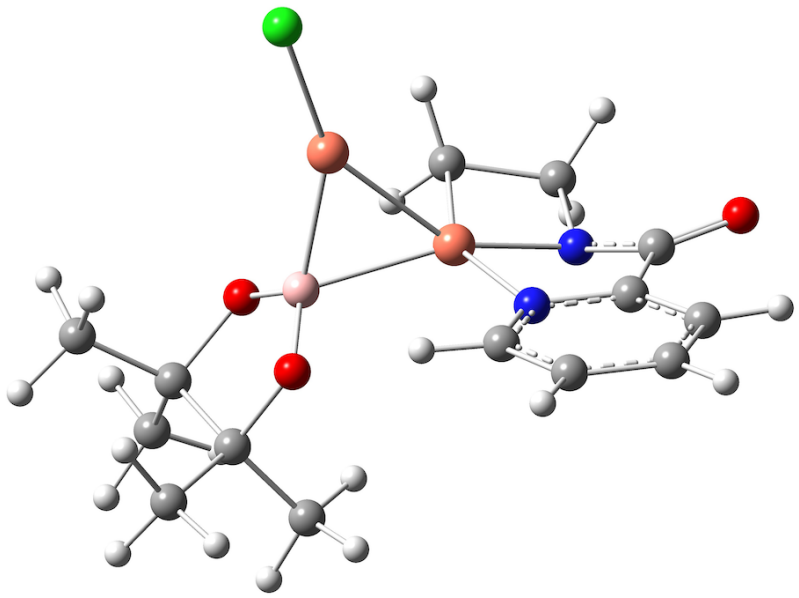
C	0.158449	-1.875530	-1.799364
N	1.177813	-2.151507	-0.192739
C	2.575439	-2.219641	-0.165330
O	3.210548	-3.226336	-0.456653
C	0.486481	-3.108989	-1.039983
C	3.251533	-0.963670	0.316683
C	4.618944	-0.944954	0.582719
C	5.196648	0.263138	0.983094
C	4.394646	1.401031	1.078492
C	3.032573	1.298848	0.777161
N	2.478500	0.133325	0.419603
Cu	-0.232301	1.879015	-0.435811
H	5.195621	-1.855789	0.462987
H	6.258819	0.315522	1.205347
H	2.369342	2.159556	0.793564
H	4.806890	2.361023	1.372606
H	1.140416	-3.838518	-1.520667
H	-0.355437	-3.583639	-0.533154
H	0.865850	-1.550291	-2.556450
Cu	0.489332	-0.325566	-0.164282
B	-1.537726	0.365377	0.000118
O	-2.441902	-0.108101	-0.946355
O	-2.058080	0.258686	1.279466
C	-3.726169	-0.314924	-0.282235
C	-3.287616	-0.523107	1.209731
Cl	0.708874	3.794117	-0.712525
H	-0.850785	-1.473877	-1.837696
C	-4.266972	0.007119	2.251963
H	-5.234585	-0.501994	2.165358
H	-3.871715	-0.175707	3.256556
H	-4.424391	1.082460	2.142961
C	-2.897082	-1.972135	1.531387
H	-2.409302	-1.998504	2.510720

H	-3.772108	-2.630715	1.557991
H	-2.186966	-2.359593	0.792893
C	-4.546394	0.961964	-0.502516
H	-4.633373	1.146457	-1.577875
H	-5.553660	0.868552	-0.081905
H	-4.054565	1.828869	-0.050469
C	-4.420516	-1.511245	-0.925846
H	-5.348122	-1.750712	-0.392315
H	-4.675023	-1.275935	-1.964612
H	-3.781577	-2.398236	-0.926259

Electronic Energy = -1760.69923010 (Hartree/Particle)
Dipole Moment (Debye): 6.6275
index 0
Harmonic frequencies
Number of imaginary frequencies= 1
Negatives Eigenvalues: -250.419

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.334219
(Hartree/Particle)
Thermal correction to Energy= 0.359120
Thermal correction to Enthalpy= 0.360064
Thermal correction to Gibbs Free Energy= 0.277475
Sum of electronic and zero-point Energies= -1760.365011
Sum of electronic and thermal Energies= -1760.340110
Sum of electronic and thermal Enthalpies= -1760.339166
Sum of electronic and thermal Free Energies= -1760.421755
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1761.00756245
Corrected Free Energy = -1760.73008735



I2 Substrate: N-(2-picolinoyl)-aziridine

CARTESIAN COORDINATES

C	0.543509	1.455816	-2.310895
N	2.104637	-0.048611	-1.870806

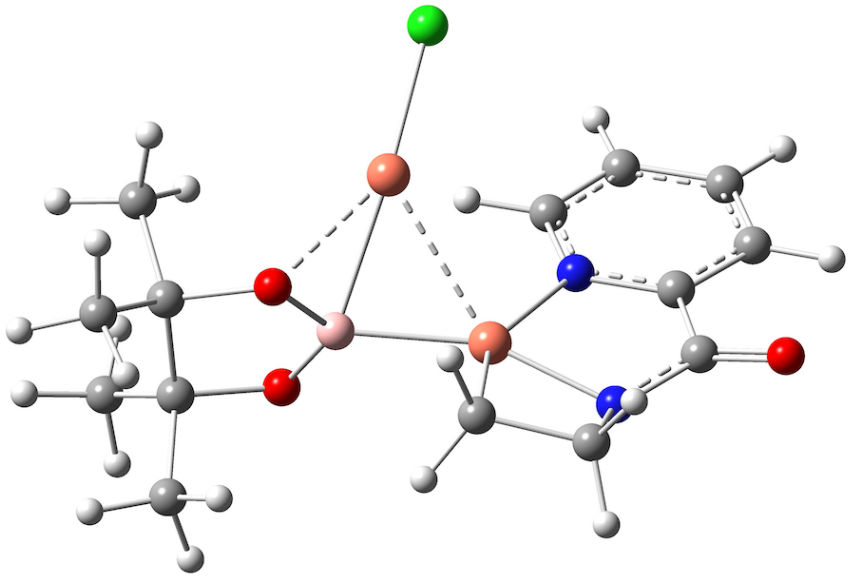
C	3.287260	-0.323275	-1.266037
O	4.417673	-0.139136	-1.715004
C	1.864794	0.955508	-2.902785
C	3.055005	-0.938667	0.108640
C	4.074158	-1.539606	0.839542
C	3.775369	-2.044123	2.107926
C	2.474954	-1.924015	2.605367
C	1.508043	-1.294462	1.820276
N	1.802992	-0.820415	0.602439
Cu	-0.458564	1.784597	0.688350
H	5.068024	-1.587504	0.406843
H	4.548755	-2.520715	2.703950
H	0.479943	-1.162525	2.140318
H	2.208916	-2.301270	3.587548
H	2.652474	1.717742	-2.932501
H	1.765370	0.513248	-3.901323
H	0.521328	2.477400	-1.931132
Cu	0.699510	0.280272	-0.699454
B	-1.352322	0.114069	-0.054363
O	-2.340004	0.250280	-1.001195
O	-1.554022	-0.974534	0.770287
C	-3.429572	-0.657036	-0.628467
C	-2.672002	-1.745028	0.214403
Cl	-0.467064	3.492789	1.951594
H	-0.385623	1.152621	-2.792270
C	-3.471396	-2.341264	1.367137
H	-4.369158	-2.844911	0.989530
H	-2.862571	-3.081605	1.896689
H	-3.774293	-1.575285	2.084423
C	-2.043988	-2.851813	-0.640328
H	-1.369330	-3.444885	-0.014724
H	-2.807126	-3.518226	-1.056270
H	-1.458743	-2.430806	-1.464494
C	-4.422248	0.169898	0.196150
H	-4.751044	1.026453	-0.400151
H	-5.302051	-0.422024	0.470564
H	-3.956674	0.554897	1.108865
C	-4.086587	-1.172658	-1.903955
H	-4.847731	-1.924876	-1.664828
H	-4.576554	-0.344794	-2.426400
H	-3.355987	-1.617257	-2.583879

Electronic Energy = -1760.71306275 (Hartree/Particle)
Dipole Moment (Debye): 8.7512
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.335220
(Hartree/Particle)
Thermal correction to Energy= 0.360420
Thermal correction to Enthalpy= 0.361364
Thermal correction to Gibbs Free Energy= 0.277322
Sum of electronic and zero-point Energies= -1760.377842
Sum of electronic and thermal Energies= -1760.352643
Sum of electronic and thermal Enthalpies= -1760.351698
Sum of electronic and thermal Free Energies= -1760.435740

PCM-SP (solvent=THF;6-311+g(2d,p)) = -1761.02236686
Corrected Free Energy = -1760.74504404



TS4 Substrate: N-(2-picolinoyl)-aziridine

CARTESIAN COORDINATES

N	-2.100287	0.290725	0.754959
C	-3.304581	-0.267376	0.488042
C	-4.494711	0.384427	0.789447
C	-4.436181	1.638037	1.403426
C	-3.190828	2.205166	1.678578
C	-2.039532	1.502252	1.325043
C	-3.276817	-1.615858	-0.222265
O	-4.277090	-2.082718	-0.770962
Cu	-0.629187	-0.936290	0.034329
N	-2.041223	-2.150160	-0.140512
C	-1.435672	-3.119524	-1.044920
C	-0.022934	-2.511278	-1.036204
B	1.314173	-0.396091	0.194877
Cu	0.421379	1.168822	-0.997942
Cl	-0.444760	3.077071	-1.372780
O	2.222218	-0.164770	-0.837061
C	3.520002	0.175727	-0.208055
C	4.628738	-0.365023	-1.101572
O	1.924814	-0.492018	1.414822
C	3.377565	-0.528203	1.187689
C	3.776938	-2.007380	1.168451
C	3.580121	1.702623	-0.127722
C	4.058843	0.198857	2.341183
H	-5.429809	-0.098000	0.524619
H	-5.349944	2.170829	1.651955
H	-1.047815	1.915593	1.465416
H	-3.100928	3.185473	2.134624
H	-1.473886	-4.144496	-0.653981
H	0.736604	-3.061981	-0.479514
H	0.357459	-2.120650	-1.980098
H	4.542088	2.040202	0.271445
H	3.452028	2.119648	-1.131238
H	2.777559	2.101949	0.500639

```
 H                 4.633481    0.176872   -2.052530
 H                 5.604508   -0.223509   -0.622083
 H                 4.494832   -1.427528   -1.316479
 H                 3.899168   -0.355742    3.271266
 H                 5.138647    0.269122    2.164137
 H                 3.658680    1.206303    2.474533
 H                 4.860638   -2.126730    1.064208
 H                 3.464644   -2.471159    2.109120
 H                 3.287200   -2.540970    0.347218
 H                -1.903336   -3.110968   -2.037872

 Electronic Energy =  -1760.70515508 (Hartree/Particle)
 Dipole Moment (Debye):      7.3206
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -78.759

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                          0.334875
(Hartree/Particle)
 Thermal correction to Energy=                   0.359345
 Thermal correction to Enthalpy=                 0.360290
 Thermal correction to Gibbs Free Energy=        0.278794
 Sum of electronic and zero-point Energies=          -1760.370280
 Sum of electronic and thermal Energies=             -1760.345810
 Sum of electronic and thermal Enthalpies=           -1760.344866
 Sum of electronic and thermal Free Energies=        -1760.426361
 PCM-SP (solvent=THF;6-311+g(2d,p)) = -1761.01401254
 Corrected Free Energy =  -1760.73521846

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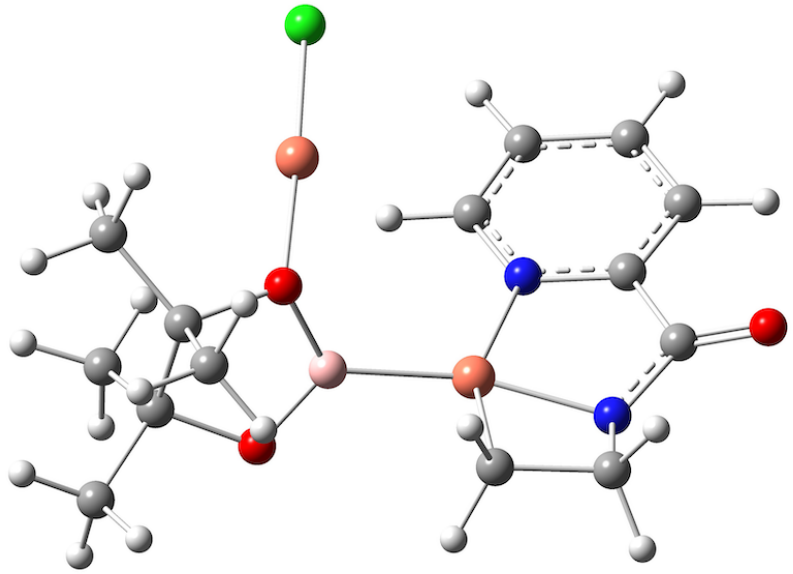

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I3     Substrate: N-(2-picolinoyl)-aziridine

 CARTESIAN COORDINATES

 C                -1.891963   -3.351253   -0.697271
 Cu               -0.856482   -1.243462    0.283068
```

B	1.064280	-0.843109	0.325983
O	1.734952	-0.056576	-0.652584
C	3.198178	-0.351491	-0.529570
C	3.283065	-0.759259	0.975253
O	1.966229	-1.361454	1.207323
Cu	1.013390	1.742606	-0.713238
Cl	0.276893	3.709918	-0.604308
C	-0.399450	-2.999230	-0.521252
N	-2.447133	-2.199304	0.008223
C	-3.500874	-1.453234	-0.370113
C	-3.361709	-0.043993	0.203375
C	-4.422494	0.853988	0.221136
C	-4.206817	2.143880	0.714117
C	-2.933727	2.498173	1.161417
C	-1.913870	1.549129	1.099766
N	-2.124105	0.309219	0.634976
O	-4.462426	-1.765434	-1.079059
H	-5.381479	0.525345	-0.165739
H	-5.018118	2.866393	0.735811
H	-0.900542	1.790849	1.397389
H	-2.710504	3.495717	1.523793
H	-2.166952	-4.305404	-0.228580
H	0.151638	-3.591230	0.211044
H	0.169613	-2.856325	-1.441823
C	3.997043	0.880633	-0.926124
H	5.067407	0.684590	-0.794243
H	3.820360	1.118251	-1.979937
H	3.732456	1.758574	-0.331652
C	3.455589	-1.505105	-1.500178
H	3.155314	-1.200181	-2.507242
H	4.517980	-1.768354	-1.519507
H	2.881692	-2.395321	-1.224818
C	3.395236	0.441301	1.920811
H	3.223255	0.100324	2.946019
H	4.388503	0.899302	1.868155
H	2.646518	1.205985	1.685682
C	4.349143	-1.802222	1.289799
H	5.344859	-1.422544	1.032008
H	4.335589	-2.028547	2.360462
H	4.174620	-2.733072	0.745231
H	-2.206601	-3.382176	-1.748629

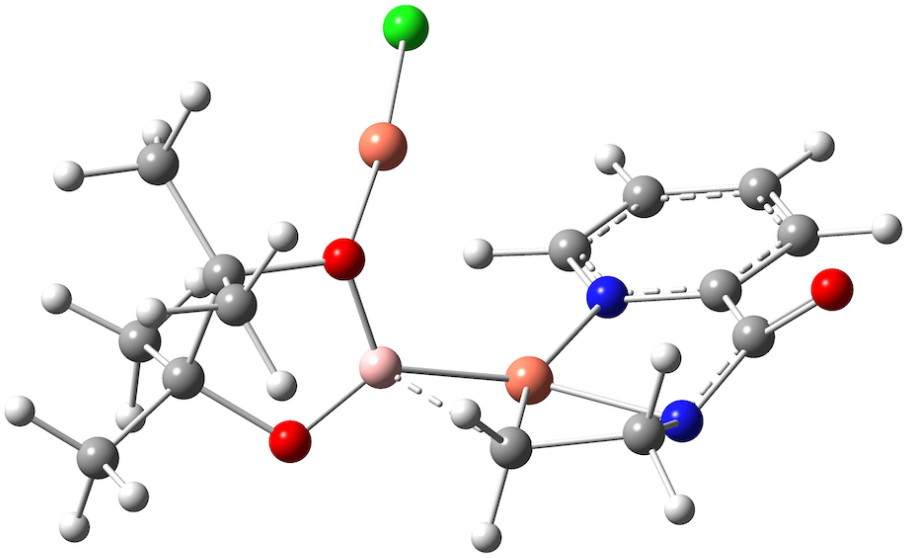
Electronic Energy = -1760.71525541 (Hartree/Particle)
Dipole Moment (Debye): 7.2813
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.335833
(Hartree/Particle)
Thermal correction to Energy= 0.360675
Thermal correction to Enthalpy= 0.361619
Thermal correction to Gibbs Free Energy= 0.278963
Sum of electronic and zero-point Energies= -1760.379422
Sum of electronic and thermal Energies= -1760.354581
Sum of electronic and thermal Enthalpies= -1760.353637
Sum of electronic and thermal Free Energies= -1760.436292

PCM-SP (solvent=THF;6-311+g(2d,p)) = -1761.02421944
Corrected Free Energy = -1760.74525603

TS5 Substrate: N-(2-picolinoyl)-aziridine



CARTESIAN COORDINATES

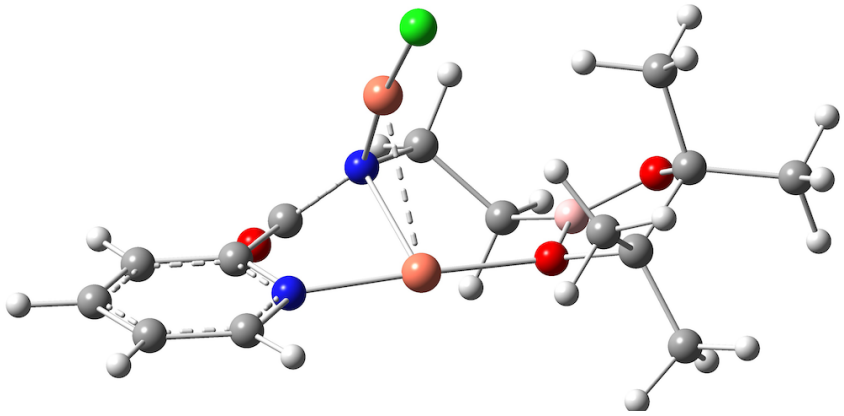
C	-0.970595	-3.159042	-0.728286
Cu	-0.681748	-1.094072	0.591138
B	1.247819	-0.880856	0.331049
O	1.731145	-0.084541	-0.744432
C	3.220107	-0.012842	-0.592490
C	3.369381	-0.225359	0.951699
O	2.229658	-1.091504	1.259199
Cu	0.603790	1.513936	-0.784849
Cl	-0.440746	3.337481	-0.689218
C	0.373003	-2.650978	-0.104653
N	-1.983416	-2.411904	0.019840
C	-2.984521	-1.767115	-0.600969
C	-3.288180	-0.441246	0.109069
C	-4.524490	0.190349	0.017202
C	-4.695337	1.438409	0.618727
C	-3.613286	2.038029	1.266442
C	-2.392608	1.368249	1.290509
N	-2.238881	0.153872	0.739020
O	-3.584613	-2.043437	-1.649469
H	-5.315525	-0.304580	-0.536113
H	-5.655031	1.945794	0.568359
H	-1.505967	1.814823	1.723787
H	-3.693628	3.021300	1.717733
H	-1.041709	-4.249836	-0.605718
H	0.662475	-3.232283	0.774952
H	1.189914	-2.667179	-0.832395
C	3.713414	1.324088	-1.123895
H	4.796081	1.403220	-0.973006
H	3.510617	1.397876	-2.196892
H	3.234327	2.172490	-0.628940

C	3.769704	-1.166850	-1.431538
H	3.419361	-1.060411	-2.462640
H	4.864241	-1.155726	-1.434294
H	3.440566	-2.138777	-1.052056
C	3.187389	1.062068	1.762946
H	3.094154	0.800850	2.821233
H	4.045500	1.731456	1.643721
H	2.281856	1.602194	1.465599
C	4.645576	-0.949275	1.366891
H	5.527717	-0.374925	1.060865
H	4.667787	-1.056268	2.455749
H	4.704801	-1.947777	0.927861
H	-1.023925	-2.940027	-1.803051

Electronic Energy = -1760.70833509 (Hartree/Particle)
Dipole Moment (Debye): 8.2841
index 0
Harmonic frequencies
Number of imaginary frequencies= 1
Negatives Eigenvalues: -142.730

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.335397
(Hartree/Particle)
Thermal correction to Energy= 0.359422
Thermal correction to Enthalpy= 0.360366
Thermal correction to Gibbs Free Energy= 0.280878
Sum of electronic and zero-point Energies= -1760.372938
Sum of electronic and thermal Energies= -1760.348914
Sum of electronic and thermal Enthalpies= -1760.347969
Sum of electronic and thermal Free Energies= -1760.427457
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1761.02086132
Corrected Free Energy = -1760.73998323



P2 Substrate: N-(2-picolinoyl)-aziridine

CARTESIAN COORDINATES

C	-0.070191	-2.352295	-1.352086
Cu	-0.378070	0.106828	0.976671
B	1.890236	-1.540129	0.161698
O	3.181716	-1.408897	-0.240285
C	3.635354	-0.041736	0.027538

C	2.692794	0.413978	1.198690
O	1.498603	-0.436267	0.947713
Cu	-0.535985	0.493520	-1.572702
Cl	0.084588	2.462996	-2.067859
C	0.925930	-2.718295	-0.212518
N	-0.968834	-1.258650	-0.947311
C	-2.159055	-1.637799	-0.424154
C	-2.959638	-0.528077	0.243425
C	-4.347951	-0.481046	0.114322
C	-5.057745	0.527274	0.762329
C	-4.363095	1.446728	1.554880
C	-2.983664	1.317673	1.671667
N	-2.294312	0.355063	1.028223
O	-2.640013	-2.780931	-0.381210
H	-4.836087	-1.237015	-0.490762
H	-6.136760	0.596306	0.655771
H	-2.396570	1.991029	2.286716
H	-4.876732	2.245716	2.079734
H	-0.659066	-3.237519	-1.612411
H	0.331563	-3.032394	0.656206
H	1.521664	-3.582869	-0.533113
C	3.420477	0.749261	-1.265265
H	3.798339	1.772599	-1.173540
H	3.960994	0.250191	-2.075483
H	2.363310	0.807732	-1.541051
C	5.114693	-0.090214	0.394635
H	5.693346	-0.419716	-0.473790
H	5.469188	0.906015	0.683342
H	5.308743	-0.785597	1.214794
C	2.258040	1.872066	1.150333
H	1.598425	2.087957	1.999313
H	3.131803	2.528754	1.228064
H	1.720170	2.108411	0.228460
C	3.187024	0.022985	2.591185
H	4.048826	0.630659	2.884991
H	2.383656	0.189974	3.316082
H	3.471822	-1.032984	2.633024
H	0.483532	-2.036776	-2.242350

Electronic Energy = -1760.81585981 (Hartree/Particle)
Dipole Moment (Debye): 6.7494
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.338359
(Hartree/Particle)
Thermal correction to Energy= 0.362615
Thermal correction to Enthalpy= 0.363559
Thermal correction to Gibbs Free Energy= 0.284403
Sum of electronic and zero-point Energies= -1760.477501
Sum of electronic and thermal Energies= -1760.453245
Sum of electronic and thermal Enthalpies= -1760.452300
Sum of electronic and thermal Free Energies= -1760.531457
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1761.12387972
Corrected Free Energy = -1760.83947691

SUBSTITUTION OF CHLORIDE WITH ALKOXIDE ANION (REF 30, MAIN TEXT, TABLE S1)

Complex-2 (Ref 33) Substrate: N-(2picolinoyl)-aziridine
                    Alkoxide = Methoxide

CARTESIAN COORDINATES

C	-0.464538	-2.792596	1.058214
N	-1.116269	-2.175923	-0.157270
C	-2.543619	-2.319220	-0.242166
O	-3.100970	-3.377926	-0.459882
C	-0.314904	-3.406339	-0.280158
C	-3.286800	-1.030181	-0.056949
C	-4.672964	-1.030943	0.098084
C	-5.314324	0.196614	0.284344
C	-4.550389	1.364076	0.309722
C	-3.162554	1.283824	0.138230
N	-2.553861	0.101696	-0.047749
Cu	0.241600	1.978102	0.022459
H	-5.213830	-1.970914	0.074152
H	-6.392614	0.237162	0.411147
H	-2.510978	2.164106	0.150794
H	-5.012156	2.335394	0.458040
H	-0.871682	-4.313852	-0.496958
H	0.608539	-3.257898	-0.830603
H	-1.147921	-3.267452	1.758528
Cu	-0.500919	-0.149243	-0.313134
B	1.516709	0.314551	-0.096922
O	2.035613	-0.386974	1.002319
O	2.486252	0.430162	-1.087831
C	3.479001	-0.490521	0.841162
C	3.647278	-0.360006	-0.714065
H	0.331677	-2.183407	1.477890
C	4.093146	0.682082	1.618098
H	3.764199	0.626540	2.660738
H	5.188363	0.652361	1.595165
H	3.756441	1.640454	1.210791
C	4.907617	0.372339	-1.168292
H	5.806951	-0.154120	-0.825449
H	4.932729	0.418421	-2.262158
H	4.933541	1.396327	-0.789028
C	3.946014	-1.817318	1.434517
H	5.018142	-1.965371	1.256949
H	3.776575	-1.817263	2.516724
H	3.403117	-2.664631	1.007352
C	3.524134	-1.699977	-1.453184
H	3.439406	-1.505537	-2.526992
H	4.395918	-2.341158	-1.280588
H	2.625145	-2.237939	-1.136011
O	-0.816721	3.459516	0.309901
C	-0.652954	4.699784	-0.318707
H	-1.501627	5.365669	-0.073895
H	0.266820	5.221530	0.005907
H	-0.607396	4.623563	-1.422336

Electronic Energy = -1415.60696054 (Hartree/Particle)
Dipole Moment (Debye): 6.3125

```
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.375106
(Hartree/Particle)
 Thermal correction to Energy=                    0.402580
 Thermal correction to Enthalpy=                  0.403525
 Thermal correction to Gibbs Free Energy=         0.314215
 Sum of electronic and zero-point Energies=          -1415.231855
 Sum of electronic and thermal Energies=             -1415.204380
 Sum of electronic and thermal Enthalpies=           -1415.203436
 Sum of electronic and thermal Free Energies=        -1415.292746
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1415.91385033
 Corrected Free Energy =  -1415.59963579
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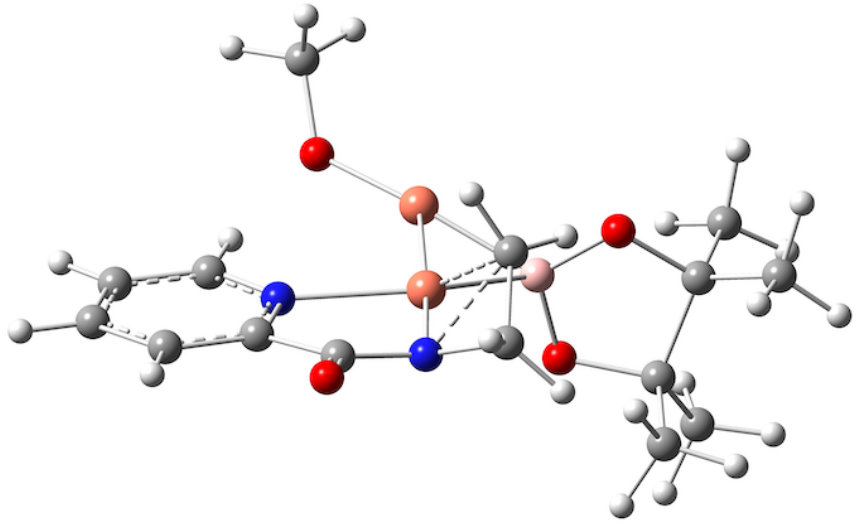

TS3 (Ref 33) Substrate: N-(2picolinoyl)-aziridine
              Alkoxide = Methoxide

CARTESIAN COORDINATES

C	0.076705	-1.911054	-1.736694
N	1.109200	-2.186978	-0.153108
C	2.506041	-2.298574	-0.147079
O	3.098689	-3.337804	-0.413726
C	0.375026	-3.143560	-0.963419
C	3.235525	-1.050953	0.273543
C	4.608110	-1.073735	0.512445
C	5.236698	0.128148	0.850143
C	4.478970	1.298481	0.906794
C	3.106914	1.241154	0.633579
N	2.506033	0.077408	0.343464
Cu	-0.166547	1.881830	-0.196704
H	5.148759	-2.009674	0.421572
H	6.303885	0.149621	1.053602
H	2.470776	2.129079	0.609462
H	4.933854	2.252998	1.153017

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 H                0.998713   -3.900983   -1.440844
 H               -0.470773   -3.582894   -0.432283
 H                0.778115   -1.627448   -2.515509
 Cu               0.467511   -0.347000   -0.129975
 B               -1.565016    0.440770    0.043228
 O               -2.441865    0.046484   -0.969632
 O               -2.140077    0.233980    1.290602
 C               -3.749317   -0.197782   -0.372437
 C               -3.370682   -0.523362    1.114738
 H               -0.916310   -1.468631   -1.760724
 C               -4.386078   -0.063796    2.156735
 H               -5.354514   -0.552554    1.993967
 H               -4.032047   -0.328410    3.158564
 H               -4.528700    1.018710    2.126082
 C               -3.009467   -1.998362    1.339643
 H               -2.557105   -2.104913    2.330488
 H               -3.891689   -2.645724    1.284993
 H               -2.277447   -2.337833    0.599406
 C               -4.554489    1.099177   -0.523542
 H               -4.600424    1.366016   -1.584208
 H               -5.577351    0.983188   -0.148315
 H               -4.073891    1.924003    0.011718
 C               -4.428468   -1.334266   -1.131451
 H               -5.378012   -1.604333   -0.653847
 H               -4.640222   -1.018087   -2.158388
 H               -3.796954   -2.225592   -1.175690
 O                0.882489    3.378967   -0.108019
 C                1.018278    4.351025   -1.106879
 H                0.079342    4.905180   -1.289085
 H                1.778963    5.096030   -0.810885
 H                1.337048    3.927046   -2.078549

 Electronic Energy =  -1415.57769795 (Hartree/Particle)
 Dipole Moment (Debye):      4.3192
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -256.540

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.373554
(Hartree/Particle)
 Thermal correction to Energy=                    0.400500
 Thermal correction to Enthalpy=                  0.401444
 Thermal correction to Gibbs Free Energy=         0.313876
 Sum of electronic and zero-point Energies=          -1415.204144
 Sum of electronic and thermal Energies=             -1415.177198
 Sum of electronic and thermal Enthalpies=           -1415.176254
 Sum of electronic and thermal Free Energies=        -1415.263822
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1415.88517817
 Corrected Free Energy =  -1415.57130222

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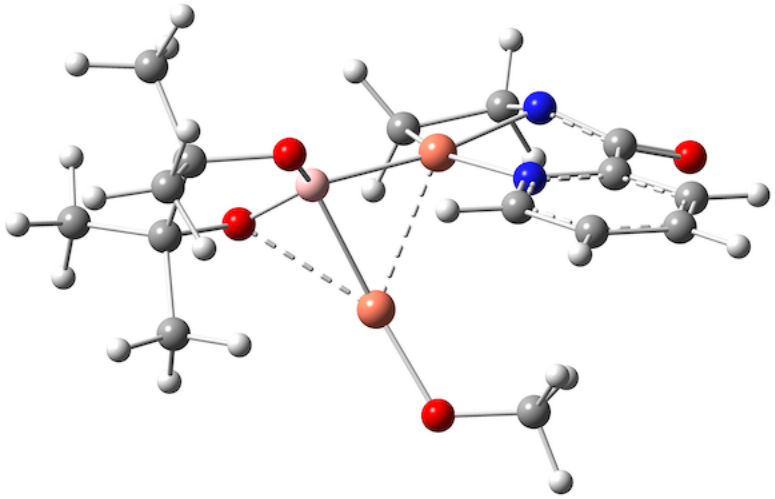

TS4 (Ref 33) Substrate: N-(2picolinoyl)-aziridine
              Alkoxide = Methoxide

CARTESIAN COORDINATES

N	1.706603	0.775618	-0.827387
C	3.011617	0.438676	-0.730982
C	4.012582	1.405205	-0.724480
C	3.646817	2.747619	-0.839603
C	2.293610	3.083542	-0.941902
C	1.345120	2.061957	-0.920991
C	3.306366	-1.049201	-0.551871
O	4.408826	-1.442929	-0.165122
Cu	0.590499	-0.897140	-0.559400
N	2.212470	-1.778379	-0.859665
C	1.868574	-3.097927	-0.332490
C	0.368220	-2.830052	-0.133445
B	-1.340697	-0.306285	-0.341275
Cu	-0.362419	-0.091775	1.566672
O	-2.325852	-0.841334	0.477652
C	-3.539487	-0.018120	0.294797
C	-4.753006	-0.929373	0.431668
O	-1.839054	0.614395	-1.230673
C	-3.305322	0.573457	-1.141679
C	-3.784069	-0.347873	-2.268635
C	-3.522605	1.034608	1.406508
C	-3.835083	1.988831	-1.343242
H	5.042819	1.083366	-0.613924
H	4.405869	3.525082	-0.837922
H	0.277290	2.249514	-0.971401
H	1.972292	4.117077	-1.021636
H	2.081383	-3.906774	-1.043557
H	-0.307437	-3.246634	-0.882039
H	-0.028959	-2.921054	0.877297
H	-4.422525	1.657743	1.377284
H	-3.480164	0.528801	2.375994
H	-2.641338	1.680290	1.332765
H	-4.819989	-1.302079	1.458652
H	-5.671964	-0.374524	0.208138
H	-4.691452	-1.789981	-0.238162
H	-3.616582	2.322031	-2.362970
H	-4.921820	2.014895	-1.199749
H	-3.373656	2.694369	-0.648562

H	-4.877725	-0.388435	-2.313463
H	-3.411098	0.036131	-3.223180
H	-3.400793	-1.365109	-2.139370
H	2.395824	-3.313668	0.605105
O	0.467593	0.841271	2.879802
C	1.841915	1.103366	2.747055
H	2.448794	0.191108	2.605927
H	2.068136	1.776929	1.899563
H	2.205161	1.600706	3.662560

Electronic Energy = -1415.58241718 (Hartree/Particle)
Dipole Moment (Debye): 8.0259
index 0
Harmonic frequencies
Number of imaginary frequencies= 1
Negatives Eigenvalues: -83.050

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.374539
(Hartree/Particle)
Thermal correction to Energy= 0.400817
Thermal correction to Enthalpy= 0.401761
Thermal correction to Gibbs Free Energy= 0.316848
Sum of electronic and zero-point Energies= -1415.207878
Sum of electronic and thermal Energies= -1415.181601
Sum of electronic and thermal Enthalpies= -1415.180656
Sum of electronic and thermal Free Energies= -1415.265569
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1415.89420375
Corrected Free Energy = -1415.57735557

Complex-2 (ref 33) Substrate: N-(2picolinoyl)-aziridine
Alkoxide = t-Butoxide

CARTESIAN COORDINATES

C	0.401004	-3.365476	0.920998
N	-0.409839	-2.836051	-0.239141
C	-1.768830	-3.297598	-0.314443
O	-2.075960	-4.442393	-0.586147
C	0.646803	-3.839994	-0.458783
C	-2.781486	-2.224736	-0.046025
C	-4.127899	-2.550203	0.118389
C	-5.027850	-1.514004	0.381783
C	-4.549095	-0.206256	0.470956
C	-3.183249	0.040901	0.285867
N	-2.325081	-0.957998	0.025995
Cu	-0.025720	1.499994	0.190731
H	-4.441331	-3.585871	0.042220
H	-6.084277	-1.727875	0.518174
H	-2.747944	1.043424	0.345841
H	-5.216078	0.624671	0.679427
H	0.304728	-4.834865	-0.730421
H	1.495145	-3.448608	-1.010967
H	-0.135649	-4.028847	1.595413
Cu	-0.274453	-0.717028	-0.262774
B	1.589648	0.179761	-0.031200

```
 O                 2.280417   -0.436075    1.023645
 O                 2.484026    0.567451   -1.023765
 C                 3.704136   -0.187205    0.845447
 C                 3.805027    0.053454   -0.702219
 H                 1.049097   -2.618361    1.371589
 C                 4.039575    1.059413    1.675665
 H                 3.753402    0.878628    2.716726
 H                 5.110286    1.290389    1.642742
 H                 3.478823    1.929283    1.319797
 C                 4.849854    1.081242   -1.129760
 H                 5.854075    0.764303   -0.822247
 H                 4.841009    1.183900   -2.220032
 H                 4.643837    2.063593   -0.698923
 C                 4.483258   -1.392206    1.366309
 H                 5.555929   -1.274257    1.170398
 H                 4.342412   -1.482611    2.448825
 H                 4.145887   -2.322966    0.902623
 C                 3.981679   -1.241532   -1.507563
 H                 3.830355   -1.021906   -2.569127
 H                 4.982546   -1.668196   -1.376820
 H                 3.240345   -1.989249   -1.208319
 O                -1.377936    2.703727    0.563543
 C                -1.599636    3.903380   -0.135814
 C                -0.373303    4.829474   -0.002876
 H                -0.164754    5.014655    1.057344
 H                 0.505805    4.337162   -0.440176
 H                -0.520045    5.793615   -0.509049
 C                -2.833765    4.586395    0.485819
 H                -3.068465    5.540883   -0.004237
 H                -3.707421    3.927817    0.397868
 H                -2.655990    4.771290    1.551591
 C                -1.864566    3.611487   -1.628838
 H                -0.992668    3.107432   -2.065893
 H                -2.726587    2.939782   -1.730053
 H                -2.065586    4.525413   -2.204715

 Electronic Energy =  -1533.57718343 (Hartree/Particle)
 Dipole Moment (Debye):      6.6515
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.459879
(Hartree/Particle)
 Thermal correction to Energy=                    0.490966
 Thermal correction to Enthalpy=                  0.491910
 Thermal correction to Gibbs Free Energy=         0.394036
 Sum of electronic and zero-point Energies=          -1533.117305
 Sum of electronic and thermal Energies=             -1533.086217
 Sum of electronic and thermal Enthalpies=           -1533.085273
 Sum of electronic and thermal Free Energies=        -1533.183147
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1533.91623820
 Corrected Free Energy =  -1533.52220177

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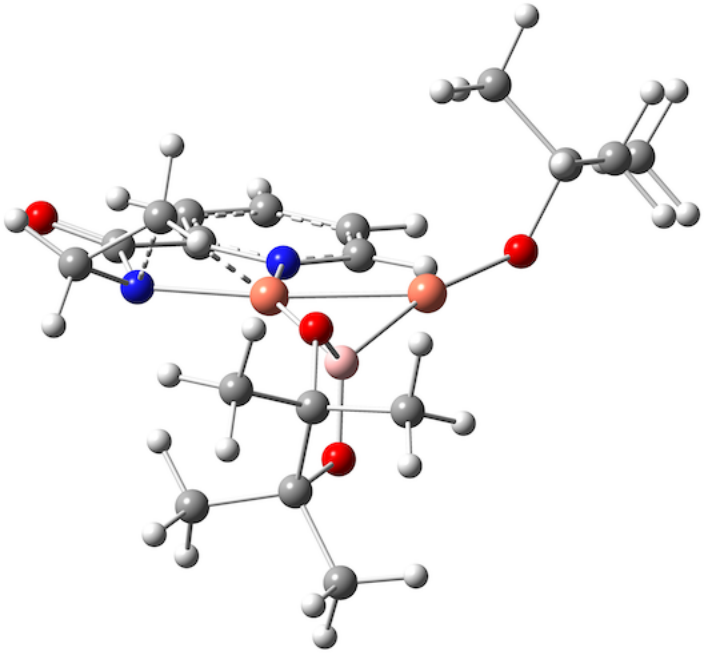

TS3 (Ref 33) Substrate: N-(2picolinoyl)-aziridine
Alkoxide = t-Butoxide

CARTESIAN COORDINATES

C	0.487855	-1.951451	1.933296
N	-0.351896	-2.729425	0.402550
C	-1.685449	-3.159464	0.387427
O	-2.047379	-4.244651	0.827376
C	0.524325	-3.333965	1.391324
C	-2.647156	-2.205393	-0.269065
C	-3.966053	-2.579974	-0.518254
C	-4.824078	-1.631280	-1.081769
C	-4.340174	-0.349242	-1.345301
C	-3.006440	-0.046629	-1.047476
N	-2.181252	-0.972349	-0.537698
Cu	-0.024474	1.471402	-0.205755
H	-4.292244	-3.582086	-0.261541
H	-5.857331	-1.888041	-1.298913
H	-2.584131	0.951871	-1.173208
H	-4.979589	0.419055	-1.769069
H	0.057440	-4.121926	1.984363
H	1.480062	-3.648605	0.969188
H	-0.308841	-1.708299	2.629854
Cu	-0.138033	-0.823954	0.060066
B	1.678003	0.381806	-0.200974
O	2.559451	0.341090	0.881421
O	2.356301	0.140699	-1.388398
C	3.921401	0.318967	0.361304
C	3.711255	-0.286892	-1.070446
H	1.353476	-1.294194	1.899211
C	4.659862	0.241304	-2.142334
H	5.700706	0.009961	-1.884766
H	4.430803	-0.231570	-3.103037
H	4.560357	1.321836	-2.267606
C	3.696375	-1.821969	-1.083213
H	3.340045	-2.164421	-2.059692
H	4.694036	-2.239347	-0.907643

```
 H                3.012304   -2.212000   -0.322121
 C                4.409932    1.772955    0.339726
 H                4.332425    2.187588    1.349863
 H                5.453681    1.841676    0.013641
 H                3.791822    2.384867   -0.324583
 C                4.788503   -0.517614    1.297794
 H                5.800429   -0.629288    0.890159
 H                4.865110   -0.022297    2.271557
 H                4.367230   -1.513750    1.457326
 O               -1.401342    2.652335   -0.491361
 C               -1.970754    3.477877    0.495901
 C               -3.107925    4.281331   -0.163807
 H               -3.600418    4.958351    0.546885
 H               -2.708080    4.873003   -0.995236
 H               -3.862161    3.595388   -0.569680
 C               -2.542177    2.617193    1.644662
 H               -3.289792    1.916689    1.252324
 H               -1.733869    2.027727    2.097891
 H               -3.012944    3.226262    2.428305
 C               -0.908282    4.444351    1.057049
 H               -0.096109    3.868051    1.520319
 H               -0.479264    5.035145    0.239488
 H               -1.322831    5.129329    1.809366

 Electronic Energy =  -1533.54822187 (Hartree/Particle)
 Dipole Moment (Debye):      4.4280
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -253.913

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.458451
(Hartree/Particle)
 Thermal correction to Energy=                    0.488885
 Thermal correction to Enthalpy=                  0.489829
 Thermal correction to Gibbs Free Energy=         0.395081
 Sum of electronic and zero-point Energies=          -1533.089770
 Sum of electronic and thermal Energies=             -1533.059337
 Sum of electronic and thermal Enthalpies=           -1533.058393
 Sum of electronic and thermal Free Energies=        -1533.153141
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1533.88806121
 Corrected Free Energy =   -1533.49298034

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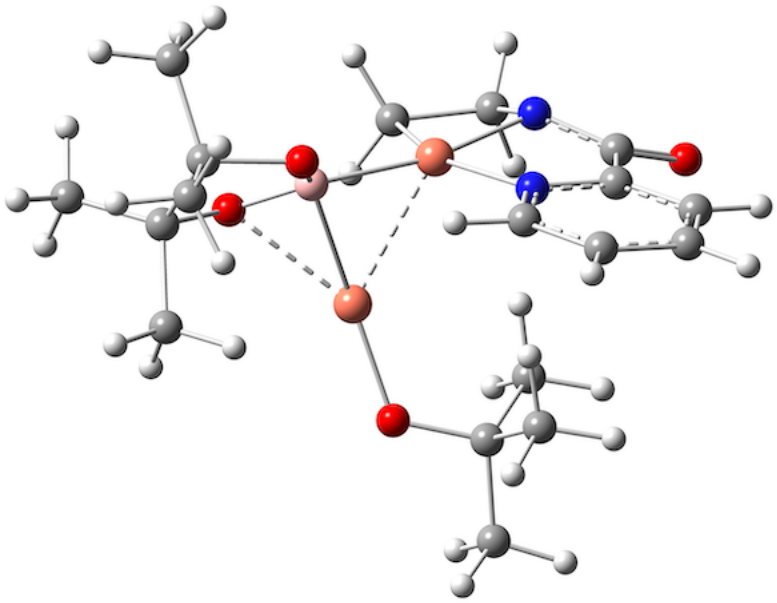

TS4 (Ref 33) Substrate: N-(2picolinoyl)-aziridine
              Alkoxide = t-Butoxide

CARTESIAN COORDINATES

N	-1.293969	-1.581325	0.622329
C	-2.607927	-1.672634	0.315693
C	-3.557067	-1.998636	1.278848
C	-3.127430	-2.257569	2.582000
C	-1.765214	-2.175073	2.883662
C	-0.873322	-1.822130	1.871510
C	-2.989372	-1.321918	-1.121688
O	-4.161483	-1.115969	-1.443492
Cu	-0.299703	-0.853978	-0.988754
N	-1.881981	-1.275899	-1.887888
C	-1.675746	-0.519465	-3.118809
C	-0.199812	-0.173063	-2.867060
B	1.581539	-0.467829	-0.359054
Cu	0.488290	1.408248	-0.193404
O	2.467606	0.493828	-0.831458
C	3.677733	0.435851	0.019541
C	4.881532	0.765252	-0.853993
O	2.172151	-1.319144	0.543145
C	3.615676	-1.041958	0.547372
C	4.256620	-2.058998	-0.402785
C	3.493792	1.491666	1.112419
C	4.134097	-1.233167	1.968348
H	-4.601669	-2.026160	0.986581
H	-3.846006	-2.513370	3.355899
H	0.194004	-1.717792	2.037697
H	-1.395828	-2.365112	3.886357
H	-1.845245	-1.115851	-4.025293
H	0.537122	-0.798390	-3.373537
H	0.077337	0.880660	-2.874199
H	4.380661	1.558813	1.751177
H	3.325563	2.466002	0.643543
H	2.622087	1.273898	1.737964
H	4.823080	1.807334	-1.183570
H	5.809925	0.637699	-0.284739
H	4.924366	0.130201	-1.741611

```
 H                4.040984   -2.285467    2.255887
 H                5.192566   -0.953906    2.030286
 H                3.571758   -0.632499    2.686837
 H                5.347495   -1.961307   -0.414566
 H                4.001767   -3.068677   -0.066173
 H                3.882923   -1.937970   -1.424547
 H               -2.319328    0.367975   -3.162154
 O               -0.400853    2.797304    0.564166
 C               -1.802012    2.805041    0.731651
 C               -2.518032    2.370780   -0.562501
 H               -2.202925    3.014454   -1.392370
 H               -2.244451    1.337606   -0.812744
 H               -3.610959    2.414939   -0.474656
 C               -2.195731    1.858263    1.883321
 H               -1.683659    2.161477    2.803999
 H               -3.278937    1.851029    2.064493
 H               -1.877368    0.838714    1.639234
 C               -2.201196    4.250410    1.084639
 H               -3.282026    4.343307    1.254225
 H               -1.673574    4.569249    1.990926
 H               -1.913630    4.924959    0.269914

 Electronic Energy =  -1533.55523236 (Hartree/Particle)
 Dipole Moment (Debye):      8.6247
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:            -85.071

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.459589
(Hartree/Particle)
 Thermal correction to Energy=                    0.489407
 Thermal correction to Enthalpy=                  0.490351
 Thermal correction to Gibbs Free Energy=         0.398846
 Sum of electronic and zero-point Energies=          -1533.095644
 Sum of electronic and thermal Energies=             -1533.065826
 Sum of electronic and thermal Enthalpies=           -1533.064881
 Sum of electronic and thermal Free Energies=        -1533.156387
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1533.89881221
 Corrected Free Energy =  -1533.49996685

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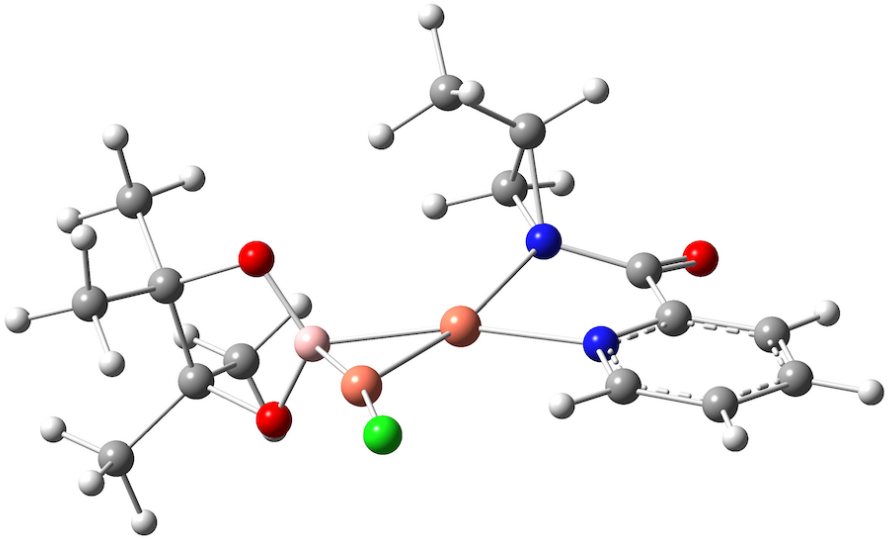


SUBSTRATE: N-(2-PICOLINOYL)-METHYL AZIRIDINE

Complex-2 Substrate: N-(2-picolinoyl)-methyl aziridine

CARTESIAN COORDINATES

C	-1.087225	-2.709815	1.493532
N	-1.279327	-2.050241	0.135376
C	-2.613626	-2.128474	-0.378018
O	-3.132381	-3.156041	-0.771487
C	-0.537778	-3.320086	0.260848
C	-3.319844	-0.805188	-0.389961
C	-4.693401	-0.736458	-0.621802
C	-5.302288	0.521071	-0.609400
C	-4.518751	1.651552	-0.372655
C	-3.144100	1.497504	-0.162898
N	-2.562083	0.289555	-0.172630
Cu	0.396799	2.030615	0.177744
H	-5.250379	-1.649475	-0.802870
H	-6.370685	0.614489	-0.782370
H	-2.482336	2.344121	0.011588
H	-4.952717	2.646350	-0.355643
H	-1.023495	-4.199195	-0.154152
H	0.522277	-3.205389	0.054132
C	-0.255933	-1.977807	2.513419
H	0.024414	-2.672803	3.315050
H	0.654049	-1.562353	2.071241
Cu	-0.513246	-0.063033	-0.073272
B	1.521662	0.267394	-0.138902
O	2.293574	-0.272330	0.892179
O	2.227188	0.242703	-1.335895
C	3.664502	-0.402379	0.415643
C	3.463910	-0.498260	-1.138041
Cl	-0.381468	4.015674	0.513368
C	4.403737	0.868607	0.855018
H	4.324501	0.965835	1.942413
H	5.464702	0.831791	0.583773
H	3.954620	1.759573	0.405162
C	4.294498	-1.631495	1.065165
H	5.300406	-1.807330	0.665108

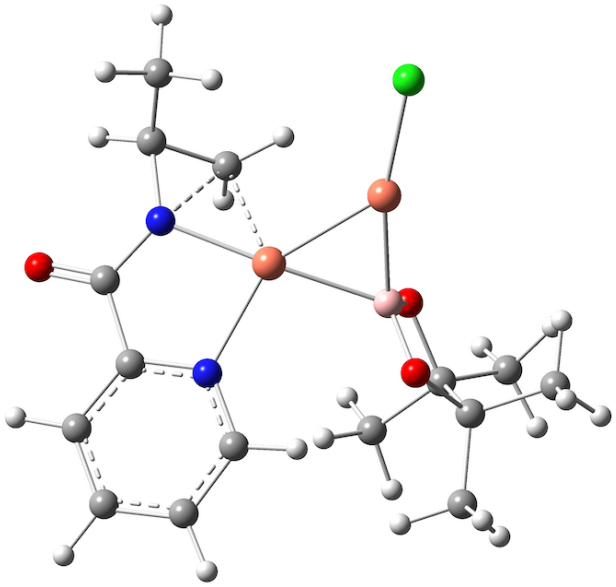
H	4.379330	-1.474591	2.145744
H	3.692664	-2.529061	0.900577
C	4.564045	0.152230	-1.972613
H	5.531460	-0.326840	-1.777921
H	4.333817	0.040952	-3.037399
H	4.650475	1.219635	-1.757810
C	3.203397	-1.928218	-1.631035
H	2.867455	-1.888542	-2.672015
H	4.106630	-2.546238	-1.577730
H	2.415657	-2.407387	-1.040726
H	-2.005618	-3.167583	1.861582
H	-0.827635	-1.155798	2.959016

Electronic Energy = -1800.05719595 (Hartree/Particle)
Dipole Moment (Debye): 8.7936
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.363783
(Hartree/Particle)
Thermal correction to Energy= 0.390722
Thermal correction to Enthalpy= 0.391666
Thermal correction to Gibbs Free Energy= 0.303896
Sum of electronic and zero-point Energies= -1799.693413
Sum of electronic and thermal Energies= -1799.666474
Sum of electronic and thermal Enthalpies= -1799.665530
Sum of electronic and thermal Free Energies= -1799.753300
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1800.37640687
Corrected Free Energy = -1800.07251092

PATH: ANTI_MARKOVNIKOV



TS3 Substrate: N-(2-picolinoyl)-methyl aziridine

Path: anti-Markovnikov

CARTESIAN COORDINATES

C	-1.758973	-1.317001	1.715715
N	-2.649497	-0.334468	0.327132
C	-3.153594	0.954571	0.487109
O	-4.191008	1.231398	1.079642
C	-3.152548	-1.386208	1.205525
C	-2.346226	2.015010	-0.223906
C	-2.830827	3.314046	-0.368579
C	-2.036131	4.244547	-1.042759
C	-0.788872	3.848972	-1.531938
C	-0.368842	2.532724	-1.322117
N	-1.139624	1.642352	-0.686756
Cu	0.600545	-2.181951	-0.629164
H	-3.801752	3.566093	0.044125
H	-2.385421	5.263661	-1.183176
H	0.597017	2.161612	-1.652390
H	-0.146865	4.542602	-2.066065
H	-3.920605	-1.023555	1.892746
H	-1.516336	-0.601406	2.495363
Cu	-0.747683	-0.349472	-0.111093
B	1.372404	-0.365828	-0.026433
O	2.104313	0.424744	-0.905892
O	1.844853	-0.228674	1.272567
C	3.290905	0.903979	-0.202147
C	2.829088	0.847026	1.296519
H	-1.062002	-2.132270	1.539001
C	-3.541792	-2.659879	0.474734
H	-3.735072	-3.461498	1.196856
H	-4.449437	-2.493588	-0.114733
Cl	0.248859	-4.251017	-1.059405
C	3.924315	0.488319	2.296263
H	4.727281	1.235083	2.272900
H	3.507526	0.465246	3.308623
H	4.352208	-0.494374	2.086273
C	2.082781	2.108180	1.753144
H	1.622853	1.913195	2.727357
H	2.759530	2.963789	1.854500
H	1.285728	2.370920	1.050305
C	4.421664	-0.079405	-0.529072
H	4.544516	-0.129161	-1.615503
H	5.371298	0.237798	-0.084288
H	4.183331	-1.085997	-0.171748
C	3.636302	2.297932	-0.718839
H	4.482800	2.716169	-0.161251
H	3.918916	2.239612	-1.775275
H	2.791511	2.985851	-0.629506
H	-2.737564	-2.983890	-0.195698

Electronic Energy = -1800.02257319 (Hartree/Particle)
Dipole Moment (Debye): 11.1955
index 0
Harmonic frequencies
Number of imaginary frequencies= 1
Negatives Eigenvalues: -267.288

THERMOCHEMICAL DATA

```
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.362067
(Hartree/Particle)
 Thermal correction to Energy=                    0.388523
 Thermal correction to Enthalpy=                  0.389467
 Thermal correction to Gibbs Free Energy=         0.302924
 Sum of electronic and zero-point Energies=          -1799.660506
 Sum of electronic and thermal Energies=             -1799.634050
 Sum of electronic and thermal Enthalpies=           -1799.633106
 Sum of electronic and thermal Free Energies=        -1799.719649
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1800.34339657
 Corrected Free Energy =  -1800.04047238
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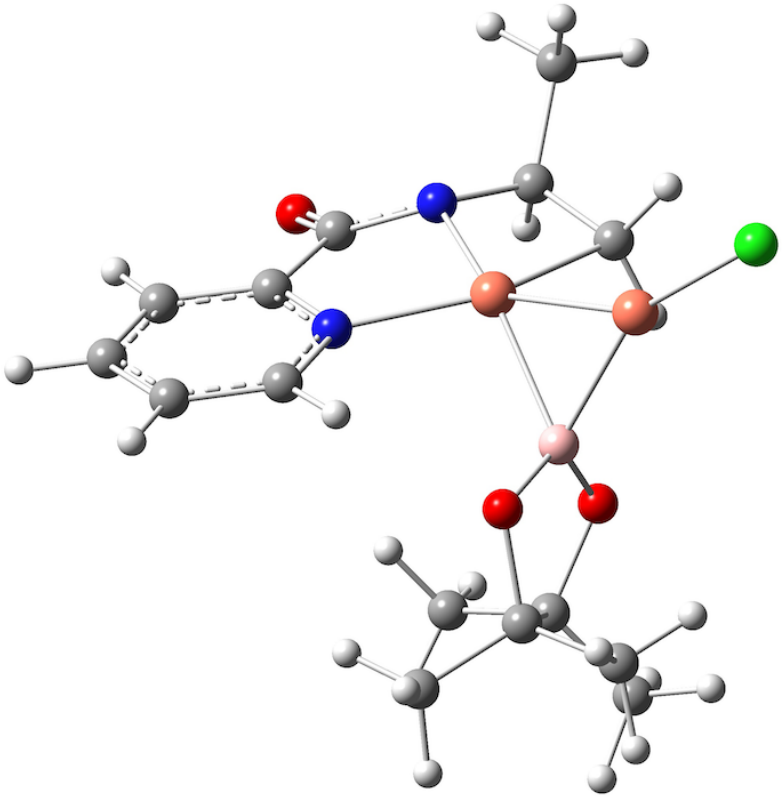


I2 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: anti-Markovnikov

CARTESIAN COORDINATES

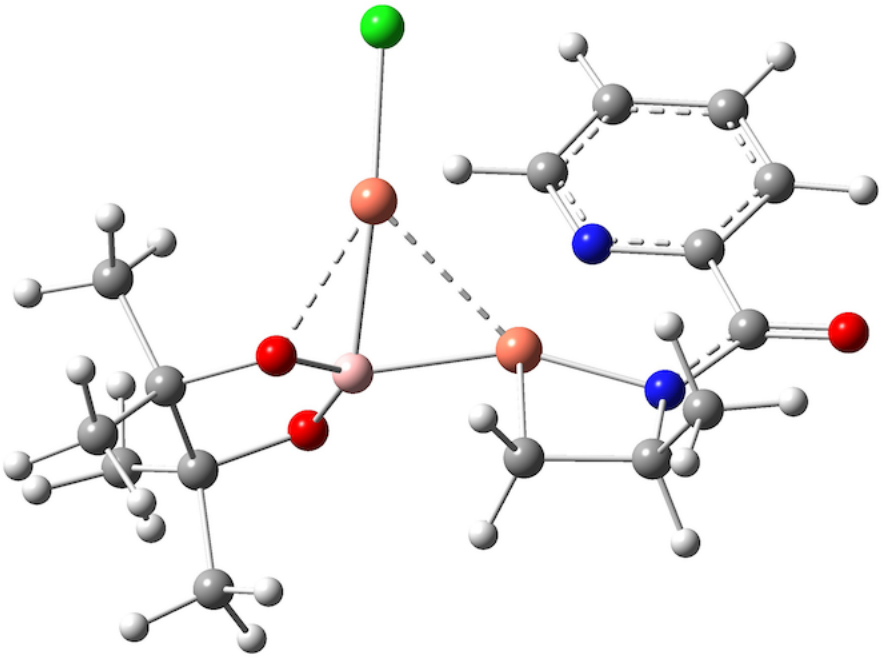
C	0.873396	2.141956	1.320868
N	2.503962	0.880601	0.506059
C	3.211326	-0.272038	0.562793
O	4.158559	-0.541918	1.302724
C	2.357484	1.856565	1.586552
C	2.688991	-1.269389	-0.462527
C	3.414094	-2.393933	-0.842724
C	2.853658	-3.263868	-1.780961
C	1.582560	-2.989954	-2.292789
C	0.902978	-1.857436	-1.842334
N	1.453252	-1.020083	-0.951015
Cu	-1.174951	1.873924	-0.767374

H	4.388790	-2.559462	-0.395702
H	3.399357	-4.145044	-2.107059
H	-0.101567	-1.610240	-2.166588
H	1.114830	-3.641885	-3.023688
H	2.506464	1.374986	2.562610
H	0.145721	1.837976	2.072339
Cu	0.739945	0.681587	-0.063080
B	-1.313175	0.044332	0.100537
O	-1.852197	-0.947869	-0.690732
O	-1.560950	-0.159024	1.441506
C	-2.735210	-1.754466	0.158140
C	-2.129582	-1.501785	1.584546
H	0.644507	3.097970	0.847345
C	3.281183	3.060898	1.450625
H	3.059204	3.803447	2.227450
H	4.325981	2.748559	1.552801
Cl	-2.105846	3.580840	-1.633514
C	-3.142920	-1.484113	2.722833
H	-3.651705	-2.452592	2.797253
H	-2.630365	-1.293126	3.671233
H	-3.893178	-0.703267	2.580316
C	-0.953257	-2.427644	1.919089
H	-0.456844	-2.059399	2.822320
H	-1.289443	-3.453919	2.101315
H	-0.216622	-2.438020	1.109034
C	-4.147333	-1.186138	-0.015926
H	-4.413398	-1.214202	-1.076996
H	-4.884061	-1.771729	0.544551
H	-4.198369	-0.144337	0.315233
C	-2.672138	-3.200555	-0.321854
H	-3.249527	-3.851192	0.345457
H	-3.102083	-3.274677	-1.326171
H	-1.643757	-3.568144	-0.362765
H	3.151301	3.530825	0.468648

Electronic Energy = -1800.03669862 (Hartree/Particle)
Dipole Moment (Debye): 9.5825
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.363337
(Hartree/Particle)
Thermal correction to Energy= 0.389975
Thermal correction to Enthalpy= 0.390919
Thermal correction to Gibbs Free Energy= 0.304038
Sum of electronic and zero-point Energies= -1799.673362
Sum of electronic and thermal Energies= -1799.646724
Sum of electronic and thermal Enthalpies= -1799.645780
Sum of electronic and thermal Free Energies= -1799.732660
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1800.35758090
Corrected Free Energy = -1800.05354228



TS4 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: anti-Markovnikov

CARTESIAN COORDINATES

N	1.970245	-0.690627	0.757446
C	3.221220	-0.172112	0.717847
C	4.337076	-0.935838	1.038944
C	4.154277	-2.268784	1.416483
C	2.862737	-2.796199	1.450887
C	1.791264	-1.972593	1.105352
C	3.347982	1.279674	0.261586
O	4.447550	1.804202	0.063215
Cu	0.621791	0.725407	0.162524
N	2.123101	1.813776	0.142765
C	1.613239	3.005727	-0.517792
C	0.144565	2.524862	-0.562388
B	-1.358847	0.327620	0.279536
Cu	-0.601814	-1.075698	-1.177419
Cl	0.119440	-2.953817	-1.870786
O	-2.295520	0.350218	-0.752997
C	-3.609243	0.012432	-0.158351
C	-4.679926	0.784440	-0.918548
O	-1.946657	0.262555	1.513287
C	-3.393211	0.453604	1.332335
C	-3.667953	1.941630	1.574121
C	-3.795015	-1.496145	-0.336152
C	-4.120435	-0.402589	2.362643
H	5.315031	-0.470157	0.974044
H	5.009145	-2.889820	1.669877
H	0.772182	-2.339329	1.071331
H	2.677714	-3.831161	1.718793
H	1.731166	3.895943	0.117789
H	-0.547901	3.017608	0.122142
H	-0.287461	2.371651	-1.552452
H	-4.776889	-1.819547	0.024479
H	-3.713647	-1.744285	-1.398796

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 H              -3.020837   -2.059392    0.194719
 H              -4.740488    0.415515   -1.947266
 H              -5.658465    0.641009   -0.445263
 H              -4.461037    1.853983   -0.953444
 H              -3.905593   -0.029428    3.369006
 H              -5.204137   -0.355019    2.202615
 H              -3.803851   -1.446759    2.313880
 H              -4.739055    2.163839    1.520290
 H              -3.306423    2.211264    2.571172
 H              -3.145337    2.566412    0.842338
 C               2.222363    3.272231   -1.893408
 H               1.738998    4.137603   -2.363829
 H               3.294824    3.467284   -1.802086
 H               2.086435    2.398124   -2.542600

 Electronic Energy =  -1800.02788397 (Hartree/Particle)
 Dipole Moment (Debye):      7.1813
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:            -81.232

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.362842
(Hartree/Particle)
 Thermal correction to Energy=                    0.388810
 Thermal correction to Enthalpy=                  0.389755
 Thermal correction to Gibbs Free Energy=         0.304384
 Sum of electronic and zero-point Energies=          -1799.665041
 Sum of electronic and thermal Energies=             -1799.639074
 Sum of electronic and thermal Enthalpies=           -1799.638129
 Sum of electronic and thermal Free Energies=        -1799.723500
 PCM-SP (solvent=THF;6-311+g(2d,p)) = -1800.34679723
 Corrected Free Energy =  -1800.04241326
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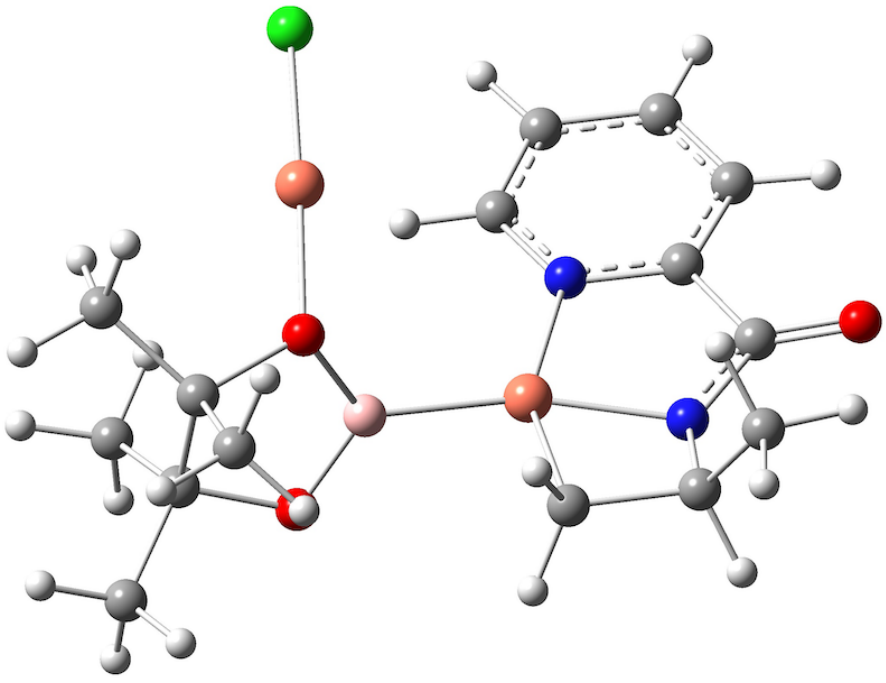

I3 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: anti-Markovnikov

CARTESIAN COORDINATES

C	2.577785	-3.289328	1.822923
C	2.144467	-3.060149	0.375581
Cu	0.872765	-0.973755	-0.383087
B	-1.080189	-0.781058	-0.426512
O	-1.843789	-0.192454	0.622188
C	-3.265187	-0.620158	0.429787
C	-3.288794	-0.853458	-1.113989
O	-1.913070	-1.282121	-1.383498
Cu	-1.305629	1.651651	0.884445
Cl	-0.751655	3.677840	0.988057
C	0.617349	-2.850619	0.204623
N	2.543454	-1.769039	-0.176239
C	3.616938	-0.992021	0.019846
C	3.280173	0.438958	-0.405913
C	4.253994	1.428646	-0.466844
C	3.878326	2.727181	-0.822559
C	2.538202	2.995672	-1.101177
C	1.614798	1.953761	-1.016240
N	1.977021	0.707768	-0.678533
O	4.735487	-1.282325	0.458610
H	5.275405	1.157505	-0.220519
H	4.619983	3.519934	-0.870371
H	0.558886	2.121672	-1.190972
H	2.193520	3.992323	-1.354832
H	2.507641	-3.888020	-0.251805
H	0.139210	-3.410769	-0.600822
H	0.035844	-2.885408	1.128927
H	2.186821	-4.246313	2.190973
H	3.668781	-3.293284	1.899003
C	-4.194221	0.467161	0.947799
H	-5.236361	0.180462	0.765552
H	-4.057970	0.593441	2.026553
H	-4.014092	1.432357	0.467984
C	-3.411159	-1.901301	1.252476
H	-3.157327	-1.688548	2.295382
H	-4.439823	-2.273886	1.214428
H	-2.742432	-2.687896	0.889500
C	-3.518641	0.432231	-1.915638
H	-3.301470	0.234497	-2.969518
H	-4.555348	0.774864	-1.831900
H	-2.857472	1.237669	-1.576888
C	-4.234013	-1.957518	-1.573435
H	-5.267354	-1.717875	-1.296186
H	-4.184854	-2.052125	-2.662649
H	-3.966784	-2.923114	-1.137946
H	2.194876	-2.484718	2.463875

Electronic Energy = -1800.03753226 (Hartree/Particle)
Dipole Moment (Debye): 7.2974
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

```
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.363855
(Hartree/Particle)
 Thermal correction to Energy=                    0.390129
 Thermal correction to Enthalpy=                  0.391074
 Thermal correction to Gibbs Free Energy=         0.305216
 Sum of electronic and zero-point Energies=          -1799.673677
 Sum of electronic and thermal Energies=             -1799.647403
 Sum of electronic and thermal Enthalpies=           -1799.646459
 Sum of electronic and thermal Free Energies=        -1799.732316
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1800.35648856
 Corrected Free Energy =  -1800.05127230
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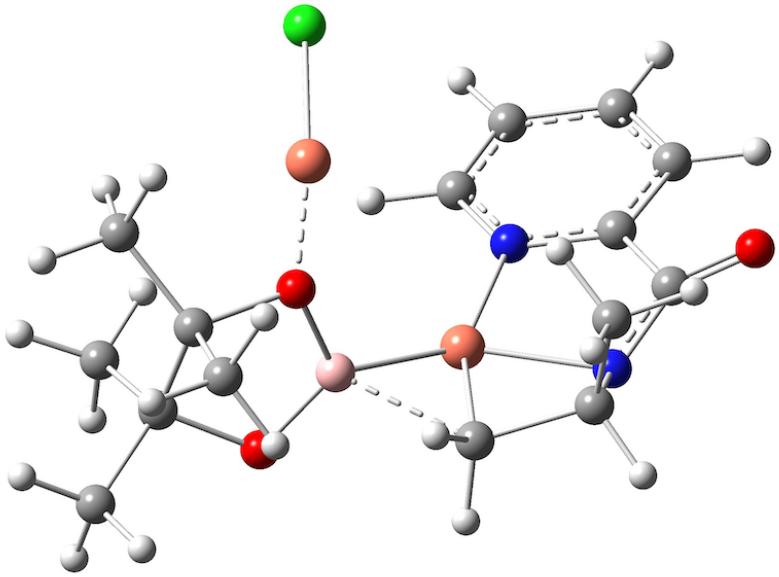

TS5 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: anti-Markovnikov

CARTESIAN COORDINATES

C	0.977814	-3.035306	0.386676
Cu	0.653820	-0.855318	-0.747011
B	-1.286738	-0.749970	-0.506433
O	-1.802250	-0.127463	0.665187
C	-3.288971	-0.066826	0.507551
C	-3.420860	-0.072614	-1.053041
O	-2.257746	-0.861486	-1.463431
Cu	-0.681246	1.449849	0.927619
Cl	0.371123	3.262312	1.105575
C	-0.348440	-2.526551	-0.285329
N	1.968500	-2.181067	-0.279532
C	3.069740	-1.642627	0.258913
C	3.289402	-0.229136	-0.309612
C	4.522536	0.410034	-0.225071
C	4.642438	1.722945	-0.684332
C	3.516058	2.373693	-1.190994
C	2.304596	1.686957	-1.221857
N	2.197492	0.415344	-0.805581
O	3.848496	-2.072126	1.122618

```
 H                5.351309   -0.134954    0.214322
 H                5.598068    2.237938   -0.632961
 H                1.388445    2.162224   -1.550679
 H                3.557032    3.403773   -1.529134
 H                1.106741   -4.100759    0.135878
 H               -0.533240   -3.005131   -1.251385
 H               -1.215104   -2.681959    0.364310
 C               -3.814148    1.176594    1.208451
 H               -4.895564    1.260347    1.051486
 H               -3.628389    1.105623    2.284746
 H               -3.340755    2.091076    0.842386
 C               -3.819695   -1.334515    1.177730
 H               -3.479866   -1.360611    2.217456
 H               -4.914211   -1.347357    1.169666
 H               -3.464953   -2.238973    0.674688
 C               -3.263762    1.317215   -1.679819
 H               -3.157033    1.204822   -2.762808
 H               -4.137799    1.945262   -1.479028
 H               -2.372670    1.830892   -1.302590
 C               -4.675902   -0.762523   -1.576328
 H               -5.574130   -0.254357   -1.206594
 H               -4.686089   -0.723102   -2.669911
 H               -4.715256   -1.812010   -1.275630
 C                0.938609   -2.880857    1.910528
 H                0.147965   -3.508160    2.341213
 H                1.900318   -3.161158    2.346744
 H                0.738713   -1.834512    2.177592

 Electronic Energy =  -1800.02970367 (Hartree/Particle)
 Dipole Moment (Debye):      8.3826
 index           1
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -138.424

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.363414
(Hartree/Particle)
 Thermal correction to Energy=                    0.388806
 Thermal correction to Enthalpy=                  0.389750
 Thermal correction to Gibbs Free Energy=         0.307359
 Sum of electronic and zero-point Energies=          -1799.666290
 Sum of electronic and thermal Energies=             -1799.640898
 Sum of electronic and thermal Enthalpies=           -1799.639953
 Sum of electronic and thermal Free Energies=        -1799.722347
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1800.35173892
 Corrected Free Energy =  -1800.04438225

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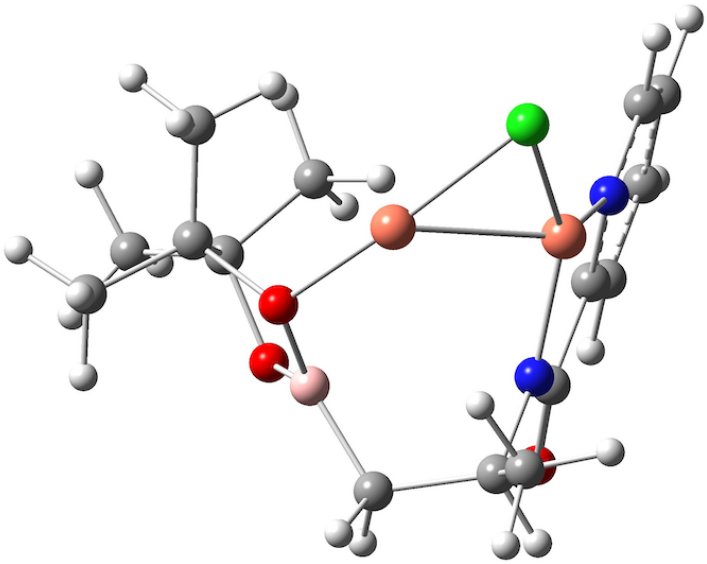

P2 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: anti-Markovnikov

CARTESIAN COORDINATES

C	-0.117690	-0.765279	2.675057
Cu	-1.073780	-1.474893	-0.163789
B	1.561516	0.717258	1.299491
O	2.256625	0.001471	0.271957
C	2.798695	1.030777	-0.668094
C	1.758161	2.178763	-0.470664
O	1.394989	2.015643	0.927497
Cu	1.356519	-1.556731	-0.501793
Cl	0.028793	-2.920989	-1.562432
C	1.137384	0.167765	2.703338
N	-0.965938	-0.480102	1.512674
C	-1.765092	0.593837	1.609327
C	-2.633696	0.840852	0.379470
C	-3.468647	1.960681	0.332379
C	-4.246804	2.177298	-0.804622
C	-4.169001	1.269863	-1.865294
C	-3.310166	0.177598	-1.740347
N	-2.563051	-0.032911	-0.646993
O	-1.862462	1.387158	2.566853
H	-3.481700	2.625844	1.188847
H	-4.905183	3.040227	-0.864782
H	-3.208678	-0.559162	-2.533312
H	-4.758201	1.399473	-2.768248
H	-0.698752	-0.553834	3.581822
H	0.896694	1.051640	3.304469
H	1.973886	-0.349146	3.194784
C	2.876775	0.456822	-2.075851
H	3.265252	1.220234	-2.759752
H	3.562235	-0.397126	-2.098751
H	1.904239	0.130643	-2.453777
C	4.197263	1.363198	-0.144359
H	4.795323	0.447194	-0.110695
H	4.699069	2.081104	-0.800880

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 H                 4.156195    1.784978    0.864443
 C                 0.476703    1.983473   -1.290345
 H                -0.283695    2.677899   -0.921525
 H                 0.647496    2.181445   -2.353838
 H                 0.078590    0.969755   -1.177212
 C                 2.321569    3.581874   -0.667380
 H                 2.701372    3.704686   -1.688503
 H                 1.528322    4.318126   -0.505240
 H                 3.128047    3.794151    0.038572
 C                 0.273565   -2.243489    2.689371
 H                 0.803768   -2.496397    3.615611
 H                -0.617253   -2.875645    2.605831
 H                 0.932082   -2.495772    1.845766

 Electronic Energy =  -1800.12533328 (Hartree/Particle)
 Dipole Moment (Debye):      6.8363
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.365152
(Hartree/Particle)
 Thermal correction to Energy=                    0.391099
 Thermal correction to Enthalpy=                  0.392044
 Thermal correction to Gibbs Free Energy=         0.308863
 Sum of electronic and zero-point Energies=          -1799.760182
 Sum of electronic and thermal Energies=             -1799.734234
 Sum of electronic and thermal Enthalpies=           -1799.733290
 Sum of electronic and thermal Free Energies=        -1799.816471
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1800.44170581
 Corrected Free Energy =  -1800.13284353
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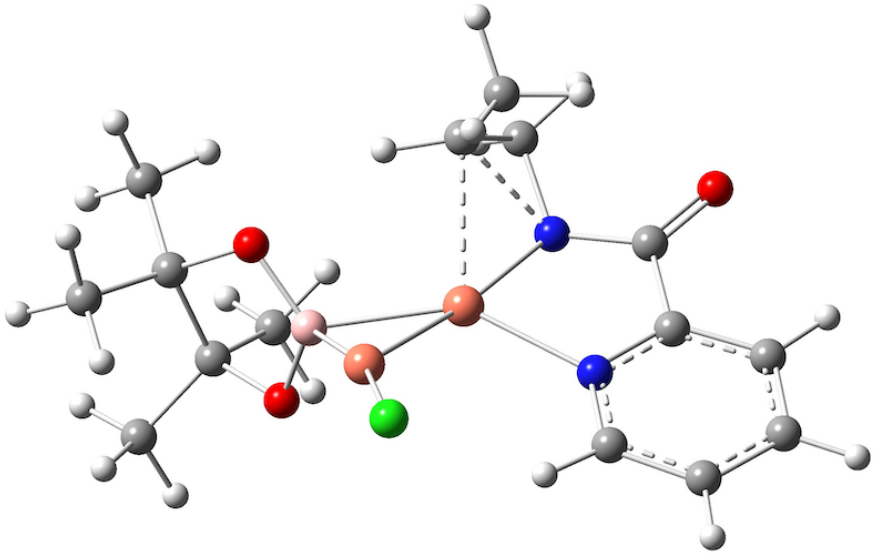
PATH: MARKOVNIKOV



TS3 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: Markovnikov

CARTESIAN COORDINATES

C	-0.160621	-1.906567	1.640076
N	-1.190145	-2.092050	-0.028784
C	-2.577668	-2.125931	-0.094738
O	-3.258891	-3.112122	0.175901
C	-0.546306	-3.084798	0.818246
C	-3.211070	-0.842051	-0.568326
C	-4.567554	-0.784256	-0.881687
C	-5.107446	0.449584	-1.254738
C	-4.282346	1.575204	-1.274700
C	-2.934807	1.433101	-0.930046
N	-2.415826	0.242906	-0.601988
Cu	0.283401	1.875339	0.478912
H	-5.165402	-1.686890	-0.816288
H	-6.159749	0.531835	-1.512392
H	-2.254992	2.279508	-0.884483
H	-4.666914	2.554283	-1.542212
H	-1.240306	-3.794114	1.275906
H	0.278584	-3.594155	0.315160
Cu	-0.450071	-0.278240	-0.013664
B	1.582732	0.388204	-0.074917
O	2.462828	-0.171389	0.850326
O	2.136856	0.385228	-1.344919
C	3.760238	-0.336519	0.201326
C	3.355197	-0.415387	-1.312012
Cl	-0.676595	3.737318	0.968738
H	0.866591	-1.551076	1.595503
C	-1.008454	-1.440604	2.777451
H	-0.631729	-1.926985	3.692674
H	-0.932919	-0.358815	2.923390
C	2.956730	-1.828197	-1.761065
H	2.492603	-1.767255	-2.750297
H	3.825158	-2.493288	-1.822422
H	2.224415	-2.266566	-1.074430
C	4.365313	0.185852	-2.284079
H	5.324789	-0.341481	-2.217922
H	3.992071	0.091606	-3.309106
H	4.532255	1.246413	-2.083077
C	4.586851	0.908439	0.545863
H	4.649952	1.002244	1.634591
H	5.603028	0.839214	0.142328
H	4.113698	1.815117	0.156261
C	4.428150	-1.589873	0.758771
H	5.366412	-1.794269	0.229286
H	4.659433	-1.444795	1.819358
H	3.781480	-2.466706	0.669443
H	-2.058370	-1.722831	2.655482

Electronic Energy = -1800.02714147 (Hartree/Particle)
Dipole Moment (Debye): 6.4129
index 1
Number of imaginary frequencies= 1
Negatives Eigenvalues: -190.930

THERMOCHEMICAL DATA

```
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.362121
(Hartree/Particle)
 Thermal correction to Energy=                    0.388657
 Thermal correction to Enthalpy=                  0.389601
 Thermal correction to Gibbs Free Energy=         0.303194
 Sum of electronic and zero-point Energies=          -1799.665020
 Sum of electronic and thermal Energies=             -1799.638484
 Sum of electronic and thermal Enthalpies=           -1799.637540
 Sum of electronic and thermal Free Energies=        -1799.723947
 PCM-SP (solvent=THF;6-311+g(2d,p)) = -1800.34663554
 Corrected Free Energy =   -1800.04344107
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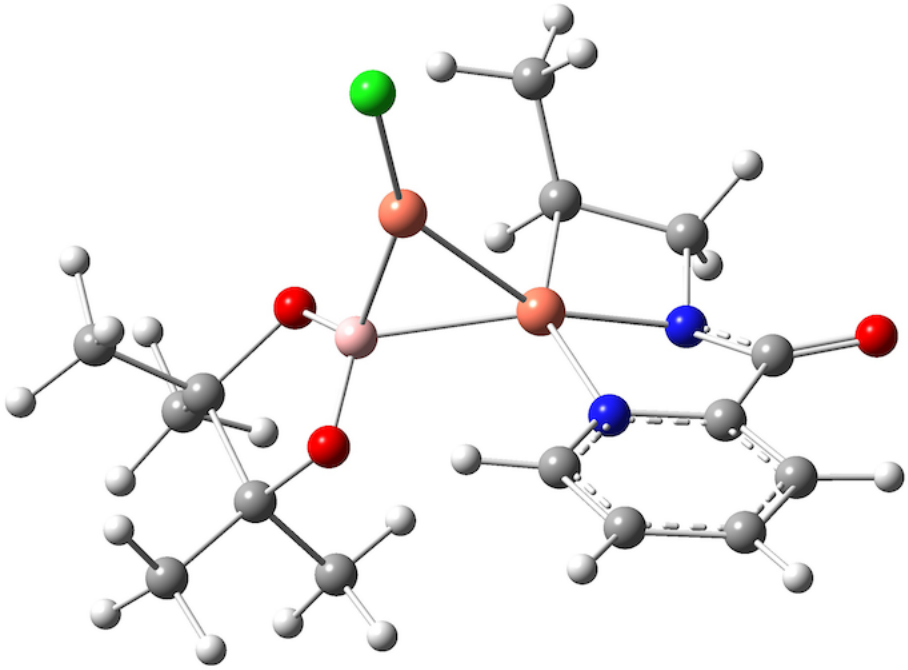

I2 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: Markovnikov

CARTESIAN COORDINATES

C	-0.394249	-1.593597	-2.133975
N	-1.977476	-0.078973	-1.875421
C	-3.189006	0.299998	-1.400605
O	-4.286754	0.105715	-1.921992
C	-1.703020	-1.160293	-2.806068
C	-3.039332	1.053451	-0.085581
C	-4.088590	1.756407	0.496931
C	-3.863247	2.394447	1.719818
C	-2.604772	2.303441	2.320696
C	-1.606030	1.567171	1.681643
N	-1.830325	0.963981	0.507819
Cu	0.398391	-1.444889	1.167350
H	-5.047600	1.779500	-0.010100
H	-4.661485	2.952551	2.201358
H	-0.607876	1.446070	2.090201

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 H              -2.396534    2.783422    3.271482
 H              -2.476798   -1.938698   -2.781389
 H              -1.585086   -0.817724   -3.842509
 Cu             -0.647259   -0.288024   -0.596675
 B               1.391171   -0.050528    0.066788
 O               2.418136   -0.435105   -0.766617
 O               1.585977    1.212366    0.592868
 C               3.508122    0.528166   -0.594194
 C               2.739274    1.802712   -0.092156
 Cl              0.168055   -2.816333    2.777292
 H               0.515373   -1.195961   -2.587136
 C              -0.287233   -3.003572   -1.615908
 H              -1.121946   -3.262782   -0.956228
 H              -0.319555   -3.696450   -2.474131
 C               2.168411    2.658512   -1.229132
 H               1.481047    3.397994   -0.806300
 H               2.960340    3.188655   -1.769017
 H               1.607213    2.045201   -1.941883
 C               3.504842    2.669405    0.901204
 H               4.425774    3.051863    0.445156
 H               2.889262    3.525482    1.196638
 H               3.765550    2.111887    1.803596
 C               4.453896   -0.065471    0.456036
 H               4.789339   -1.049661    0.114831
 H               5.333533    0.569947    0.605357
 H               3.946660   -0.197630    1.416915
 C               4.224245    0.692221   -1.930369
 H               4.990237    1.473775   -1.861057
 H               4.717648   -0.246689   -2.201645
 H               3.529342    0.953737   -2.732016
 H               0.645828   -3.166586   -1.070516

 Electronic Energy =  -1800.03685215 (Hartree/Particle)
 Dipole Moment (Debye):      7.8243
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.363284
(Hartree/Particle)
 Thermal correction to Energy=                    0.390038
 Thermal correction to Enthalpy=                  0.390982
 Thermal correction to Gibbs Free Energy=         0.303141
 Sum of electronic and zero-point Energies=          -1799.673568
 Sum of electronic and thermal Energies=             -1799.646814
 Sum of electronic and thermal Enthalpies=           -1799.645870
 Sum of electronic and thermal Free Energies=        -1799.733711
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1800.35676461
 Corrected Free Energy =   -1800.05362346

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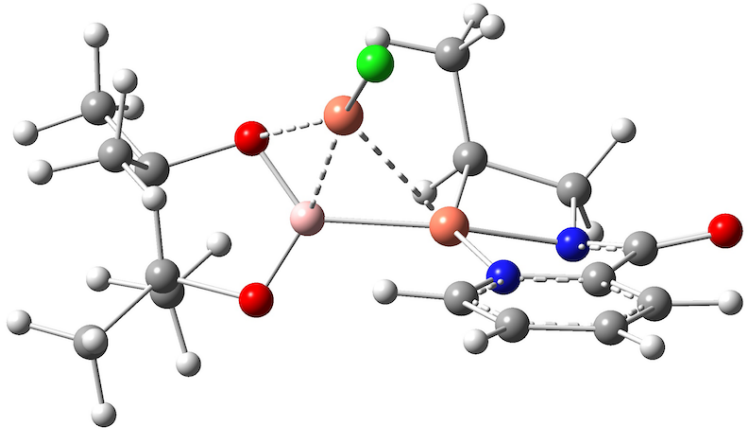


TS4 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: Markovnikov

CARTESIAN COORDINATES

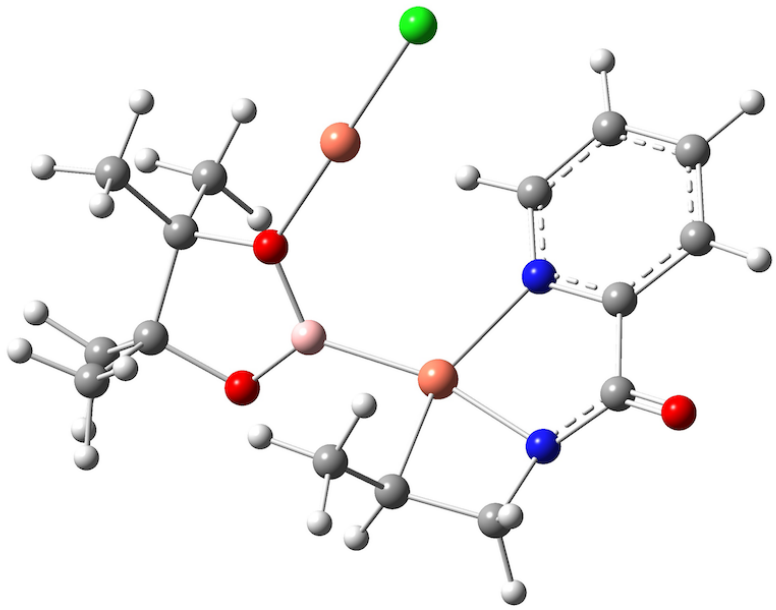
N	2.043960	-0.513115	0.831478
C	3.276094	0.028346	0.698996
C	4.429482	-0.707834	0.946183
C	4.300664	-2.037184	1.356122
C	3.025580	-2.589926	1.487773
C	1.916688	-1.793544	1.202394
C	3.327838	1.465365	0.194904
O	4.376960	1.980285	-0.198708
Cu	0.634487	0.863847	0.214330
N	2.100578	2.019708	0.255738
C	1.605442	3.149767	-0.508679
C	0.197421	2.585220	-0.771824
B	-1.309955	0.321497	0.346155
Cu	-0.470663	-1.010133	-1.165287
Cl	0.533387	-2.712062	-1.948726
O	-2.252446	0.212520	-0.681451
C	-3.521272	-0.252613	-0.073496
C	-4.670559	0.379590	-0.847697
O	-1.891552	0.217067	1.581360
C	-3.349745	0.244899	1.404243
C	-3.785615	1.699325	1.612409
C	-3.540793	-1.776007	-0.215728
C	-3.977091	-0.660347	2.458291
H	5.391504	-0.228694	0.797146
H	5.183653	-2.637899	1.556442
H	0.904736	-2.180386	1.240531
H	2.882755	-3.624438	1.782163
H	1.602463	4.082249	0.071190
H	-4.481020	-2.196656	0.155400
H	-3.433112	-2.038780	-1.272612
H	-2.709364	-2.237653	0.326532
H	-4.692393	-0.018626	-1.867087
H	-5.627173	0.142640	-0.367263
H	-4.569248	1.465433	-0.908806
H	-3.800437	-0.242216	3.454314
H	-5.060161	-0.734198	2.303855
H	-3.549508	-1.665071	2.432409
H	-4.874774	1.801774	1.558743
H	-3.453261	2.030480	2.600994

H	-3.335254	2.359963	0.864265
H	2.175976	3.318793	-1.432641
C	-0.140344	2.249048	-2.206475
H	0.638038	1.628188	-2.664334
H	-1.095603	1.725126	-2.289959
H	-0.198847	3.182544	-2.790232
H	-0.605884	3.077540	-0.220315

Electronic Energy = -1800.02792406 (Hartree/Particle)
Dipole Moment (Debye): 7.6917
index 0
Harmonic frequencies
Number of imaginary frequencies= 1
Negatives Eigenvalues: -82.020

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.363138
(Hartree/Particle)
Thermal correction to Energy= 0.389075
Thermal correction to Enthalpy= 0.390020
Thermal correction to Gibbs Free Energy= 0.305246
Sum of electronic and zero-point Energies= -1799.664786
Sum of electronic and thermal Energies= -1799.638849
Sum of electronic and thermal Enthalpies= -1799.637904
Sum of electronic and thermal Free Energies= -1799.722678
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1800.34779585
Corrected Free Energy = -1800.04254979



I3 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: Markovnikov

CARTESIAN COORDINATES

N	1.929477	-0.266595	0.910762
C	3.196659	0.026109	0.530825
C	4.223969	-0.905395	0.636390

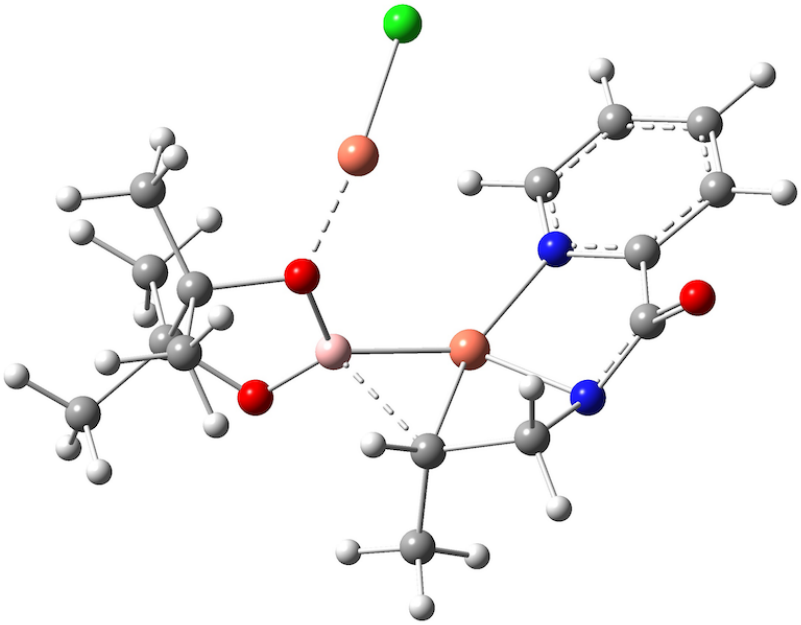
C	3.937961	-2.167786	1.161555
C	2.632848	-2.460595	1.558735
C	1.654564	-1.479016	1.410398
C	3.418273	1.405606	-0.084362
O	4.454277	1.677867	-0.697846
Cu	0.711937	1.304926	0.362896
N	2.346652	2.186277	0.147739
C	1.920214	3.336509	-0.634493
C	0.412127	3.012296	-0.655240
B	-1.201238	0.817754	0.405110
Cu	-0.666254	-1.841094	-0.865156
Cl	0.466756	-3.497035	-1.483125
O	-1.715865	-0.375680	-0.165072
C	-3.125254	-0.553350	0.290347
C	-3.910528	-1.224721	-0.827597
O	-2.226595	1.533668	0.952782
C	-3.512794	0.930328	0.596910
C	-4.030013	1.688651	-0.630205
C	-3.060293	-1.450247	1.528234
C	-4.467820	1.104054	1.773316
H	5.212132	-0.624108	0.287568
H	4.719182	-2.918070	1.245703
H	0.618690	-1.665443	1.674333
H	2.360692	-3.436696	1.945375
H	2.152346	4.290590	-0.142285
H	-4.063636	-1.673457	1.904775
H	-2.575082	-2.394848	1.259307
H	-2.480473	-0.981342	2.329223
H	-3.541270	-2.244545	-0.981429
H	-4.971558	-1.282447	-0.559143
H	-3.815444	-0.684951	-1.771958
H	-4.680606	2.168035	1.916339
H	-5.415414	0.587796	1.579486
H	-4.039698	0.718353	2.701191
H	-5.031318	1.349323	-0.915966
H	-4.079264	2.755223	-0.390918
H	-3.362152	1.562824	-1.487720
H	2.367951	3.349413	-1.638201
C	-0.193975	2.761190	-2.019234
H	0.357062	1.989166	-2.567858
H	-1.242673	2.456245	-1.955873
H	-0.143674	3.685568	-2.617348
H	-0.202339	3.636653	-0.003395

Electronic Energy = -1800.03653571 (Hartree/Particle)
Dipole Moment (Debye): 8.8354
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.363978
(Hartree/Particle)
Thermal correction to Energy= 0.390383
Thermal correction to Enthalpy= 0.391327
Thermal correction to Gibbs Free Energy= 0.304940
Sum of electronic and zero-point Energies= -1799.672558
Sum of electronic and thermal Energies= -1799.646152

Sum of electronic and thermal Enthalpies= -1799.645208
Sum of electronic and thermal Free Energies= -1799.731596
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1800.35759687
Corrected Free Energy = -1800.05265716



TS5 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: Markovnikov

CARTESIAN COORDINATES

C	0.709728	2.906877	-1.048611
Cu	0.614894	1.068904	0.589712
B	-1.299127	0.728479	0.296749
O	-1.654433	-0.141069	-0.773337
C	-3.132654	-0.360112	-0.680011
C	-3.368754	-0.128029	0.850278
O	-2.335529	0.855337	1.180298
Cu	-0.372549	-1.619071	-0.720429
Cl	0.821985	-3.339922	-0.519811
C	-0.548898	2.530941	-0.196989
N	1.815604	2.345359	-0.270894
C	2.790361	1.641074	-0.867206
C	3.212113	0.454122	0.008174
C	4.469071	-0.135867	-0.085775
C	4.746359	-1.268627	0.680510
C	3.745319	-1.804724	1.493493
C	2.496860	-1.189595	1.509786
N	2.242020	-0.079495	0.798919
O	3.285856	1.760898	-1.997597
H	5.191824	0.298655	-0.768136
H	5.724529	-1.739492	0.631343
H	1.666704	-1.598924	2.073217
H	3.908673	-2.703550	2.078661
H	0.750321	4.001616	-1.165677
H	-1.425262	2.444515	-0.850461
C	-3.466340	-1.752196	-1.194023

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 H              -4.541101   -1.937293   -1.085038
 H              -3.211039   -1.829719   -2.255469
 H              -2.925905   -2.535842   -0.657310
 C              -3.759636    0.711825   -1.572261
 H              -3.354833    0.618539   -2.584469
 H              -4.846158    0.588040   -1.620163
 H              -3.548966    1.721412   -1.206832
 C              -3.094459   -1.371196    1.703383
 H              -3.074374   -1.077377    2.757080
 H              -3.875242   -2.126536    1.567379
 H              -2.127319   -1.823533    1.458383
 C              -4.727193    0.473628    1.193610
 H              -5.534062   -0.193757    0.869262
 H              -4.806240    0.604343    2.277264
 H              -4.866966    1.449993    0.724028
 C              -0.810851    3.528060    0.933153
 H               0.097697    3.693462    1.520959
 H              -1.101771    4.493651    0.495966
 H              -1.608280    3.195577    1.602378
 H               0.664971    2.467879   -2.054677

 Electronic Energy =  -1800.02666080 (Hartree/Particle)
 Dipole Moment (Debye):      8.6356
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -143.049

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.363669
(Hartree/Particle)
 Thermal correction to Energy=                    0.389141
 Thermal correction to Enthalpy=                  0.390085
 Thermal correction to Gibbs Free Energy=         0.307696
 Sum of electronic and zero-point Energies=          -1799.662992
 Sum of electronic and thermal Energies=             -1799.637520
 Sum of electronic and thermal Enthalpies=           -1799.636576
 Sum of electronic and thermal Free Energies=        -1799.718964
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1800.35044651
 Corrected Free Energy =   -1800.04274971

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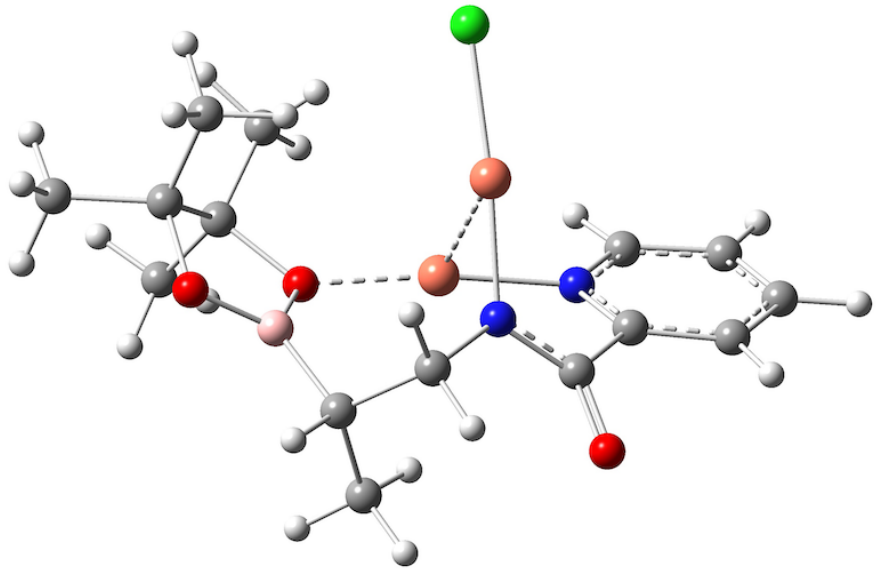


P2 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: Markovnikov

CARTESIAN COORDINATES

C	-0.071125	1.952779	1.759067
Cu	-0.387242	-0.018054	-0.964649
B	1.911430	1.392783	0.177509
O	3.199224	1.161057	0.544167
C	3.635264	-0.127104	-0.000813
C	2.682442	-0.322711	-1.234822
O	1.502691	0.476932	-0.813087
Cu	-0.541361	-0.882801	1.454538
Cl	0.058004	-2.913554	1.609404
C	0.981534	2.521149	0.758422
N	-0.962647	0.958963	1.136070
C	-2.191803	1.395492	0.766261
C	-2.977228	0.438783	-0.123422
C	-4.364611	0.350993	-0.006133
C	-5.066710	-0.507014	-0.849763
C	-4.365328	-1.233825	-1.816727
C	-2.987110	-1.069778	-1.903873
N	-2.305104	-0.255453	-1.075129
O	-2.721428	2.487233	1.020806
H	-4.857239	0.959324	0.744228
H	-6.144725	-0.607402	-0.759179
H	-2.395295	-1.594846	-2.645800
H	-4.872346	-1.910803	-2.496697
H	-0.666239	2.782655	2.156970
H	1.628242	3.186480	1.348758
C	3.417396	-1.162994	1.104657
H	3.778891	-2.150982	0.801854
H	3.971474	-0.847802	1.994270
H	2.361660	-1.261497	1.374029
C	5.113594	-0.019870	-0.359903
H	5.699514	0.120160	0.553682
H	5.455819	-0.940004	-0.847523
H	5.312247	0.825834	-1.022648
C	2.223753	-1.753880	-1.477710
H	1.557544	-1.783928	-2.348222

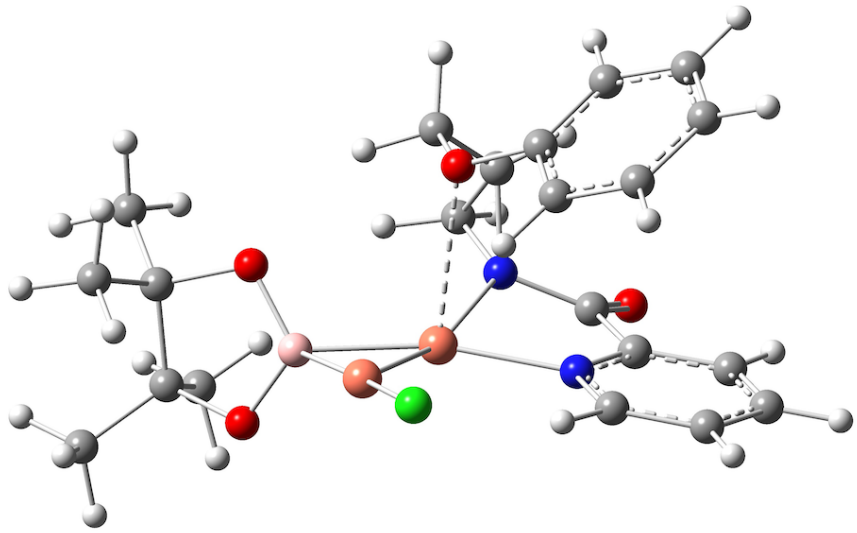
H	3.085861	-2.395620	-1.691446
H	1.684819	-2.161184	-0.618210
C	3.178973	0.332879	-2.523174
H	4.030889	-0.214844	-2.938532
H	2.370774	0.326720	-3.261805
H	3.478726	1.371756	-2.353358
C	0.307700	3.353227	-0.353533
H	-0.359840	2.736681	-0.967663
H	-0.301911	4.155651	0.076081
H	1.050132	3.803251	-1.024334
H	0.447177	1.476576	2.598487

Electronic Energy = -1800.13343971 (Hartree/Particle)
Dipole Moment (Debye): 6.9196
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.366778
(Hartree/Particle)
Thermal correction to Energy= 0.392409
Thermal correction to Enthalpy= 0.393353
Thermal correction to Gibbs Free Energy= 0.311753
Sum of electronic and zero-point Energies= -1799.766661
Sum of electronic and thermal Energies= -1799.741031
Sum of electronic and thermal Enthalpies= -1799.740087
Sum of electronic and thermal Free Energies= -1799.821687
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1800.45193594
Corrected Free Energy = -1800.14018323

SUBSTRATE: 1c



Complex-2 Substrate: 1c

CARTESIAN COORDINATES

C	-0.675681	-2.517430	1.139506

```
 N              -0.432016   -2.201179   -0.310580
 C              -1.535437   -2.522324   -1.171984
 O              -1.810629   -3.654713   -1.517914
 C               0.271995   -3.322403    0.323363
 C              -2.316464   -1.319282   -1.602499
 C              -3.592535   -1.461115   -2.145870
 C              -4.289292   -0.303807   -2.502135
 C              -3.683483    0.937935   -2.309055
 C              -2.394078    0.991380   -1.770933
 N              -1.727688   -0.118935   -1.428000
 Cu             0.833851    2.030227   -0.401055
 H              -4.013040   -2.453091   -2.271067
 H              -5.289730   -0.372946   -2.919638
 H              -1.872960    1.930400   -1.597296
 H              -4.192925    1.861066   -2.566739
 H              -0.025342   -4.320214    0.012045
 H               1.337243   -3.142118    0.438163
 H              -1.646657   -2.975014    1.316127
 C              -0.210824   -1.476625    2.143267
 H              -0.460860   -1.810209    3.160258
 H               0.868345   -1.331853    2.065798
 O              -0.736407   -0.181682    1.879816
 C              -2.073765    0.099188    2.023030
 C              -2.450303    1.375413    1.580329
 C              -3.024113   -0.774918    2.561703
 C              -3.782791    1.767219    1.670248
 H              -1.691728    2.036763    1.169444
 C              -4.362337   -0.364396    2.644305
 H              -2.744078   -1.755564    2.932025
 C              -4.750022    0.899137    2.197414
 H              -4.064148    2.758875    1.325185
 H              -5.098319   -1.044714    3.065803
 H              -5.789077    1.209490    2.265522
 Cu             0.189212   -0.147938   -0.676365
 B               2.138701    0.364279   -0.230853
 O               2.592316   -0.109124    1.006430
 O               3.171758    0.337051   -1.160214
 C               4.045003   -0.201506    0.958281
 C               4.311314   -0.355442   -0.580075
 Cl             -0.294217    3.879461   -0.448615
 C               4.588959    1.109561    1.541243
 H               4.188747    1.240583    2.551666
 H               5.683325    1.102916    1.596782
 H               4.270833    1.967270    0.940568
 C               4.489262   -1.384273    1.814838
 H               5.572531   -1.535423    1.734771
 H               4.248997   -1.189967    2.865745
 H               3.987932   -2.309503    1.517935
 C               5.594766    0.300397   -1.082312
 H               6.472124   -0.142531   -0.594956
 H               5.688444    0.147777   -2.162619
 H               5.593935    1.376389   -0.894447
 C               4.234630   -1.809234   -1.068026
 H               4.223965   -1.814799   -2.162478
 H               5.091412   -2.399168   -0.723402
 H               3.313205   -2.289366   -0.721977

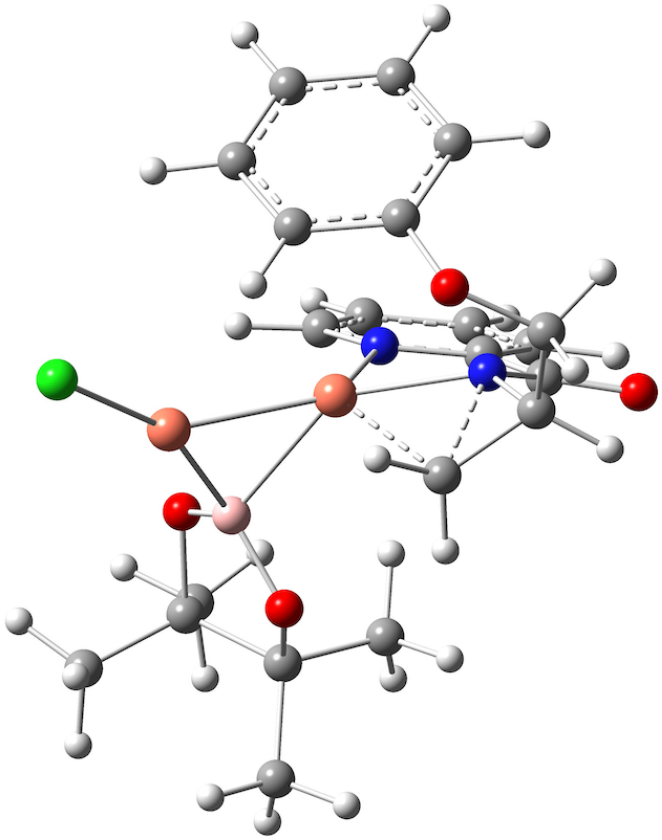
Electronic Energy =  -2106.33708712 (Hartree/Particle)
Dipole Moment (Debye):      8.9849
index           0
```

```
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.450209
(Hartree/Particle)
 Thermal correction to Energy=                    0.482319
 Thermal correction to Enthalpy=                  0.483263
 Thermal correction to Gibbs Free Energy=         0.383962
 Sum of electronic and zero-point Energies=          -2105.886878
 Sum of electronic and thermal Energies=             -2105.854768
 Sum of electronic and thermal Enthalpies=           -2105.853824
 Sum of electronic and thermal Free Energies=        -2105.953125
 PCM-SP (solvent=THF;6-311+g(2d,p)) =    -2106.73911105
 Corrected Free Energy =  -2106.35514893
```

PATH: ANTI_MARKOVNIKOV



TS3 Substrate: 1c
Path: anti-Markovnikov

CARTESIAN COORDINATES

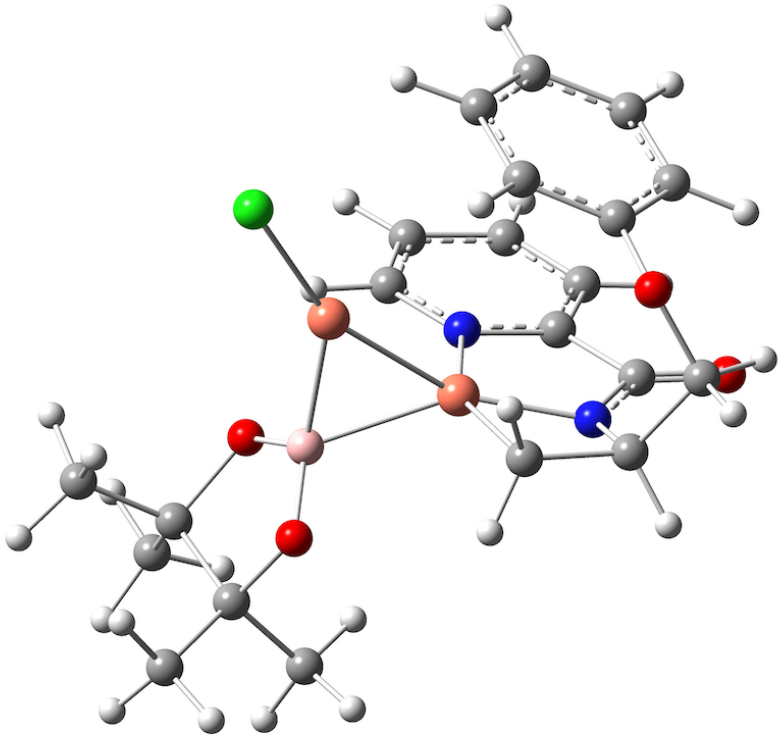
C	-0.939688	0.028723	2.339981
N	-1.423217	1.330809	1.138654
C	-0.898309	2.604318	0.919365
O	-1.123135	3.571763	1.640774
C	-1.995004	1.062073	2.443570

C	-0.112207	2.740730	-0.356306
C	0.348875	3.987204	-0.780848
C	1.082851	4.050986	-1.966591
C	1.344807	2.872669	-2.671151
C	0.868578	1.663316	-2.161227
N	0.143678	1.609923	-1.037686
Cu	0.136511	-2.333519	-0.203162
H	0.133632	4.863855	-0.179649
H	1.452393	5.005127	-2.331839
H	1.080744	0.709440	-2.632014
H	1.914669	2.882407	-3.595015
H	-1.814171	1.863169	3.165469
H	0.046986	0.211354	2.751928
Cu	-0.341206	-0.045167	0.123862
B	1.590508	-0.961121	0.139814
O	2.498910	-0.745689	-0.887758
O	2.164013	-0.669447	1.375345
C	3.816703	-0.535938	-0.299235
C	3.454674	-0.029718	1.141185
H	-1.223014	-0.999818	2.131932
C	-3.461233	0.637461	2.444179
H	-3.746775	0.342171	3.458564
H	-4.081705	1.493632	2.152378
O	-3.715304	-0.508041	1.641302
C	-3.664212	-0.397643	0.261020
C	-3.096085	-1.482167	-0.412953
C	-4.153191	0.702384	-0.450919
C	-2.980357	-1.453589	-1.805647
H	-2.734723	-2.337779	0.147841
C	-4.035741	0.719399	-1.843961
H	-4.602907	1.545293	0.063499
C	-3.443042	-0.348516	-2.527207
H	-2.509986	-2.298253	-2.300953
H	-4.410073	1.578438	-2.395727
H	-3.349729	-0.321108	-3.609511
Cl	-0.756515	-4.256818	-0.573978
C	4.421278	-0.458722	2.240323
H	5.427023	-0.068251	2.043127
H	4.084848	-0.063661	3.204873
H	4.476871	-1.546422	2.322462
C	3.208557	1.484053	1.206981
H	2.761298	1.730865	2.175688
H	4.140887	2.049818	1.103851
H	2.516902	1.804487	0.422483
C	4.526194	-1.895385	-0.305733
H	4.558645	-2.272695	-1.332563
H	5.552465	-1.814845	0.069538
H	3.983551	-2.625665	0.302473
C	4.577618	0.466848	-1.162487
H	5.539998	0.721381	-0.702447
H	4.775005	0.028932	-2.146680
H	4.006041	1.386812	-1.309566

Electronic Energy = -2106.30303380 (Hartree/Particle)
Dipole Moment (Debye): 11.4790
index 1
Number of imaginary frequencies= 1
Negatives Eigenvalues: -279.645

THERMOCHEMICAL DATA

```
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.448004
(Hartree/Particle)
 Thermal correction to Energy=                    0.479707
 Thermal correction to Enthalpy=                  0.480651
 Thermal correction to Gibbs Free Energy=         0.381979
 Sum of electronic and zero-point Energies=          -2105.855030
 Sum of electronic and thermal Energies=             -2105.823327
 Sum of electronic and thermal Enthalpies=           -2105.822383
 Sum of electronic and thermal Free Energies=        -2105.921054
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -2106.70700049
 Corrected Free Energy =  -2106.32502069
```



I2 Substrate: 1c
Path: anti-Markovnikov

CARTESIAN COORDINATES

C	-0.283339	-0.873174	2.354926
N	-1.396000	0.898409	1.698411
C	-2.231250	1.811555	1.175858
O	-3.250876	2.286255	1.683143
C	-1.507183	-0.047942	2.793760
C	-1.760038	2.208110	-0.217429
C	-2.411621	3.180882	-0.966555
C	-1.956610	3.443826	-2.260614
C	-0.867303	2.726886	-2.761813
C	-0.258153	1.770567	-1.948485
N	-0.700879	1.527112	-0.708070
Cu	0.776041	-1.696960	-0.578191

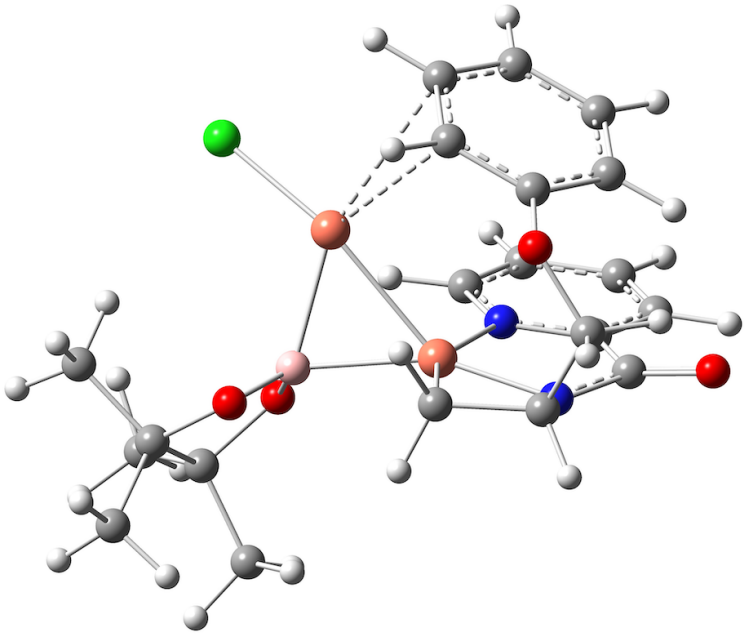
```
 H              -3.261154    3.691718   -0.525185
 H              -2.448636    4.194512   -2.873100
 H               0.602034    1.190994   -2.264664
 H              -0.489295    2.899543   -3.764370
 H              -1.379483    0.436734    3.773751
 H               0.655213   -0.694154    2.876973
 Cu             -0.098904    0.134248    0.630504
 B               1.966812   -0.218746    0.131727
 O               2.506183    0.635197   -0.809763
 O               2.808401   -0.428521    1.199036
 C               3.928362    0.790766   -0.486892
 C               3.943525    0.485868    1.053915
 H              -0.460189   -1.915965    2.097661
 C              -2.827646   -0.837854    2.839763
 H              -2.865246   -1.415004    3.768373
 H              -3.669326   -0.137162    2.829079
 O              -2.940000   -1.825212    1.809180
 C              -3.120957   -1.430968    0.499478
 C              -2.367964   -2.114352   -0.463444
 C              -4.027792   -0.439717    0.109253
 C              -2.481784   -1.773026   -1.813943
 H              -1.697077   -2.908552   -0.150879
 C              -4.130517   -0.102725   -1.243795
 H              -4.618551    0.092789    0.845926
 C              -3.356627   -0.756083   -2.209356
 H              -1.863337   -2.298608   -2.535829
 H              -4.822169    0.682585   -1.538842
 H              -3.440714   -0.480680   -3.257179
 Cl              0.822977   -3.480758   -1.755720
 C               3.619879    1.709924    1.918964
 H               3.449143    1.381485    2.949084
 H               4.444144    2.431235    1.917379
 H               2.712530    2.212884    1.568257
 C               5.199650   -0.214329    1.559610
 H               6.083736    0.409632    1.382008
 H               5.115979   -0.390856    2.636889
 H               5.345786   -1.179342    1.069496
 C               4.359062    2.201954   -0.870712
 H               5.393449    2.384933   -0.556339
 H               4.307726    2.320551   -1.958039
 H               3.715532    2.958640   -0.415610
 C               4.678354   -0.252497   -1.322517
 H               4.453264   -0.088463   -2.380878
 H               5.761442   -0.172184   -1.180482
 H               4.361771   -1.268427   -1.066974

 Electronic Energy =  -2106.32252478 (Hartree/Particle)
 Dipole Moment (Debye):      8.6048
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.449823
(Hartree/Particle)
 Thermal correction to Energy=                    0.481425
 Thermal correction to Enthalpy=                  0.482369
 Thermal correction to Gibbs Free Energy=         0.384450
```

```
 Sum of electronic and zero-point Energies=          -2105.872702
 Sum of electronic and thermal Energies=             -2105.841100
 Sum of electronic and thermal Enthalpies=           -2105.840155
 Sum of electronic and thermal Free Energies=        -2105.938075
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -2106.72339381
 Corrected Free Energy =  -2106.33894402
```



TS4a Substrate: 1c
Path: anti-Markovnikov

CARTESIAN COORDINATES

C	2.660184	2.131518	-1.777140
C	1.723007	2.827917	-1.002036
C	1.656489	2.613450	0.382520
C	2.557616	1.723888	1.001747
C	3.524163	1.066490	0.235847
C	3.555349	1.263544	-1.149457
O	2.441203	1.611210	2.361643
C	2.701716	0.363947	3.026877
C	1.602986	-0.693372	2.801663
Cu	0.216913	-0.542848	0.661100
B	-1.787492	-0.046869	0.272021
O	-2.692477	0.361046	1.220751
C	-4.017865	-0.059683	0.753052
C	-3.665331	-1.286609	-0.167750
O	-2.311967	-0.954868	-0.623247
Cu	-0.540191	1.442483	-0.449974
Cl	-1.619551	2.608662	-1.936964
C	0.197037	-0.090774	2.595477
N	1.647472	-1.374862	1.511890
C	2.656400	-1.832971	0.757398
C	2.207622	-1.928965	-0.700134
C	2.992643	-2.522740	-1.681697
C	2.536640	-2.509905	-3.002836
C	1.315167	-1.901166	-3.301648
C	0.580452	-1.323334	-2.265496

```
 N                1.025849   -1.344003   -1.002153
 O                3.810684   -2.119061    1.096819
 H                3.939526   -2.965798   -1.390546
 H                3.129823   -2.965149   -3.791385
 H               -0.374882   -0.832173   -2.421367
 H                0.932962   -1.865423   -4.316675
 H                1.658116   -1.401631    3.642687
 H               -0.629737   -0.663498    3.015268
 H                0.081009    0.982505    2.723939
 H                2.721156    0.638211    4.084949
 H                3.678739   -0.047447    2.754758
 H                0.969158    3.177412    1.008822
 H                4.229472    0.385756    0.697506
 H                1.040938    3.531570   -1.466979
 H                4.296724    0.727503   -1.736690
 H                2.692070    2.278100   -2.852466
 C               -4.610891    1.128257   -0.011571
 H               -5.625819    0.907390   -0.360225
 H               -4.655226    1.991578    0.659885
 H               -3.986740    1.407639   -0.865110
 C               -4.869887   -0.397324    1.971908
 H               -5.048523    0.510603    2.556876
 H               -5.841155   -0.799358    1.659524
 H               -4.380635   -1.127859    2.620939
 C               -4.556030   -1.444442   -1.394985
 H               -4.233251   -2.314661   -1.976442
 H               -5.598967   -1.601081   -1.094516
 H               -4.503088   -0.564671   -2.039885
 C               -3.548296   -2.611612    0.593499
 H               -4.528162   -2.970198    0.926936
 H               -3.109574   -3.364703   -0.068953
 H               -2.896846   -2.508200    1.467489

 Electronic Energy =  -2106.32217014 (Hartree/Particle)
 Dipole Moment (Debye):      4.8578
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:            -14.406

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.450137
(Hartree/Particle)
 Thermal correction to Energy=                    0.480568
 Thermal correction to Enthalpy=                  0.481512
 Thermal correction to Gibbs Free Energy=         0.389003
 Sum of electronic and zero-point Energies=          -2105.872033
 Sum of electronic and thermal Energies=             -2105.841602
 Sum of electronic and thermal Enthalpies=           -2105.840658
 Sum of electronic and thermal Free Energies=        -2105.933167
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -2106.72148533
 Corrected Free Energy =  -2106.33248219

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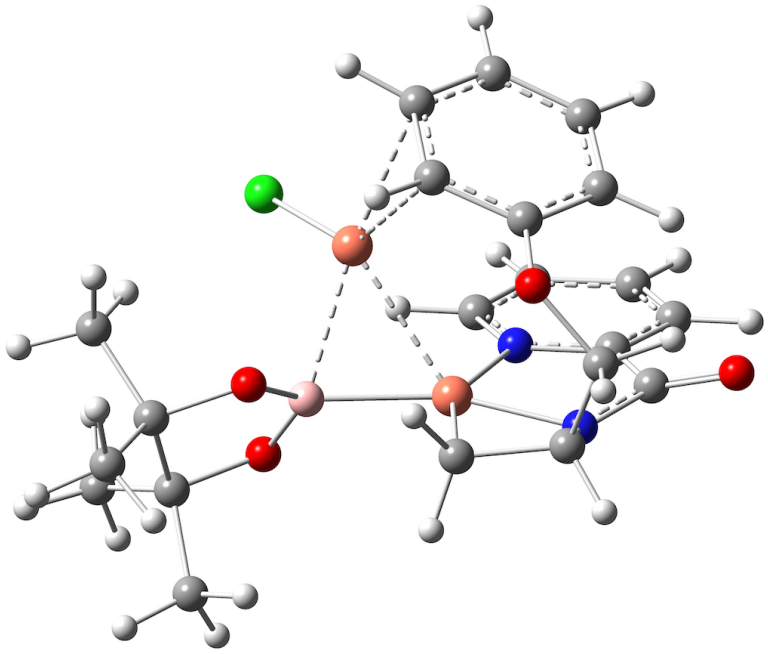

I3a Substrate: 1c
Path: anti-Markovnikov

CARTESIAN COORDINATES

C	2.159132	1.378848	2.728342
C	0.953236	0.727009	3.047906
C	0.739034	-0.603004	2.631879
C	1.765017	-1.299385	1.943310
C	2.968601	-0.655902	1.653292
C	3.146301	0.682066	2.035613
O	1.488869	-2.605038	1.667989
C	2.050154	-3.276880	0.524879
C	1.353440	-2.895621	-0.795316
Cu	0.242587	-0.605690	-0.838832
B	-1.699531	-0.236807	-0.369641
O	-2.505148	-0.891604	0.538049
C	-3.890561	-0.484890	0.268614
C	-3.810342	-0.005840	-1.232468
O	-2.402474	0.373796	-1.374995
Cu	-0.416858	0.783836	1.140867
Cl	-1.191633	2.841412	1.137121
C	-0.140429	-2.545851	-0.610157
N	1.743211	-1.606450	-1.353298
C	2.927275	-0.992976	-1.443394
C	2.706824	0.509344	-1.598573
C	3.738087	1.370514	-1.953727
C	3.468715	2.738641	-2.051610
C	2.179911	3.200559	-1.780642
C	1.196006	2.280649	-1.413124
N	1.460635	0.968720	-1.326818
O	4.067009	-1.475969	-1.383221
H	4.721215	0.949848	-2.138505
H	4.255573	3.434217	-2.331185
H	0.189270	2.583986	-1.145914
H	1.930208	4.255185	-1.834822
H	1.526865	-3.723051	-1.501555

```
 H              -0.775292   -2.823435   -1.453569
 H              -0.598010   -2.758249    0.352202
 H               1.868067   -4.333743    0.736582
 H               3.129114   -3.115045    0.445333
 H              -0.142248   -1.160620    2.940262
 H               3.759158   -1.169065    1.119029
 H               0.210772    1.229326    3.661990
 H               4.082185    1.174388    1.784363
 H               2.305607    2.414157    3.017558
 C              -4.224680    0.634279    1.258488
 H              -5.265043    0.959711    1.149092
 H              -4.087741    0.255353    2.276904
 H              -3.562941    1.494336    1.130920
 C              -4.788699   -1.695059    0.508323
 H              -4.764151   -1.964321    1.569295
 H              -5.825656   -1.460770    0.239644
 H              -4.465017   -2.564446   -0.068974
 C              -4.663731    1.215225   -1.559011
 H              -4.536985    1.480117   -2.613905
 H              -5.724982    1.001599   -1.383503
 H              -4.369863    2.076369   -0.955215
 C              -4.055485   -1.126195   -2.249384
 H              -5.103471   -1.445127   -2.251318
 H              -3.801794   -0.758739   -3.248768
 H              -3.425354   -1.996723   -2.039035

 Electronic Energy =  -2106.32353478 (Hartree/Particle)
 Dipole Moment (Debye):      1.8400
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.450115
(Hartree/Particle)
 Thermal correction to Energy=                    0.481459
 Thermal correction to Enthalpy=                  0.482404
 Thermal correction to Gibbs Free Energy=         0.386793
 Sum of electronic and zero-point Energies=          -2105.873420
 Sum of electronic and thermal Energies=             -2105.842075
 Sum of electronic and thermal Enthalpies=           -2105.841131
 Sum of electronic and thermal Free Energies=        -2105.936742
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -2106.72173924
 Corrected Free Energy =   -2106.33494643

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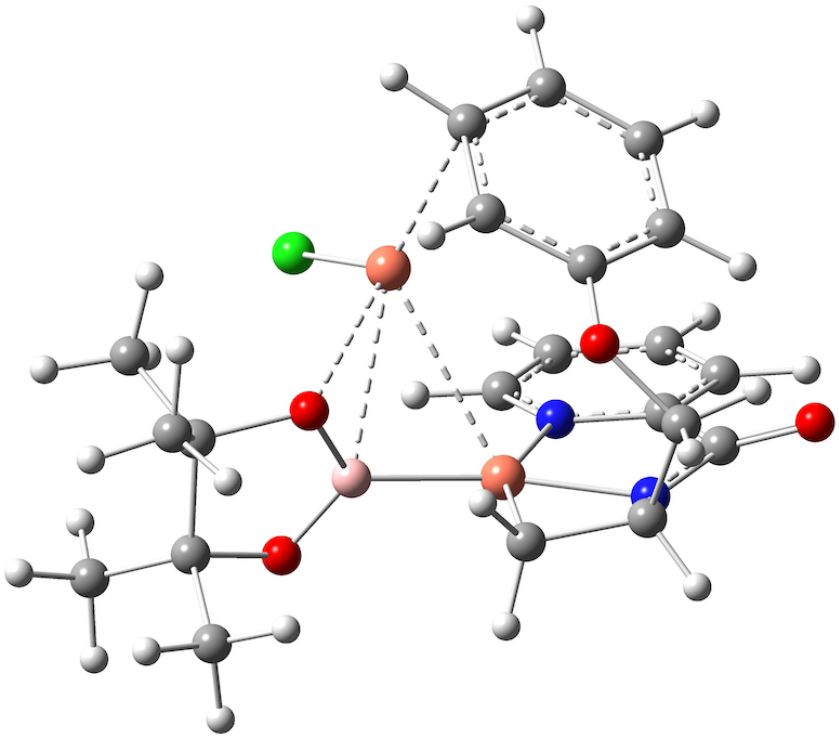

TS4b Substrate: 1c
Path: anti-Markovnikov

CARTESIAN COORDINATES

C	-1.974853	-1.635708	2.888312
C	-0.654161	-1.179125	3.077791
C	-0.295134	0.136154	2.698227
C	-1.288613	1.009766	2.173894
C	-2.593421	0.549897	1.993873
C	-2.918660	-0.770095	2.346047
O	-0.859899	2.280692	1.958525
C	-1.557986	3.205639	1.104072
C	-1.173619	3.039641	-0.376918
Cu	-0.255169	0.771107	-1.036235
B	1.643732	0.335200	-0.726511
O	2.232533	0.324009	0.528693
C	3.669639	0.039738	0.360731
C	3.893832	0.378603	-1.163703
O	2.553772	0.219678	-1.737527
Cu	0.410445	-1.205092	1.112692
Cl	0.813709	-3.112659	0.130510
C	0.306489	2.616331	-0.564946
N	-1.768220	1.892287	-1.043154
C	-2.988665	1.360848	-1.017845
C	-2.900095	-0.089403	-1.491126
C	-4.037393	-0.827835	-1.794905
C	-3.889921	-2.152319	-2.216853
C	-2.608985	-2.695856	-2.311761
C	-1.511818	-1.902121	-1.970227
N	-1.657029	-0.632202	-1.567159
O	-4.066783	1.856549	-0.652186
H	-5.004970	-0.347362	-1.692126
H	-4.762802	-2.750389	-2.465188
H	-0.500378	-2.288363	-1.976912

```
 H              -2.447168   -3.721694   -2.626266
 H              -1.417925    3.990664   -0.878139
 H               0.773386    3.028502   -1.461826
 H               0.946915    2.686791    0.311557
 H              -1.222419    4.184781    1.457196
 H              -2.642402    3.138728    1.228316
 H               0.667728    0.564437    2.966227
 H              -3.361745    1.192399    1.582261
 H               0.061978   -1.801874    3.609540
 H              -3.939274   -1.109748    2.190531
 H              -2.239456   -2.652204    3.159700
 C               3.891615   -1.431635    0.708301
 H               4.956153   -1.686219    0.662406
 H               3.535823   -1.615114    1.727609
 H               3.328987   -2.094881    0.049675
 C               4.426955    0.935100    1.337762
 H               4.190121    0.636982    2.364477
 H               5.508888    0.829999    1.194784
 H               4.158232    1.987559    1.220440
 C               4.841108   -0.565594   -1.896467
 H               4.915913   -0.265576   -2.946742
 H               5.844042   -0.524396   -1.455090
 H               4.483432   -1.596732   -1.862668
 C               4.290032    1.838137   -1.416524
 H               5.302660    2.048645   -1.055898
 H               4.256737    2.032124   -2.493201
 H               3.594477    2.528694   -0.928278

 Electronic Energy =  -2106.32190725 (Hartree/Particle)
 Dipole Moment (Debye):      2.5374
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:            -36.673

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.450034
(Hartree/Particle)
 Thermal correction to Energy=                    0.480564
 Thermal correction to Enthalpy=                  0.481508
 Thermal correction to Gibbs Free Energy=         0.387797
 Sum of electronic and zero-point Energies=          -2105.871874
 Sum of electronic and thermal Energies=             -2105.841344
 Sum of electronic and thermal Enthalpies=           -2105.840399
 Sum of electronic and thermal Free Energies=        -2105.934110
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -2106.72076964
 Corrected Free Energy =  -2106.33297239

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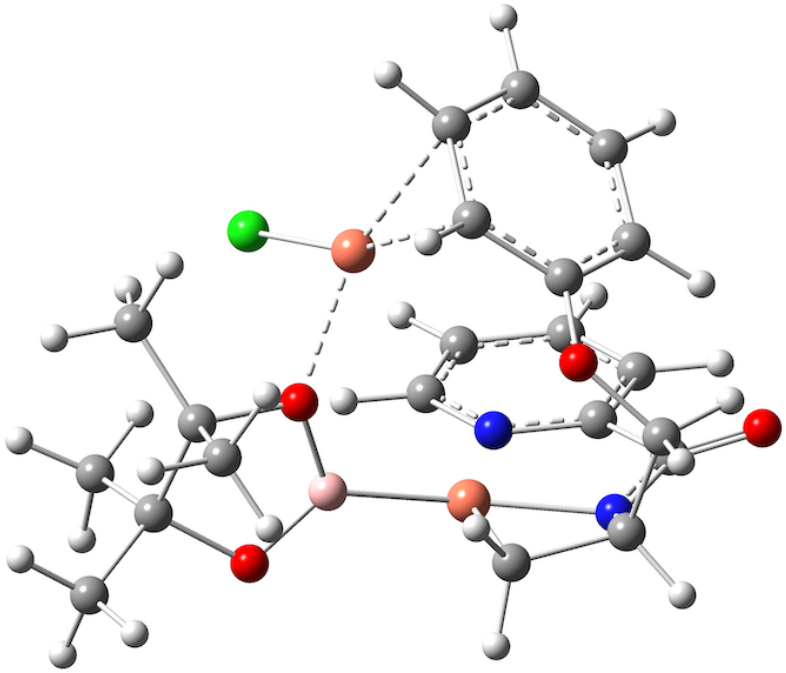

I3b Substrate: 1c
Path: anti-Markovnikov

CARTESIAN COORDINATES

C	1.754428	2.540452	2.416257
C	0.489977	2.008294	2.754929
C	0.259486	0.613870	2.669706
C	1.321433	-0.252122	2.275870
C	2.564270	0.285030	1.944938
C	2.763648	1.676104	2.014787
O	1.005827	-1.572582	2.323559
C	1.885195	-2.620910	1.872592
C	1.579296	-3.058589	0.428387
Cu	0.356585	-1.344391	-0.942199
B	-1.539943	-0.954695	-0.704466
O	-1.946179	-0.235116	0.413975
C	-3.421785	-0.295710	0.471656
C	-3.782832	-0.600131	-1.024766
O	-2.589106	-1.320377	-1.495054
Cu	-0.616164	1.538132	0.912203
Cl	-1.145271	3.028486	-0.603153
C	0.062960	-2.992337	0.101135
N	2.028692	-2.128220	-0.601764
C	3.123952	-1.376596	-0.713839
C	2.797856	-0.137759	-1.551828
C	3.788454	0.729373	-1.995419
C	3.415114	1.887237	-2.684867
C	2.061487	2.147255	-2.896521
C	1.118418	1.236940	-2.416322
N	1.480564	0.122249	-1.766047
O	4.248187	-1.526844	-0.208919
H	4.822551	0.483596	-1.776785
H	4.171290	2.582108	-3.040530
H	0.054803	1.413653	-2.514224
H	1.724215	3.046480	-3.400954
H	2.005224	-4.067867	0.306205

```
 H              -0.269346   -3.751690   -0.609561
 H              -0.610145   -2.899093    0.951842
 H               1.670097   -3.453602    2.549243
 H               2.937506   -2.344759    1.977364
 H              -0.635170    0.158638    3.087742
 H               3.386393   -0.347493    1.635982
 H              -0.262791    2.652556    3.205114
 H               3.740686    2.069915    1.747454
 H               1.921271    3.611150    2.468514
 C              -3.944020    1.030868    1.007871
 H              -5.039537    1.050566    0.969353
 H              -3.640384    1.150689    2.054250
 H              -3.547612    1.876718    0.443023
 C              -3.751252   -1.443122    1.430838
 H              -3.284420   -1.242290    2.400582
 H              -4.832180   -1.537971    1.579814
 H              -3.364226   -2.397182    1.058587
 C              -3.903395    0.660949   -1.884760
 H              -3.941013    0.365606   -2.938342
 H              -4.818994    1.213769   -1.647091
 H              -3.049019    1.328602   -1.738178
 C              -4.992209   -1.508205   -1.218231
 H              -5.890609   -1.043107   -0.795113
 H              -5.162046   -1.668184   -2.287731
 H              -4.846960   -2.484267   -0.749007

 Electronic Energy =  -2106.32816499 (Hartree/Particle)
 Dipole Moment (Debye):      2.6979
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.450490
(Hartree/Particle)
 Thermal correction to Energy=                    0.481544
 Thermal correction to Enthalpy=                  0.482488
 Thermal correction to Gibbs Free Energy=         0.388415
 Sum of electronic and zero-point Energies=          -2105.877675
 Sum of electronic and thermal Energies=             -2105.846621
 Sum of electronic and thermal Enthalpies=           -2105.845677
 Sum of electronic and thermal Free Energies=        -2105.939750
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -2106.72721471
 Corrected Free Energy =  -2106.33879995

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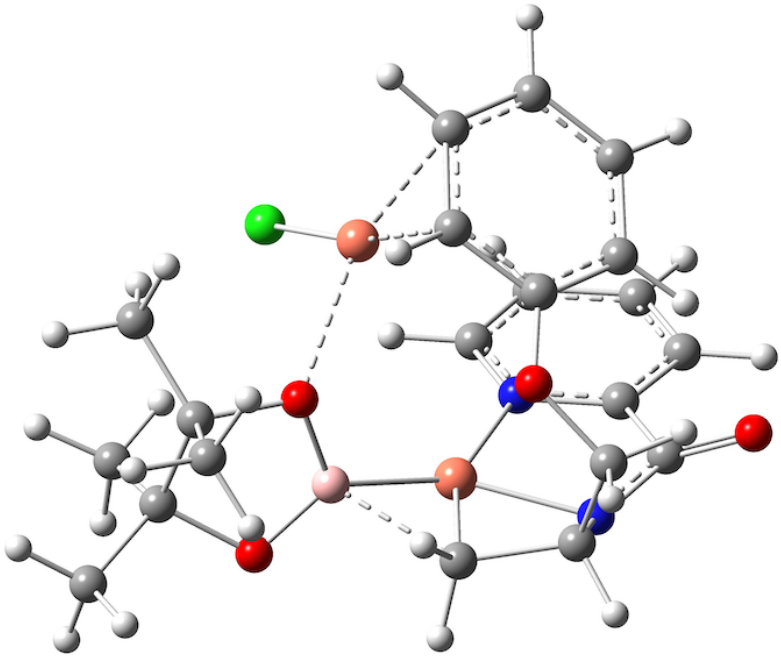

TS5 Substrate: 1c
Path: anti-Markovnikov

CARTESIAN COORDINATES

C	1.827383	2.705139	2.263997
C	0.464807	2.420218	2.492870
C	0.011318	1.079558	2.513008
C	0.942024	0.017735	2.317520
C	2.289352	0.310892	2.103049
C	2.713366	1.650439	2.076926
O	0.394947	-1.219992	2.411009
C	1.124655	-2.440841	2.174690
C	0.927827	-2.981615	0.742473
Cu	0.321747	-1.245030	-0.933674
B	-1.585258	-1.072687	-0.471139
O	-1.984959	-0.108835	0.438447
C	-3.457610	-0.038173	0.379985
C	-3.752363	-0.623664	-1.048845
O	-2.613048	-1.527800	-1.252520
Cu	-0.494460	1.788107	0.566962
Cl	-0.873969	2.849401	-1.286681
C	-0.516976	-2.686208	0.195337
N	1.755564	-2.374141	-0.291773
C	2.949485	-1.803390	-0.208164
C	3.028158	-0.634152	-1.205054
C	4.247694	-0.065834	-1.560709
C	4.260945	1.053577	-2.395945
C	3.048615	1.589539	-2.832745
C	1.859885	0.983867	-2.424083
N	1.849957	-0.103777	-1.637278
O	3.905775	-2.009775	0.566032
H	5.154474	-0.508768	-1.162170
H	5.203189	1.507427	-2.692221
H	0.890359	1.389625	-2.688413
H	3.009747	2.471557	-3.463854
H	1.073425	-4.073579	0.807091

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 H              -0.828551   -3.453147   -0.518225
 H              -1.255957   -2.610644    0.996913
 H               0.681506   -3.145610    2.884566
 H               2.188266   -2.334546    2.399794
 H              -0.986103    0.820868    2.859124
 H               3.019221   -0.473932    1.951586
 H              -0.218188    3.221634    2.765748
 H               3.766956    1.851933    1.902124
 H               2.169232    3.734619    2.238697
 C              -3.882213    1.410382    0.583758
 H              -4.965470    1.510905    0.448438
 H              -3.638249    1.726748    1.604376
 H              -3.369422    2.079720   -0.109707
 C              -3.964429   -0.923327    1.522601
 H              -3.543206   -0.563798    2.466882
 H              -5.056742   -0.890290    1.594931
 H              -3.658259   -1.965998    1.388898
 C              -3.688490    0.428348   -2.159146
 H              -3.693077   -0.082454   -3.127483
 H              -4.554255    1.098294   -2.116711
 H              -2.779579    1.032507   -2.087575
 C              -5.033696   -1.444133   -1.150788
 H              -5.904262   -0.822399   -0.910405
 H              -5.150813   -1.813950   -2.174374
 H              -5.020597   -2.305849   -0.478920

 Electronic Energy =  -2106.32405558 (Hartree/Particle)
 Dipole Moment (Debye):      3.1867
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -115.830

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.449998
(Hartree/Particle)
 Thermal correction to Energy=                    0.480427
 Thermal correction to Enthalpy=                  0.481371
 Thermal correction to Gibbs Free Energy=         0.389242
 Sum of electronic and zero-point Energies=          -2105.874058
 Sum of electronic and thermal Energies=             -2105.843629
 Sum of electronic and thermal Enthalpies=           -2105.842685
 Sum of electronic and thermal Free Energies=        -2105.934814
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -2106.72383744
 Corrected Free Energy =  -2106.33459586

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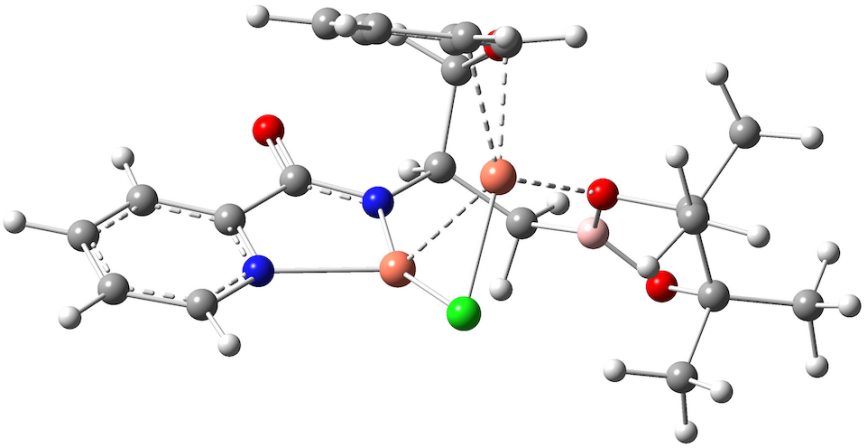


P2 Substrate: 1c
Path: anti-Markovnikov

CARTESIAN COORDINATES

C	1.483707	3.382353	-1.148678
C	0.086295	3.321469	-1.072899
C	-0.547765	2.732736	0.047943
C	0.242956	2.171721	1.091331
C	1.642399	2.255121	1.011962
C	2.241094	2.862351	-0.094962
O	-0.457786	1.624229	2.106575
C	0.160079	0.678326	3.006171
C	0.293310	-0.752204	2.450505
Cu	0.829147	-1.040192	-0.576212
B	-2.154864	-1.000968	1.149092
O	-2.247122	0.107197	0.312047
C	-3.642163	0.190348	-0.153850
C	-4.095409	-1.303924	-0.047703
O	-3.286501	-1.779233	1.063118
Cu	-0.599910	0.950224	-1.058064
Cl	-0.242868	-0.723498	-2.525857
C	-1.045360	-1.454650	2.171870
N	1.211877	-0.872004	1.315155
C	2.513125	-0.777159	1.630550
C	3.484473	-0.961462	0.474920
C	4.861855	-0.870677	0.698019
C	5.729625	-1.023020	-0.383858
C	5.198662	-1.254038	-1.656265
C	3.811162	-1.326170	-1.791461
N	2.979335	-1.188514	-0.751906
O	2.992745	-0.523103	2.759702
H	5.211395	-0.683380	1.707251
H	6.805176	-0.960543	-0.238656
H	3.338815	-1.496662	-2.756095
H	5.839223	-1.375348	-2.524844
H	0.754060	-1.284440	3.298776
H	-0.810631	-2.494136	1.899992
H	-1.586432	-1.546714	3.128850
H	-0.512788	0.667773	3.868644
H	1.137525	1.036607	3.336277
H	-1.615603	2.845956	0.218558
H	2.264456	1.827621	1.788771
H	-0.527060	3.773047	-1.847650

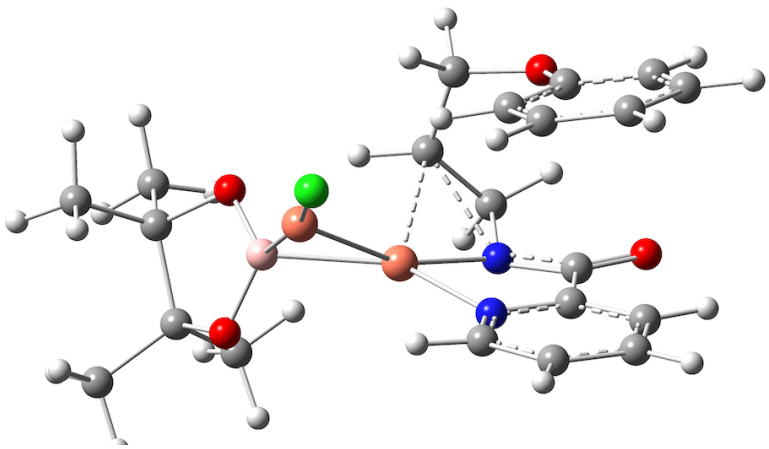
H	3.326295	2.906001	-0.137821
H	1.966554	3.825331	-2.013817
C	-3.671689	0.771002	-1.562967
H	-4.696547	0.759266	-1.951610
H	-3.332130	1.813267	-1.547560
H	-3.031360	0.211848	-2.248011
C	-4.364049	1.121465	0.826001
H	-3.852114	2.088597	0.847467
H	-5.403584	1.286128	0.523322
H	-4.354904	0.713783	1.841580
C	-3.706986	-2.137233	-1.274938
H	-3.847852	-3.196509	-1.037752
H	-4.332429	-1.889932	-2.139843
H	-2.658429	-1.981342	-1.547046
C	-5.568154	-1.502121	0.296575
H	-6.206914	-1.059257	-0.476944
H	-5.790385	-2.572673	0.351214
H	-5.821305	-1.055409	1.261207

Electronic Energy = -2106.41494402 (Hartree/Particle)
Dipole Moment (Debye): 4.5968
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.452033
(Hartree/Particle)
Thermal correction to Energy= 0.482922
Thermal correction to Enthalpy= 0.483866
Thermal correction to Gibbs Free Energy= 0.390290
Sum of electronic and zero-point Energies= -2105.962911
Sum of electronic and thermal Energies= -2105.932022
Sum of electronic and thermal Enthalpies= -2105.931078
Sum of electronic and thermal Free Energies= -2106.024654
PCM-SP (solvent=THF;6-311+g(2d,p)) = -2106.81097231
Corrected Free Energy = -2106.42068229

PATH: MARKOVNIKOV



TS3 Substrate: 1c
Path: Markovnikov

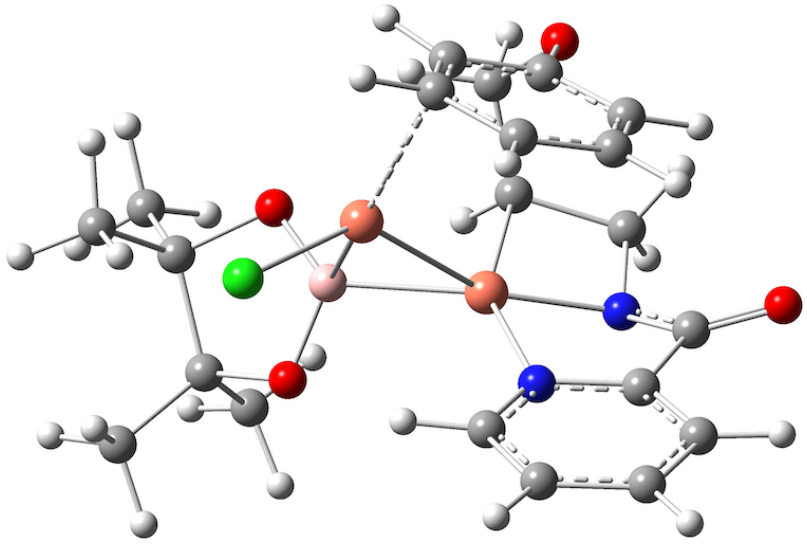
CARTESIAN COORDINATES

C	-0.299954	-2.133977	-0.903735
N	0.505324	-2.010048	0.797575
C	1.846446	-1.927262	1.194917
O	2.590148	-2.897131	1.256590
C	0.119273	-3.189824	0.042762
C	2.286174	-0.561469	1.647054
C	3.573990	-0.358022	2.136036
C	3.940959	0.935722	2.512240
C	3.019513	1.973200	2.370023
C	1.754605	1.684792	1.852050
N	1.398629	0.440133	1.515330
Cu	-0.853872	1.806031	-0.488126
H	4.256808	-1.198063	2.192231
H	4.939124	1.132201	2.893344
H	1.016169	2.458557	1.667193
H	3.271381	2.995202	2.634664
H	0.965987	-3.806960	-0.261248
H	-0.678178	-3.772059	0.510047
Cu	-0.300795	-0.224979	0.498804
B	-2.286793	0.418879	0.002206
O	-2.954982	-0.296066	-0.992306
O	-3.108434	0.615078	1.100267
C	-4.367932	-0.367920	-0.630241
C	-4.309996	-0.193431	0.927324
Cl	0.328855	3.505234	-1.087284
H	-1.355090	-1.876269	-0.970107
C	0.506557	-1.775499	-2.120919
H	0.150643	-2.460237	-2.909203
H	0.280354	-0.759938	-2.455587
O	1.888525	-2.023258	-1.984725
C	2.763000	-0.986923	-1.705146
C	2.403725	0.358664	-1.595944
C	4.094176	-1.381518	-1.520397
C	3.386896	1.312045	-1.307936
H	1.381499	0.703522	-1.701163
C	5.063870	-0.422375	-1.235396
H	4.340343	-2.436381	-1.589952
C	4.716718	0.931344	-1.128985
H	3.076124	2.349204	-1.218146
H	6.095076	-0.735568	-1.091914
H	5.475109	1.676415	-0.904362
C	-4.057282	-1.509015	1.676643
H	-3.822598	-1.281918	2.721155
H	-4.934570	-2.164660	1.649817
H	-3.202771	-2.046141	1.250741
C	-5.494292	0.547725	1.539571
H	-6.428522	0.006103	1.347598
H	-5.360030	0.626477	2.623358
H	-5.585346	1.559218	1.137424
C	-5.066105	0.794131	-1.347219
H	-4.884134	0.708211	-2.423144
H	-6.147842	0.779764	-1.174425
H	-4.668756	1.757835	-1.013860
C	-4.927489	-1.703125	-1.111884
H	-5.964622	-1.828874	-0.778783
H	-4.914462	-1.736171	-2.206474
H	-4.339774	-2.546510	-0.739907

Electronic Energy = -2106.31037510 (Hartree/Particle)
Dipole Moment (Debye): 5.6783
index 0
Harmonic frequencies
Number of imaginary frequencies= 1
Negatives Eigenvalues: -222.555

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.448491
(Hartree/Particle)
Thermal correction to Energy= 0.480080
Thermal correction to Enthalpy= 0.481024
Thermal correction to Gibbs Free Energy= 0.383276
Sum of electronic and zero-point Energies= -2105.861884
Sum of electronic and thermal Energies= -2105.830295
Sum of electronic and thermal Enthalpies= -2105.829351
Sum of electronic and thermal Free Energies= -2105.927099
PCM-SP (solvent=THF;6-311+g(2d,p)) = -2106.71119542
Corrected Free Energy = -2106.3279193



I2 Substrate: 1c
Path: Markovnikov

CARTESIAN COORDINATES

C	-0.057418	2.570992	0.108653
N	1.571234	1.948037	-1.305556
C	2.820716	1.454063	-1.405226
O	3.894834	2.053311	-1.287525
C	1.182839	3.157450	-0.586313
C	2.773586	-0.045025	-1.677522
C	3.885741	-0.750732	-2.122126
C	3.772507	-2.130266	-2.310966
C	2.557308	-2.760342	-2.035000
C	1.488624	-1.991053	-1.571418
N	1.602749	-0.664901	-1.403404

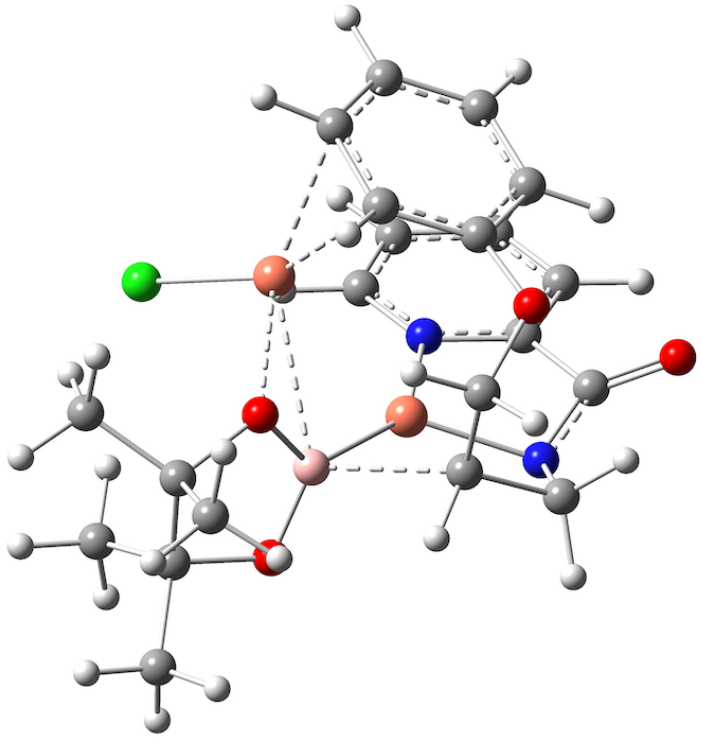
Cu	-0.359946	-1.014285	0.968246
H	4.808386	-0.208028	-2.297597
H	4.623906	-2.705900	-2.662962
H	0.533115	-2.429834	-1.300477
H	2.432438	-3.831190	-2.159423
H	1.952722	3.485566	0.120944
H	0.948792	3.988366	-1.264598
Cu	0.318941	0.730882	-0.612939
B	-1.638840	0.122467	-0.245235
O	-2.562874	0.710847	0.595742
O	-2.197208	-0.367266	-1.398998
C	-3.891275	0.313646	0.112551
C	-3.609916	0.012528	-1.407845
Cl	-1.088680	-3.084695	0.905591
H	-1.013835	2.855380	-0.333353
C	-0.126923	2.635171	1.619910
H	-0.333626	3.670328	1.922057
H	-0.935588	2.000568	1.993088
O	1.126199	2.340094	2.265144
C	1.539717	1.032027	2.277203
C	2.803608	0.737344	1.766100
C	0.735607	0.006662	2.821969
C	3.263253	-0.585393	1.769994
H	3.401169	1.536872	1.340628
C	1.217176	-1.317127	2.833636
H	-0.198766	0.258648	3.317955
C	2.477280	-1.615025	2.288688
H	4.236440	-0.804321	1.339847
H	0.617278	-2.101071	3.284962
H	2.825163	-2.643263	2.269858
C	-3.720580	1.246901	-2.310310
H	-3.327770	0.998937	-3.301743
H	-4.761606	1.569188	-2.419635
H	-3.134558	2.083363	-1.914327
C	-4.410704	-1.150007	-1.984621
H	-5.485486	-0.942072	-1.921312
H	-4.148451	-1.291523	-3.038217
H	-4.197498	-2.081012	-1.454904
C	-4.859730	1.463844	0.366357
H	-5.835990	1.239652	-0.079251
H	-5.001517	1.602082	1.443413
H	-4.491940	2.404210	-0.051025
C	-4.297427	-0.922388	0.921121
H	-4.309126	-0.657632	1.983876
H	-5.298171	-1.268577	0.641358
H	-3.584009	-1.740022	0.786862

Electronic Energy = -2106.32541596 (Hartree/Particle)
Dipole Moment (Debye): 2.1292
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.450402
(Hartree/Particle)
Thermal correction to Energy= 0.481773
Thermal correction to Enthalpy= 0.482717

```
 Thermal correction to Gibbs Free Energy=          0.387207
 Sum of electronic and zero-point Energies=          -2105.875014
 Sum of electronic and thermal Energies=             -2105.843643
 Sum of electronic and thermal Enthalpies=           -2105.842699
 Sum of electronic and thermal Free Energies=        -2105.938209
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -2106.72471889
 Corrected Free Energy =  -2106.33751193
```



TS4=TS5 Substrate: 1c
Path: Markovnikov

CARTESIAN COORDINATES

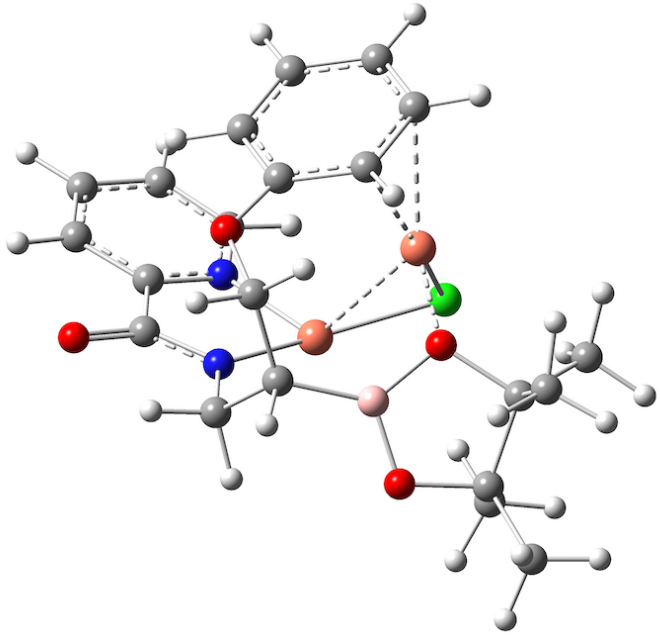
C	-0.489118	2.369361	0.359369
N	1.484755	2.314936	-1.004360
C	2.752835	1.988157	-0.748233
O	3.649341	2.600000	-0.141840
C	0.691116	3.241829	-0.214445
C	3.027961	0.571130	-1.270638
C	4.315673	0.141887	-1.580054
C	4.508268	-1.172390	-2.009566
C	3.407150	-2.027129	-2.095285
C	2.148229	-1.541479	-1.740944
N	1.965666	-0.273000	-1.340373
Cu	-0.378771	-1.434918	0.626164
H	5.132527	0.847587	-1.470317
H	5.502663	-1.526051	-2.270020
H	1.263170	-2.169534	-1.749382
H	3.511073	-3.058471	-2.417449
H	1.258439	3.697927	0.608589
H	0.286074	4.040688	-0.846966
Cu	0.320256	0.792853	-0.704347
B	-1.622878	0.746999	-0.340274

O	-2.289373	0.115562	0.687472
O	-2.418016	1.041838	-1.409794
C	-3.713757	0.020914	0.314745
C	-3.693660	0.331938	-1.239394
Cl	-0.928354	-3.044566	-0.739170
H	-1.452883	2.830369	0.119779
C	-0.416264	2.205897	1.878280
H	-0.535966	3.197480	2.329153
H	-1.212954	1.561229	2.255836
O	0.871516	1.777137	2.339867
C	1.217768	0.459166	2.270308
C	2.557506	0.177824	2.002885
C	0.302588	-0.596180	2.527433
C	3.001739	-1.149939	1.986120
H	3.227823	1.004174	1.787364
C	0.778672	-1.932399	2.524639
H	-0.688843	-0.373252	2.912080
C	2.128611	-2.206330	2.239475
H	4.045298	-1.350957	1.759457
H	0.118699	-2.736595	2.841133
H	2.477655	-3.233731	2.222237
C	-4.806231	1.263267	-1.714662
H	-4.689760	1.446717	-2.787206
H	-5.787136	0.801662	-1.551690
H	-4.782834	2.228472	-1.203030
C	-3.628404	-0.912986	-2.125571
H	-4.567117	-1.475988	-2.081941
H	-3.463257	-0.596675	-3.160530
H	-2.808201	-1.573212	-1.835801
C	-4.424448	1.085826	1.153778
H	-5.503614	1.084385	0.968628
H	-4.256907	0.875409	2.215073
H	-4.037895	2.087964	0.940556
C	-4.192653	-1.378458	0.682042
H	-4.156081	-1.504800	1.769580
H	-5.228655	-1.526826	0.356552
H	-3.560143	-2.144723	0.228670

Electronic Energy = -2106.31540616 (Hartree/Particle)
Dipole Moment (Debye): 4.4348
index 0
Harmonic frequencies
Number of imaginary frequencies= 1
Negatives Eigenvalues: -148.079

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.449959
(Hartree/Particle)
Thermal correction to Energy= 0.480696
Thermal correction to Enthalpy= 0.481640
Thermal correction to Gibbs Free Energy= 0.388353
Sum of electronic and zero-point Energies= -2105.865447
Sum of electronic and thermal Energies= -2105.834710
Sum of electronic and thermal Enthalpies= -2105.833766
Sum of electronic and thermal Free Energies= -2105.927053
PCM-SP (solvent=THF;6-311+g(2d,p)) = -2106.71773050
Corrected Free Energy = -2106.32937735



P2 Substrate: 1c
Path: Markovnikov

CARTESIAN COORDINATES

C	1.072742	-1.770882	1.701063
N	-0.940251	-1.857041	0.164318
C	-2.235096	-2.099564	0.446090
O	-2.695818	-2.900337	1.285298
C	0.027140	-2.629699	0.936395
C	-3.239210	-1.269419	-0.345865
C	-4.604080	-1.359113	-0.052577
C	-5.498297	-0.555947	-0.760907
C	-5.007411	0.312522	-1.741259
C	-3.631597	0.334201	-1.975340
N	-2.776615	-0.439757	-1.297414
Cu	0.579201	1.445785	-0.100120
H	-4.921399	-2.049181	0.721426
H	-6.564099	-0.603774	-0.551474
H	-3.185993	0.989787	-2.720346
H	-5.670388	0.955144	-2.313387
H	-0.508770	-3.261430	1.653840
H	0.582167	-3.292953	0.259516
Cu	-0.612655	-0.495797	-1.150102
B	2.126607	-1.095298	0.743675
O	2.411161	0.261094	0.577951
O	3.003599	-1.882216	0.047360
C	3.725866	0.353295	-0.090319
C	3.814418	-1.035729	-0.817896
Cl	0.180208	1.274535	-2.305330
H	1.712482	-2.523346	2.198415
C	0.483178	-0.981160	2.889972
H	0.230323	-1.687102	3.685299
H	1.209717	-0.266652	3.298508
O	-0.777460	-0.334769	2.651956
C	-0.896286	0.894393	2.119627

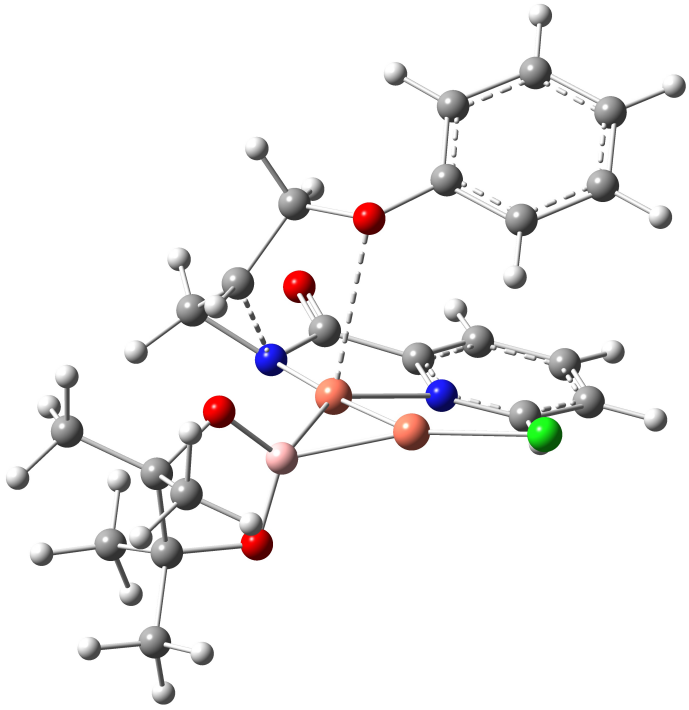
```
 C              -2.199825    1.273792    1.757026
 C               0.171006    1.815750    1.948765
 C              -2.451140    2.542257    1.237365
 H              -2.994826    0.547786    1.888915
 C              -0.108502    3.099610    1.404986
 H               1.150535    1.609553    2.366724
 C              -1.414653    3.463178    1.049463
 H              -3.468006    2.805844    0.959697
 H               0.697086    3.827026    1.340710
 H              -1.611434    4.444236    0.629346
 C               5.220816   -1.623534   -0.890682
 H               5.185663   -2.590429   -1.402387
 H               5.884558   -0.960380   -1.457994
 H               5.646950   -1.783044    0.102794
 C               3.153177   -1.047868   -2.198699
 H               3.734914   -0.471578   -2.926169
 H               3.088600   -2.083628   -2.546510
 H               2.140640   -0.638430   -2.159723
 C               4.749771    0.524497    1.036404
 H               5.761316    0.650419    0.636809
 H               4.495004    1.416719    1.617782
 H               4.747675   -0.336709    1.712456
 C               3.732592    1.567585   -1.009142
 H               3.627171    2.483063   -0.415829
 H               4.683999    1.622863   -1.550591
 H               2.918262    1.534358   -1.734816

 Electronic Energy =  -2106.40715696 (Hartree/Particle)
 Dipole Moment (Debye):      6.9395
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.452124
(Hartree/Particle)
 Thermal correction to Energy=                    0.483169
 Thermal correction to Enthalpy=                  0.484114
 Thermal correction to Gibbs Free Energy=         0.389808
 Sum of electronic and zero-point Energies=          -2105.955033
 Sum of electronic and thermal Energies=             -2105.923987
 Sum of electronic and thermal Enthalpies=           -2105.923043
 Sum of electronic and thermal Free Energies=        -2106.017349
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -2106.80650319
 Corrected Free Energy =  -2106.41669523
```

TS3-B and correponding intermediate I3-B Ref 34 (main text)



TS3-B (Ref 34) Substrate: 1c
Path: Markovnikov

CARTESIAN COORDINATES

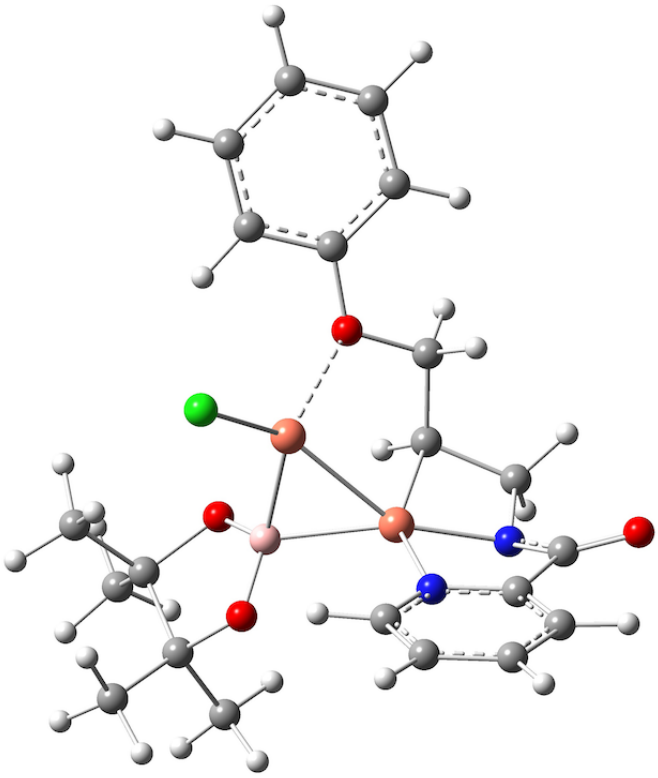
C	0.307167	-1.789726	1.469768
N	-0.124300	-2.388471	-0.375046
C	-1.426480	-2.679262	-0.769972
O	-1.991829	-3.743583	-0.531902
C	0.404440	-3.107495	0.772249
C	-2.105535	-1.573850	-1.536112
C	-3.362010	-1.767478	-2.104850
C	-3.976231	-0.682631	-2.736276
C	-3.321267	0.548565	-2.759474
C	-2.066305	0.660748	-2.153289
N	-1.472673	-0.385768	-1.566648
Cu	0.717306	1.809347	-0.334041
H	-3.834073	-2.740929	-2.027526
H	-4.956690	-0.795970	-3.190328
H	-1.527935	1.603916	-2.111060
H	-3.769233	1.419731	-3.226821
H	-0.243078	-3.909665	1.136877
H	1.422777	-3.463202	0.606676
Cu	0.298143	-0.494479	-0.401520
B	2.211347	0.433584	-0.093348
O	2.813493	0.208233	1.141766
O	3.121133	0.268171	-1.124469
C	4.256861	0.134498	0.935320
C	4.346387	-0.296360	-0.570903
Cl	-0.323420	3.661415	-0.721303
H	1.202765	-1.237785	1.747666
C	-0.980254	-1.448232	2.157016
H	-1.796404	-2.066333	1.766062
H	-0.868980	-1.672865	3.232324
O	-1.249900	-0.064943	1.972179

C	-2.561047	0.357867	1.899331
C	-3.644027	-0.360137	2.418124
C	-2.757795	1.588588	1.261593
C	-4.937287	0.161018	2.277978
H	-3.498152	-1.301007	2.939271
C	-4.049363	2.095313	1.136874
H	-1.902971	2.129266	0.867304
C	-5.147867	1.383139	1.637474
H	-5.778284	-0.396986	2.682011
H	-4.192914	3.050499	0.638483
H	-6.153713	1.781276	1.534986
C	4.254791	-1.814623	-0.775269
H	4.111001	-2.020822	-1.840353
H	5.164782	-2.323802	-0.439223
H	3.398326	-2.231424	-0.234938
C	5.537905	0.270838	-1.336074
H	6.480045	-0.065126	-0.886017
H	5.509710	-0.077566	-2.373709
H	5.523228	1.362911	-1.347527
C	4.810612	1.539920	1.200083
H	4.526441	1.848106	2.211176
H	5.903202	1.561743	1.122582
H	4.392518	2.266598	0.496608
C	4.841073	-0.863821	1.930195
H	5.912127	-1.009722	1.745715
H	4.718782	-0.483506	2.949840
H	4.343159	-1.835104	1.868628

Electronic Energy = -2106.30448992 (Hartree/Particle)
Dipole Moment (Debye): 6.6327
index 1
Number of imaginary frequencies= 1
Negatives Eigenvalues: -164.577

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.448288
(Hartree/Particle)
Thermal correction to Energy= 0.480008
Thermal correction to Enthalpy= 0.480953
Thermal correction to Gibbs Free Energy= 0.382024
Sum of electronic and zero-point Energies= -2105.856202
Sum of electronic and thermal Energies= -2105.824481
Sum of electronic and thermal Enthalpies= -2105.823537
Sum of electronic and thermal Free Energies= -2105.922465
PCM-SP (solvent=THF;6-311+g(2d,p)) = -2106.70645868
Corrected Free Energy = -2106.32443378



I2-B (Ref 34) Substrate: 1c
Path: Markovnikov

CARTESIAN COORDINATES

C	0.508959	-0.951067	-2.166175
N	-1.263181	-2.261577	-1.729352
C	-1.587622	-3.352998	-0.999813
O	-1.427235	-4.541536	-1.286086
C	-0.234266	-2.168476	-2.756774
C	-2.215215	-2.927481	0.327868
C	-2.889162	-3.817871	1.156593
C	-3.386137	-3.348743	2.376072
C	-3.180704	-2.014016	2.734832
C	-2.478477	-1.182109	1.861366
N	-2.021116	-1.637908	0.687838
Cu	0.681220	0.416354	0.758278
H	-2.996755	-4.849077	0.836685
H	-3.920445	-4.019545	3.043404
H	-2.264826	-0.140616	2.078295
H	-3.543870	-1.619573	3.678337
H	0.382014	-3.075950	-2.832679
H	-0.667072	-1.962838	-3.742067
Cu	-0.838395	-0.753486	-0.700583
B	-0.814301	1.311144	-0.302817
O	-0.301958	2.287962	-1.124943
O	-2.013663	1.665341	0.275806
C	-1.035438	3.520284	-0.811288
C	-2.409554	2.955984	-0.297503
Cl	1.139317	1.205019	2.709054
H	0.516270	-0.033412	-2.755428
C	1.851245	-1.318316	-1.584617
H	1.796908	-2.282005	-1.060772

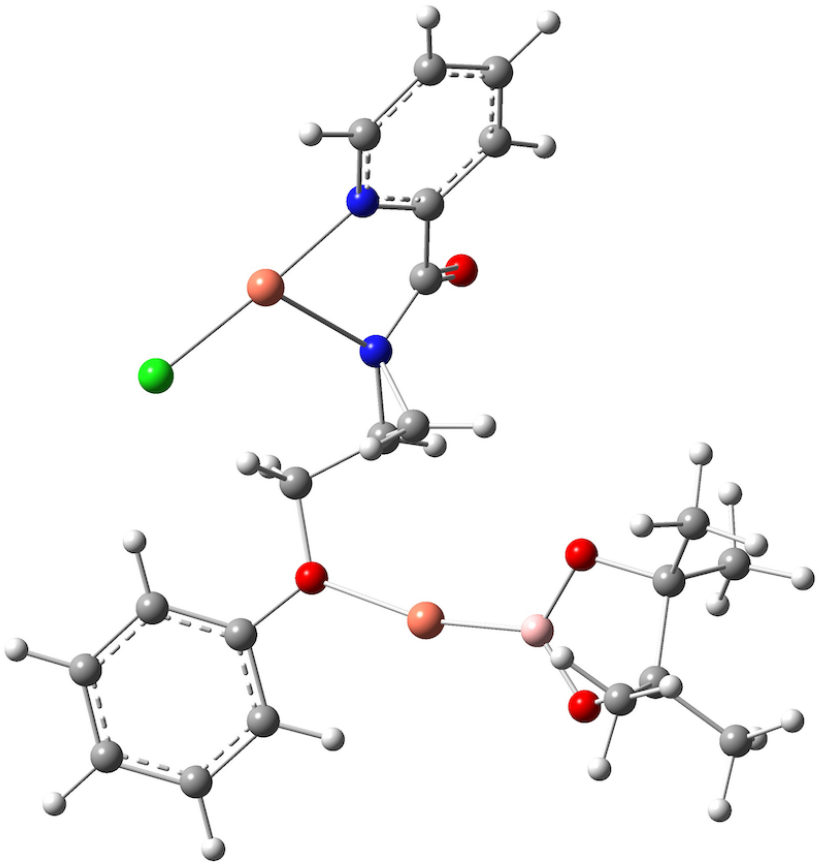
```
 H                2.570810   -1.415022   -2.413444
 O                2.318903   -0.308549   -0.683772
 C                3.642540   -0.352308   -0.262236
 C                4.511079   -1.412355   -0.537006
 C                4.068556    0.746248    0.492210
 C                5.826927   -1.353822   -0.057973
 H                4.187484   -2.279645   -1.101040
 C                5.377333    0.785145    0.966337
 H                3.359351    1.534299    0.723753
 C                6.266629   -0.261626    0.689854
 H                6.502638   -2.177870   -0.272096
 H                5.700223    1.635347    1.560895
 H                7.287002   -0.226919    1.061115
 C               -3.402295    2.644669   -1.422288
 H               -4.236881    2.068327   -1.010460
 H               -3.800513    3.561975   -1.869411
 H               -2.931868    2.046158   -2.209220
 C               -3.072797    3.781492    0.799028
 H               -3.291712    4.793223    0.437028
 H               -4.017125    3.312673    1.095359
 H               -2.435985    3.853604    1.683443
 C               -0.227765    4.238457    0.276109
 H                0.780843    4.429406   -0.103835
 H               -0.685032    5.197432    0.543177
 H               -0.132105    3.622364    1.175857
 C               -1.120000    4.367473   -2.075340
 H               -1.738928    5.255355   -1.898787
 H               -0.117614    4.701338   -2.362126
 H               -1.542960    3.806045   -2.911973

 Electronic Energy =  -2106.31437690 (Hartree/Particle)
 Dipole Moment (Debye):      3.9688
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.449496
(Hartree/Particle)
 Thermal correction to Energy=                    0.481514
 Thermal correction to Enthalpy=                  0.482458
 Thermal correction to Gibbs Free Energy=         0.381930
 Sum of electronic and zero-point Energies=          -2105.864881
 Sum of electronic and thermal Energies=             -2105.832863
 Sum of electronic and thermal Enthalpies=           -2105.831918
 Sum of electronic and thermal Free Energies=        -2105.932447
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -2106.71642467
 Corrected Free Energy =   -2106.33449477
```

PATH: ANTI-OPENING. TS-ANTI and the corresponding minima: Complex-ANTI and intermediate I-ANTI (Ref 35 main text)



Complex-ANTI (Ref 35) Substrate: 1c

CARTESIAN COORDINATES

C	-0.530065	0.642188	1.258186
N	-1.836307	0.158957	0.855423
C	-2.620921	-0.649634	1.669422
O	-2.510553	-0.746241	2.881582
C	-0.635360	-0.337330	0.132573
C	-3.719808	-1.357982	0.917332
C	-4.309111	-2.489386	1.481823
C	-5.328212	-3.141615	0.788718
C	-5.732845	-2.630434	-0.445569
C	-5.109124	-1.485224	-0.937710
N	-4.118765	-0.852977	-0.277117
Cu	2.231466	0.517867	0.292361
H	-3.957012	-2.830176	2.449377
H	-5.797712	-4.028693	1.203795
H	-5.402124	-1.042360	-1.883491
H	-6.523758	-3.099745	-1.021777
B	2.850331	-1.294343	-0.057517
O	4.135623	-1.744986	-0.312077
O	1.949510	-2.366317	-0.075815
C	4.072686	-3.134461	-0.740838
C	2.707210	-3.609543	-0.131192
H	-0.309394	-1.356868	0.319053
H	-0.548085	0.017374	-0.891159
H	-0.143118	0.272996	2.206290
C	-0.282934	2.094681	0.930792
H	-0.825522	2.359066	0.018716
H	-0.590969	2.753133	1.750933

```
  O                1.145236    2.247915    0.732599
  C                1.634477    3.533407    0.498175
  C                2.993089    3.728716    0.760693
  C                0.835782    4.567345    0.006139
  C                3.562100    4.979790    0.524268
  H                3.583634    2.898829    1.139909
  C                1.421720    5.819088   -0.218115
  H               -0.211858    4.411791   -0.226152
  C                2.777852    6.032218    0.037217
  H                4.619172    5.131169    0.725320
  H                0.805208    6.625379   -0.606138
  H                3.221955    7.006942   -0.143857
  Cu              -3.341995    0.785494   -1.005406
  Cl              -2.604011    2.537813   -1.964477
  C                4.080800   -3.125632   -2.276158
  H                4.974792   -2.595791   -2.620303
  H                4.098252   -4.141864   -2.686799
  H                3.205474   -2.600054   -2.670919
  C                5.304830   -3.867045   -0.215221
  H                5.247530   -4.938009   -0.446815
  H                6.204024   -3.461588   -0.691092
  H                5.414007   -3.746396    0.865194
  C                1.935917   -4.618565   -0.978595
  H                2.520807   -5.536343   -1.116814
  H                0.999531   -4.884778   -0.475358
  H                1.686968   -4.210994   -1.961360
  C                2.830637   -4.118754    1.311782
  H                1.826556   -4.238177    1.732765
  H                3.342977   -5.086641    1.356850
  H                3.375212   -3.402574    1.935031

 Electronic Energy =  -2106.30357832 (Hartree/Particle)
 Dipole Moment (Debye):      7.6683
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.449832
(Hartree/Particle)
 Thermal correction to Energy=                    0.482532
 Thermal correction to Enthalpy=                  0.483476
 Thermal correction to Gibbs Free Energy=         0.378741
 Sum of electronic and zero-point Energies=          -2105.853746
 Sum of electronic and thermal Energies=             -2105.821046
 Sum of electronic and thermal Enthalpies=           -2105.820102
 Sum of electronic and thermal Free Energies=        -2105.924837
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -2106.70537461
 Corrected Free Energy =  -2106.32663329

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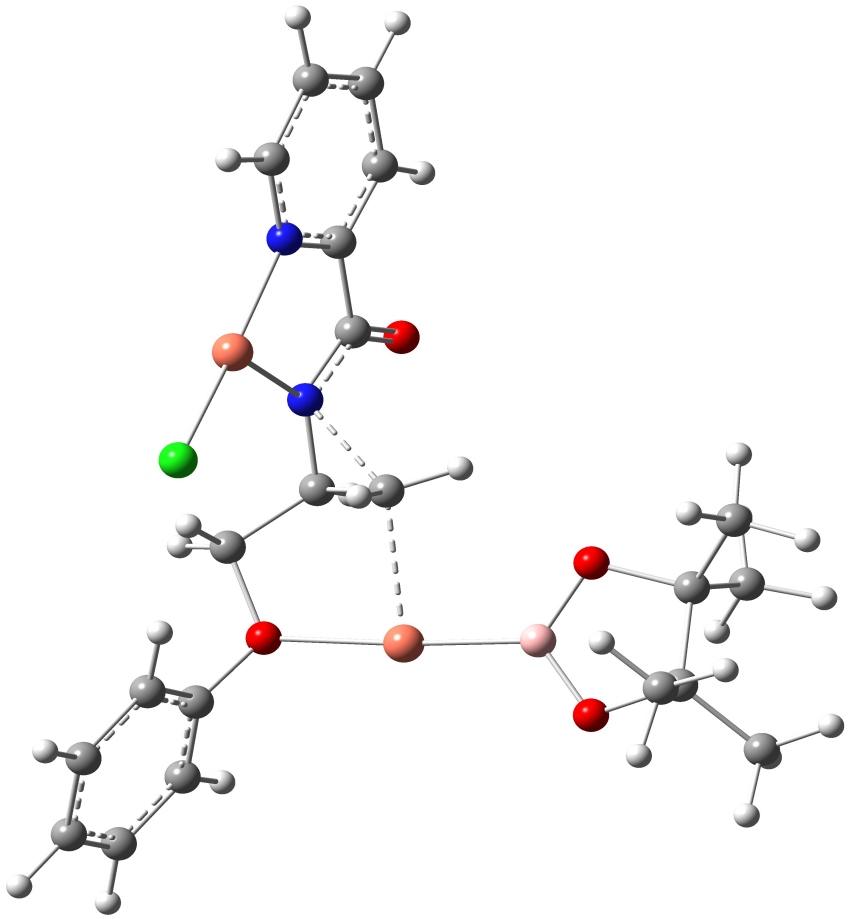

TS-ANTI (Ref 35) Substrate: 1c
Path: anti-Markovnikov

CARTESIAN COORDINATES

C	0.749321	0.642419	-1.470800
N	1.999441	0.203127	-0.899466
C	2.706054	-0.772974	-1.566444
O	2.428491	-1.276487	-2.656195
C	0.277393	-0.285548	-0.415727
C	3.957394	-1.191754	-0.823493
C	4.794979	-2.156873	-1.385523
C	5.950190	-2.536110	-0.702670
C	6.231432	-1.937492	0.526792
C	5.345676	-0.982905	1.025899
N	4.231648	-0.610142	0.369993
Cu	-1.915096	0.432228	-0.585254
H	4.519104	-2.584999	-2.342863
H	6.617376	-3.284432	-1.121156
H	5.517698	-0.491081	1.977465
H	7.117973	-2.198925	1.095942
B	-2.669768	-1.309688	-0.104701
O	-4.005133	-1.548146	0.147224
O	-1.912966	-2.462894	0.034051
C	-4.131232	-2.891824	0.708693
C	-2.825686	-3.592892	0.188257
H	0.170005	-1.340163	-0.637690

```
 H                0.276586    0.035752    0.622041
 H                0.551829    0.311027   -2.492424
 C                0.451269    2.106578   -1.209662
 H                0.904737    2.412881   -0.263882
 H                0.790205    2.754003   -2.024678
 O               -1.001527    2.202949   -1.120577
 C               -1.519477    3.421567   -0.647300
 C               -2.417219    4.096002   -1.471385
 C               -1.182489    3.890328    0.623018
 C               -2.997360    5.281523   -1.009594
 H               -2.653795    3.686658   -2.448998
 C               -1.763049    5.082012    1.065974
 H               -0.487070    3.338250    1.250078
 C               -2.668469    5.777129    0.256166
 H               -3.702550    5.815606   -1.640713
 H               -1.509435    5.459676    2.052642
 H               -3.118206    6.700078    0.611950
 Cu               2.941048    0.704754    1.097341
 Cl               1.700973    1.989016    2.312967
 C               -2.984185   -4.222020   -1.201978
 H               -1.995777   -4.506446   -1.577287
 H               -3.614113   -5.117983   -1.168142
 H               -3.422650   -3.510677   -1.909049
 C               -2.201149   -4.596278    1.153544
 H               -2.899087   -5.416285    1.362144
 H               -1.296448   -5.023156    0.707427
 H               -1.921098   -4.125227    2.098622
 C               -5.436861   -3.506602    0.212915
 H               -5.523555   -4.548137    0.546090
 H               -6.284992   -2.945564    0.619126
 H               -5.506756   -3.479741   -0.877008
 C               -4.167242   -2.728082    2.233731
 H               -4.993608   -2.060569    2.497817
 H               -4.320914   -3.688963    2.737690
 H               -3.240030   -2.280368    2.605231

 Electronic Energy =  -2106.29170211 (Hartree/Particle)
 Dipole Moment (Debye):      4.4089
 index           1
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -368.166

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.448483
(Hartree/Particle)
 Thermal correction to Energy=                    0.480537
 Thermal correction to Enthalpy=                  0.481481
 Thermal correction to Gibbs Free Energy=         0.380349
 Sum of electronic and zero-point Energies=          -2105.843219
 Sum of electronic and thermal Energies=             -2105.811165
 Sum of electronic and thermal Enthalpies=           -2105.810221
 Sum of electronic and thermal Free Energies=        -2105.911353
 PCM-SP (solvent=THF;6-311+g(2d,p)) = -2106.69111316
 Corrected Free Energy =  -2106.310764052
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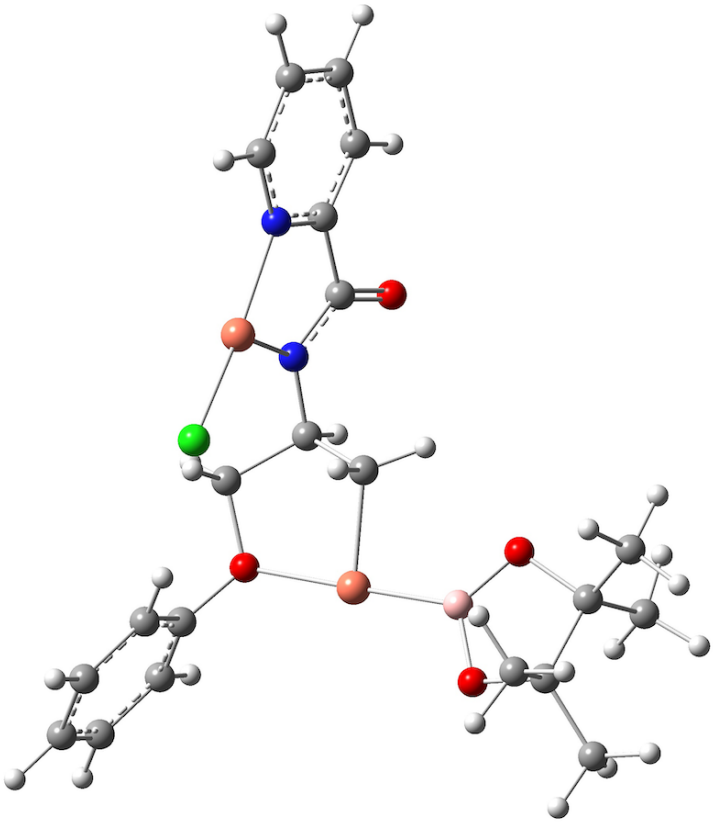


I-ANTI (Ref 35) Substrate: 1c
Path: anti-Markovnikov

CARTESIAN COORDINATES

C	0.870390	0.483220	-1.391602
N	2.163295	0.148304	-0.863028
C	2.891909	-0.789973	-1.503370
O	2.635123	-1.379778	-2.567586
C	0.012736	-0.433938	-0.515526
C	4.186542	-1.101449	-0.766692
C	5.167254	-1.883078	-1.379666
C	6.346795	-2.158255	-0.688183
C	6.506738	-1.649025	0.602734
C	5.476443	-0.885490	1.151537
N	4.340703	-0.612882	0.486959
Cu	-1.760464	0.423450	-0.784135
H	4.976409	-2.254938	-2.380450
H	7.126934	-2.760550	-1.146143
H	5.544872	-0.474916	2.154092
H	7.405974	-1.839122	1.180715
B	-2.602849	-1.273764	-0.269085
O	-3.894121	-1.184739	0.179168
O	-2.103652	-2.543617	-0.270648
C	-4.236650	-2.497121	0.758239
C	-3.218893	-3.451063	0.030454
H	0.040428	-1.480861	-0.807503
H	0.142433	-0.270237	0.558583
H	0.750683	0.227880	-2.451365
C	0.601585	1.961569	-1.132569
H	0.924892	2.221517	-0.122864
H	1.084493	2.605867	-1.872072

O	-0.852806	2.165049	-1.241774
C	-1.369796	3.351751	-0.685853
C	-2.100466	4.184701	-1.529969
C	-1.194000	3.634822	0.669746
C	-2.678032	5.342253	-0.998931
H	-2.207418	3.921161	-2.578064
C	-1.770673	4.800235	1.182216
H	-0.616275	2.967726	1.306160
C	-2.511859	5.651731	0.354910
H	-3.251827	6.001070	-1.645064
H	-1.639753	5.035814	2.234649
H	-2.958234	6.553833	0.764252
Cu	2.767511	0.464167	1.169616
Cl	1.336044	1.443179	2.504410
C	-2.686910	-4.597144	0.883765
H	-3.508313	-5.250351	1.201400
H	-1.980776	-5.194541	0.298232
H	-2.165293	-4.231553	1.770958
C	-3.726108	-3.974791	-1.317437
H	-2.897288	-4.456557	-1.845232
H	-4.527072	-4.709613	-1.182616
H	-4.100373	-3.160071	-1.945657
C	-5.706708	-2.779725	0.472706
H	-5.974603	-3.786030	0.816274
H	-6.331542	-2.057929	1.008436
H	-5.935051	-2.700874	-0.592556
C	-3.992703	-2.376814	2.265923
H	-4.597808	-1.554231	2.659383
H	-4.275670	-3.297290	2.787881
H	-2.942602	-2.159121	2.484695

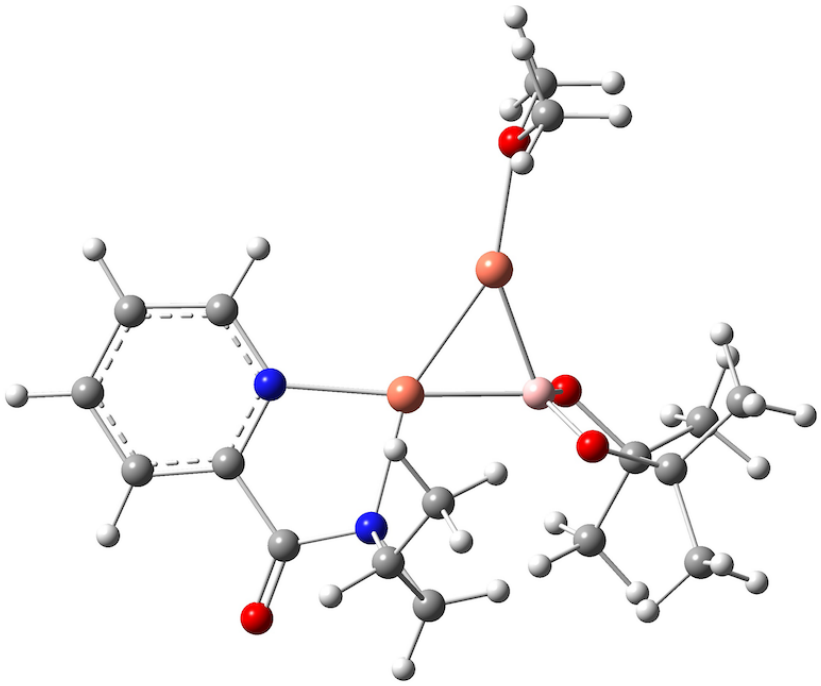
Electronic Energy = -2106.29855042 (Hartree/Particle)
Dipole Moment (Debye): 4.8348
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.449219
(Hartree/Particle)
Thermal correction to Energy= 0.481494
Thermal correction to Enthalpy= 0.482438
Thermal correction to Gibbs Free Energy= 0.380654
Sum of electronic and zero-point Energies= -2105.849331
Sum of electronic and thermal Energies= -2105.817057
Sum of electronic and thermal Enthalpies= -2105.816113
Sum of electronic and thermal Free Energies= -2105.917897
PCM-SP (solvent=THF;6-311+g(2d,p)) = -2106.70346197
Corrected Free Energy = -2106.32280855

MODEL: [Az-(Cu)2-Bpin]+/Et2O

SUBSTRATE: N-(2-PICOLINOYL)-METHYL AZIRIDINE



Complex-3 Substrate: N-(2-picolinoyl)-methyl aziridine

CARTESIAN COORDINATES

C	-1.622828	-2.024526	2.067654
N	-1.634373	-1.650290	0.586061
C	-2.920781	-1.735007	-0.032439
O	-3.503346	-2.773999	-0.262503
C	-1.027365	-2.916992	1.050105
C	-3.494921	-0.391474	-0.384133
C	-4.831857	-0.281133	-0.764719
C	-5.334804	0.984322	-1.074148
C	-4.481917	2.086885	-0.998723
C	-3.151618	1.886600	-0.623648
N	-2.664364	0.674298	-0.319376
Cu	0.947242	1.800979	0.156688
H	-5.444890	-1.174806	-0.810273
H	-6.372484	1.106273	-1.369936
H	-2.445156	2.708560	-0.567791
H	-4.831799	3.087196	-1.232769
H	-1.552506	-3.825486	0.768996
H	0.053315	-2.914088	0.949190
C	-0.805652	-1.160460	2.990741
H	-0.663354	-1.685524	3.942945
H	0.176536	-0.946576	2.560435
Cu	-0.702231	0.172544	0.022006
B	1.308136	-0.220973	-0.175610
O	1.875196	-1.050364	0.774563
O	1.841024	-0.422532	-1.430556
C	3.045029	-1.694165	0.157435
C	2.697105	-1.614414	-1.372602
C	4.258412	-0.845567	0.553975
H	4.314497	-0.791679	1.645614
H	5.190617	-1.281199	0.180554
H	4.170398	0.174663	0.165507
C	3.180497	-3.105550	0.717114

```
 H                4.012817   -3.628842    0.232995
 H                3.385786   -3.060820    1.791434
 H                2.273736   -3.696218    0.567509
 C                3.892455   -1.399642   -2.294478
 H                4.596018   -2.235799   -2.209405
 H                3.552979   -1.344598   -3.333430
 H                4.422050   -0.473021   -2.062121
 C                1.840844   -2.783234   -1.872497
 H                1.484522   -2.556505   -2.881810
 H                2.416587   -3.713658   -1.909704
 H                0.965057   -2.938180   -1.234536
 H               -2.610052   -2.315554    2.425265
 H               -1.322988   -0.216858    3.199391
 O                1.572752    3.670284    0.377573
 C                2.232441    4.326414   -0.726013
 H                3.310902    4.134849   -0.687419
 H                1.810673    3.908406   -1.641204
 H                2.035915    5.403058   -0.678657
 C                2.009796    4.141289    1.669142
 H                3.078182    3.936560    1.803448
 H                1.816329    5.216585    1.749058
 H                1.427450    3.600703    2.416660

 Electronic Energy =  -1494.66752736 (Hartree/Particle)
 Dipole Moment (Debye):      6.5515
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.445587
(Hartree/Particle)
 Thermal correction to Energy=                    0.476418
 Thermal correction to Enthalpy=                  0.477363
 Thermal correction to Gibbs Free Energy=         0.379819
 Sum of electronic and zero-point Energies=          -1494.221940
 Sum of electronic and thermal Energies=             -1494.191109
 Sum of electronic and thermal Enthalpies=           -1494.190165
 Sum of electronic and thermal Free Energies=        -1494.287708
 PCM-SP (solvent=THF;6-311+g(2d,p)) = -1495.03244674
 Corrected Free Energy =  -1494.65262738

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PATH: ANTI_MARKOVNIKOV
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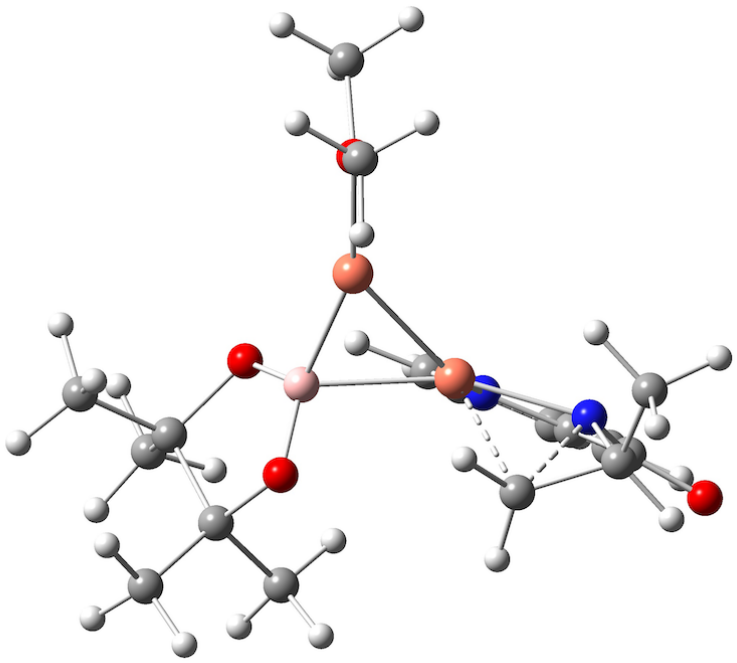

TS6 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: anti-markovnikov

CARTESIAN COORDINATES

C	-0.519753	-1.705512	2.098655
N	-1.719718	-2.022773	0.601200
C	-2.995355	-1.471731	0.395808
O	-4.003184	-1.879996	0.950359
C	-1.498241	-2.791461	1.821734
C	-3.040690	-0.386718	-0.649237
C	-4.254505	0.077438	-1.150180
C	-4.228434	1.095576	-2.107426
C	-2.998119	1.618888	-2.511181
C	-1.827458	1.111109	-1.941894
N	-1.856035	0.122734	-1.038155
Cu	1.981935	-0.858003	-0.428744
H	-5.179916	-0.354950	-0.785013
H	-5.154679	1.476381	-2.527602
H	-0.843833	1.498488	-2.187151
H	-2.938516	2.409737	-3.252164
H	-2.375483	-2.792596	2.473371
H	-0.844070	-0.817819	2.633829
Cu	-0.333172	-0.793036	0.063376
B	1.061889	0.841975	0.192948
O	1.058368	1.890486	-0.697158
O	0.952632	1.252091	1.503048
C	1.151060	3.137260	0.083044
C	0.615447	2.686069	1.489779
H	0.548843	-1.902779	2.067133
C	-0.943630	-4.185011	1.587081
H	-0.623849	-4.629252	2.536527
H	-1.710626	-4.827488	1.143777
C	1.288237	3.354821	2.682209
H	1.124357	4.438083	2.653733
H	0.860112	2.971006	3.613512
H	2.363488	3.164827	2.700114

```
 C              -0.910379    2.760797    1.617866
 H              -1.215735    2.258963    2.541564
 H              -1.257633    3.797781    1.661980
 H              -1.404421    2.261070    0.778622
 C               2.629940    3.534851    0.087982
 H               2.974456    3.640730   -0.945239
 H               2.783503    4.488742    0.602556
 H               3.245018    2.772351    0.576786
 C               0.310877    4.201599   -0.613891
 H               0.290343    5.121860   -0.019333
 H               0.747717    4.437747   -1.589415
 H              -0.717762    3.868413   -0.771322
 H              -0.085759   -4.149322    0.905038
 O               3.361647   -2.111517   -1.077823
 C               4.444972   -2.553912   -0.233470
 H               4.656621   -3.609277   -0.436225
 H               5.336814   -1.944269   -0.417279
 H               4.114077   -2.431505    0.798944
 C               3.638435   -2.244064   -2.488692
 H               2.744799   -1.913405   -3.019858
 H               4.494284   -1.617113   -2.762803
 H               3.844412   -3.294376   -2.720994

 Electronic Energy =  -1494.63027914 (Hartree/Particle)
 Dipole Moment (Debye):      4.9667
 index           1
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -218.939

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.443468
(Hartree/Particle)
 Thermal correction to Energy=                    0.473912
 Thermal correction to Enthalpy=                  0.474856
 Thermal correction to Gibbs Free Energy=         0.378379
 Sum of electronic and zero-point Energies=          -1494.186811
 Sum of electronic and thermal Energies=             -1494.156367
 Sum of electronic and thermal Enthalpies=           -1494.155423
 Sum of electronic and thermal Free Energies=        -1494.251900
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1494.99838714
 Corrected Free Energy =  -1494.62000800

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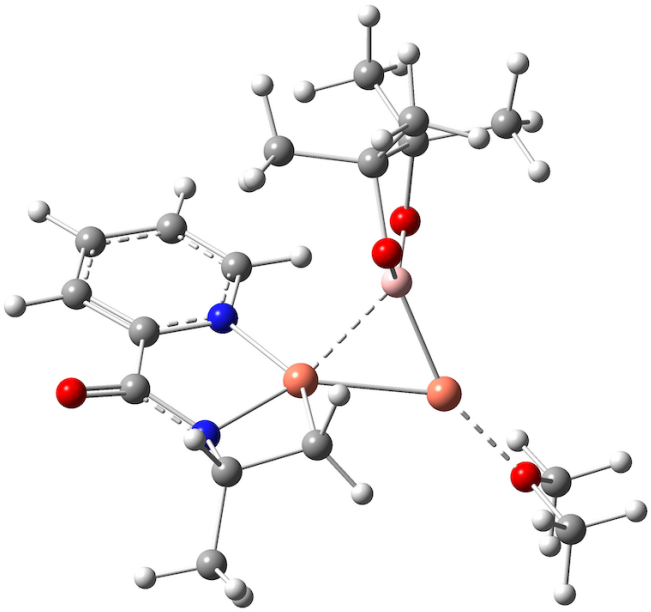

I4 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: anti-markovnikov

CARTESIAN COORDINATES

C	-0.062028	-2.001004	-1.752783
N	1.753341	-1.993420	-0.575061
C	2.983136	-1.418280	-0.382117
O	4.003913	-1.698031	-0.996859
C	1.327208	-2.625282	-1.822674
C	2.954379	-0.402353	0.740642
C	4.116387	0.086603	1.326314
C	3.998336	1.034123	2.346793
C	2.726734	1.468135	2.730198
C	1.608305	0.949359	2.076509
N	1.727403	0.028766	1.107499
Cu	-1.966066	-0.792231	0.433375
H	5.075211	-0.277581	0.972147
H	4.885035	1.430387	2.832972
H	0.600248	1.279466	2.299837
H	2.595456	2.202660	3.518193
H	1.905548	-2.242211	-2.672862
H	-0.313732	-1.201991	-2.449388
Cu	0.344827	-0.885595	-0.095731
B	-1.004531	0.854947	-0.243478
O	-1.024645	1.916502	0.621517
O	-0.806096	1.213386	-1.550870
C	-1.027522	3.148409	-0.197301
C	-0.421140	2.640006	-1.555985
H	-0.886819	-2.667617	-1.497809
C	1.375893	-4.145541	-1.787769
H	0.938095	-4.560918	-2.703743
H	2.412269	-4.489441	-1.712392
C	-0.998498	3.292098	-2.805458
H	-0.801736	4.370097	-2.796002
H	-0.525661	2.868517	-3.696815
H	-2.076193	3.134557	-2.885096
C	1.110591	2.658003	-1.591227
H	1.454262	2.109901	-2.473756

```
 H                1.494413    3.681147   -1.651002
 H                1.535996    2.176745   -0.705038
 C               -2.488846    3.590973   -0.302729
 H               -2.891567    3.738874    0.703897
 H               -2.577820    4.533828   -0.851482
 H               -3.099208    2.835681   -0.808368
 C               -0.194168    4.200046    0.525115
 H               -0.101918    5.101267   -0.091295
 H               -0.683076    4.479723    1.463607
 H                0.808916    3.834537    0.756945
 H                0.819416   -4.528156   -0.923835
 O               -3.418709   -1.934754    1.095072
 C               -4.371119   -2.556540    0.204661
 H               -4.549977   -3.587601    0.527299
 H               -5.307444   -1.987852    0.204326
 H               -3.928182   -2.548745   -0.792378
 C               -3.853824   -1.897223    2.472678
 H               -4.768279   -1.300084    2.557718
 H               -4.029237   -2.919087    2.824891
 H               -3.049285   -1.437309    3.048025

 Electronic Energy =  -1494.63618139 (Hartree/Particle)
 Dipole Moment (Debye):      7.4110
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.444581
(Hartree/Particle)
 Thermal correction to Energy=                    0.475281
 Thermal correction to Enthalpy=                  0.476226
 Thermal correction to Gibbs Free Energy=         0.379534
 Sum of electronic and zero-point Energies=          -1494.191600
 Sum of electronic and thermal Energies=             -1494.160900
 Sum of electronic and thermal Enthalpies=           -1494.159956
 Sum of electronic and thermal Free Energies=        -1494.256648
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1495.00805742
 Corrected Free Energy =  -1494.62852403

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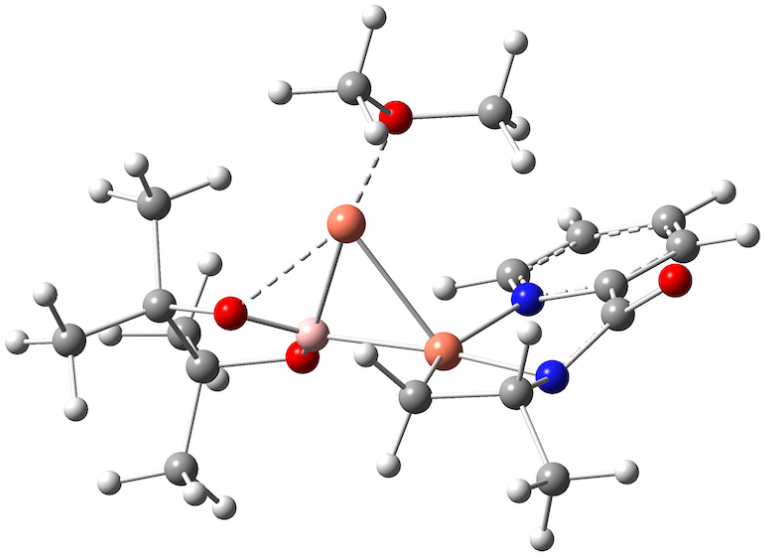


TS7 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: anti-markovnikov

CARTESIAN COORDINATES

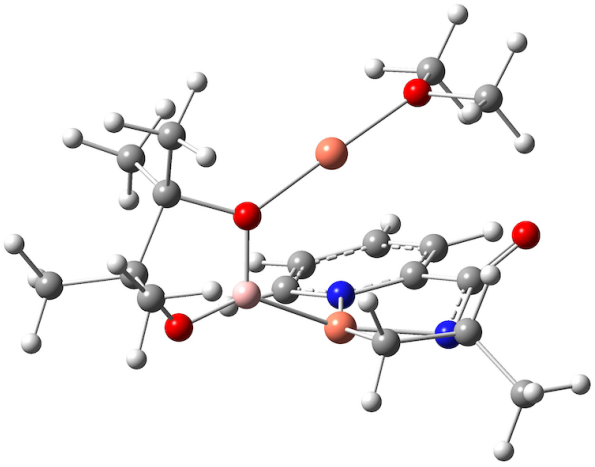
N	-1.341523	1.690711	-0.070809
C	-2.684775	1.534832	-0.119351
C	-3.502407	2.443409	-0.781734
C	-2.910435	3.562834	-1.373802
C	-1.523400	3.724743	-1.301954
C	-0.763043	2.755033	-0.648428
C	-3.209900	0.271926	0.547683
O	-4.284303	-0.233400	0.224959
Cu	-0.562472	0.093511	0.886909
N	-2.319811	-0.181747	1.469437
C	-2.235886	-1.576381	1.921501
C	-0.707266	-1.660718	1.857030
B	1.462592	0.134015	0.448949
Cu	0.431260	-1.188648	-0.888183
O	2.363783	-0.895944	0.217601
C	3.673057	-0.258370	-0.116340
C	4.782175	-1.139407	0.439383
O	2.050516	1.356521	0.527906
C	3.518661	1.142944	0.575730
C	3.905101	1.144256	2.056170
C	3.730811	-0.194077	-1.643313
C	4.186280	2.295649	-0.162979
H	-4.571130	2.258782	-0.817415
H	-3.522486	4.300528	-1.884668
H	0.317634	2.811055	-0.565052
H	-1.033003	4.584801	-1.746180
H	-0.182884	-1.438534	2.790043
H	4.683342	0.220136	-1.986966
H	3.633915	-1.206263	-2.049235
H	2.919230	0.420683	-2.048309
H	4.802071	-2.095663	-0.092327
H	5.753718	-0.652405	0.298711
H	4.645185	-1.342891	1.503165
H	4.019044	3.229122	0.382641
H	5.267521	2.129226	-0.227008

H	3.791654	2.415976	-1.174536
H	4.988740	1.053170	2.180345
H	3.584812	2.087833	2.507353
H	3.422265	0.325597	2.599449
O	-0.689347	-2.076670	-2.220289
C	-0.553617	-3.499652	-2.439165
H	-0.985002	-3.756069	-3.412089
H	0.514781	-3.719563	-2.435495
H	-1.060676	-4.053788	-1.641053
C	-2.067504	-1.621729	-2.246827
H	-2.621747	-2.032478	-1.396887
H	-2.040318	-0.533938	-2.180929
H	-2.527580	-1.927980	-3.191290
H	-2.702179	-2.243221	1.183174
H	-0.255068	-2.500671	1.329066
C	-2.845078	-1.820622	3.296219
H	-3.925950	-1.647315	3.261933
H	-2.668238	-2.853344	3.620507
H	-2.407946	-1.138705	4.034511

Electronic Energy = -1494.62665898 (Hartree/Particle)
Dipole Moment (Debye): 6.1152
index 1
Number of imaginary frequencies= 1
Negatives Eigenvalues: -54.390

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.444377
(Hartree/Particle)
Thermal correction to Energy= 0.474024
Thermal correction to Enthalpy= 0.474969
Thermal correction to Gibbs Free Energy= 0.382269
Sum of electronic and zero-point Energies= -1494.182282
Sum of electronic and thermal Energies= -1494.152635
Sum of electronic and thermal Enthalpies= -1494.151690
Sum of electronic and thermal Free Energies= -1494.244390
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1494.99926829
Corrected Free Energy = -1494.61699931



I5 Substrate: N-(2-picolinoyl)-methyl aziridine

Path: anti-markovnikov

CARTESIAN COORDINATES

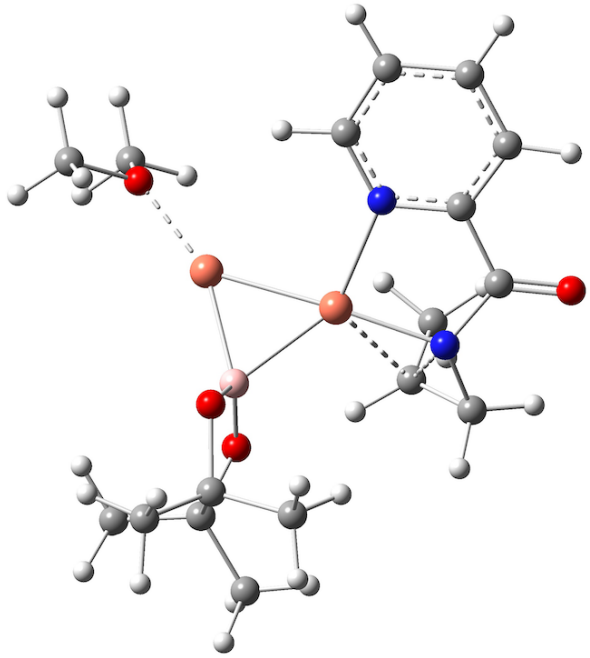
N	-1.434097	-1.638047	-0.767203
C	-2.649461	-1.148160	-0.417649
C	-3.636065	-1.965398	0.125796
C	-3.373430	-3.329660	0.270682
C	-2.122259	-3.829460	-0.104622
C	-1.170744	-2.945663	-0.610968
C	-2.808743	0.359624	-0.587834
O	-3.539707	0.998669	0.187096
Cu	-0.340116	-0.082714	-1.448442
N	-2.013303	0.805357	-1.574585
C	-1.473320	2.176900	-1.619696
C	0.016351	1.823660	-1.825586
B	1.530134	-0.243412	-0.914414
Cu	0.338963	0.680745	1.525958
O	1.788771	0.174682	0.426023
C	3.169524	-0.285741	0.802068
C	3.770533	0.747484	1.740781
O	2.665175	-0.685046	-1.490635
C	3.819084	-0.374396	-0.621639
C	4.382676	0.959057	-1.118187
C	2.986785	-1.633639	1.496175
C	4.843619	-1.491428	-0.773607
H	-4.583933	-1.521771	0.412717
H	-4.132990	-3.996244	0.669090
H	-0.179343	-3.273734	-0.907490
H	-1.883479	-4.883650	-0.009003
H	3.946115	-2.026369	1.845797
H	2.334704	-1.506119	2.367775
H	2.530730	-2.370203	0.828033
H	3.223816	0.753912	2.690726
H	4.813707	0.494663	1.958524
H	3.738274	1.752842	1.316107
H	5.240187	-1.485872	-1.792840
H	5.679521	-1.339826	-0.081336
H	4.405353	-2.474245	-0.587125
H	5.287801	1.236537	-0.568746
H	4.638018	0.862060	-2.177016
H	3.650472	1.767358	-1.018880
H	-1.623902	2.670902	-0.649855
H	0.354515	1.849430	-2.864799
O	-1.128337	1.206688	2.594277
C	-1.710505	2.532993	2.434893
H	-2.496308	2.491043	1.675962
H	-2.108224	2.851620	3.403412
H	-0.899964	3.196632	2.130444
C	-2.098750	0.221998	3.046172
H	-1.570055	-0.728874	3.127626
H	-2.468293	0.528838	4.029712
H	-2.913205	0.161182	2.319473
C	-2.076999	3.030513	-2.729071
H	-3.145715	3.183838	-2.543538
H	-1.586443	4.010205	-2.778216
H	-1.963316	2.531049	-3.697910
H	0.729527	2.315747	-1.162369

Electronic Energy = -1494.63850993 (Hartree/Particle)
Dipole Moment (Debye): 6.7992
index 0
Harmonic frequencies
Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.445809
(Hartree/Particle)
Thermal correction to Energy= 0.475584
Thermal correction to Enthalpy= 0.476528
Thermal correction to Gibbs Free Energy= 0.384442
Sum of electronic and zero-point Energies= -1494.192701
Sum of electronic and thermal Energies= -1494.162926
Sum of electronic and thermal Enthalpies= -1494.161982
Sum of electronic and thermal Free Energies= -1494.254068
PCM-SP (solvent=THF;6-311+g(2d,p)) = -1495.01084685
Corrected Free Energy = -1494.62640492

PATH: MARKOVNIKOV



TS6 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: markovnikov

CARTESIAN COORDINATES

C	-0.207839	-1.111433	2.371665
N	-1.256211	-1.980627	0.910721
C	-2.640289	-1.948111	0.759195
O	-3.432390	-2.569946	1.455146
C	-0.735294	-2.488354	2.172693
C	-3.104664	-1.122357	-0.417849
C	-4.402095	-1.243019	-0.912000

C	-4.769734	-0.458747	-2.008001
C	-3.835881	0.422796	-2.559042
C	-2.564921	0.497990	-1.986265
N	-2.210552	-0.261058	-0.940778
Cu	0.437545	1.820116	0.175225
H	-5.086838	-1.937735	-0.437564
H	-5.768660	-0.535792	-2.427154
H	-1.798579	1.164872	-2.371501
H	-4.081311	1.039468	-3.417809
H	-1.510656	-2.810036	2.872385
H	0.019425	-3.264003	2.028047
Cu	-0.460280	-0.358051	0.193814
B	1.575895	0.185087	-0.221178
O	2.542670	-0.164502	0.694833
O	1.833476	-0.288448	-1.483571
C	3.654995	-0.781104	-0.052551
C	2.937527	-1.258266	-1.366179
H	0.853032	-0.935684	2.203752
C	-0.978055	-0.109178	3.165886
H	-0.699108	-0.246028	4.224384
H	-0.733493	0.919644	2.885710
C	2.273567	-2.633656	-1.236696
H	1.638340	-2.806184	-2.110595
H	3.018330	-3.434107	-1.186005
H	1.638166	-2.686288	-0.345726
C	3.786544	-1.185293	-2.628915
H	4.664277	-1.834910	-2.534957
H	3.201488	-1.525749	-3.488801
H	4.125484	-0.166975	-2.831192
C	4.687211	0.325900	-0.284997
H	4.990293	0.740782	0.681247
H	5.578394	-0.062798	-0.787953
H	4.271361	1.136990	-0.891581
C	4.244722	-1.897115	0.801391
H	5.016449	-2.437982	0.242075
H	4.708840	-1.473358	1.697552
H	3.481829	-2.612436	1.118139
H	-2.058352	-0.265877	3.090474
O	-0.167776	3.669906	0.538758
C	-1.235795	4.254974	-0.233158
H	-0.826514	4.800894	-1.090949
H	-1.865066	3.431499	-0.575153
H	-1.818698	4.929383	0.403447
C	0.728137	4.642986	1.118499
H	0.162030	5.311173	1.776202
H	1.467053	4.087178	1.697643
H	1.223030	5.216378	0.326624

Electronic Energy = -1494.63033337 (Hartree/Particle)
Dipole Moment (Debye): 6.6498
index 1
Number of imaginary frequencies= 1
Negatives Eigenvalues: -149.298

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.443409
(Hartree/Particle)
Thermal correction to Energy= 0.474038

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 Thermal correction to Enthalpy=                  0.474982
 Thermal correction to Gibbs Free Energy=         0.377125
 Sum of electronic and zero-point Energies=          -1494.186925
 Sum of electronic and thermal Energies=             -1494.156296
 Sum of electronic and thermal Enthalpies=           -1494.155351
 Sum of electronic and thermal Free Energies=        -1494.253208
 PCM-SP (solvent=THF;6-311+g(2d,p)) = -1495.00034032
 Corrected Free Energy =  -1494.62321195
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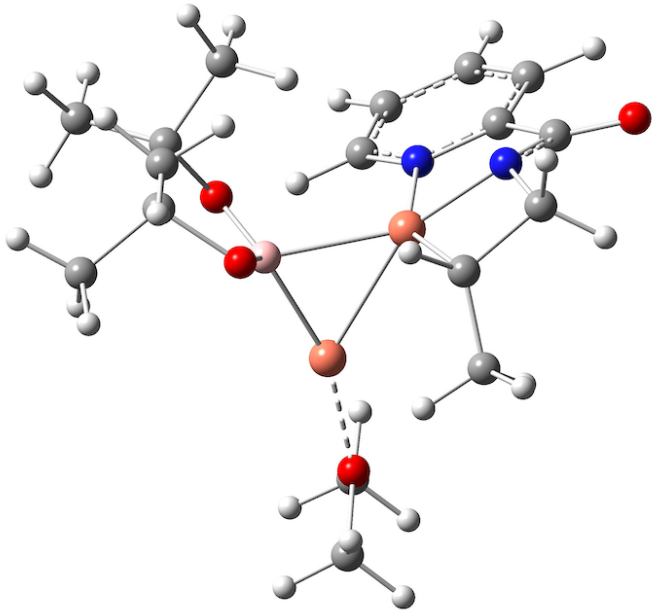

I4 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: markovnikov

CARTESIAN COORDINATES

C	-0.357889	0.490724	2.648771
N	-1.809593	-0.875464	1.805430
C	-3.039872	-1.069525	1.238066
O	-4.100541	-1.151938	1.844122
C	-1.574261	-0.302065	3.117428
C	-2.934576	-1.236452	-0.266082
C	-3.978053	-1.742480	-1.033700
C	-3.781757	-1.878209	-2.411055
C	-2.556353	-1.501981	-2.969169
C	-1.564841	-0.985581	-2.133491
N	-1.762154	-0.854831	-0.814331
Cu	0.484806	1.747456	-0.420414
H	-4.906384	-2.018050	-0.544085
H	-4.571933	-2.277743	-3.040103
H	-0.585071	-0.690279	-2.495722
H	-2.365706	-1.608013	-4.032304
H	-2.404575	0.327787	3.459406
H	-1.360878	-1.056073	3.883533
Cu	-0.585827	-0.066793	0.673700
B	1.469040	0.009017	-0.128314
O	2.430936	-0.111671	0.836529

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 O                 1.579317   -0.912136   -1.138298
 C                 3.413238   -1.103945    0.351664
 C                 2.563683   -1.919743   -0.689027
 H                 0.612248    0.025605    2.829238
 C                -0.399096    1.990898    2.748313
 H                -1.301183    2.409965    2.288970
 H                -0.425101    2.266180    3.815878
 C                 1.740045   -3.047697   -0.058957
 H                 1.035787   -3.433872   -0.802031
 H                 2.379901   -3.871827    0.271309
 H                 1.161179   -2.688516    0.799227
 C                 3.335576   -2.421652   -1.901717
 H                 4.130810   -3.107130   -1.587661
 H                 2.662812   -2.967337   -2.570721
 H                 3.784953   -1.601077   -2.465225
 C                 4.556465   -0.305746   -0.280413
 H                 4.965709    0.383546    0.464318
 H                 5.361175   -0.967438   -0.616185
 H                 4.208565    0.281368   -1.136670
 C                 3.909262   -1.906942    1.547605
 H                 4.571820   -2.714005    1.215011
 H                 4.476926   -1.257141    2.220759
 H                 3.083867   -2.345585    2.113007
 H                 0.484272    2.454017    2.298235
 O                 0.021816    3.576142   -0.971194
 C                -0.639535    3.844954   -2.226717
 H                -1.402509    4.616094   -2.076981
 H                 0.093408    4.171816   -2.972489
 H                -1.109496    2.912777   -2.543604
 C                 0.659228    4.735891   -0.391944
 H                 1.444747    5.103322   -1.061239
 H                -0.091624    5.514128   -0.219567
 H                 1.093114    4.419371    0.557556

 Electronic Energy =  -1494.63510643 (Hartree/Particle)
 Dipole Moment (Debye):      7.3136
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.444520
(Hartree/Particle)
 Thermal correction to Energy=                    0.475391
 Thermal correction to Enthalpy=                  0.476335
 Thermal correction to Gibbs Free Energy=         0.378135
 Sum of electronic and zero-point Energies=          -1494.190586
 Sum of electronic and thermal Energies=             -1494.159715
 Sum of electronic and thermal Enthalpies=           -1494.158771
 Sum of electronic and thermal Free Energies=        -1494.256972
 PCM-SP (solvent=THF;6-311+g(2d,p)) = -1495.00722031
 Corrected Free Energy =  -1494.62908588

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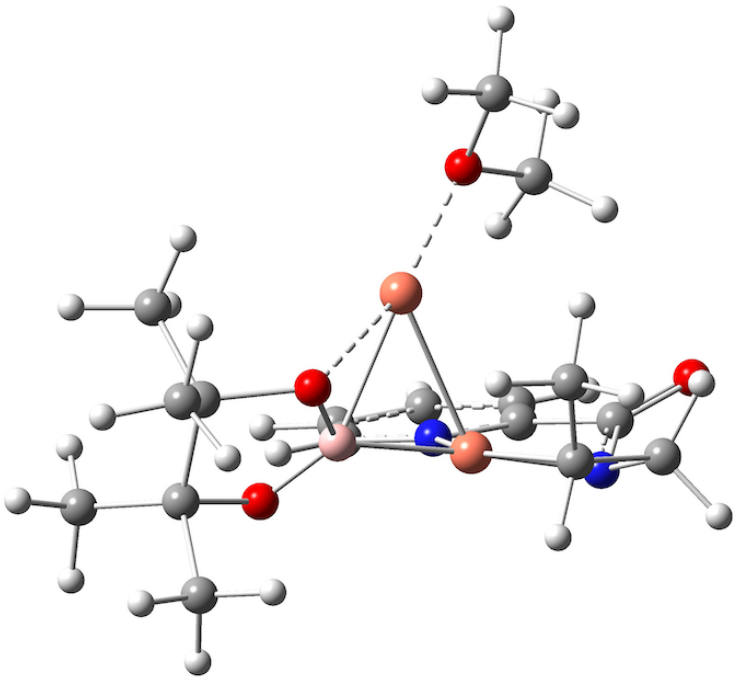

TS7 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: markovnikov

CARTESIAN COORDINATES

N	-1.591252	1.537604	-0.111311
C	-2.915977	1.277911	-0.037970
C	-3.849470	2.030045	-0.742960
C	-3.394139	3.103632	-1.513588
C	-2.023728	3.376030	-1.569155
C	-1.144791	2.557762	-0.859103
C	-3.297987	0.082106	0.823876
O	-4.362111	-0.516763	0.670703
Cu	-0.607052	0.125341	0.986720
N	-2.302648	-0.200995	1.700358
C	-2.101730	-1.487937	2.354725
C	-0.573848	-1.510556	2.218384
B	1.354694	0.277164	0.428169
Cu	0.413875	-1.317192	-0.729786
O	2.276754	-0.739005	0.161304
C	3.511188	-0.086433	-0.374204
C	4.712858	-0.884832	0.108310
O	1.905767	1.516272	0.338504
C	3.374811	1.356516	0.227484
C	3.930458	1.484012	1.647769
C	3.387197	-0.139685	-1.897509
C	3.904895	2.470608	-0.666192
H	-4.899163	1.764239	-0.671618
H	-4.098613	3.721605	-2.062871
H	-0.069253	2.706705	-0.864758
H	-1.637410	4.206010	-2.151900
H	4.274522	0.276168	-2.383904
H	3.286102	-1.184198	-2.211440
H	2.508560	0.415148	-2.245277
H	4.711556	-1.878395	-0.350549
H	5.640502	-0.378260	-0.180934

```
 H                4.708274   -1.009937    1.192759
 H                3.759632    3.437034   -0.174486
 H                4.978128    2.337552   -0.843458
 H                3.392634    2.499216   -1.630719
 H                5.024058    1.438984    1.649942
 H                3.624021    2.447746    2.064450
 H                3.547894    0.693862    2.302012
 O               -0.757111   -2.426913   -1.819069
 C               -0.381420   -2.849147   -3.148787
 H               -0.648082   -2.075912   -3.878157
 H                0.697965   -3.005530   -3.138598
 H               -0.892338   -3.787989   -3.385964
 C               -2.186526   -2.247252   -1.652459
 H               -2.698202   -3.177263   -1.918286
 H               -2.361374   -2.013830   -0.603352
 H               -2.536236   -1.422409   -2.282299
 H               -2.603761   -2.310758    1.829976
 H               -0.166766   -2.356778    1.661201
 C                0.240912   -1.126482    3.429535
 H                0.133938   -1.918913    4.188091
 H                1.304019   -1.022386    3.194680
 H               -0.117220   -0.195341    3.880580
 H               -2.440048   -1.491288    3.399123

 Electronic Energy =  -1494.62566448 (Hartree/Particle)
 Dipole Moment (Debye):      6.8825
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:            -59.462

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.444587
(Hartree/Particle)
 Thermal correction to Energy=                    0.474370
 Thermal correction to Enthalpy=                  0.475314
 Thermal correction to Gibbs Free Energy=         0.381934
 Sum of electronic and zero-point Energies=          -1494.181077
 Sum of electronic and thermal Energies=             -1494.151295
 Sum of electronic and thermal Enthalpies=           -1494.150351
 Sum of electronic and thermal Free Energies=        -1494.243731
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1494.99785619
 Corrected Free Energy =  -1494.61592271

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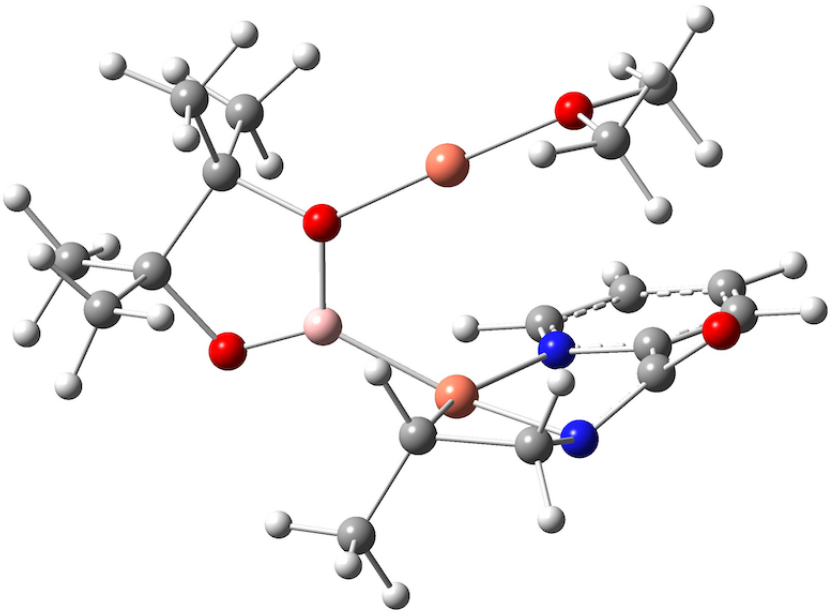

I5 Substrate: N-(2-picolinoyl)-methyl aziridine
Path: markovnikov

CARTESIAN COORDINATES

N	1.627319	1.413291	0.948592
C	2.809399	0.923798	0.502038
C	3.916954	0.813098	1.337781
C	3.809360	1.259183	2.657036
C	2.589732	1.774491	3.107582
C	1.514402	1.824378	2.221765
C	2.801745	0.434396	-0.942610
O	3.526810	-0.515149	-1.282304
Cu	0.318347	1.318076	-0.611509
N	1.888566	1.109135	-1.659743
C	1.233792	0.552823	-2.847430
C	-0.239100	0.828294	-2.473132
B	-1.482074	0.846121	-0.018148
Cu	-0.185738	-1.702856	0.099528
O	-1.671105	-0.546841	0.234083
C	-2.999604	-0.730145	0.911462
C	-3.583639	-2.056304	0.452871
O	-2.633252	1.513691	0.203163
C	-3.738346	0.554249	0.400583
C	-4.396175	0.373366	-0.969732
C	-2.708214	-0.735204	2.410394
C	-4.717401	1.153968	1.401721
H	4.834301	0.392156	0.939136
H	4.663713	1.207806	3.325964
H	0.541075	2.202804	2.518669
H	2.469266	2.132541	4.124852
H	1.528361	1.074953	-3.767162
H	-3.623204	-0.904972	2.985617
H	-2.007699	-1.545968	2.640064
H	-2.262130	0.209543	2.734962
H	-2.974254	-2.884938	0.831389

```
 H              -4.596449   -2.178500    0.851411
 H              -3.628030   -2.128637   -0.635767
 H              -5.180854    2.045238    0.969204
 H              -5.511567    0.436373    1.636952
 H              -4.221684    1.447823    2.329420
 H              -5.273291   -0.278411   -0.907222
 H              -4.719265    1.351043   -1.338018
 H              -3.696641   -0.049597   -1.698702
 H               1.453059   -0.514812   -2.974850
 O               1.313575   -2.839247   -0.081794
 C               1.746176   -3.267299   -1.405794
 H               2.457277   -2.538571   -1.804251
 H               2.201338   -4.258378   -1.314443
 H               0.849405   -3.327285   -2.024168
 C               2.412684   -2.766437    0.867854
 H               1.990764   -2.426442    1.814732
 H               2.833451   -3.770048    0.985246
 H               3.163312   -2.064810    0.494764
 H              -0.873195   -0.061969   -2.474843
 C              -0.886963    2.030090   -3.127885
 H              -1.011968    1.829757   -4.203449
 H              -1.869725    2.252060   -2.702218
 H              -0.258885    2.922188   -3.033276

 Electronic Energy =  -1494.63626144 (Hartree/Particle)
 Dipole Moment (Debye):      6.3941
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.446040
(Hartree/Particle)
 Thermal correction to Energy=                    0.475915
 Thermal correction to Enthalpy=                  0.476860
 Thermal correction to Gibbs Free Energy=         0.384339
 Sum of electronic and zero-point Energies=          -1494.190221
 Sum of electronic and thermal Energies=             -1494.160346
 Sum of electronic and thermal Enthalpies=           -1494.159402
 Sum of electronic and thermal Free Energies=        -1494.251923
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1495.00833143
 Corrected Free Energy =  -1494.62399296

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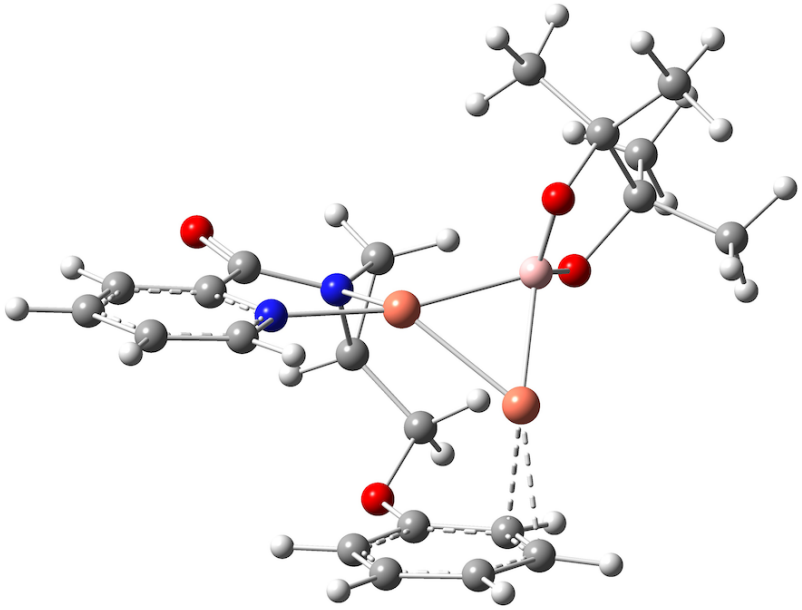
MODEL: [Az-(Cu)2-Bpin]+



SUBSTRATE: 1c

Complex-4 Substrate: 1c

CARTESIAN COORDINATES

C	-0.752006	-0.888987	2.640171
N	-0.723731	-1.508100	1.256852
C	-1.831681	-2.383315	0.993373
O	-2.083445	-3.375334	1.643643
C	0.227233	-1.943225	2.309504
C	-2.664487	-1.962356	-0.183873
C	-3.893055	-2.580490	-0.416932
C	-4.649106	-2.172392	-1.517892
C	-4.145894	-1.169037	-2.347536
C	-2.901776	-0.608245	-2.050518
N	-2.174349	-0.992845	-0.990466
Cu	0.535840	1.854037	-0.589879
H	-4.229995	-3.359860	0.257974
H	-5.610827	-2.632135	-1.724887
H	-2.461207	0.165344	-2.670810
H	-4.697968	-0.826064	-3.216699
H	0.069069	-2.936844	2.719276
H	1.247587	-1.650900	2.078128
H	-1.614743	-1.190585	3.231554
C	-0.371901	0.564190	2.739267
H	-0.094320	0.801741	3.772332
H	0.475554	0.771198	2.079813
O	-1.524208	1.354828	2.384622
C	-1.426943	2.256444	1.369414
C	-2.537511	2.394180	0.527561
C	-0.271907	3.039374	1.142745
C	-2.481158	3.247135	-0.578666
H	-3.422383	1.802133	0.738083
C	-0.219733	3.890552	0.012176
H	0.540671	3.038307	1.863101
C	-1.320968	3.976376	-0.862607

```
  H              -3.345711    3.332332   -1.230633
  H               0.637822    4.545979   -0.122159
  H              -1.276081    4.631672   -1.726204
  Cu             -0.326354   -0.308026   -0.534819
  B               1.707464    0.122023   -0.577131
  O               2.435831    0.037622    0.601424
  O               2.360311   -0.455787   -1.636602
  C               3.785269   -0.440057    0.249650
  C               3.517451   -1.189166   -1.103190
  C               4.659328    0.808726    0.095346
  H               4.631539    1.382638    1.026995
  H               5.700233    0.542269   -0.113692
  H               4.295447    1.449783   -0.714124
  C               4.303181   -1.316873    1.383729
  H               5.278195   -1.742281    1.120707
  H               4.429631   -0.716265    2.290366
  H               3.621984   -2.140654    1.610474
  C               4.651765   -1.113760   -2.118206
  H               5.559076   -1.575247   -1.711644
  H               4.371650   -1.655056   -3.027076
  H               4.877831   -0.081999   -2.395900
  C               3.054554   -2.638808   -0.916649
  H               2.692911   -3.022416   -1.875331
  H               3.873152   -3.279875   -0.574152
  H               2.233188   -2.703259   -0.194178

 Electronic Energy =  -1645.88840862 (Hartree/Particle)
 Dipole Moment (Debye):      3.6725
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.449779
(Hartree/Particle)
 Thermal correction to Energy=                    0.479705
 Thermal correction to Enthalpy=                  0.480649
 Thermal correction to Gibbs Free Energy=         0.387147
 Sum of electronic and zero-point Energies=          -1645.438629
 Sum of electronic and thermal Energies=             -1645.408704
 Sum of electronic and thermal Enthalpies=           -1645.407759
 Sum of electronic and thermal Free Energies=        -1645.501262
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1646.28883721
 Corrected Free Energy =  -1645.90169059

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PATH: ANTI_MARKOVNIKOV
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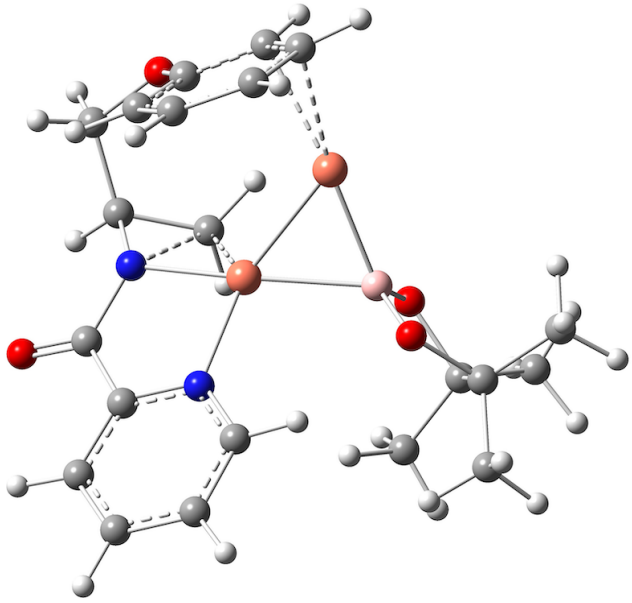

TS8 Substrate: 1c
Path: anti-markovnikov

CARTESIAN COORDINATES

C	-1.277074	0.149042	2.278648
N	-1.854696	1.299599	0.810837
C	-1.640396	2.680957	0.672199
O	-2.326525	3.523218	1.229023
C	-2.567346	0.835535	1.989605
C	-0.548881	3.036966	-0.303171
C	-0.360611	4.350409	-0.725053
C	0.675869	4.612387	-1.626511
C	1.485642	3.559950	-2.058088
C	1.240543	2.272662	-1.570855
N	0.239217	2.024814	-0.717163
Cu	-0.325657	-1.971591	-0.458528
H	-1.011819	5.130347	-0.344861
H	0.848500	5.623455	-1.983365
H	1.843507	1.413943	-1.850620
H	2.296981	3.725459	-2.759752
H	-2.832336	1.652986	2.667214
H	-0.530535	0.681534	2.859852
Cu	-0.321519	0.272325	0.252444
B	1.417622	-0.983334	0.079124
O	2.369566	-0.759766	-0.889861
O	1.955733	-1.056744	1.344820
C	3.692109	-0.907189	-0.256103
C	3.363276	-0.633654	1.254940
H	-1.199309	-0.931678	2.218539
C	-3.796407	-0.040742	1.730080
H	-4.320224	-0.206185	2.674236
H	-4.482345	0.463891	1.041589
O	-3.470203	-1.365789	1.286235
C	-3.086709	-1.632951	0.008661
C	-2.390104	-2.855323	-0.153411
C	-3.327754	-0.818266	-1.104073
C	-1.907129	-3.227485	-1.426612
H	-2.300850	-3.519888	0.701404

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 C              -2.838197   -1.195802   -2.361604
 H              -3.857996    0.119762   -0.997592
 C              -2.114142   -2.378107   -2.534592
 H              -1.445542   -4.203187   -1.561062
 H              -3.021181   -0.546662   -3.212803
 H              -1.738013   -2.659272   -3.512433
 C               4.181533   -1.444821    2.252135
 H               5.247532   -1.211882    2.149109
 H               3.876050   -1.195563    3.273137
 H               4.043620   -2.518775    2.110262
 C               3.378995    0.853969    1.625747
 H               2.954352    0.975687    2.627192
 H               4.397967    1.253534    1.634701
 H               2.777604    1.444122    0.925928
 C               4.147135   -2.342874   -0.534891
 H               4.159273   -2.510012   -1.616219
 H               5.154456   -2.522979   -0.146049
 H               3.464687   -3.070925   -0.084677
 C               4.647825    0.091704   -0.898940
 H               5.623053    0.062140   -0.400064
 H               4.797838   -0.165010   -1.952411
 H               4.265452    1.114095   -0.846585

 Electronic Energy =  -1645.85590322 (Hartree/Particle)
 Dipole Moment (Debye):      2.0153
 index           1
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -217.650

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.448034
(Hartree/Particle)
 Thermal correction to Energy=                    0.477323
 Thermal correction to Enthalpy=                  0.478267
 Thermal correction to Gibbs Free Energy=         0.387322
 Sum of electronic and zero-point Energies=          -1645.407869
 Sum of electronic and thermal Energies=             -1645.378580
 Sum of electronic and thermal Enthalpies=           -1645.377636
 Sum of electronic and thermal Free Energies=        -1645.468581
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1646.25760073
 Corrected Free Energy =   -1645.87027851

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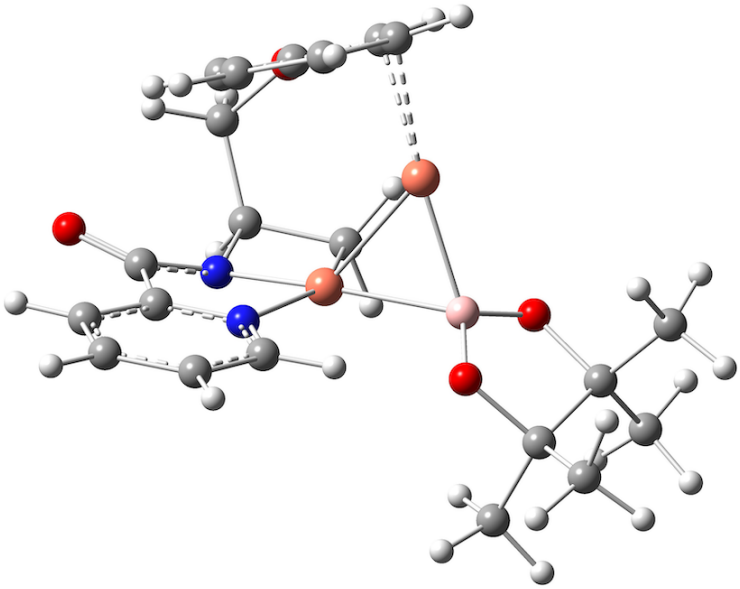

I6 Substrate: 1c
Path: anti-markovnikov

CARTESIAN COORDINATES

C	1.767079	-0.951000	3.032536
C	1.035503	-2.092204	2.639836
C	1.279393	-2.688790	1.379925
C	2.260972	-2.136945	0.513205
C	3.030585	-1.048557	0.945850
C	2.770333	-0.462663	2.190903
O	2.378861	-2.754096	-0.684820
C	2.822173	-2.055014	-1.870897
C	1.763436	-1.090717	-2.453697
Cu	0.170367	0.141797	-0.811250
B	-1.807140	-0.184354	0.018670
O	-2.684467	-1.087722	-0.509987
C	-4.046551	-0.559165	-0.277293
C	-3.775387	0.981531	-0.118490
O	-2.386633	0.996511	0.398479
Cu	-0.285272	-1.174645	1.080928
C	0.314629	-1.427363	-2.074194
N	1.691249	0.238478	-1.860256
C	2.672767	1.056243	-1.411480
C	2.119501	2.087336	-0.445807
C	2.866378	3.177242	-0.016027
C	2.288624	4.059134	0.902671
C	0.992126	3.814664	1.362490
C	0.307616	2.691684	0.894437
N	0.868678	1.853600	0.010148
O	3.868475	0.988837	-1.692129
H	3.871122	3.309830	-0.404314
H	2.842200	4.925219	1.253689
H	-0.701835	2.444774	1.205125
H	0.511377	4.479487	2.072767
H	1.934322	-1.042479	-3.537944
H	-0.442975	-1.179274	-2.817603
H	0.118615	-2.348443	-1.532926
H	2.994650	-2.865416	-2.581233
H	3.766527	-1.531671	-1.703063

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 H                0.799458   -3.621063    1.091303
 H                3.811300   -0.642354    0.313052
 H                0.348815   -2.570083    3.335379
 H                3.365438    0.391543    2.501049
 H                1.577694   -0.489587    3.995960
 C               -4.550461   -1.229791    1.003774
 H               -5.582454   -0.938397    1.222623
 H               -4.519541   -2.315792    0.874443
 H               -3.925696   -0.968544    1.864552
 C               -4.918299   -0.941210   -1.466719
 H               -5.040434   -2.027965   -1.502393
 H               -5.912040   -0.489837   -1.368287
 H               -4.480354   -0.617123   -2.413264
 C               -4.670887    1.694902    0.885752
 H               -4.406125    2.755875    0.932480
 H               -5.719499    1.621305    0.576343
 H               -4.573438    1.274041    1.888848
 C               -3.735141    1.739381   -1.448354
 H               -4.735500    1.826295   -1.883659
 H               -3.346474    2.747583   -1.275561
 H               -3.082939    1.241458   -2.173510

 Electronic Energy =  -1645.86109934 (Hartree/Particle)
 Dipole Moment (Debye):      4.5232
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.449619
(Hartree/Particle)
 Thermal correction to Energy=                    0.478914
 Thermal correction to Enthalpy=                  0.479858
 Thermal correction to Gibbs Free Energy=         0.389413
 Sum of electronic and zero-point Energies=          -1645.411480
 Sum of electronic and thermal Energies=             -1645.382185
 Sum of electronic and thermal Enthalpies=           -1645.381241
 Sum of electronic and thermal Free Energies=        -1645.471686
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1646.26400759
 Corrected Free Energy =  -1645.87459425

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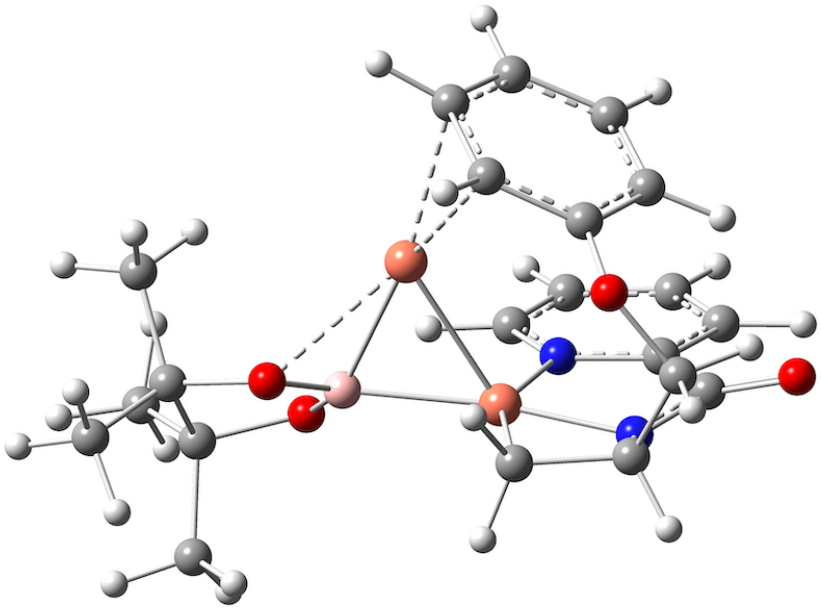

TS9 Substrate: 1c
Path: anti-markovnikov

CARTESIAN COORDINATES

N	0.980383	1.907399	0.001226
C	2.304504	2.038867	-0.242523
C	3.053556	3.066137	0.317922
C	2.405402	3.994029	1.138924
C	1.034843	3.858486	1.374067
C	0.350477	2.792986	0.787385
C	2.926147	0.973514	-1.131166
O	4.144960	0.824751	-1.225917
Cu	0.277715	0.268838	-0.951907
N	1.961026	0.238917	-1.720737
C	1.996916	-1.063031	-2.370089
C	0.483799	-1.298119	-2.212571
C	2.895454	-2.139040	-1.720988
O	2.261450	-2.842107	-0.627205
C	2.039887	-2.251971	0.568403
C	0.921635	-2.756060	1.288990
C	0.562179	-2.170591	2.528919
C	1.315476	-1.096006	3.045358
C	2.450787	-0.664890	2.352772
C	2.824267	-1.235878	1.130724
Cu	-0.473932	-1.193648	0.804863
O	-2.572137	-1.002215	-0.359773
C	-3.916106	-0.494263	0.025031
C	-4.964483	-1.311508	-0.716740
B	-1.722900	0.084580	-0.376139
O	-2.365234	1.280832	-0.263284
C	-3.817974	1.014338	-0.402057
C	-4.160702	1.260928	-1.872900
C	-4.025143	-0.703417	1.537265
C	-4.565920	1.986094	0.501406
H	4.115453	3.116705	0.099302
H	2.961321	4.813121	1.585961
H	-0.713996	2.634013	0.922671
H	0.497458	4.563644	1.999791

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 H                2.311692   -0.980840   -3.420230
 H               -0.129081   -0.993868   -3.061818
 H                0.153726   -2.225886   -1.752346
 H                3.083336   -2.934024   -2.444781
 H                3.852823   -1.705311   -1.421362
 H                0.434315   -3.657925    0.924103
 H                3.704294   -0.871608    0.613525
 H               -0.235166   -2.615897    3.119777
 H                3.061674    0.133612    2.764258
 H                1.039011   -0.644888    3.992530
 H               -5.008539   -0.401835    1.910308
 H               -3.885069   -1.765364    1.762570
 H               -3.260105   -0.131505    2.074577
 H               -4.948816   -2.347004   -0.363393
 H               -5.963370   -0.902307   -0.527762
 H               -4.787845   -1.316547   -1.794140
 H               -4.432964    3.008536    0.135011
 H               -5.638236    1.760360    0.494867
 H               -4.207446    1.943263    1.532481
 H               -5.233994    1.142796   -2.051923
 H               -3.877319    2.283381   -2.139382
 H               -3.620534    0.574033   -2.532401

 Electronic Energy =  -1645.86006202 (Hartree/Particle)
 Dipole Moment (Debye):      5.4811
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:            -31.689

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.449488
(Hartree/Particle)
 Thermal correction to Energy=                    0.477931
 Thermal correction to Enthalpy=                  0.478875
 Thermal correction to Gibbs Free Energy=         0.391230
 Sum of electronic and zero-point Energies=          -1645.410574
 Sum of electronic and thermal Energies=             -1645.382131
 Sum of electronic and thermal Enthalpies=           -1645.381187
 Sum of electronic and thermal Free Energies=        -1645.468832
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1646.26274602
 Corrected Free Energy =  -1645.87151600

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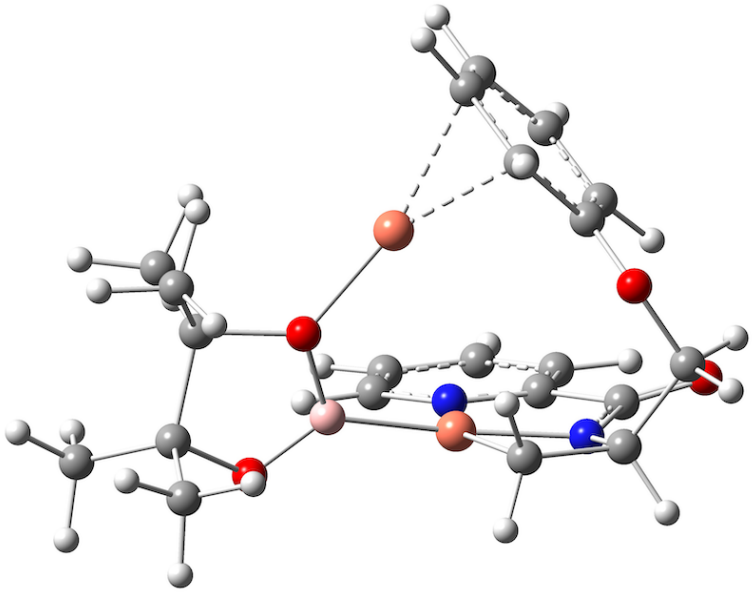

I7 Substrate: 1c
Path: anti-markovnikov

CARTESIAN COORDINATES

N	1.323786	-2.078771	-0.246752
C	2.666406	-1.894885	-0.181564
C	3.540813	-2.621378	-0.981687
C	3.017370	-3.579132	-1.854764
C	1.634563	-3.772759	-1.905967
C	0.817203	-2.995438	-1.085445
C	3.160862	-0.829299	0.795439
O	4.323782	-0.411191	0.763951
Cu	0.408279	-0.838101	1.057134
N	2.142415	-0.445324	1.571418
C	1.920724	0.659521	2.490742
C	0.372327	0.566223	2.474035
C	2.512082	2.029495	2.096743
O	1.645216	2.821533	1.248361
C	1.492941	2.585728	-0.066151
C	0.382424	3.259728	-0.664173
C	0.121940	3.087368	-2.052014
C	0.946985	2.253367	-2.829939
C	2.049245	1.640519	-2.228477
C	2.331073	1.796897	-0.865512
Cu	-1.002117	1.728850	-0.677451
O	-2.098605	0.301640	-0.018178
C	-3.479145	-0.088086	-0.459443
C	-4.357292	1.151851	-0.403149
B	-1.520627	-0.800369	0.675197
O	-2.465521	-1.739232	0.912464
C	-3.801176	-1.200804	0.593973
C	-4.369791	-0.652890	1.905582
C	-3.330341	-0.600768	-1.890796
C	-4.661834	-2.339888	0.061678
H	4.604564	-2.423280	-0.896932
H	3.678411	-4.169066	-2.483152
H	-0.262973	-3.102012	-1.079827
H	1.190954	-4.511567	-2.565411

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 H                2.333362    0.423746    3.482470
 H               -0.076723    0.118427    3.361245
 H               -0.161361    1.458586    2.149137
 H                2.606647    2.653440    2.987117
 H                3.501214    1.904775    1.647544
 H               -0.112314    4.040588   -0.087771
 H                3.206915    1.319967   -0.443042
 H               -0.652636    3.686276   -2.525979
 H                2.716978    1.027443   -2.827503
 H                0.749785    2.127238   -3.889248
 H               -4.303184   -0.866507   -2.314894
 H               -2.891482    0.186887   -2.513989
 H               -2.677892   -1.477759   -1.936473
 H               -4.025980    1.879598   -1.153356
 H               -5.395642    0.888797   -0.631523
 H               -4.327147    1.629416    0.578216
 H               -4.829120   -3.072410    0.856477
 H               -5.637453   -1.962204   -0.264713
 H               -4.185489   -2.853499   -0.776372
 H               -5.393984   -0.289699    1.773439
 H               -4.382020   -1.456010    2.647677
 H               -3.755660    0.163411    2.299944

 Electronic Energy =  -1645.86850731 (Hartree/Particle)
 Dipole Moment (Debye):      7.3570
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.449876
(Hartree/Particle)
 Thermal correction to Energy=                    0.479002
 Thermal correction to Enthalpy=                  0.479946
 Thermal correction to Gibbs Free Energy=         0.389496
 Sum of electronic and zero-point Energies=          -1645.418631
 Sum of electronic and thermal Energies=             -1645.389506
 Sum of electronic and thermal Enthalpies=           -1645.388562
 Sum of electronic and thermal Free Energies=        -1645.479011
 PCM-SP (solvent=THF;6-311+g(2d,p)) =   -1646.27329686
 Corrected Free Energy =  -1645.88380055

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PATH: MARKOVNIKOV
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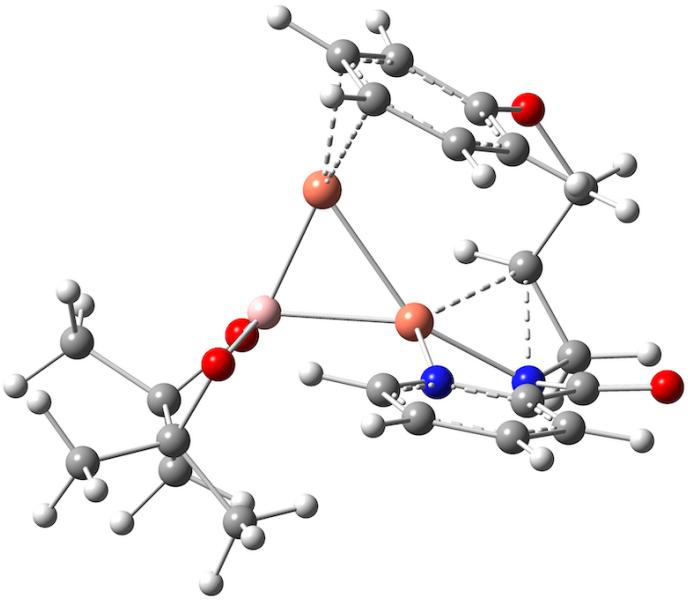

TS8 Substrate: 1c
Path: Markovnikov

CARTESIAN COORDINATES

C	1.303245	-0.774821	2.519760
N	1.099895	1.139769	2.023652
C	2.143063	1.837370	1.402146
O	3.215448	2.099559	1.931126
C	1.386728	0.493161	3.294479
C	1.807906	2.288702	0.001752
C	2.590731	3.228503	-0.665976
C	2.218776	3.589358	-1.964779
C	1.098618	2.990074	-2.547193
C	0.384219	2.037285	-1.814962
N	0.735633	1.707992	-0.567438
Cu	-0.233174	-1.783257	-0.630598
H	3.458067	3.652190	-0.170891
H	2.795320	4.328564	-2.513276
H	-0.492860	1.528376	-2.203897
H	0.777264	3.255036	-3.549597
H	2.368831	0.736704	3.707867
Cu	0.131029	0.140906	0.685551
B	-1.790751	-0.575125	-0.107235
O	-2.632392	-0.841451	0.941650
O	-2.328893	0.299136	-1.024538
C	-3.940642	-0.235209	0.627510
C	-3.544991	0.870384	-0.415585
H	0.426581	-1.412146	2.611825
C	-4.570904	1.119998	-1.513448
H	-5.516613	1.464013	-1.079412
H	-4.207389	1.897693	-2.192765
H	-4.763493	0.219265	-2.100201
C	-3.107048	2.190119	0.230151
H	-2.666853	2.835073	-0.536691
H	-3.955733	2.717144	0.677113
H	-2.350922	2.022023	1.004931
C	-4.801825	-1.355325	0.036635
H	-4.861431	-2.177376	0.756235

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 H              -5.817806   -1.004599   -0.171388
 H              -4.369874   -1.743922   -0.891243
 C              -4.550223    0.288158    1.922414
 H              -5.482594    0.825526    1.714778
 H              -4.781734   -0.549658    2.587332
 H              -3.869333    0.961340    2.448429
 C               2.603710   -1.412157    2.123628
 H               3.342449   -0.665540    1.812104
 H               2.999723   -1.884955    3.034272
 O               2.472143   -2.486074    1.195929
 C               2.289929   -2.208783   -0.127107
 C               2.872803   -1.125500   -0.800346
 C               1.476786   -3.128421   -0.836491
 C               2.616245   -0.938345   -2.164087
 H               3.520870   -0.430991   -0.277641
 C               1.223140   -2.915654   -2.208075
 H               1.143717   -4.030268   -0.327489
 C               1.782417   -1.808778   -2.869951
 H               3.070545   -0.092570   -2.671840
 H               0.622141   -3.636496   -2.754707
 H               1.581039   -1.647391   -3.923773
 H               0.590822    0.652364    4.022748

 Electronic Energy =  -1645.85266128 (Hartree/Particle)
 Dipole Moment (Debye):      2.7354
 index           1
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -168.079

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.447730
(Hartree/Particle)
 Thermal correction to Energy=                    0.477240
 Thermal correction to Enthalpy=                  0.478184
 Thermal correction to Gibbs Free Energy=         0.385894
 Sum of electronic and zero-point Energies=          -1645.404931
 Sum of electronic and thermal Energies=             -1645.375421
 Sum of electronic and thermal Enthalpies=           -1645.374477
 Sum of electronic and thermal Free Energies=        -1645.466767
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1646.25513609
 Corrected Free Energy =  -1645.86924181

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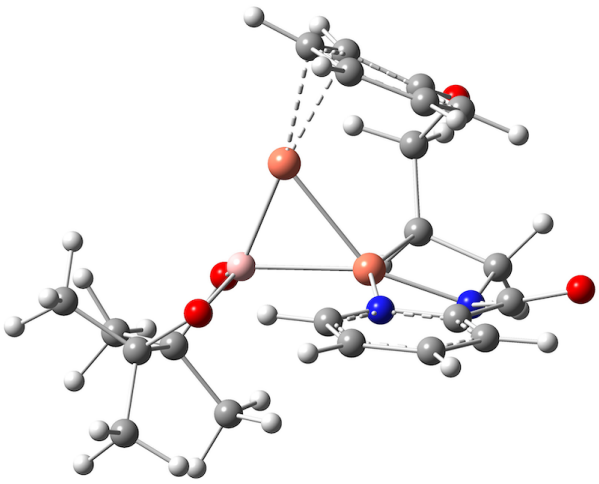

I6 Substrate: 1c
Path: Markovnikov

CARTESIAN COORDINATES

C	-0.400877	1.540152	2.053085
N	-1.335375	-0.429743	2.182612
C	-2.413971	-1.165678	1.772516
O	-3.542630	-1.114419	2.247875
C	-1.439197	0.828390	2.913207
C	-2.045302	-2.100135	0.637668
C	-2.844747	-3.172053	0.258324
C	-2.422017	-3.967004	-0.811634
C	-1.227468	-3.655219	-1.466917
C	-0.490130	-2.549064	-1.040940
N	-0.899811	-1.797403	-0.009194
Cu	0.151703	1.126694	-1.258914
H	-3.766496	-3.359875	0.799383
H	-3.015576	-4.819780	-1.128247
H	0.445719	-2.250805	-1.502135
H	-0.866087	-4.256374	-2.295003
H	-2.438897	1.269240	2.841541
H	-1.162897	0.727776	3.968420
Cu	-0.204076	-0.046291	0.762754
B	1.736913	0.258179	-0.274238
O	2.593016	0.977573	0.511551
O	2.295451	-0.868357	-0.817027
C	3.801308	0.146707	0.708675
C	3.748455	-0.813800	-0.534808
H	0.619200	1.554331	2.444066
C	-0.787223	2.853305	1.405542
H	-0.892875	3.600512	2.203694
H	-0.010192	3.198535	0.715675
O	-2.079508	2.827293	0.772564
C	-2.159651	2.226261	-0.451173
C	-3.070849	1.179994	-0.624553
C	-1.361284	2.661315	-1.540336
C	-3.143129	0.513021	-1.854364
H	-3.693015	0.883633	0.214554
C	-1.427151	1.961215	-2.768582
H	-0.788959	3.582481	-1.456077
C	-2.308206	0.871957	-2.915802
H	-3.845892	-0.306873	-1.970859

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 H              -0.855614    2.322212   -3.619823
 H              -2.357696    0.341815   -3.861368
 C               4.237101   -2.233229   -0.275459
 H               4.155783   -2.826802   -1.191393
 H               5.289876   -2.222229    0.028430
 H               3.654439   -2.727790    0.504923
 C               4.404594   -0.231955   -1.789408
 H               5.494126   -0.207045   -1.688317
 H               4.153527   -0.859711   -2.649778
 H               4.051144    0.784347   -1.991710
 C               3.595571   -0.571456    2.046180
 H               4.466050   -1.181135    2.307440
 H               3.451085    0.174077    2.834135
 H               2.712111   -1.218765    2.021609
 C               5.016676    1.062552    0.765969
 H               4.961255    1.697220    1.655712
 H               5.935763    0.469065    0.828710
 H               5.079029    1.711012   -0.110516

 Electronic Energy =  -1645.85932718 (Hartree/Particle)
 Dipole Moment (Debye):      5.2390
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            0

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.449249
(Hartree/Particle)
 Thermal correction to Energy=                    0.478828
 Thermal correction to Enthalpy=                  0.479773
 Thermal correction to Gibbs Free Energy=         0.387601
 Sum of electronic and zero-point Energies=          -1645.410078
 Sum of electronic and thermal Energies=             -1645.380499
 Sum of electronic and thermal Enthalpies=           -1645.379554
 Sum of electronic and thermal Free Energies=        -1645.471727
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1646.26409937
 Corrected Free Energy =  -1645.87649919

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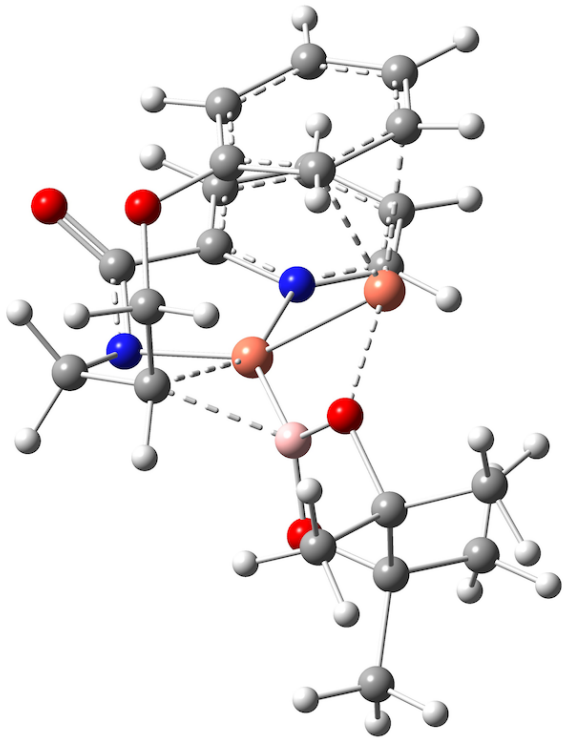

TS9 Substrate: 1c
Path: Markovnikov

CARTESIAN COORDINATES

C	0.597771	-0.676364	2.051608
N	-1.357094	-1.897916	1.399656
C	-2.644232	-1.540901	1.240642
O	-3.521502	-1.307586	2.076809
C	-0.563276	-1.604011	2.583794
C	-2.938850	-1.347152	-0.251955
C	-4.221614	-1.452440	-0.780344
C	-4.414273	-1.218681	-2.142915
C	-3.319225	-0.861538	-2.936490
C	-2.068547	-0.742155	-2.337408
N	-1.883808	-0.981052	-1.026649
Cu	0.498479	1.220316	-0.777353
H	-5.034752	-1.715115	-0.111501
H	-5.403017	-1.313256	-2.582718
H	-1.188176	-0.451402	-2.900288
H	-3.427867	-0.672435	-3.999451
H	-1.134985	-1.080317	3.359925
H	-0.144520	-2.521262	3.009869
Cu	-0.305568	-0.900470	0.171755
B	1.655566	-0.561247	0.297977
O	2.381768	0.622177	0.185946
O	2.360588	-1.664613	-0.073717
C	3.775567	0.231574	-0.190711
C	3.539180	-1.186828	-0.822660
H	1.568095	-1.117207	2.307496
C	0.551293	0.739232	2.644495
H	0.711147	0.643316	3.723404
H	1.340732	1.375482	2.238596
O	-0.735668	1.366900	2.540588

```
 C              -1.102863    1.936936    1.358194
 C              -2.424381    1.753896    0.938638
 C              -0.216436    2.724337    0.578772
 C              -2.845555    2.267443   -0.292775
 H              -3.092158    1.173895    1.568960
 C              -0.649859    3.211388   -0.683294
 H               0.732013    3.053759    0.995416
 C              -1.964486    2.962206   -1.124282
 H              -3.870324    2.098662   -0.610527
 H              -0.003964    3.883993   -1.243611
 H              -2.294602    3.346409   -2.084073
 C               4.676331   -2.177120   -0.613478
 H               4.421145   -3.134633   -1.076654
 H               5.594761   -1.804760   -1.081145
 H               4.868711   -2.354538    0.446659
 C               3.122192   -1.134281   -2.295811
 H               3.959272   -0.843925   -2.937705
 H               2.774696   -2.124639   -2.602772
 H               2.300049   -0.424745   -2.454348
 C               4.559628    0.200323    1.120126
 H               5.613810   -0.028656    0.936281
 H               4.501441    1.180661    1.602477
 H               4.162332   -0.550980    1.810072
 C               4.316934    1.289467   -1.138780
 H               4.431516    2.242043   -0.612388
 H               5.300956    0.990260   -1.515551
 H               3.654475    1.445858   -1.994187

 Electronic Energy =  -1645.83478468 (Hartree/Particle)
 Dipole Moment (Debye):      8.7563
 index           0
 Harmonic frequencies
 Number of imaginary frequencies=            1
 Negatives Eigenvalues:           -170.316

 THERMOCHEMICAL DATA

 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
 Zero-point correction=                           0.449085
(Hartree/Particle)
 Thermal correction to Energy=                    0.477711
 Thermal correction to Enthalpy=                  0.478655
 Thermal correction to Gibbs Free Energy=         0.390923
 Sum of electronic and zero-point Energies=          -1645.385699
 Sum of electronic and thermal Energies=             -1645.357074
 Sum of electronic and thermal Enthalpies=           -1645.356129
 Sum of electronic and thermal Free Energies=        -1645.443862
 PCM-SP (solvent=THF;6-311+g(2d,p)) =  -1646.24680146
 Corrected Free Energy =   -1645.85587878

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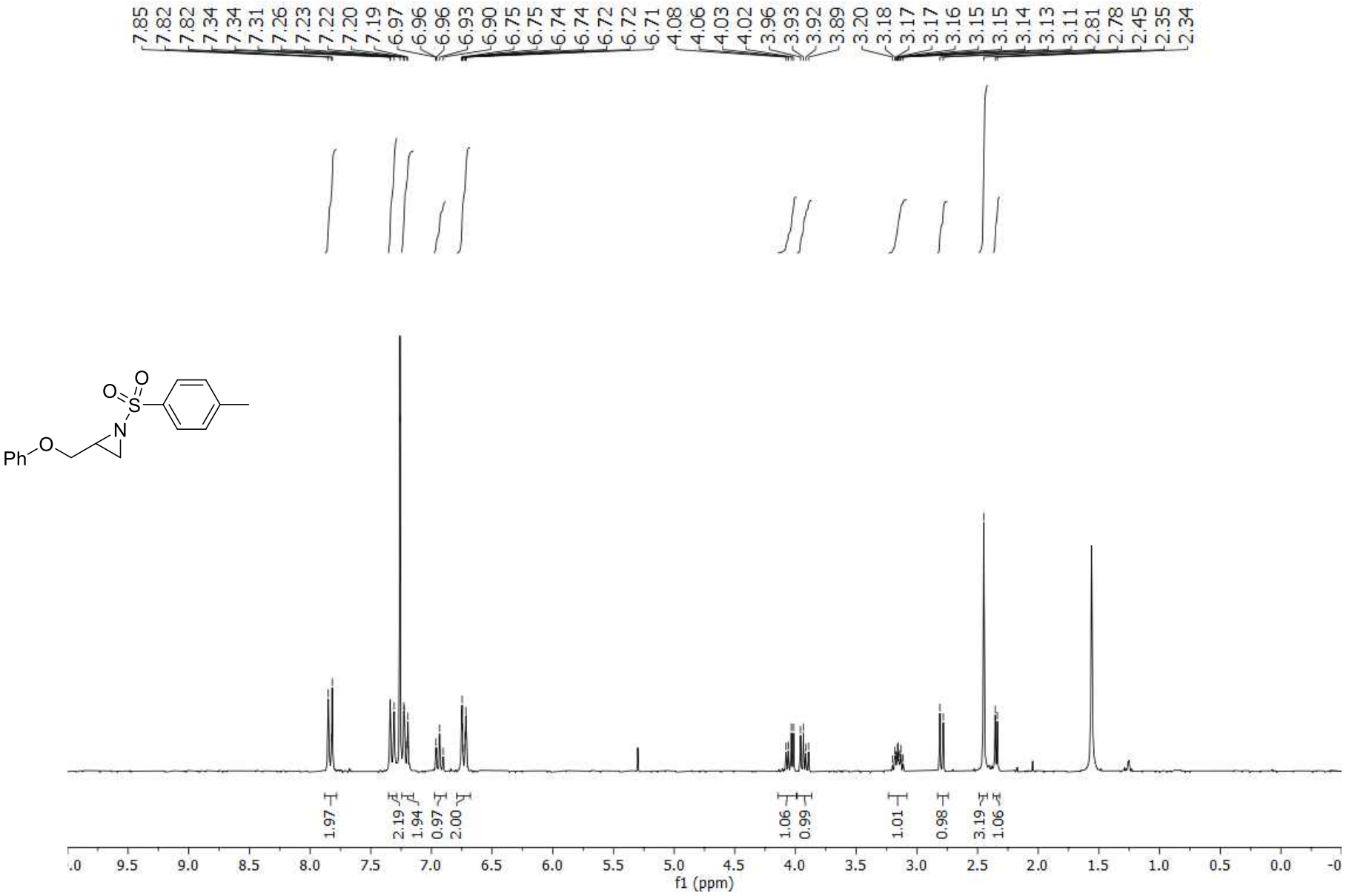
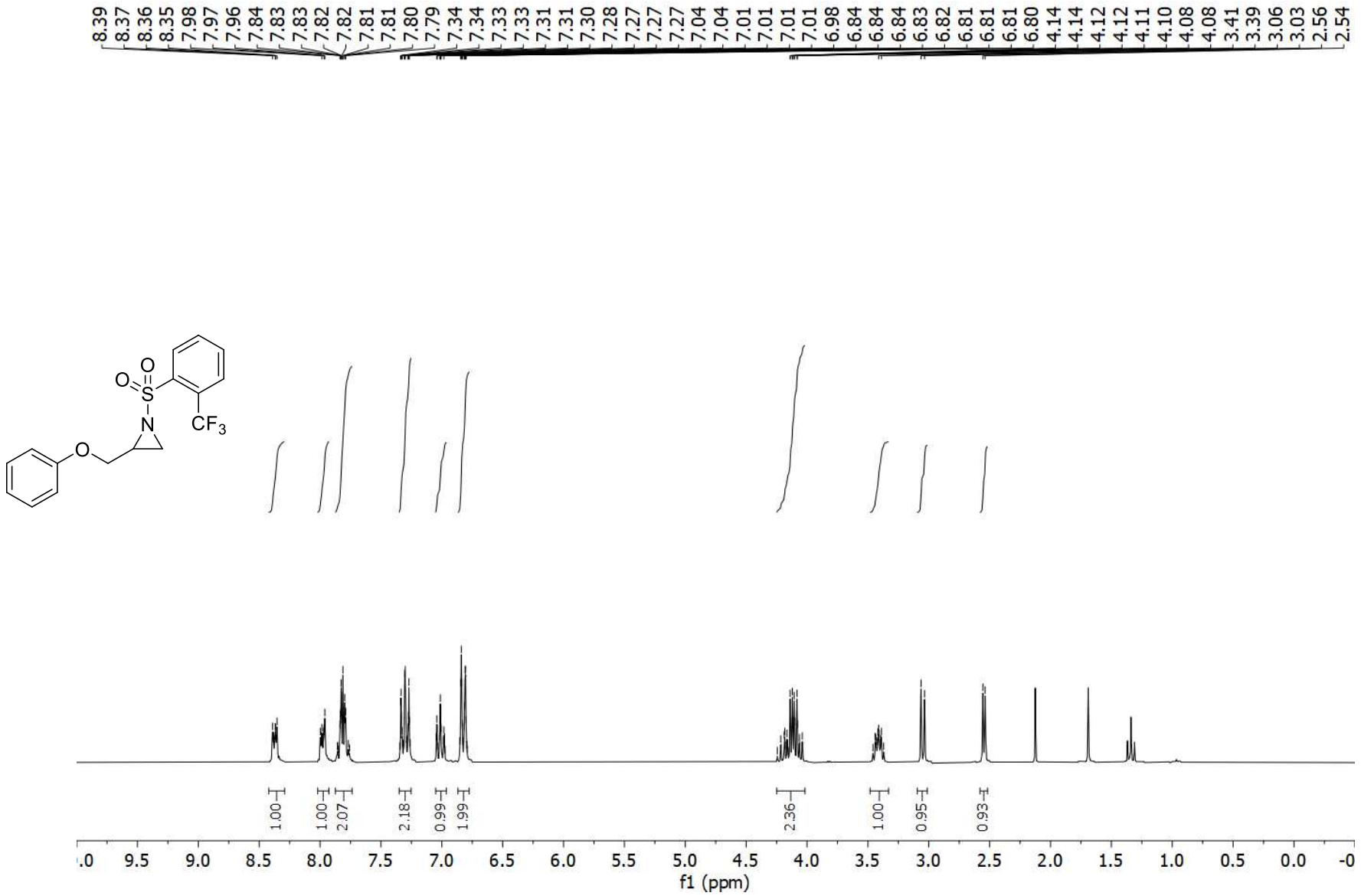
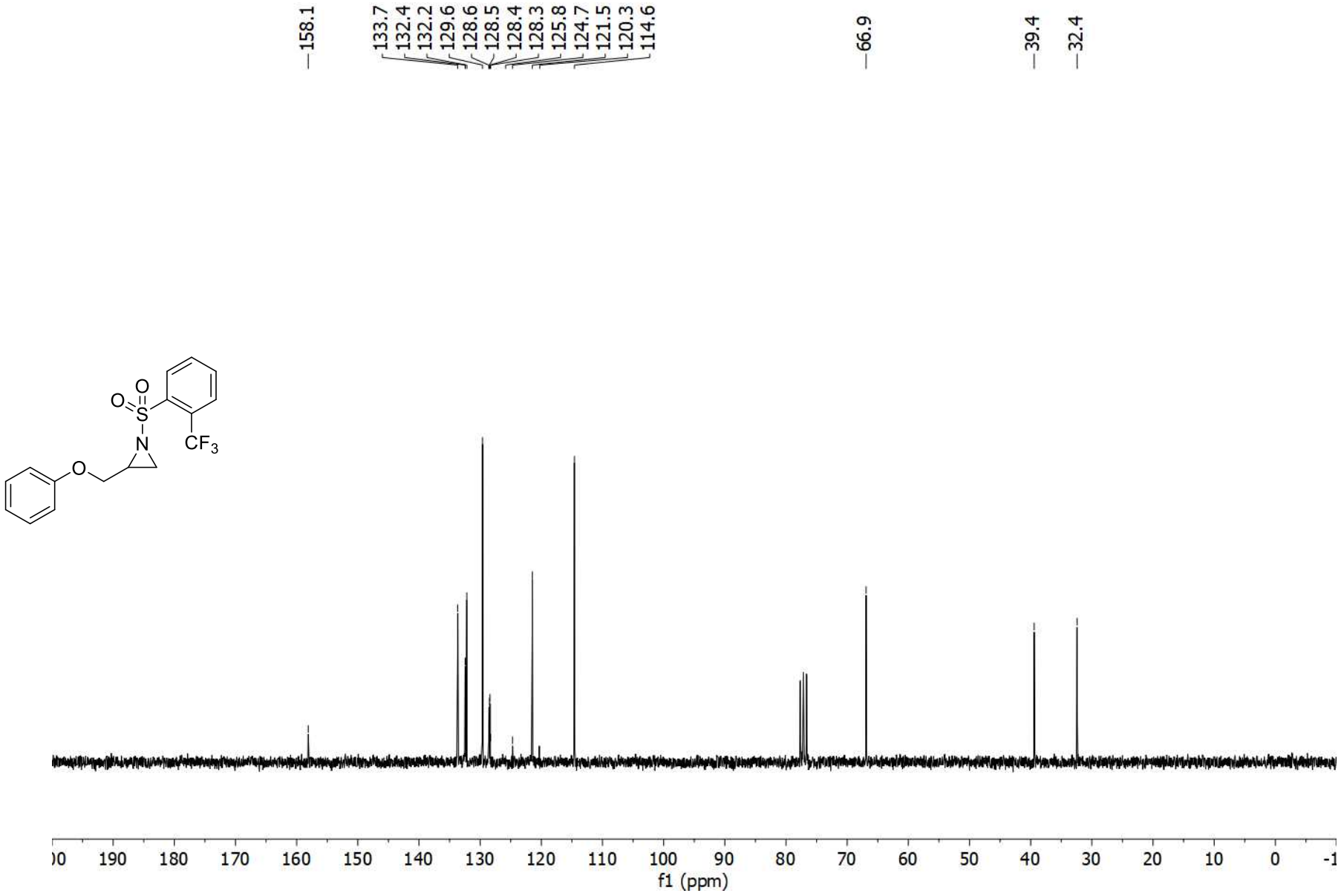
Compound **1a** ^{1}H NMR (250 MHz, $CDCl_3$)



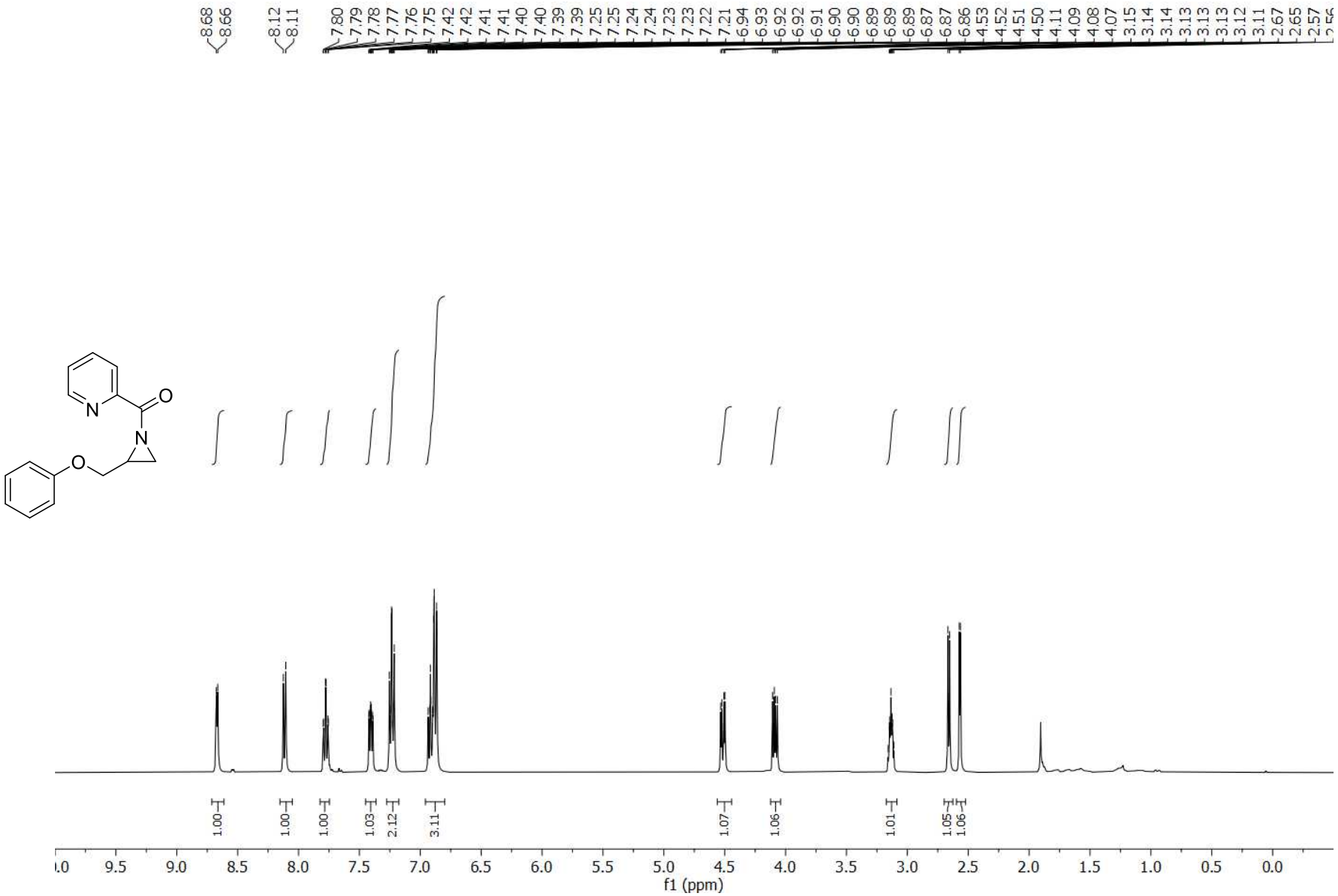
Compound **1b** ^{1}H NMR (250 MHz, $CDCl_3$)



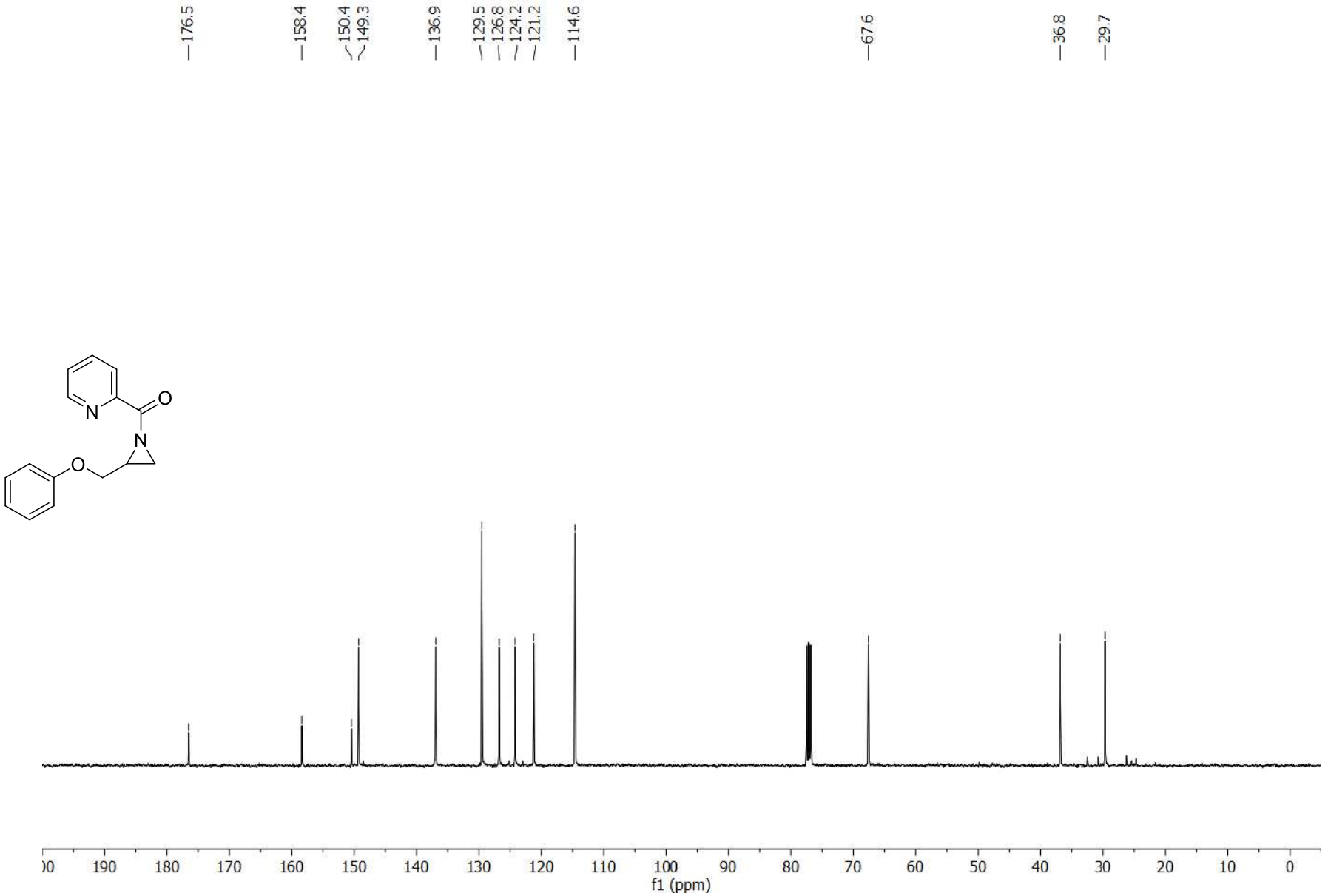
Compound **1b** ^{13}C NMR (63 MHz, $CDCl_3$)



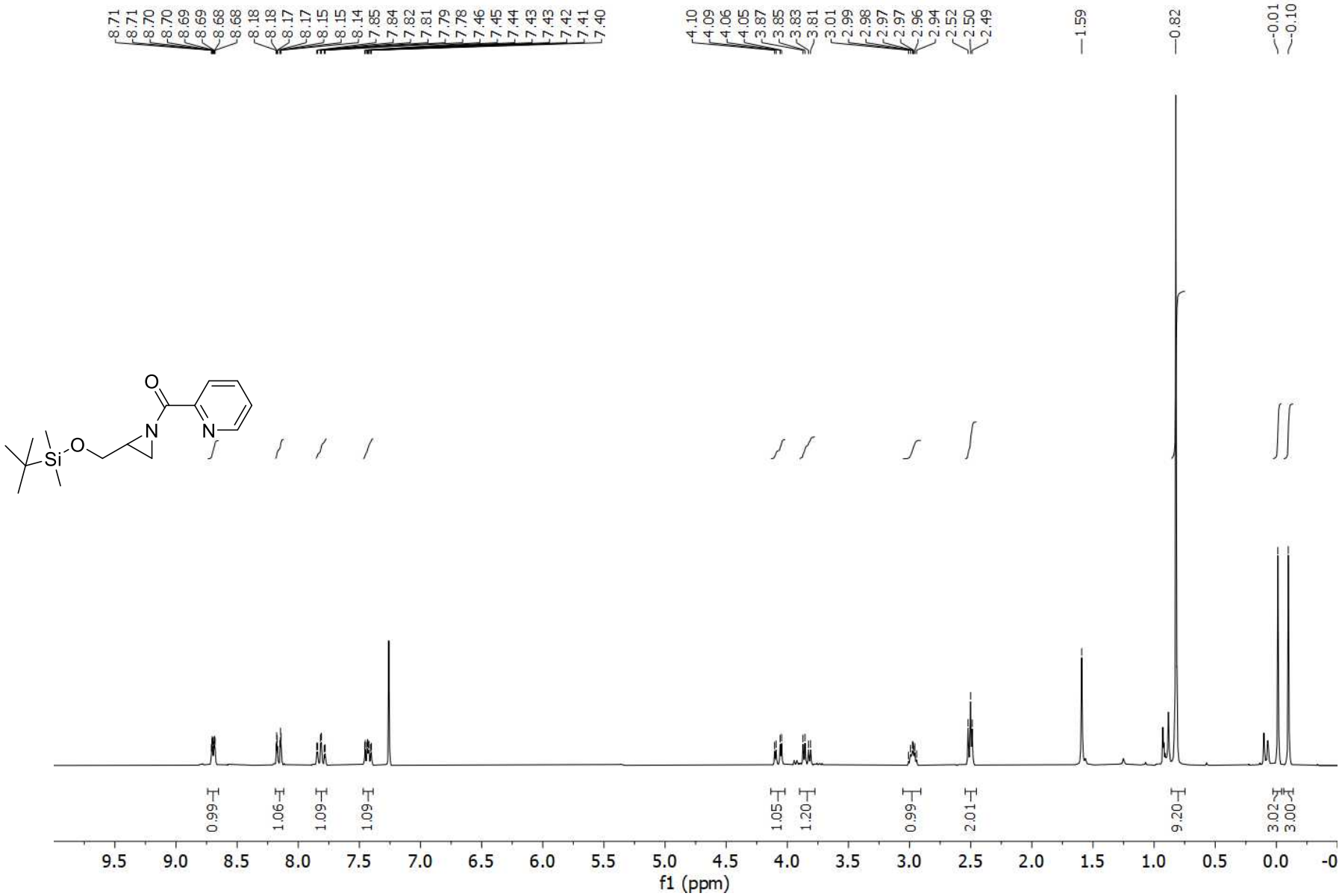
Compound **1c** ^{1}H NMR (250 MHz, $CDCl_3$)



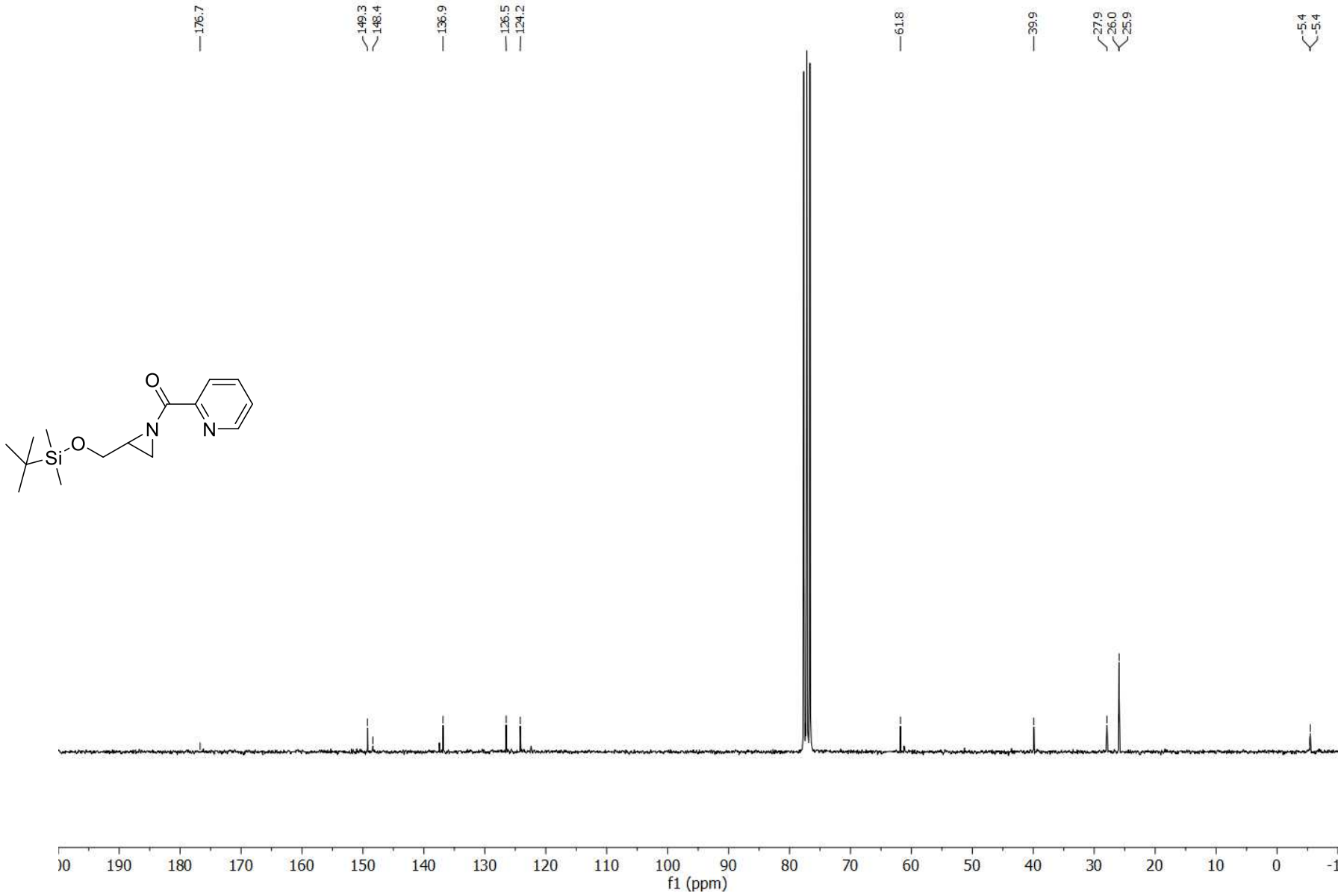
Compound **1c** ^{13}C NMR (101 MHz, $CDCl_3$)



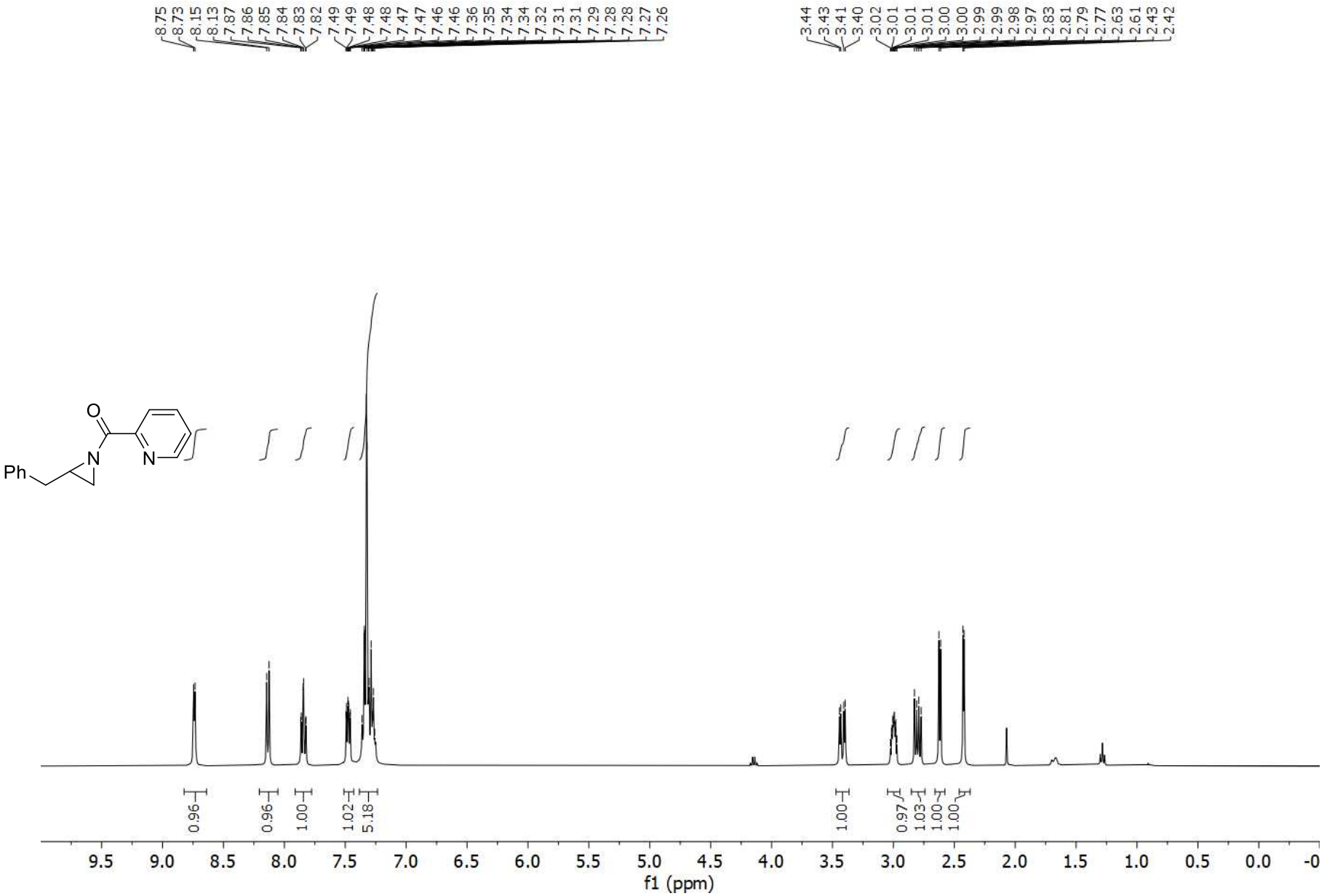
Compound **4c** ^{1}H NMR (250 MHz, $CDCl_3$)



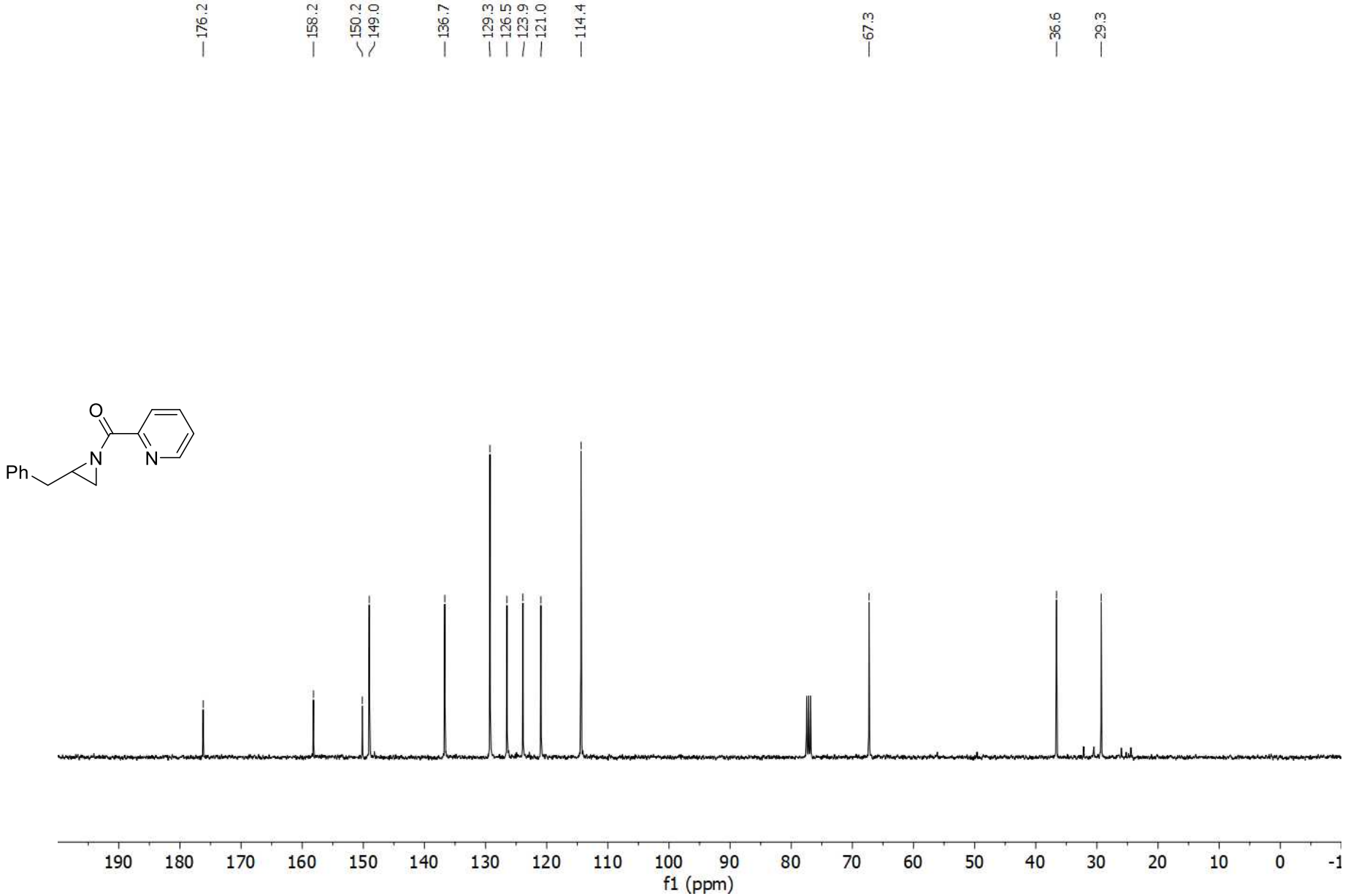
Compound **4c** ^{13}C NMR (63 MHz, $CDCl_3$)



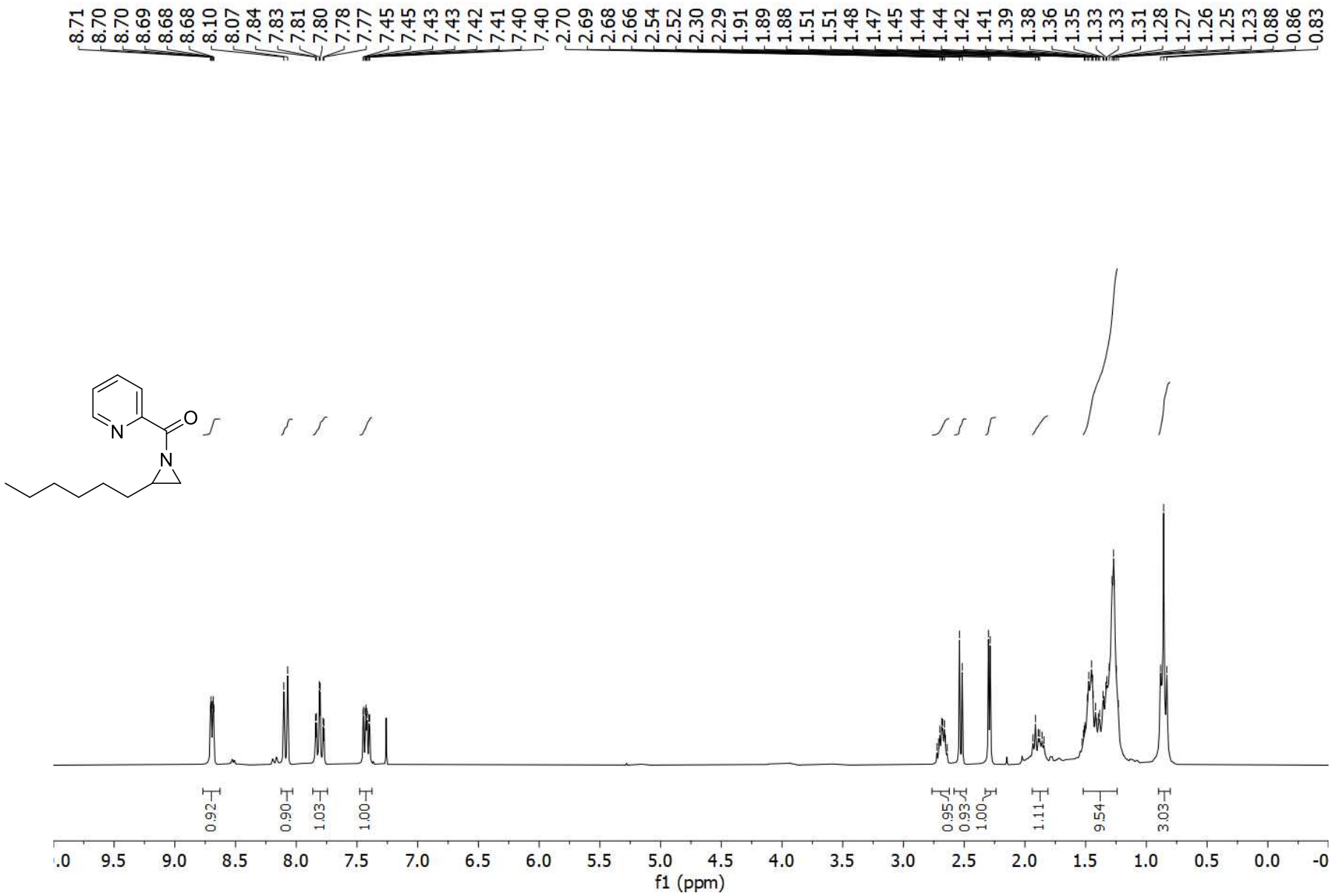
Compound **6c** ^{1}H NMR (400 MHz, $CDCl_3$)



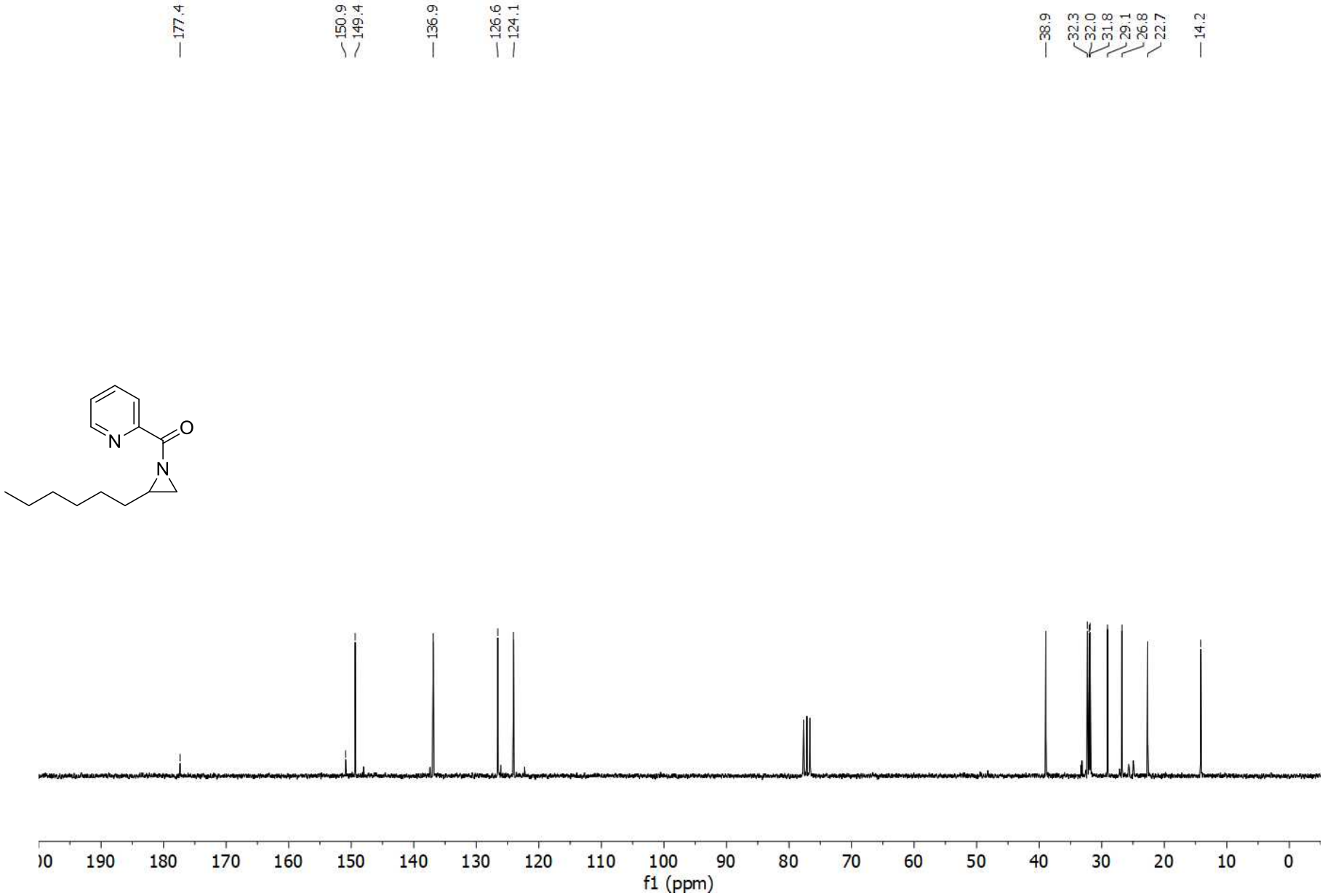
Compound **6c** ^{13}C NMR (101 MHz, $CDCl_3$)



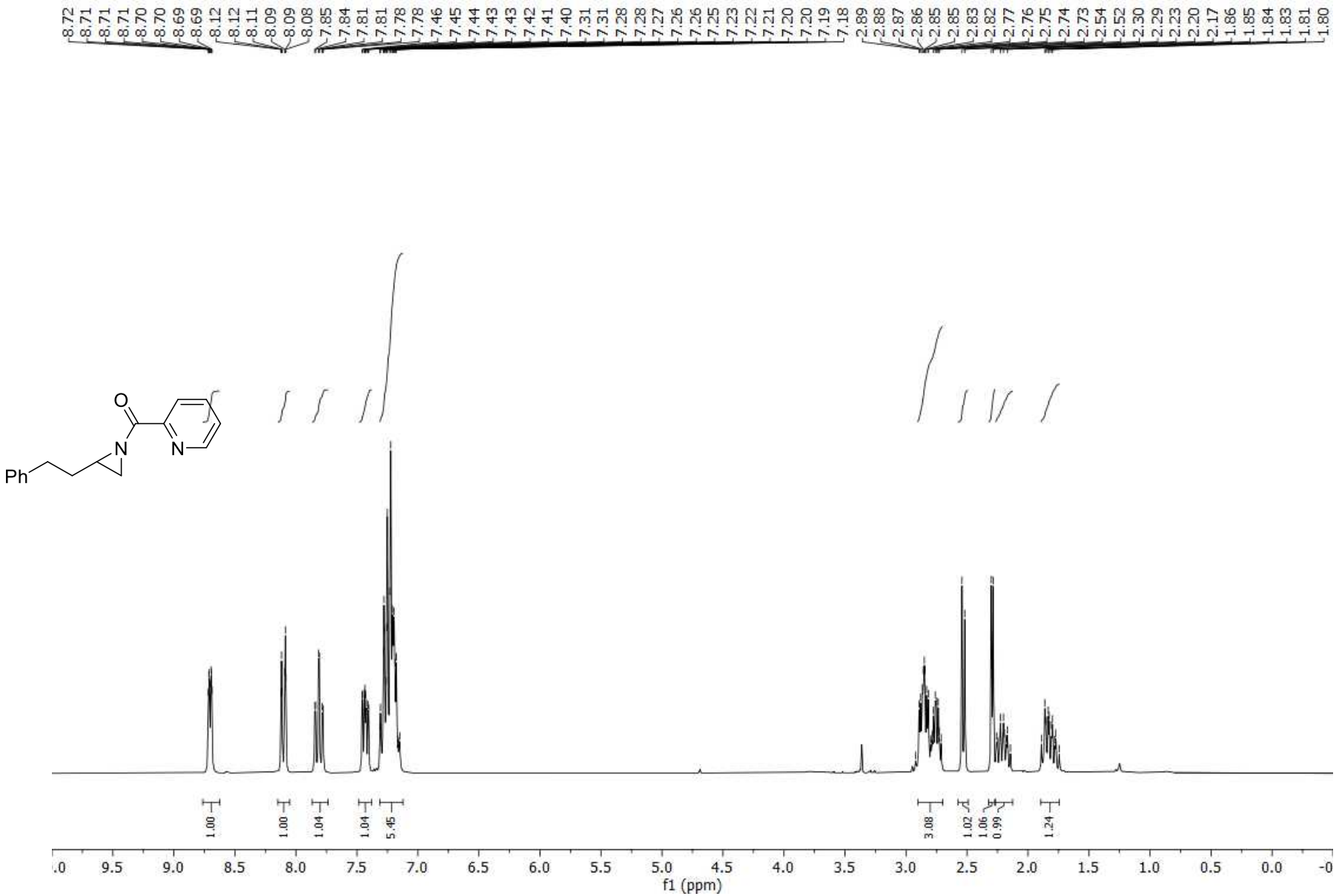
Compound **7c** ^{1}H NMR (250 MHz, $CDCl_3$)



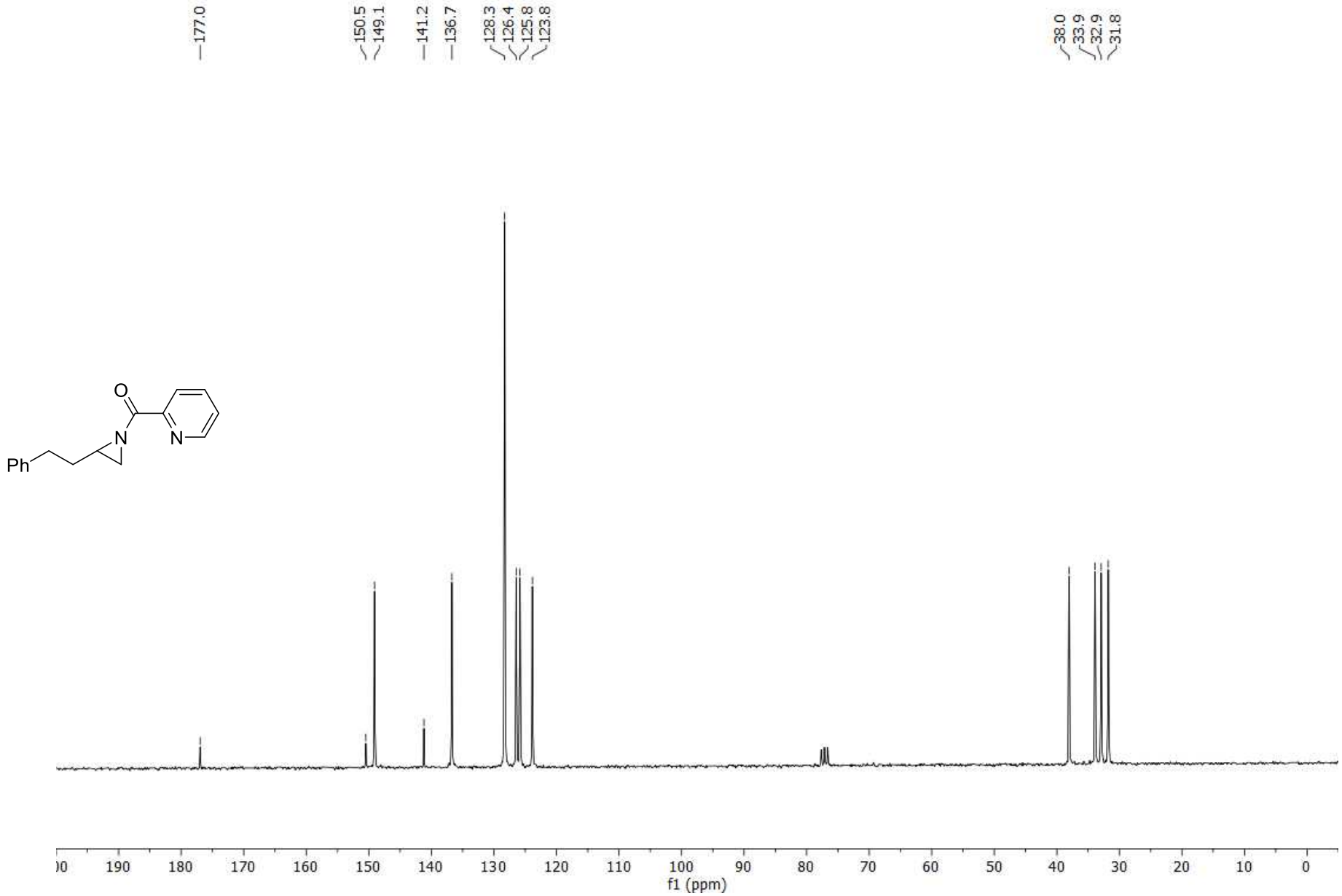
Compound **7c** ^{13}C NMR (101 MHz, $CDCl_3$)



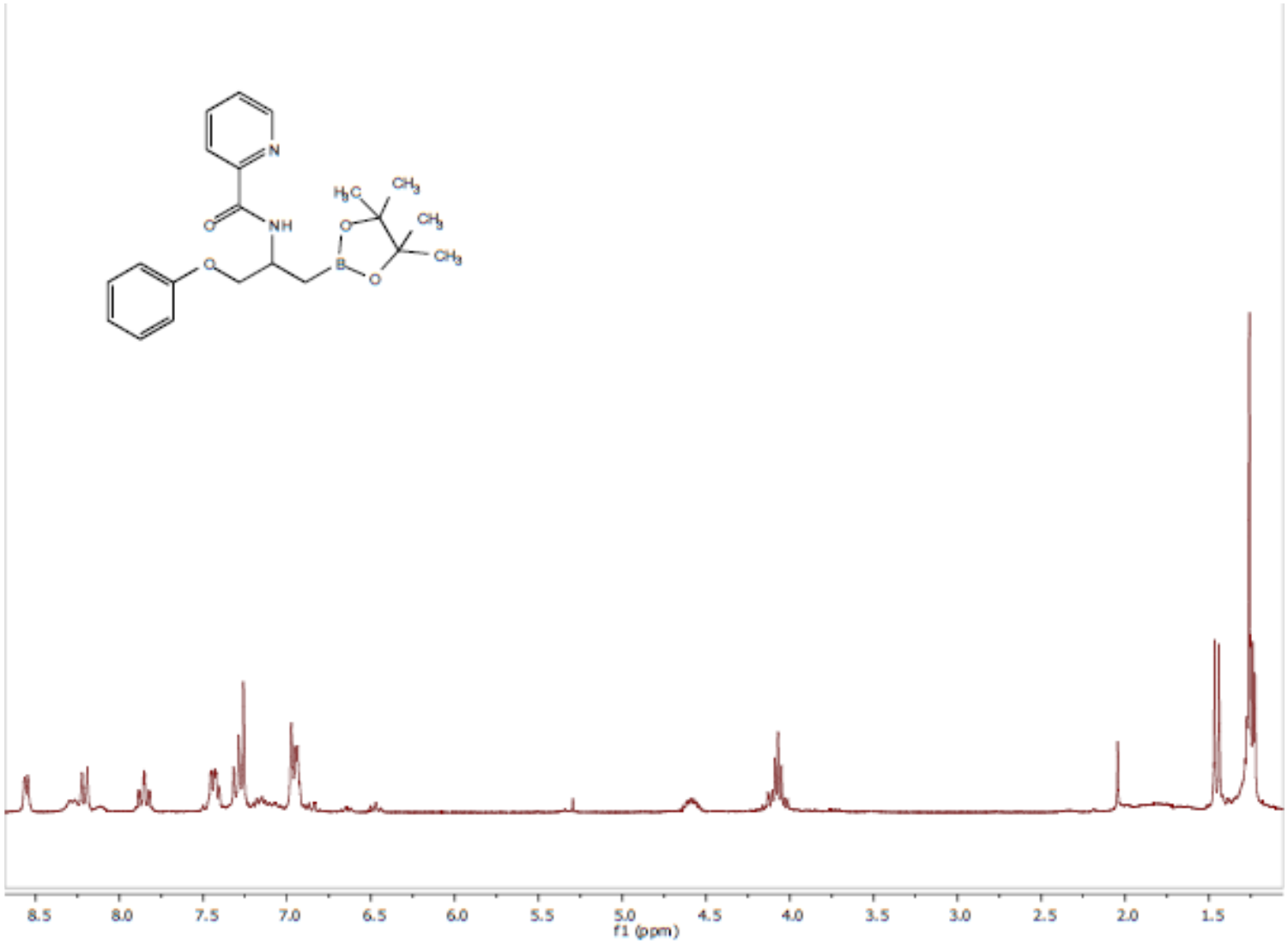
Compound **10** ^{1}H NMR (250 MHz, $CDCl_3$)



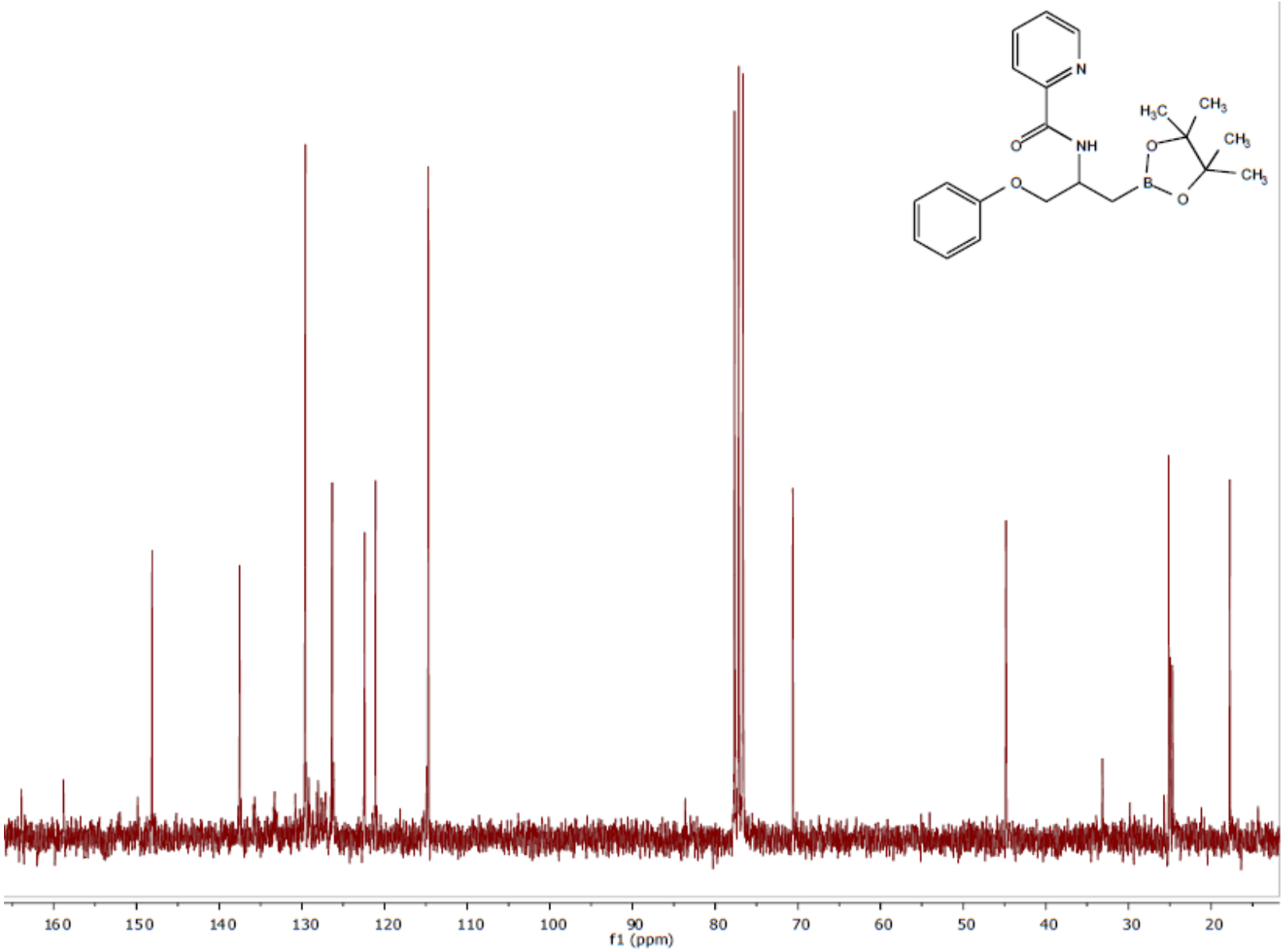
Compound **10** ^{13}C NMR (101 MHz, $CDCl_3$)



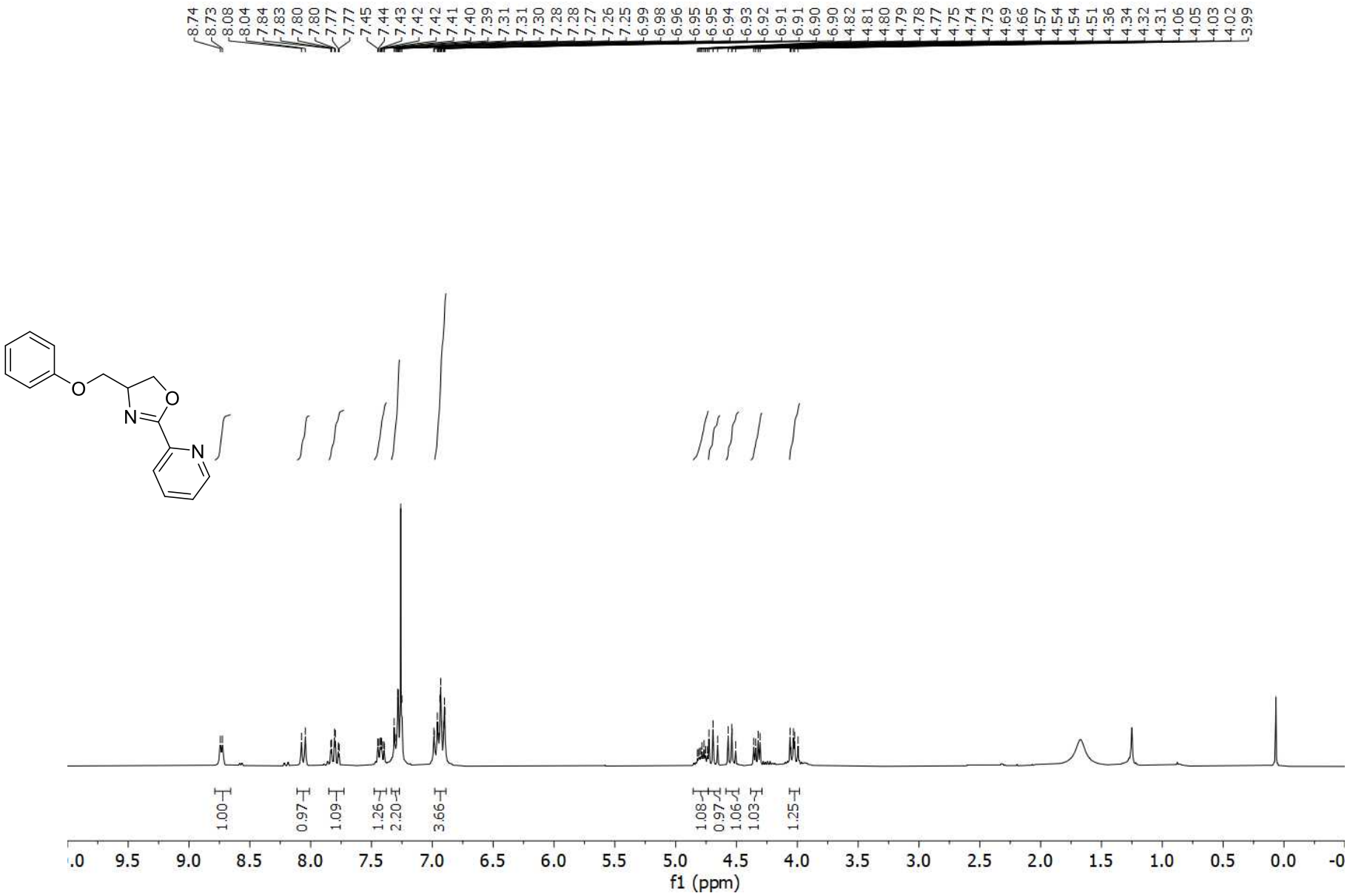
Compound **2c** ^{1}H NMR (250 MHz, $CDCl_3$)



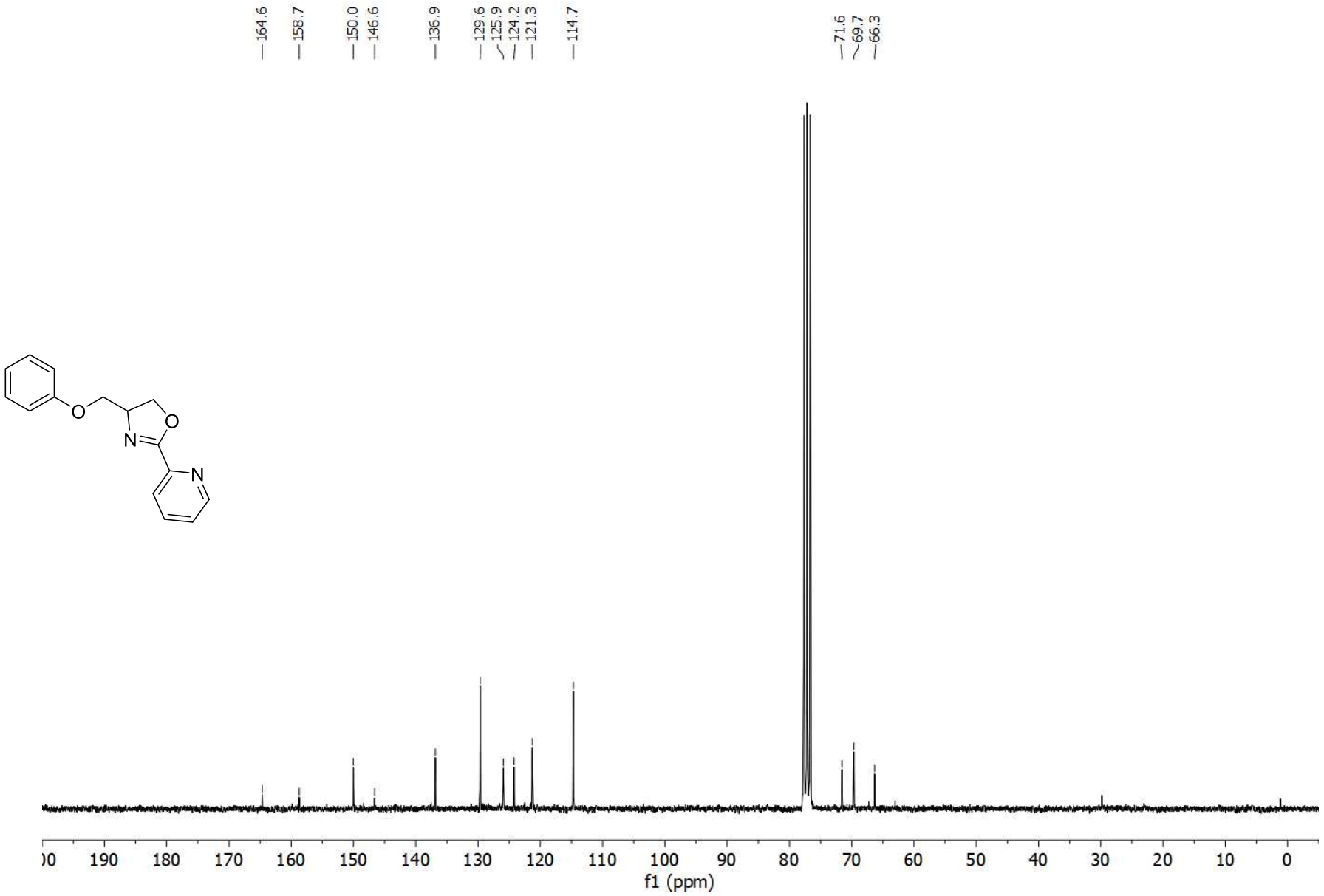
Compound **2c** ^{13}C NMR (63 MHz, $CDCl_3$)



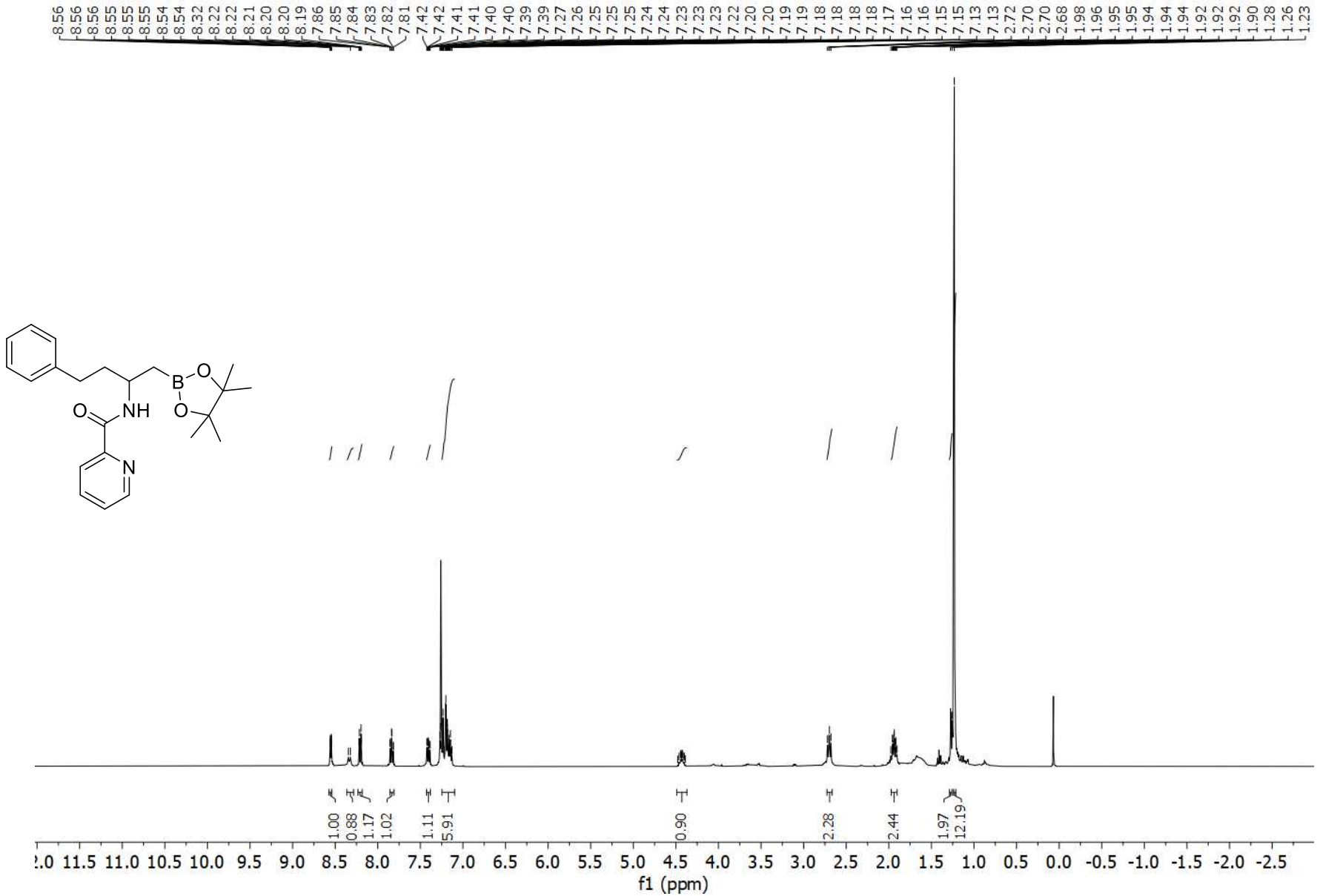
Compound **3c** ^{1}H NMR (250 MHz, $CDCl_3$)



Compound **3c** ^{13}C NMR (63 MHz, $CDCl_3$)



Compound **11** ^{1}H NMR (400 MHz, $CDCl_3$)



Compound **12** ^{1}H NMR (400 MHz, $CDCl_3$)