Cu-catalyzed [1,3]-Asymmetric Methoxy Rearrangement Reactions of *N*-Methoxyanilines; Mechanistic Insight

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Supporting Information

1. General Information

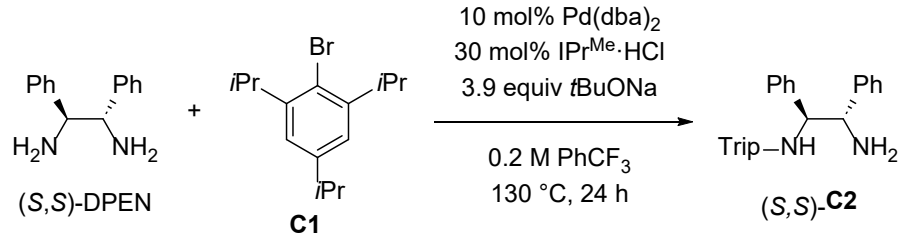
^{1}H and ^{13}C NMR spectra were recorded on a JEOL JNM-ECS600 (600 MHz for ^{1}H and 150 MHz for ^{13}C) spectrometer. Chemical shifts are reported in ppm relative to $CHCl_3$ (for ^{1}H, δ 7.26), and $CDCl_3$ (for ^{13}C, δ 77.00). ^{1}H NMR data are reported as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, sext = sextet, sept = septet, dd = double doublet, dt = double triplet, dq = double quartet, ddt = double double triplet, br = broad, m = multiplet) and coupling constants (Hz). Infrared spectra were recorded on a JASCO FT/IR-4100 spectrometer. High-resolution mass spectra analysis was performed on a Bruker Daltonics solariX FT-ICR-MS spectrometer at the Research and Analytical Center for Giant Molecules, Graduate School of Science, Tohoku University. Flash column chromatography was performed with Kanto Chemical silica gel 60N (spherical, neutral, 40-50 μm). Analytical thin layer chromatography (TLC) was performed on Merck precoated TLC plates (silica gel 60 F_{254}). All reactions were carried out under nitrogen atmosphere. Chiral stationary phase HPLC analysis was performed on a jasco LC-2000 Plus Series system with DAICEL chiral analytical column (4.6 mm Φ* 250 mm length).

Materials

Anhydrous 1,2-dichloroethane (DCE), 1,2-dioxane, ethyl acetate, and acetone were purchased from Fujifilm WAKO and used as received. Anhydrous toluene and diethyl ether were purchased from KANTO and used as received. $AgNTf_2$ was purchased from Aldrich and used as received. (*S*,*S*)-DPEN was purchased from BLDpharm.

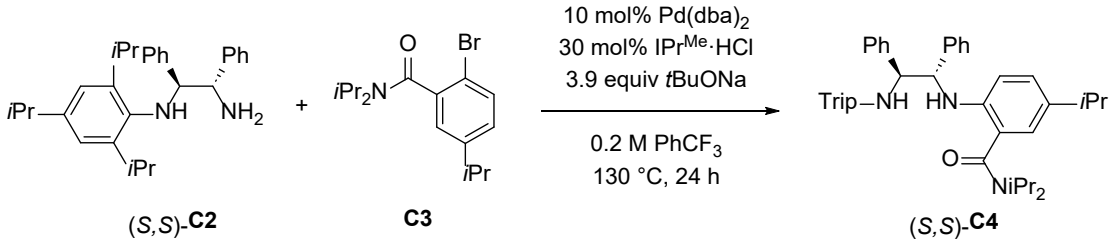
2. Synthesis of chiral NHC ligands

2-1. General procedure for the preparation of chiral NHC ligand **L1-L4**



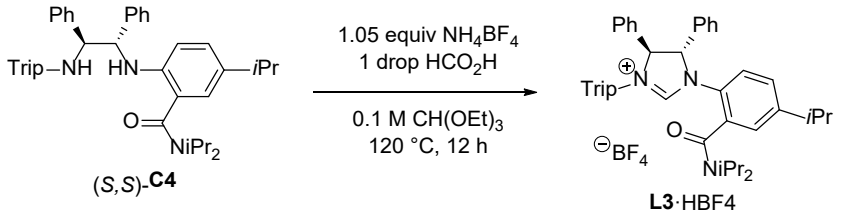
The coupling reaction between amine and arylbromide was carried out according to the reported method[1]

To an oven-dried 5 mL vial was added (*S*,*S*)-(－)-1,2-diphenyl-ethylenediamine (106 mg, 0.50 mmol, 1.0 equiv.), bis(dibenzylideneacetone)palladium(0) (28.8 mg, 0.050 mmol, 10 mol%), IPr^{Me}•HCl (68 mg, 0.15 mmol, 30 mol%) and sodium *tert*- butoxide (187mg, 1.95 mmol, 3.9 equiv.) in a glovebox. The vial was sealed and brought out of the glovebox. The vial was connected with a nitrogen line through a needle, and a solution of 1-bromo-2,4,6-triisopropylbenzene **C1** (126 μL, 0.50 mmol, 1.0 equiv.) in α,α,α-trifluorotoluene (2.5 mL) was added through the septum by a syringe. After the nitrogen line with needle was removed, the resulting mixture was placed in a pre-heated 130℃ aluminum block and stirred for 24 h. After cooling to rt, volatiles were removed under vacuum. The crude product was purified by silica gel flash column chromatography using hexane/EtOAc (2/1) as eluent to give (*S*,*S*)-**C2** (146.8 mg, 0.355 mmol, 71% yield) as a pale yellow solid.

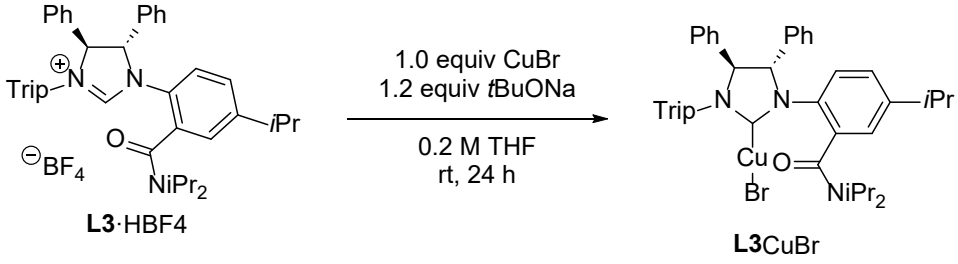


To an oven-dried vial was added (*S*,*S*)-**C2** (414.0 mg, 1.0 mmol), bis(dibenzylidene-acetone)palladium(0) (57.5 mg, 10 mol%), IPr^{Me}•HCl (135.9 mg, 30 mol%), and sodium *tert*-butoxide (374.8 mg, 3.9 equiv.) in a glovebox. The vial was sealed and brought out of the glovebox. The vial was connected with a nitrogen line through a needle, and a solution of bromoarene **C3** (652.6 mg, 2.0 equiv.) in α,α,α-trifluorotoluene (0.2 M) was added through the septum using syringe. After the nitrogen line with needle was removed, the resulting mixture was placed in a pre-heated 130℃ aluminum block and stirred for 24 h. After cooling

to rt, volatiles were removed under vacuum. the crude product was purified by silica gel flash column chromatography using hexane/EtOAc (5/1) as eluent to give the product (*S*,*S*)-**C4** (554.4 mg, 0.84 mmol, 84% yield).



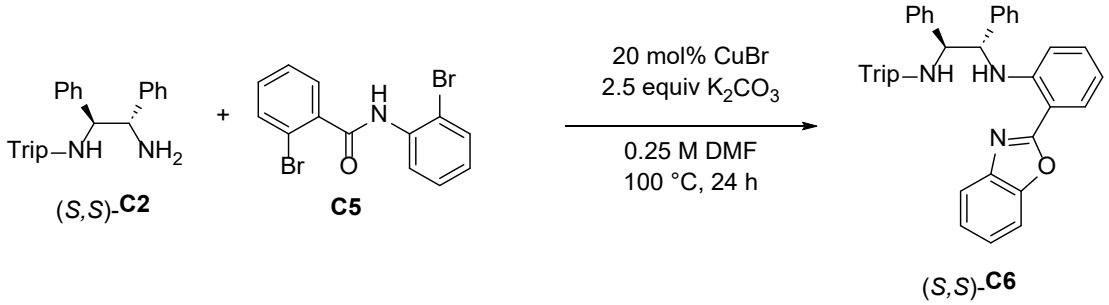
The solution of (*S*,*S*)-**C4** (554.4 mg, 0.84 mmol, 1.0 equiv.), NH_4BF_4 (92.5 mg, 1.05 equiv.) and HCOOH (1drop) in $CH(OEt_3)$ (8.4 mL) was heated at 120 ºC. The reaction mixture was stirred for 12 h and concentrated in vacuo. The residue was purified by flash silica gel column chromatography using DCM/MeOH (10/1) as eluent to give (*S*,*S*)-**L3**·HBF_4 (530.5 mg, 0.70 mmol, 83% yield).



To an oven-dried vial was added **L3**·HBF_4 (530.5 mg, 0.70 mmol), CuBr (100.4 mg, 1.0 equiv.) and ^{t}BuONa (80.7 mg, 1.2 equiv.) in a glovebox. The vial was connected with a nitrogen line through a needle, and THF (3.5 mL) was added through the septum by using syringe. The nitrogen line with needle was removed from the vial, and the resulting mixture stirred at room temperature for 24 h. Then, the reaction mixture was filtered through a short pad of Celite and concentrated in vacuo. The reaction mixture was purified by flash silica gel column chromatography using hexane/EtOAc (5/1) as eluent and recrystallization from hexane and DCM afforded **L3**CuBr (366.1 mg, 0.45 mmol, 64% yield)

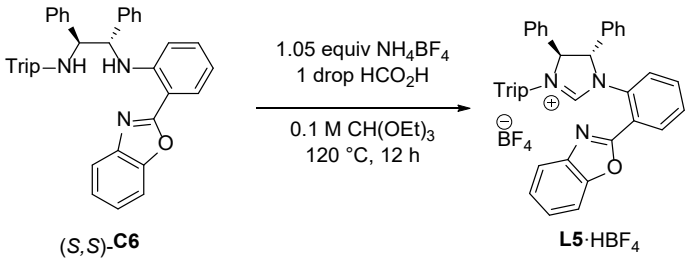
[1] Wang, H.; Lu, G.; Sormunen, G. J.; Malik, H. A.; Liu, P.; Montgomery, J. *J. Am. Chem. Soc.* **2017**, *139*, 9317– 9324

2-2. General procedure for the preparation of chiral NHC ligand **L5**

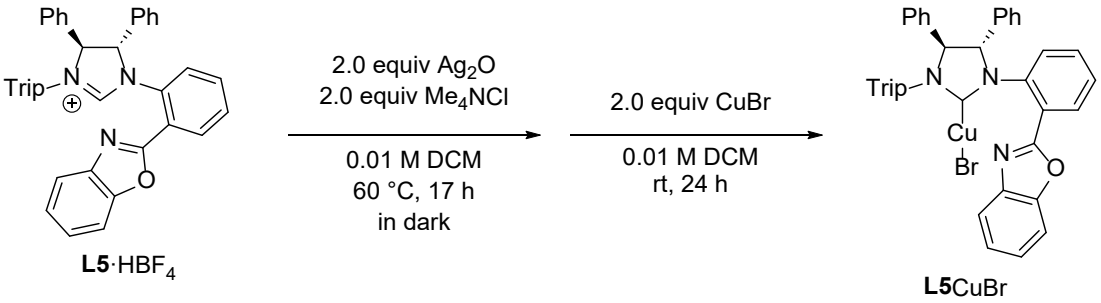


This coupling reaction was carried out according to the reported method[1].

To an oven-dried vial were added (*S*,*S*)-**C2** (414.0 mg,1.0 mmol, 1.0 equiv.), **C5** (355.0 mg, 1.0 equiv.), CuBr (28.7 mg, 20 mol%), and K_2CO_3 (345.5 mg, 2.5 equiv.) in a glovebox. The vial was sealed and brought out of the glovebox. The vial was connected with a nitrogen line through a needle, and DMF (4 mL) was added through the septum by syringe. After the nitrogen line with needle was removed, the resulting mixture was placed in a pre-heated 100℃ aluminum block and stirred for 24 h. After cooling to rt, volatiles were removed under vacuum and the crude product was purified by silica gel flash column chromatography using hexane/EtOAc (50/1 to 5/1) as eluent to give (*S*,*S*)-**C6** (340.4 mg, 0.56 mmol, 56% yield).



The solution of (*S*,*S*)-**C6** (340.4 mg, 0.56 mmol, 1.0 equiv.), NH_4BF_4 (61.6 mg, 1.05 equiv.) and HCOOH (1drop) in $CH(OEt_3)$ (5.6 mL) was heated at 120 ºC. The reaction mixture was stirred for 12 h and concentrated in vacuo. The residue was purified by flash column chromatography using DCM/MeOH (10/1) as eluent to give **L5**·HBF_4 (317.5 mg, 0.45 mmol, 80% yield).



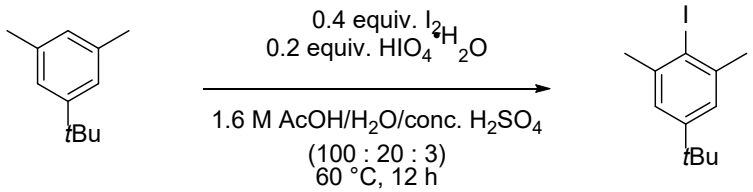
L5·HBF_4 **L5**CuBr

The preparation of Cu complex was carried out according to the reported method[2]

To an oven-dried and covered with foil vial were added **L5**·HBF_4 (317.5 mg. 0.45 mmol, 1.0 equiv.), Ag_2O (208.6 mg, 0.90 mmol, 2.0 equiv.), and Me_4NCl (xx mg, 2.0 equiv.) in a glovebox. The vial was connected with a nitrogen line through a needle, and DCM (45 mL) was added through the septum by syringe. The nitrogen line with needle was removed and the resulting mixture stirred at 60 ºC for 17 h. Then the reaction mixture was filtered through a short pad of Celite and concentrated in vacuo. In a glovebox, to an oven-dried vial covered with foil were added the reaction mixture and CuBr (129.1 mg, 0.90 mmol, 2.0 equiv.). The vial was connected with a nitrogen line through a needle, and DCM (45 mL) was added through the septum by syringe. The nitrogen line with needle was removed, and the resulting mixture stirred at room temperature for 24 h. Then, the reaction mixture was filtered through a short pad of Celite and concentrated in vacuo. The reaction mixture was purified by flash chromatography using hexane/EtOAc (5/1) as eluent and recrystallization from hexane and DCM afforded **L5**CuBr (161.6 mg, 0.21 mmol, 47% yield).

3. General procedure for preparation of starting materials 1

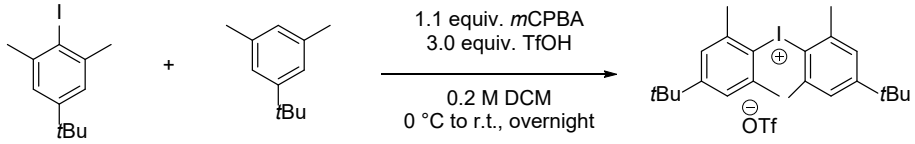
3-1 General procedure for the preparation of **1a-1d**



S-1 **S-2**

The iodonation of **S-1** was carried out according to the reported method[1].

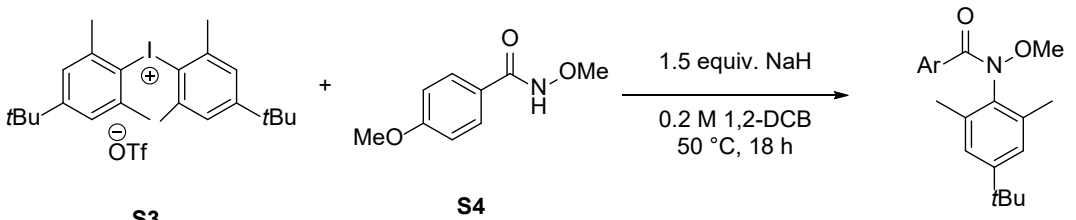
The 1.6 M solution of **S-1** (1.87 mL, 10 mmol, 1.0 equiv.), I_2 (1.02 g, 4 mmol, 0.4 equiv.), and $HIO_4 \cdot H_2O$ (0.46 g, 2 mmol, 0.2 equiv.) in the solvent mixed with AcOH (5 mL), H_2O (1 mL) and conc. H_2SO_4 (0.15 mL) was heated at 60 ºC. After stirring for 12 h, the reaction mixture sat. $NaHCO_3$ aq. Was added to the reaction mixture to quench the reaction. Then, the mixture was extracted with hexane, dried with Na_2SO_4, and concentrated in vacuo. The residue was purified by silica gel flash column chromatography using hexane as eluent to give **S2** as a colorless oil (2.82 g, 9.8 mmol, 98% yield).



S2 **S1** (1.1 equiv.) **S3**

The preparation of diaryliodonium triflate was carried out according to the reported method[2].

To a solution of **S2** (2.82 g, 9.8 mmol, 1.0 equiv.), **S1** (2.0 mL, 10.8 mmol, 1.1 equiv.), and *m*CPBA (contains *ca.* 30% water, 2.66 g, 10.8 mmol) in DCM (49 mL) was added TfOH (2.58 mL, 29.4 mmol, 3.0 equiv.) dropwise at 0 ºC. The reaction mixture warmed up to room temperature and stirred overnight. To the solution was added $NaHCO_3$ aq. to quench the reaction. The mixture was extracted with DCM, dried with Na_2SO_4, and concentrated in vacuo. The residue was washed by Et_2O to afford diaryliodonium triflate **S3** (419.0 mg, 7.0 mmol, 71% yield) as a colorless solid.



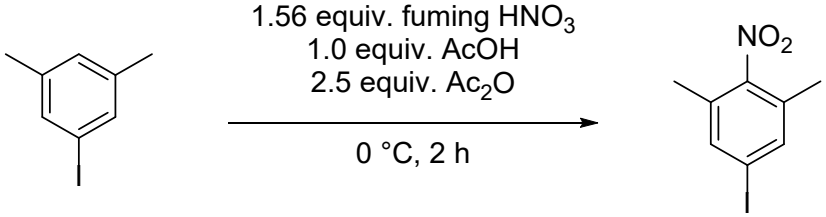
S3

S4
(1.5 equiv.)

1a
(Ar = *p*-$MeOC_6H_4$)

The amidation of diaryliodonium triflate was carried out according to the reported method[3]. The solution of **S3** (598 mg, 1.0 mmol,1.0 equiv.), **S4** (271 mg, 1.5 mmol, 1.5 equiv.) and NaH (containing *ca.* 40% mineral oil, 60 mg, 1.5 mmol) in 1,2-DCB (5 mL) was heated at 50 ºC. After stirring for 18 h, water was added to the reaction mixture to quench the reaction. The mixture was extracted with DCM, dried with Na_2SO_4, and concentrated in vacuo. The residue was purified by silica gel flash column chromatography using hexane/EtOAc (5/1) as eluent to give **1a** (266.3 mg, 0.78 mmol, 78% yield).

3-2 General procedure for the preparation of **1e** and **1f**

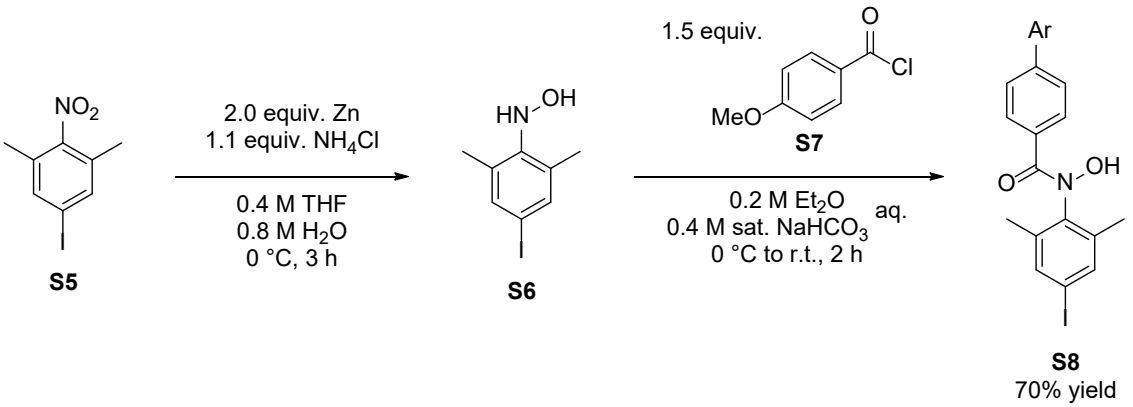


1-iodo-3,5-dimethylbenzene

S5
47% yield

The nitration of 1-iodo-3,5-dimethylbenzene was carried out according to the reported method[4].

A mixture of fuming HNO_3 (1.05 mL, 25 mmol, 1.56 equiv.), AcOH (0.950 mL, 16.7 mmol, 1.0 equiv.), Ac_2O (0.926 mL, 9.8 mmol, 0.61 equiv.) was dropped into a solution of 1-iodo-3,5-dimethylbenzene (2.99 mL, 16 mmol, 1.0 equiv.) and Ac_2O (2.78 ml, 29.4 mmol, 1.84 equiv.) at 0ºC within 2 h. The precipitate was filtered and recrystallized in methanol, and then dried to afford **S5** (2.08 g, 7.51 mmol, 47%).

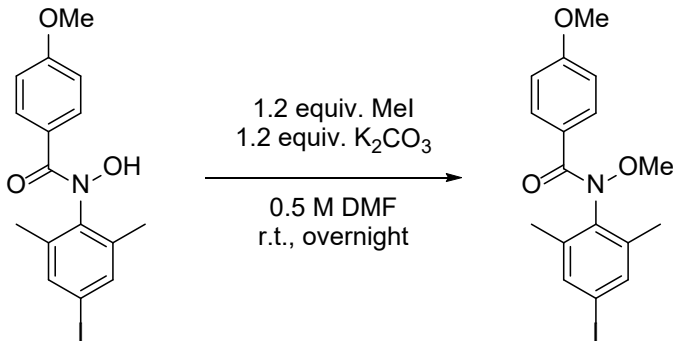


S5 **S6** **S8**
70% yield

S6 was prepared in accordance with the literature method[5].

To a solution of **S5** (2.08 g, 7.51 mmol), NH_4Cl (442 mg, 8.26 mmol) in THF (19 mL) and H_2O (9 mL) was added Zn (980 mg, 15.0 mmol) at 0 °C. The reaction mixture was stirred at 0 °C for 3 h. The reaction mixture was filtered through a short pad of Celite and extracted with Et_2O. The combined organic layers were washed with brine, dried with Na_2SO_4, and concentrated in vacuo. The residue was directly used for the next step.

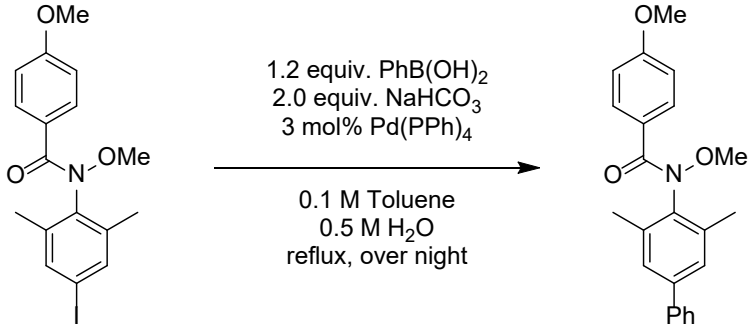
To a solution of **S6** in Et_2O (38 mL) and sat. $NaHCO_3$ aq. (19 mL) was added **S7** (1.53 ml, 11.3 mmol) dropwise at 0 °C. The reaction mixture warmed up to room temperature and stirred for 2 h. To the reaction mixture was added water to quench the reaction. The mixture was extracted with EtOAc, dried with Na_2SO_4, and concentrated in vacuo. Recrystallization from hexane/DCM afforded **S8** (2.09 g, 5.26 mmol, 70% in two steps).



S8 **S9**
74% yield

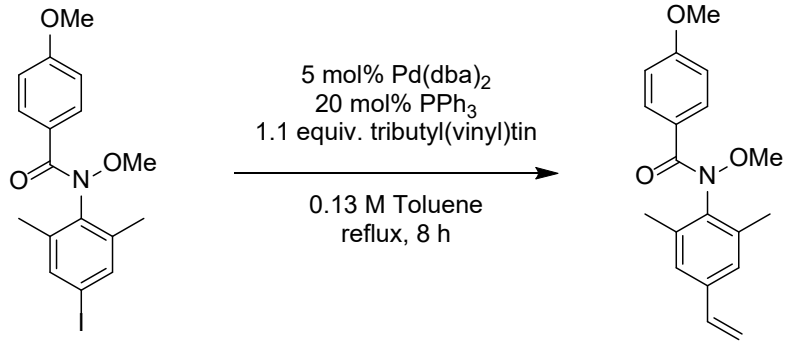
To a solution of **S8** (2.09 g, 5.26 mmol) and K_2CO_3 (872 mg, 6.31 mmol) in DMF (11 mL) was added MeI (0.48 mL, 6.31 mmol) dropwise at room temperature. After stirring overnight, water was added to the reaction mixture to quench the reaction. The mixture was extracted with Et_2O, washed with brine, dried with Na_2SO_4, and concentrated in vacuo. The residue was purified by silica gel flash column chromatography using hexane/EtOAc (2/1) as eluent

to give **S9** (1.60 g, 3.89 mmol, 74%).



S9 **1e**

To a mixture of **S9** (0.617 g, 1.5 mmol), phenylboronic acid (219.5 mg, 1.8 mmol), $NaHCO_3$ (252 mg, 3.0 mmol), $Pd(PPh_3)_4$ (52 mg, 0.045 mmol) in a 100 mL two-neck flask were added toluene (15 mL) and water (3 mL) under nitrogen atmosphere. The reaction mixture was stirred with refluxing overnight. After cooling down to room temperature, the reaction mixture was extracted with EtOAc, washed with brine, and dried with Na_2SO_4. After removing solvents in vacuo, the residue was purified by silica gel flash column chromatography using hexane/EtOAc (2/1) as eluent to give **1e** (0.448 g, 1.24 mmol, 83%).



S9 **1f**

To a mixture of **S9** (0.288 g, 0.7 mmol), PPh_3 (37 mg, 0.14 mmol) in a 50 mL round-bottom flask were added $Pd(dba)_2$ (20 mg, 0.035 mmol), toluene (5.4 mL), and tributylvinyltin (0.24 mL, 0.77 mmol) under Ar atmosphere. The reaction mixture was stirred with refluxing for 8 h. After cooling to room temperature, the reaction mixture was extracted with EtOAc, washed with brine, and dried with Na_2SO_4. After removing solvents in vacuo, the residue was purified by silica gel flash column chromatography using hexane/EtOAc (2/1) with 10 wt% potassium fluoride as eluent to give **1f** (0.198 g, 0.64 mmol, 91%).

[1] Suzuki, H.; Nakamura, K.; Goto, R. *Bull. Chem. Soc. Jpn.*, **1968**, *39*, 128-131

[2] Bielawski, M.; Olofsson, B.; *Chem. Commun.*, **2007**, 2521-2523

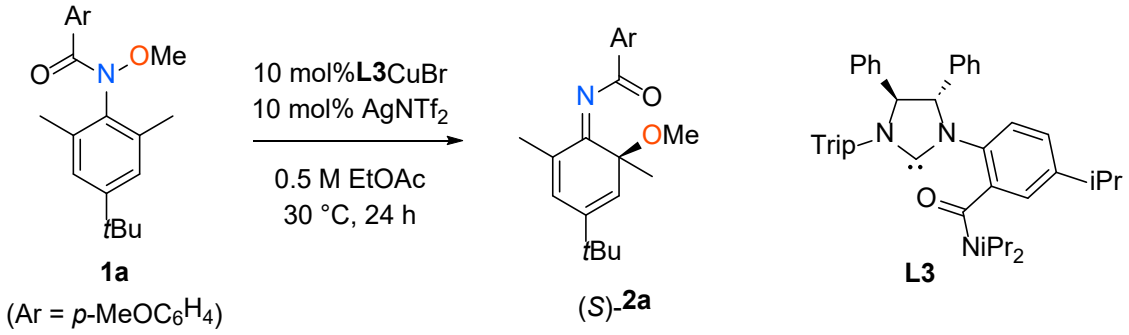
[3] Kikushima, K.; Morita, A.; Elboray, E. E.; Bae, T.; Miyamoto, N.; Kita Y.; Dohi, T. *Synthesis*,

2022, *54*, 5192-5202

[4] Jingyu Liu, Yanguo Li, Yuesheng Li, Ninghai Hu, *Journal of Applied Polymer Science*, **2008**,*109*, 700–707

[5] Porzelle, A.; Woodrow, M. D.; Tomkinson, N. C. O. *Org. Lett*. **2010**, *12*, 812

4. General procedure for copper-catalyzed reaction of 1



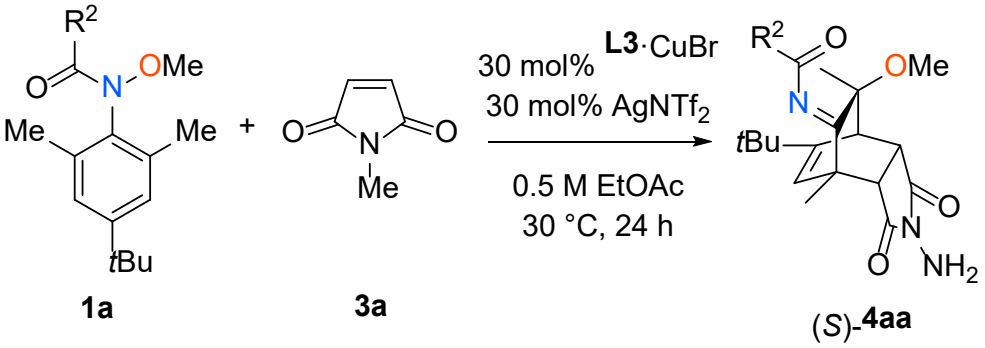
1a
(Ar = *p*-$MeOC_6H_4$)

(*S*)-**2a**

L3

To a mixture of **1a** (34.1 mg, 0.1 mmol), **L3**CuBr (24.3 mg, 0.03 mmol), and $AgNTf_2$ (11.7 mg, 0.03 mmol) in a 3 mL pressure vial was added EtOAc under argon atmosphere. After stirring at 30 °C for 24 h, the reaction mixture was passed through a short pad of silica with EtOAc (50 mL), then solvent was removed in vacuo. The crude mixture was purified by silica gel flash column chromatography using hexane/EtOAc (5/1) as eluent to give (*S*)-**2a** (23.5 mg, 0.082 mmol, 58% yield, er = 89:11) in an analytically pure form.

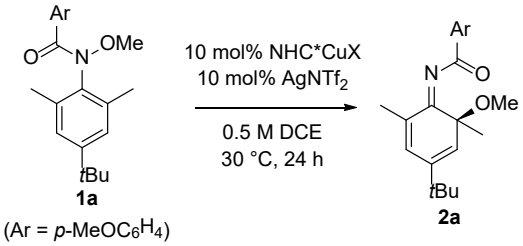
5. General procedure for copper-catalyzed reaction between 1 and 3

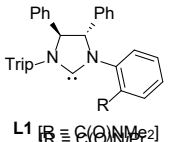


To a mixture of **1a** (34.1 mg, 0.1 mmol), **3a** (55.6 mg, 0.5 mmol), **L3**CuBr (5.34 mg, 0.03 mmol), and $AgNTf_2$ (11.7 mg, 0.03 mmol) in a 3 mL pressure vial was added EtOAc under argon atmosphere. After stirring at 30 °C for 24 h, the reaction mixture was passed through a short pad of silica with EtOAc (50 mL), then solvent was removed in vacuo. The crude mixture was purified by silica gel flash column chromatography using hexane/EtOAc (2/1) as eluent to give (*S*)-**2a** (23.5 mg, 0.082 mmol, 58% yield, er = 89:11) in an analytically pure form.

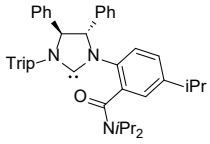
6. Screening of chiral NHC ligands

Table S1. Screening of chiral NHC ligands

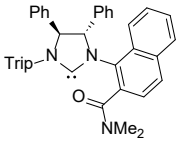




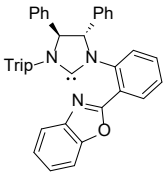
L1 [R = C(O)NMe2]
L2 [R = C(O)NPh2]
L6
L7 (R = MeO)
L8 [R = C(O)Ph]



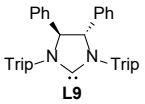
L3



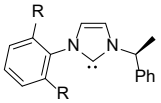
L4



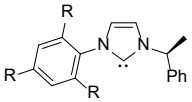
L5



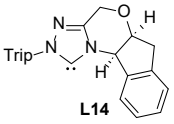
L9
(Trip: 2,4,6-triisopropylphenyl)



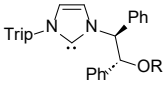
L10 (R = iPr)
L11 (R = Ph)



L12 (R = cyclohexyl)
L13 (R = cyclopentyl)



L14



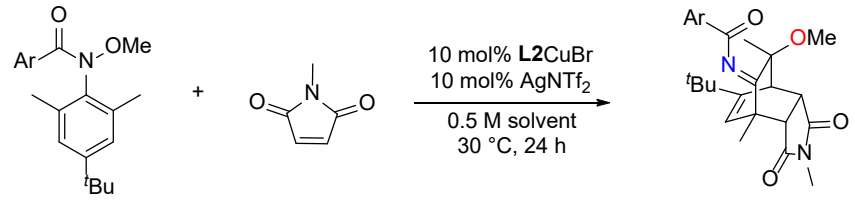
L15 (R = H)
L16 (R = Me)

Entry	NHC*	Yield / %[a]	Er	Recovery / %[a]
1	**L1**	27	82:18	70
2	**L2**	33	80:20	65
3	**L3**	31	74:26	60
4	**L4**	49	34:66	50
5	**L5**	13	82:18	85
6	**L6**	31	73:27	65
7	**L7**	10	45:55	80
8	**L8**	10	38:62	80
9	**L9**	86	44:56	<1
10	**L10**	35	45:55	65
11	**L11**	44	50:50	56
12	**L12**	<5	45:55	>95
13	**L13**	<5	46:54	>95
14	**L14**	37	25:75	63
15	**L15**	33	32:68	67
16	**L16**	36	30:70	64

[a] Yields were determined by ^{1}H NMR using CH_2Br_2 as the internal standard.

7. Solvent effect on the [1,3]-rearrangement – Diels-Alder cascade reactions

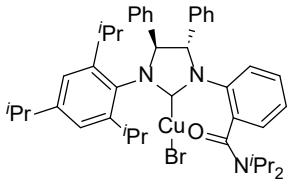
Table S2. Solvent effect



1a
Ar = 4-MeOC$_6$H$_4$

3a
(5.0 equiv.)

4aa



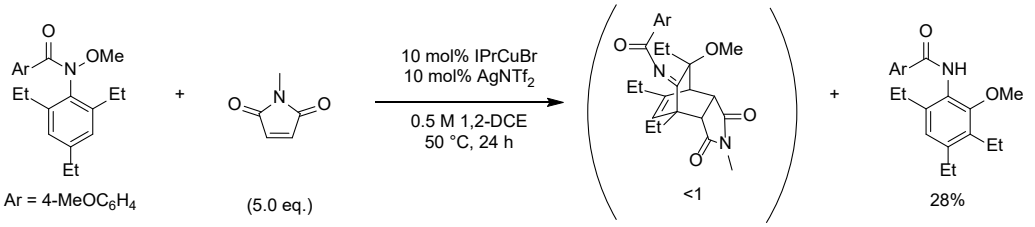
L2CuBr

Entry	solvent	**4aa** (%[a])	Er	**1a** (%[a])
1	DCE	38	80:20	44
2	toluene	23	85:15	61
3	1,4-dioxane	27	84:16	58
4	EtOAc	28	89:11	52
5	acetone	31	88:12	55
6	Et_2O	30	86:14	53
7[b]	EtOAc	33	92:8	59

[a] Yields were determined by ^{1}H NMR using CH_2Br_2 as the internal standard. [b] **L3**CuBr was used instead of **L2**CuBr.

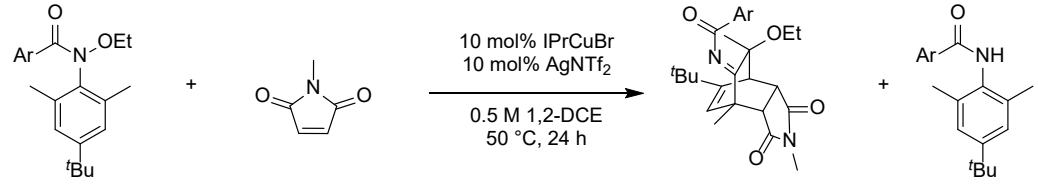
8. Unsuccessful substrates at the present stage

8-1. *ortho*-diethyl-*N*-methoxyaniline



Ar = 4-MeOC$_6$H$_4$ (5.0 eq.) <1 28%

8-2. *N*-ethoxyaniline



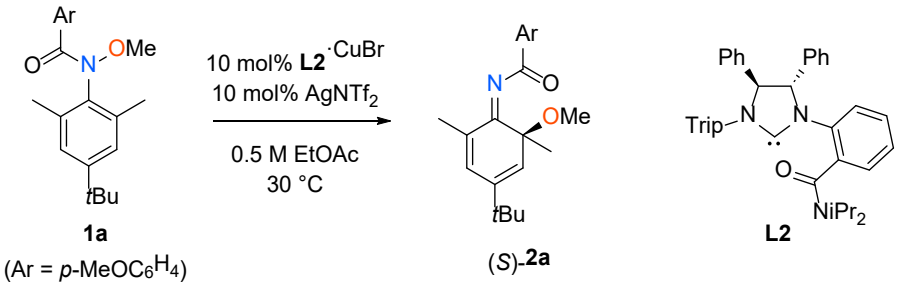
Ar = 4-MeOC$_6$H$_4$ (5.0 eq.) 22% yield 51% yield

(17% of *N*-ethoxyaniline was recovered)

9. Mechanistic Studies

9-1. Decrease of enantioselectivity by prolonging reaction time

Table S3. Prolonged reaction time



1a (Ar = *p*-$MeOC_6H_4$)

(*S*)-**2a**

L2

Entry	Time (h)	2a (%[a])	Er	1 (%[a])
1	3	24	84:16	76
2	24	33	79:21	65

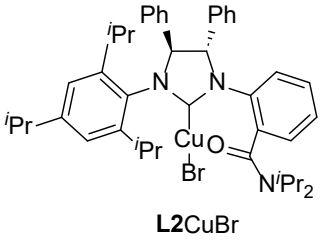
[a] Yields were determined by ^1H NMR using CH_2Br_2 as the internal standard.

9-2. Formation of Homoleptic $[(\mathbf{L2})_2Cu]^+$ catalysts

detected by HRMS

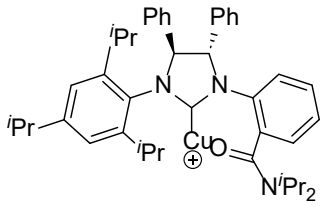
calcd for $[(\mathbf{L2})_2Cu]^+$: 1317.7668:

found: 1317.7668



L2CuBr

Cf.

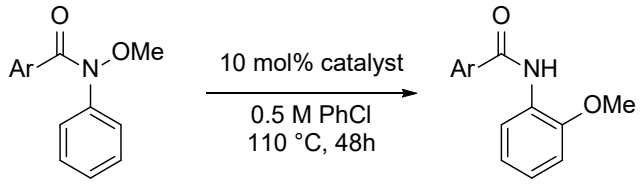


calcd for $\mathbf{L2}Cu^+$: 690.3479

found: 690.3479 (HRMS)

9-3. The reaction using homoleptic $[(IMes)_2Cu]BF_4$ catalyst

Table S4. Reactivity of homoleptic $[(IMes)_2Cu]BF_4$ catalyst



Ar = 3,4,5-$(MeO)_3C_6H_2$

Entry	Catalyst	Yield (%[a])
1	$[(IMes)_2Cu]BF_4$	<1
2	IMesCuBr, $AgNTf_2$	45

[a] Yields were determined by ^1H NMR using CH_2Br_2 as the internal standard.

10. X-ray crystallographic analysis of (*S*)-2c

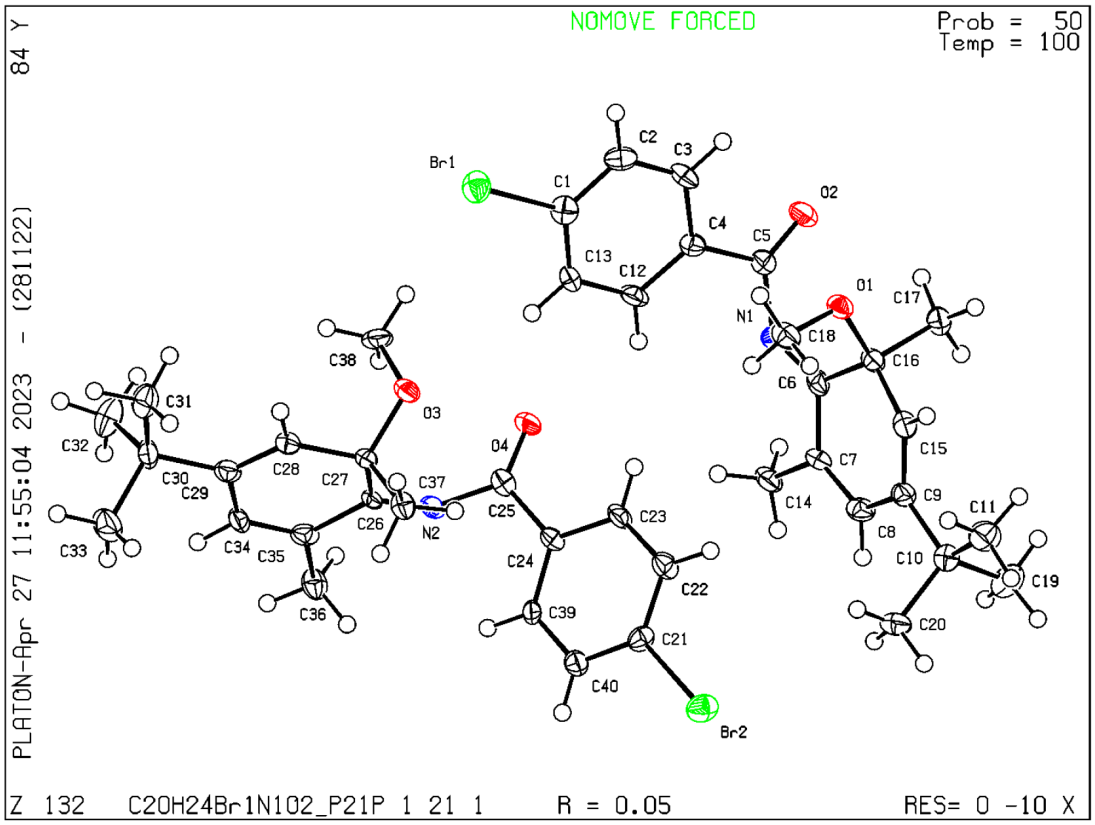


Table S5. Crystal data and structure refinement for (*S*)-2c

Identification code	mo_230426nakamura_0m
Empirical formula	$C_{40}H_{48}Br_2N_2O_4$
Formula weight	780.62
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	10.4950(6)
b/Å	15.3001(10)
c/Å	11.7177(8)
α/°	90
β/°	97.033(2)
γ/°	90
Volume/Å^3	1867.4(2)

Z	2
ρ_{calc}g/cm^3	1.388
μ/mm^{-1}	2.213
F(000)	808.0
Crystal size/mm^3	0.2 × 0.2 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.91 to 55.04
Index ranges	-13 ≤ h ≤ 13, -19 ≤ k ≤ 19, -15 ≤ l ≤ 15
Reflections collected	59545
Independent reflections	8582 [R_{int} = 0.1202, R_{sigma} = 0.0836]
Data/restraints/parameters	8582/1/445
Goodness-of-fit on F^2	1.015
Final R indexes [I>=2σ (I)]	R_1 = 0.0477, wR_2 = 0.0966
Final R indexes [all data]	R_1 = 0.0721, wR_2 = 0.1077
Largest diff. peak/hole / e Å^{-3}	0.83/-0.50
Flack parameter	0.038(8)

Table S6. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for (*S*)-2c. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Br1	9027.6(6)	2250.8(4)	5925.9(6)	30.48(19)
Br2	8813.4(6)	7771.6(4)	932.0(6)	29.59(19)
O1	8204(4)	6632(3)	7256(3)	23.1(9)
O2	5666(4)	5657(4)	7939(4)	27.8(11)
O3	7821(4)	2816(3)	2588(3)	23.1(9)
O4	5773(4)	4213(3)	2961(4)	26.0(11)
N1	5778(5)	6126(4)	6096(5)	20.6(12)
N2	5908(5)	3780(4)	1103(5)	20.6(12)
C1	8100(5)	3267(5)	6259(6)	24.0(16)
C2	8073(6)	3507(5)	7392(6)	26.8(16)
C3	7410(6)	4247(5)	7625(6)	25.9(16)
C4	6777(6)	4753(5)	6736(6)	21.1(15)

Table S6. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for (*S*)-2c. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C5	6082(6)	5561(5)	7024(6)	22.0(15)
C6	6287(5)	6863(4)	5916(6)	20.9(14)
C7	5797(5)	7344(5)	4870(5)	19.6(14)
C8	6387(6)	8087(5)	4610(6)	23.3(15)
C9	7554(6)	8436(5)	5259(6)	21.8(14)
C10	8104(6)	9270(5)	4832(6)	26.2(16)
C11	9376(6)	9530(5)	5540(7)	32.8(18)
C12	6809(6)	4486(5)	5596(6)	23.6(16)
C13	7487(6)	3748(5)	5355(6)	23.1(15)
C14	4678(6)	6959(5)	4103(6)	25.4(16)
C15	8033(6)	8017(4)	6225(6)	22.3(15)
C16	7351(5)	7287(5)	6749(5)	20.8(12)
C17	6707(6)	7694(6)	7743(6)	27.8(16)
C18	9024(6)	6283(5)	6510(6)	26.0(15)
C19	7133(7)	10013(5)	4943(8)	37.1(19)
C20	8343(7)	9177(5)	3570(6)	31.8(17)
C21	7969(5)	6715(5)	1265(6)	21.1(14)
C22	7893(6)	6497(5)	2413(6)	24.2(16)
C23	7288(6)	5727(5)	2634(6)	22.2(15)
C24	6750(5)	5190(5)	1740(6)	19.0(14)
C25	6158(6)	4339(5)	2025(6)	22.6(15)
C26	6537(5)	3133(4)	763(5)	16.4(13)
C27	7849(5)	2834(4)	1368(5)	18.9(12)
C28	8243(6)	1957(4)	965(6)	20.4(14)
C29	7661(6)	1525(5)	55(6)	22.1(15)
C30	8073(6)	622(5)	-330(6)	25.3(15)
C31	9241(7)	276(5)	438(7)	32.4(18)
C32	6937(7)	-10(5)	-279(8)	39(2)
C33	8409(8)	666(6)	-1568(7)	39(2)

Table S6. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for (*S*)-2c. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C34	6526(6)	1930(4)	-590(6)	20.6(15)
C35	6000(5)	2674(5)	-292(6)	21.8(15)
C36	4807(6)	3066(5)	-963(6)	26.1(17)
C37	8866(5)	3509(4)	1145(6)	22.8(15)
C38	6929(6)	2185(6)	2939(6)	29.1(15)
C39	6820(6)	5444(5)	621(6)	21.0(15)
C40	7425(6)	6212(5)	370(6)	22.8(15)

Table S7. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for (*S*)-2c. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\square E$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br1	29.0(3)	28.8(4)	32.5(4)	-3.0(4)	-0.5(3)	6.5(3)
Br2	28.4(3)	28.8(4)	30.5(4)	4.3(4)	-0.8(3)	-8.6(3)
O1	26(2)	26(2)	16(2)	0.7(19)	-0.2(17)	6.4(18)
O2	36(3)	32(3)	16(3)	0(2)	5(2)	4(2)
O3	29(2)	26(2)	14(2)	-1(2)	1.2(16)	-3(2)
O4	39(3)	26(3)	15(3)	0(2)	9(2)	-6(2)
N1	25(3)	19(3)	18(3)	2(2)	3(2)	4(2)
N2	24(3)	24(3)	14(3)	0(2)	3(2)	-3(2)
C1	18(3)	27(4)	28(4)	-1(3)	6(3)	0(3)
C2	24(3)	31(4)	24(4)	9(3)	-3(3)	4(3)
C3	29(3)	35(5)	12(4)	-2(3)	-1(3)	0(3)
C4	22(3)	22(4)	18(4)	2(3)	0(3)	1(3)
C5	24(3)	23(4)	19(4)	-1(3)	1(3)	0(3)
C6	21(3)	23(4)	19(4)	-5(3)	5(2)	6(3)
C7	21(3)	26(4)	12(3)	1(3)	2(2)	1(3)
C8	23(3)	28(4)	19(4)	4(3)	1(3)	7(3)
C9	25(3)	22(4)	18(4)	0(3)	5(2)	4(3)

Table S7. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for (*S*)-2c. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\square E$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C10	32(3)	23(4)	24(4)	-1(3)	4(3)	-2(3)
C11	33(4)	34(4)	32(4)	1(3)	6(3)	-9(3)
C12	29(3)	30(4)	12(4)	2(3)	-1(3)	-4(3)
C13	31(3)	22(4)	16(4)	-5(3)	4(3)	2(3)
C14	30(3)	32(4)	14(4)	-2(3)	0(3)	4(3)
C15	23(3)	23(4)	21(4)	-4(3)	1(2)	2(2)
C16	24(3)	23(3)	15(3)	-1(3)	2(2)	6(3)
C17	36(3)	24(4)	23(4)	-4(3)	2(3)	5(3)
C18	24(3)	33(4)	20(4)	0(3)	2(3)	8(3)
C19	36(4)	27(4)	48(5)	5(4)	7(3)	3(3)
C20	45(4)	31(4)	20(4)	6(3)	8(3)	-5(3)
C21	19(3)	19(4)	25(4)	2(3)	1(2)	-4(2)
C22	24(3)	29(4)	19(4)	-4(3)	1(3)	-5(3)
C23	27(3)	27(4)	12(4)	-4(3)	-1(3)	-3(3)
C24	20(3)	24(4)	13(3)	-2(3)	-1(2)	-1(3)
C25	23(3)	26(4)	19(4)	-4(3)	2(3)	-1(3)
C26	23(3)	17(3)	10(3)	-1(2)	6(2)	-3(2)
C27	26(3)	18(3)	12(3)	0(3)	2(2)	-3(3)
C28	23(3)	21(4)	17(3)	1(3)	5(2)	-1(2)
C29	26(3)	24(4)	17(3)	2(3)	4(2)	-5(3)
C30	32(3)	20(4)	24(4)	-9(3)	8(3)	-3(3)
C31	34(4)	25(4)	39(5)	-5(3)	8(3)	6(3)
C32	38(4)	23(4)	56(6)	-6(4)	4(4)	-5(3)
C33	50(4)	40(5)	28(5)	-6(4)	10(3)	13(4)
C34	27(3)	21(4)	15(3)	-6(3)	5(2)	-8(3)
C35	23(3)	25(4)	18(3)	4(3)	3(2)	-8(3)
C36	23(3)	29(4)	25(4)	-7(3)	-4(3)	-2(3)
C37	22(3)	24(4)	22(4)	-4(3)	1(3)	0(3)
C38	41(3)	25(4)	21(4)	9(3)	4(3)	-8(3)
C39	31(3)	14(4)	16(4)	-4(3)	-3(3)	3(3)

Table S7. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for (*S*)-2c. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\square E$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C40	27(3)	22(4)	19(4)	-2(3)	1(3)	5(3)

Table S8. Bond Lengths for (*S*)-2c.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C1	1.900(7)	C10	C11	1.536(9)
Br2	C21	1.907(7)	C10	C19	1.543(10)
O1	C16	1.425(7)	C10	C20	1.536(10)
O1	C18	1.404(7)	C12	C13	1.382(10)
O2	C5	1.216(8)	C15	C16	1.497(9)
O3	C27	1.434(7)	C16	C17	1.547(8)
O3	C38	1.440(8)	C21	C22	1.397(9)
O4	C25	1.230(8)	C21	C40	1.367(9)
N1	C5	1.395(9)	C22	C23	1.379(10)
N1	C6	1.276(9)	C23	C24	1.396(9)
N2	C25	1.377(9)	C24	C25	1.498(10)
N2	C26	1.279(8)	C24	C39	1.378(9)
C1	C2	1.381(10)	C26	C27	1.539(8)
C1	C13	1.383(10)	C26	C35	1.472(9)
C2	C3	1.374(10)	C27	C28	1.498(9)
C3	C4	1.398(9)	C27	C37	1.531(8)
C4	C5	1.494(10)	C28	C29	1.337(9)
C4	C12	1.402(10)	C29	C30	1.532(10)
C6	C7	1.468(9)	C29	C34	1.467(9)
C6	C16	1.534(8)	C30	C31	1.525(10)
C7	C8	1.347(10)	C30	C32	1.543(10)
C7	C14	1.508(9)	C30	C33	1.535(10)
C8	C9	1.461(9)	C34	C35	1.331(10)
C9	C10	1.511(10)	C35	C36	1.518(9)

Table S8. Bond Lengths for (*S*)-2c.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C9	C15	1.344(9)	C39	C40	1.384(10)

Table S9. Bond Angles for (*S*)-2c.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C18	O1	C16	114.2(5)	C15	C16	C6	113.7(5)
C27	O3	C38	113.0(5)	C15	C16	C17	106.5(6)
C6	N1	C5	128.0(6)	C22	C21	Br2	118.8(5)
C26	N2	C25	131.9(6)	C40	C21	Br2	118.7(5)
C2	C1	Br1	119.1(5)	C40	C21	C22	122.5(6)
C2	C1	C13	122.2(7)	C23	C22	C21	117.8(6)
C13	C1	Br1	118.7(5)	C22	C23	C24	121.0(7)
C3	C2	C1	118.7(7)	C23	C24	C25	119.0(6)
C2	C3	C4	121.0(7)	C39	C24	C23	119.0(7)
C3	C4	C5	119.4(6)	C39	C24	C25	122.0(6)
C3	C4	C12	118.9(7)	O4	C25	N2	123.4(6)
C12	C4	C5	121.7(6)	O4	C25	C24	121.7(6)
O2	C5	N1	122.7(6)	N2	C25	C24	114.2(6)
O2	C5	C4	122.5(7)	N2	C26	C27	123.6(6)
N1	C5	C4	114.1(6)	N2	C26	C35	118.1(6)
N1	C6	C7	118.0(6)	C35	C26	C27	118.3(5)
N1	C6	C16	123.8(6)	O3	C27	C26	109.8(5)
C7	C6	C16	118.2(6)	O3	C27	C28	109.7(5)
C6	C7	C14	118.0(6)	O3	C27	C37	106.5(5)
C8	C7	C6	119.2(6)	C28	C27	C26	112.8(5)
C8	C7	C14	122.8(6)	C28	C27	C37	108.9(5)
C7	C8	C9	124.7(6)	C37	C27	C26	108.9(5)
C8	C9	C10	117.8(6)	C29	C28	C27	125.2(6)
C15	C9	C8	117.9(6)	C28	C29	C30	124.2(6)
C15	C9	C10	124.3(6)	C28	C29	C34	117.7(6)

Table S9. Bond Angles for (*S*)-2c.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C9	C10	C11	112.5(6)	C34	C29	C30	118.0(6)
C9	C10	C19	108.1(5)	C29	C30	C32	107.9(5)
C9	C10	C20	110.8(6)	C29	C30	C33	110.2(6)
C11	C10	C19	107.6(6)	C31	C30	C29	112.0(6)
C11	C10	C20	108.1(6)	C31	C30	C32	109.1(7)
C20	C10	C19	109.6(6)	C31	C30	C33	108.2(6)
C13	C12	C4	120.5(7)	C33	C30	C32	109.4(6)
C12	C13	C1	118.7(7)	C35	C34	C29	124.2(6)
C9	C15	C16	123.5(6)	C26	C35	C36	116.9(6)
O1	C16	C6	109.8(5)	C34	C35	C26	120.0(6)
O1	C16	C15	112.8(4)	C34	C35	C36	123.0(6)
O1	C16	C17	106.3(5)	C24	C39	C40	121.4(6)
C6	C16	C17	107.3(5)	C21	C40	C39	118.3(7)

Table S10. Torsion Angles for (*S*)-2c.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Br1	C1	C2	C3	179.4(5)	C15	C9	C10	C11	7.2(9)
Br1	C1	C13	C12	179.8(5)	C15	C9	C10	C19	-111.5(7)
Br2	C21	C22	C23	-179.5(5)	C15	C9	C10	C20	128.3(7)
Br2	C21	C40	C39	179.7(5)	C16	C6	C7	C8	7.5(8)
O3	C27	C28	C29	133.4(6)	C16	C6	C7	C14	-175.1(5)
N1	C6	C7	C8	-174.5(6)	C18	O1	C16	C6	73.7(6)
N1	C6	C7	C14	2.9(8)	C18	O1	C16	C15	-54.3(7)
N1	C6	C16	O1	37.1(8)	C18	O1	C16	C17	-170.6(5)
N1	C6	C16	C15	164.5(6)	C21	C22	C23	C24	-1.0(9)
N1	C6	C16	C17	-78.0(8)	C22	C21	C40	C39	-2.4(9)
N2	C26	C27	O3	44.8(8)	C22	C23	C24	C25	177.1(6)
N2	C26	C27	C28	167.4(6)	C22	C23	C24	C39	-0.7(9)
N2	C26	C27	C37	-71.5(7)	C23	C24	C25	O4	22.8(9)
N2	C26	C35	C34	-170.8(6)	C23	C24	C25	N2	-166.8(6)

Table S10. Torsion Angles for (*S*)-2c.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N2	C26	C35	C36	6.2(9)	C23	C24	C39	C40	0.9(9)
C1	C2	C3	C4	-0.4(10)	C24	C39	C40	C21	0.6(9)
C2	C1	C13	C12	-1.0(10)	C25	N2	C26	C27	-1.5(11)
C2	C3	C4	C5	-179.1(6)	C25	N2	C26	C35	-178.8(6)
C2	C3	C4	C12	1.1(10)	C25	C24	C39	C40	-176.8(6)
C3	C4	C5	O2	-25.3(10)	C26	N2	C25	O4	-92.5(9)
C3	C4	C5	N1	164.3(6)	C26	N2	C25	C24	97.3(8)
C3	C4	C12	C13	-1.9(10)	C26	C27	C28	C29	10.7(8)
C4	C12	C13	C1	1.8(10)	C27	C26	C35	C34	11.7(9)
C5	N1	C6	C7	-179.8(6)	C27	C26	C35	C36	-171.3(5)
C5	N1	C6	C16	-1.9(10)	C27	C28	C29	C30	-179.2(6)
C5	C4	C12	C13	178.4(6)	C27	C28	C29	C34	-1.5(9)
C6	N1	C5	O2	82.2(9)	C28	C29	C30	C31	-0.8(9)
C6	N1	C5	C4	-107.5(7)	C28	C29	C30	C32	119.4(7)
C6	C7	C8	C9	4.1(10)	C28	C29	C30	C33	-121.3(7)
C7	C6	C16	O1	-145.0(5)	C28	C29	C34	C35	-3.7(9)
C7	C6	C16	C15	-17.6(7)	C29	C34	C35	C26	-1.8(9)
C7	C6	C16	C17	99.9(7)	C29	C34	C35	C36	-178.6(6)
C7	C8	C9	C10	178.8(6)	C30	C29	C34	C35	174.1(6)
C7	C8	C9	C15	-4.2(10)	C34	C29	C30	C31	-178.4(6)
C8	C9	C10	C11	-176.0(6)	C34	C29	C30	C32	-58.3(8)
C8	C9	C10	C19	65.3(8)	C34	C29	C30	C33	61.1(8)
C8	C9	C10	C20	-54.9(8)	C35	C26	C27	O3	-137.9(6)
C8	C9	C15	C16	-8.1(10)	C35	C26	C27	C28	-15.2(7)
C9	C15	C16	O1	144.3(6)	C35	C26	C27	C37	105.8(6)
C9	C15	C16	C6	18.4(8)	C37	C27	C28	C29	-110.4(7)
C9	C15	C16	C17	-99.5(7)	C38	O3	C27	C26	64.1(7)
C10	C9	C15	C16	168.7(6)	C38	O3	C27	C28	-60.4(6)
C12	C4	C5	O2	154.4(7)	C38	O3	C27	C37	-178.1(5)
C12	C4	C5	N1	-16.0(9)	C39	C24	C25	O4	-159.5(6)
C13	C1	C2	C3	0.3(10)	C39	C24	C25	N2	10.9(9)

Table S10. Torsion Angles for (*S*)-2c.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C14	C7	C8	C9	-173.2(6)	C40	C21	C22	C23	2.6(10)

Table S11. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for (*S*)-2c.

Atom	*x*	*y*	*z*	U(eq)
H2	8496.16	3174.49	7985.75	32
H3	7380.64	4413.37	8384.27	31
H8	6025.89	8400.57	3970.92	28
H11A	9994.34	9071.7	5502.6	49
H11B	9238.74	9623.22	6325.37	49
H11C	9691.47	10058.89	5232.95	49
H12	6371.83	4807.54	4998.27	28
H13	7529.95	3578.75	4598.24	28
H14A	4404.5	7360.38	3492.89	38
H14B	3982.1	6851.56	4545.44	38
H14C	4935.9	6418.4	3783.35	38
H15	8831.41	8188.94	6587.97	27
H17A	6077.74	8115.27	7437.29	42
H17B	7346.39	7977.01	8273.23	42
H17C	6297.22	7242.6	8134.75	42
H18A	8530.58	6119.46	5797.59	39
H18B	9452.02	5776.68	6857.12	39
H18C	9650.25	6713.22	6365.6	39
H19A	7488.05	10556.31	4722.11	56
H19B	6954.03	10050.31	5725.64	56
H19C	6352.35	9893.45	4450.58	56
H20A	7545.22	9058.46	3102.23	48
H20B	8930.5	8704.94	3500.06	48
H20C	8701.76	9710.55	3318.56	48
H22	8240.12	6860.2	3007.8	29

Table S11. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for (*S*)-2c.

Atom	*x*	*y*	*z*	U(eq)
H23	7237.19	5562.73	3391.74	27
H28	8950.11	1691.19	1381.46	24
H31A	9462.79	-292.08	174.54	49
H31B	9045.2	233.54	1215.52	49
H31C	9951.47	667.06	409.1	49
H32A	6237.59	158.88	-841.61	59
H32B	6664.31	10.91	473.53	59
H32C	7200.99	-594.11	-436.23	59
H33A	7676.67	867.95	-2069.76	59
H33B	8647.54	94.37	-1805.78	59
H33C	9112.71	1061.75	-1601.86	59
H34	6149.38	1648.23	-1249.22	25
H36A	4995.2	3645.91	-1208	39
H36B	4130.83	3091.02	-481.47	39
H36C	4541.45	2709.98	-1623.5	39
H37A	9696.19	3310.42	1480.21	34
H37B	8674.71	4057.83	1482.3	34
H37C	8866.54	3582.02	330.81	34
H38A	6076.04	2328.77	2598.91	44
H38B	6963.87	2191.41	3761.58	44
H38C	7152.41	1612.9	2690.83	44
H39	6452.28	5092.96	21.62	25
H40	7461.63	6381.91	-387.32	27

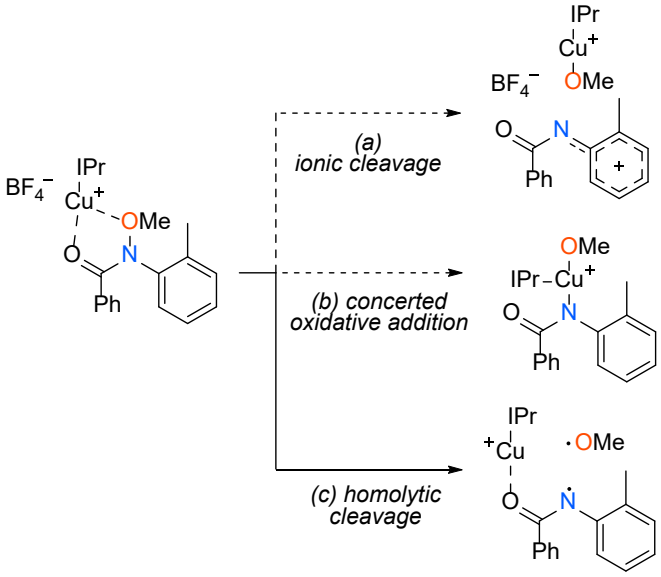
11. Computational Studies

11-1 General

Computational studies were carried out using the Gaussian 16 program package[1)] with density functional theory (DFT). The B3LYP functional, incorporating Grimme's D3 dispersion correction with Becke-Johnson damping, was employed in conjunction with the def2-SVP basis set for all atoms. Intrinsic reaction coordinate (IRC) calculations were performed for all optimized transition states to verify their connectivity to the corresponding reactants and products. Additionally, natural bond orbital (NBO) analysis was conducted using the NBO 7.0 program.[2)]

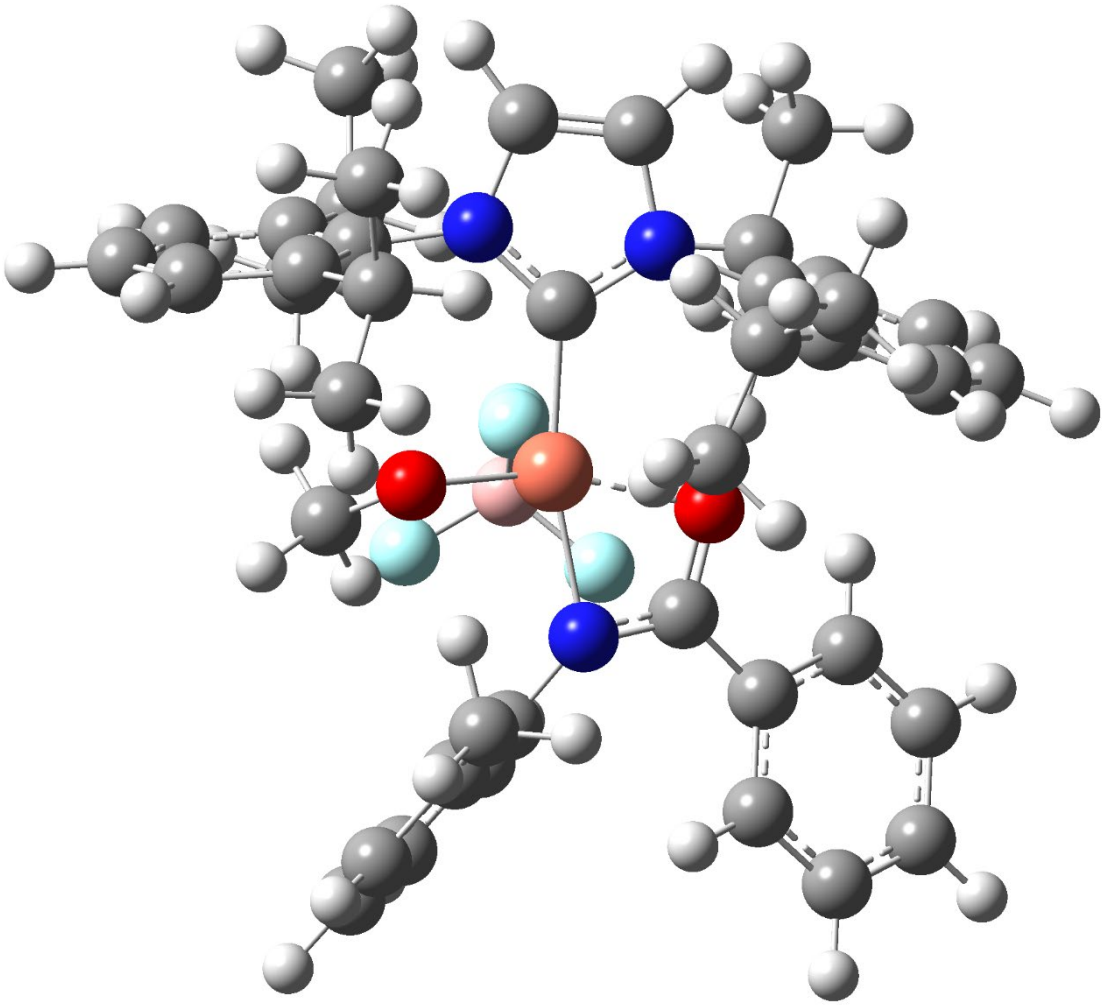
1) Gaussian 16, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2019.
2) NBO 7.0.10, E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, P. Karafiloglou, C. R. Landis, and F. Weinhold, Theoretical Chemistry Institute, University of Wisconsin, Madison, WI (2018).

11-2 Possible mechanisms for Cu-mediated N-O bond cleavage

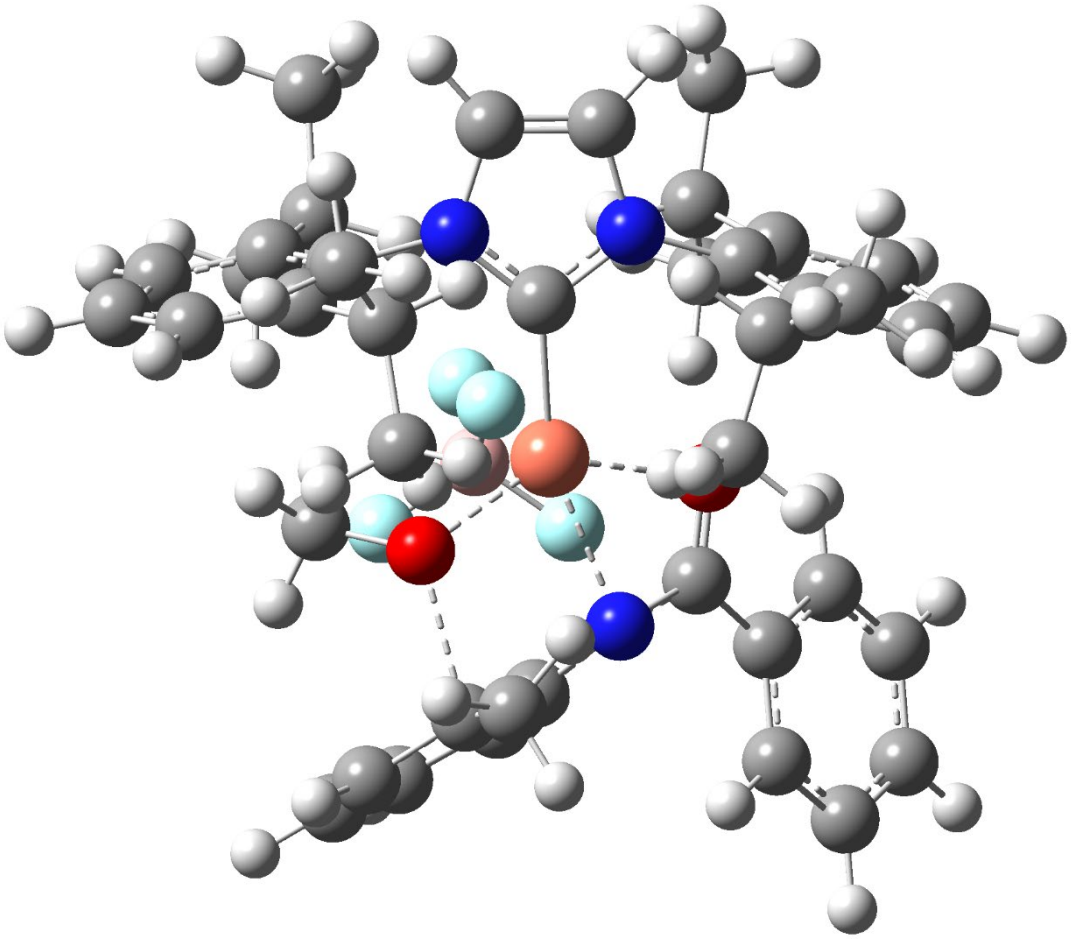


Scheme S1

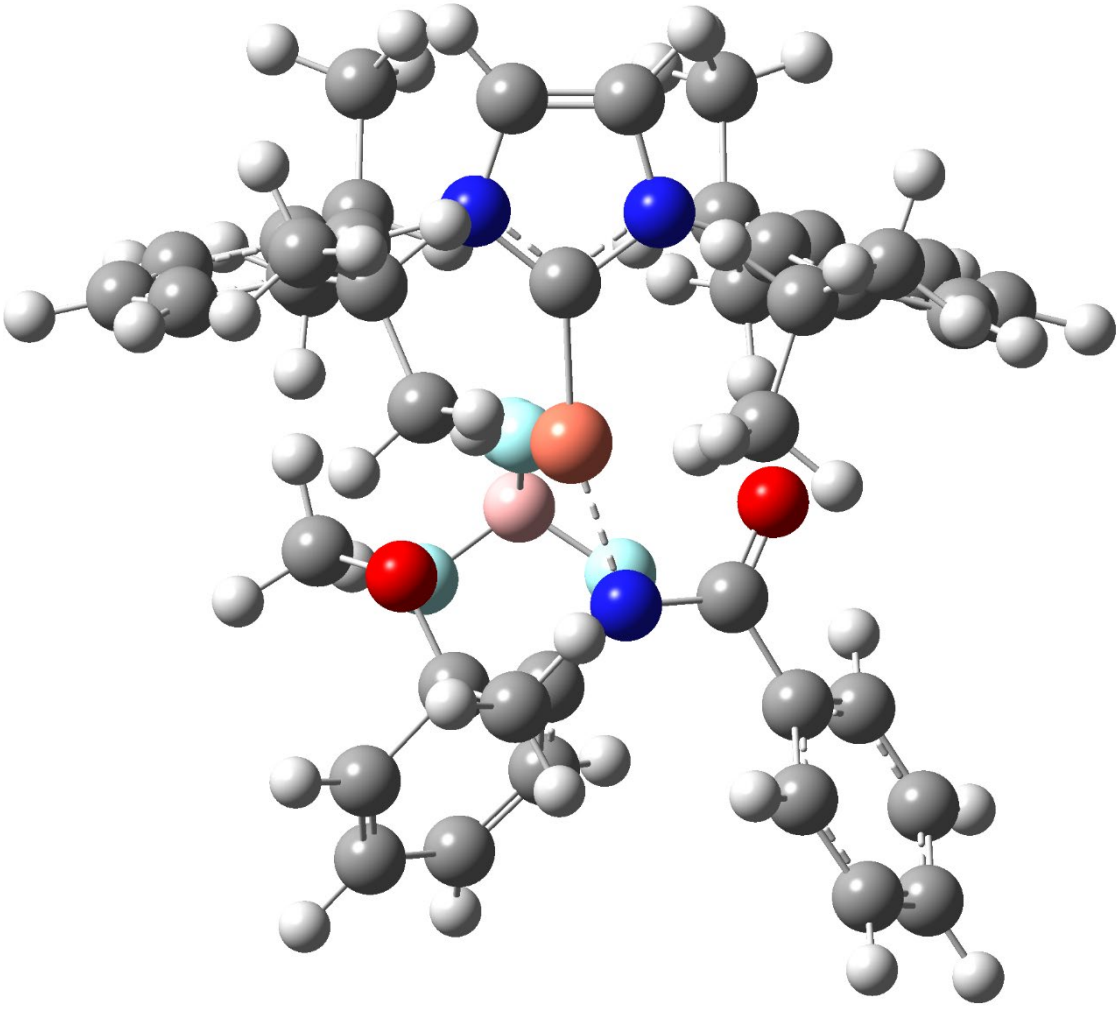
11-3 3D visualization of **IM2**, $\mathbf{TS_{2\text{-}3}}$, and **QI**



IM2



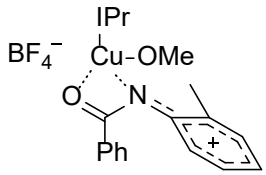
$TS_{2\text{-}3}$



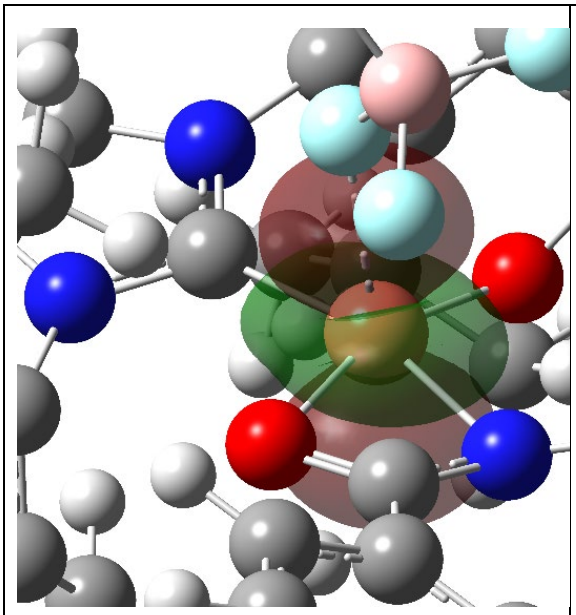
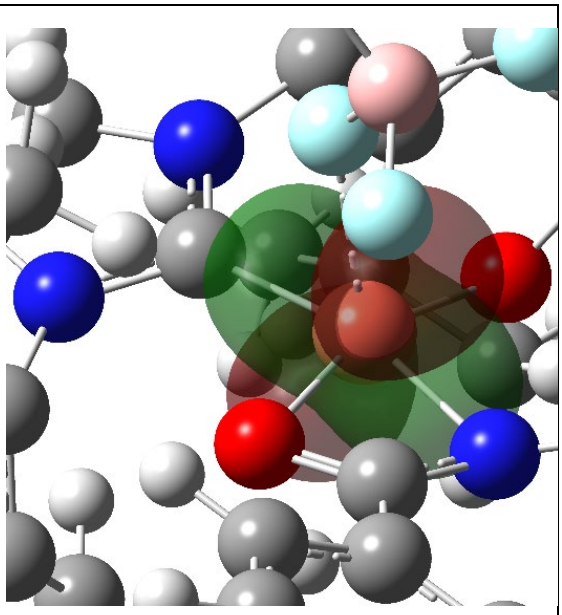
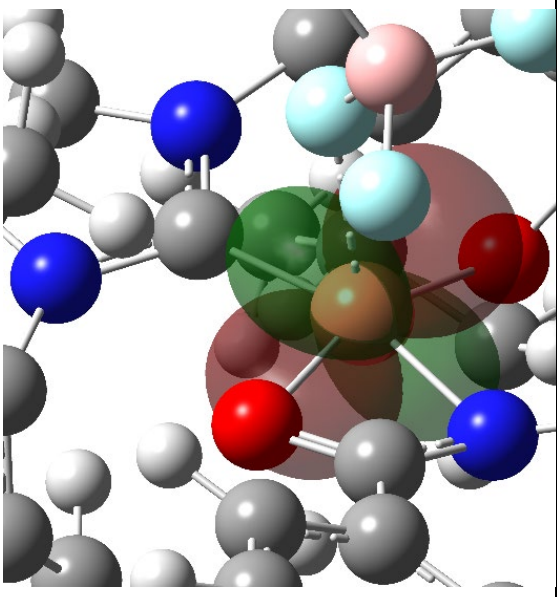
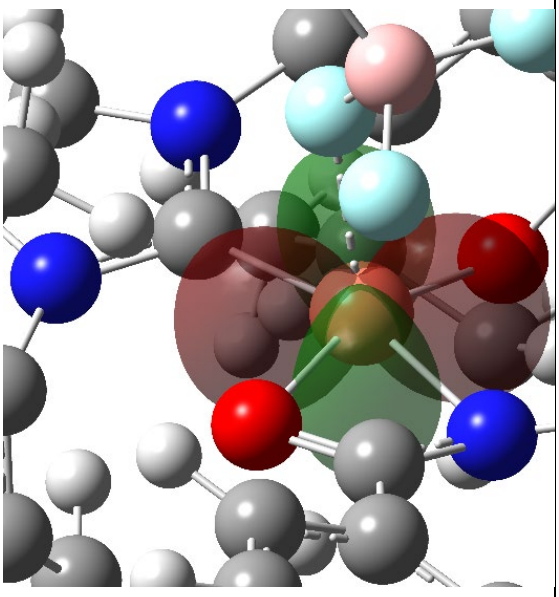
QI

11-4 NBO analysis of **IM2**

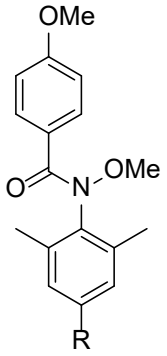
occupation number (ON) of Cu atom >1.98



IM2A

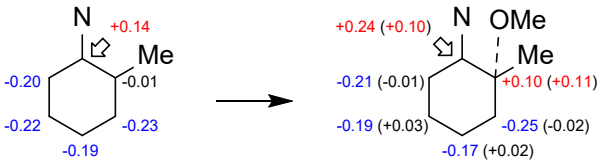
	
d_{z2}	d_{yz}
	
d_{xz}	d_{xy}

11-5 Substituent effect on the *N*-methoxyaniline in the reaction with $IPrCuBF_4$



R	N-O bond dissociation energy (kcal/mol)	ΔG of $TS_{2\text{-}3}$ (kcal/mol)
Me	24.2	27.9
H	23.8	28.6
CF_3	24.1	30.2

11-6 NBO charge distribution of **IM2** and **$TS_{2\text{-}3}$**



IM2 **$TS_{2\text{-}3}$**

11-7 Cartesian coordinates

IM2, major product

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4008.493315

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.388529	2.085862	0.212169
2	6	0	2.439477	3.043003	0.037075
3	1	0	4.452297	2.149772	0.414794
4	1	0	2.489025	4.126743	0.054325
5	6	0	1.433538	1.031283	-0.180830
6	6	0	-0.000765	3.055545	-0.422461
7	6	0	-0.757546	3.427453	0.701003
8	6	0	-0.410591	3.285127	-1.746519
9	6	0	-1.959285	4.104711	0.461724
10	6	0	-1.632031	3.943927	-1.931632
11	6	0	-2.392710	4.358129	-0.838410
12	1	0	-2.575913	4.414287	1.307292
13	1	0	-1.995405	4.133159	-2.943107
14	6	0	3.488300	-0.375657	0.193601
15	6	0	4.028954	-0.935259	-0.977695
16	6	0	3.691832	-0.915775	1.474915
17	6	0	4.833002	-2.070441	-0.833102
18	6	0	4.518295	-2.046328	1.566082
19	6	0	5.085476	-2.613929	0.427921
20	1	0	5.267099	-2.537673	-1.719111
21	1	0	4.702034	-2.494016	2.543698
22	6	0	3.053743	-0.311976	2.717410
23	1	0	2.202413	0.298217	2.389850
24	6	0	3.764558	-0.335586	-2.350125
25	1	0	2.947349	0.391362	-2.244246
26	6	0	0.396046	2.775245	-2.933231
27	1	0	1.422308	2.583677	-2.583604
28	6	0	-0.319469	3.080098	2.115833
29	1	0	0.455724	2.305125	2.044328
30	29	0	-0.018880	-0.299344	-0.401974
31	7	0	-1.696669	-1.250387	-0.852083
32	6	0	-2.394267	-0.207243	-0.423400
33	8	0	-1.650849	0.819023	-0.234571
34	6	0	-3.852415	-0.122308	-0.227676
35	6	0	-4.741223	-1.021857	-0.837448
36	6	0	-4.348773	0.927405	0.561141
37	6	0	-6.115158	-0.875053	-0.648918
38	1	0	-4.360348	-1.829806	-1.462199
39	6	0	-5.721980	1.061469	0.755064
40	1	0	-3.642272	1.615524	1.023039
41	6	0	-6.606344	0.161590	0.151182
42	1	0	-6.805692	-1.574325	-1.125522
43	1	0	-6.105636	1.868984	1.382555
44	1	0	-7.683069	0.268062	0.304281
45	6	0	-1.967840	-2.610626	-0.801446
46	6	0	-1.645278	-3.383498	-1.947951
47	6	0	-2.491728	-3.215475	0.358866
48	6	0	-1.891322	-4.756698	-1.897942
49	6	0	-2.728135	-4.587075	0.374320
50	1	0	-2.679986	-2.596665	1.234995
51	6	0	-2.426886	-5.358608	-0.751871
52	1	0	-1.658452	-5.369467	-2.772627
53	1	0	-3.128515	-5.055345	1.275740
54	1	0	-2.601071	-6.437270	-0.739277

55	8	0	1.128758	-1.638993	-0.930993
56	6	0	1.171399	-2.725088	-0.058826
57	1	0	0.201389	-2.948106	0.424996
58	1	0	1.426475	-3.622985	-0.656834
59	1	0	1.924359	-2.600133	0.735881
60	6	0	-1.064080	-2.717563	-3.163374
61	1	0	-0.894784	-3.442090	-3.972326
62	1	0	-1.730969	-1.923203	-3.536000
63	1	0	-0.111110	-2.234134	-2.902167
64	7	0	1.248596	2.373371	-0.201817
65	7	0	2.750904	0.859444	0.078528
66	1	0	-3.341641	4.874117	-1.003578
67	1	0	5.721205	-3.497831	0.520523
68	6	0	0.296707	4.300892	2.816906
69	1	0	-0.441800	5.113631	2.913310
70	1	0	0.637979	4.031547	3.828913
71	1	0	1.160114	4.699661	2.260994
72	6	0	-1.457071	2.468462	2.942102
73	1	0	-1.067765	2.084006	3.895252
74	1	0	-2.243280	3.208032	3.166834
75	1	0	-1.904879	1.615204	2.418912
76	6	0	0.493873	3.799673	-4.070584
77	1	0	-0.483888	3.979945	-4.544364
78	1	0	0.876538	4.766652	-3.709202
79	1	0	1.173037	3.432889	-4.856203
80	6	0	-0.169266	1.437320	-3.440810
81	1	0	-0.168790	0.671787	-2.652632
82	1	0	-1.210249	1.555199	-3.781195
83	1	0	0.429847	1.053117	-4.281700
84	6	0	4.999207	0.423818	-2.860779
85	1	0	5.857012	-0.256437	-2.987136
86	1	0	4.793313	0.893740	-3.836125
87	1	0	5.303094	1.216006	-2.158565
88	6	0	3.284224	-1.385704	-3.359559
89	1	0	2.402024	-1.907752	-2.964237
90	1	0	3.009599	-0.900750	-4.310340
91	1	0	4.066102	-2.128674	-3.584244
92	6	0	4.046260	0.601055	3.455611
93	1	0	3.566449	1.053082	4.338051
94	1	0	4.923453	0.029920	3.801552
95	1	0	4.411557	1.417821	2.813889
96	6	0	2.477786	-1.376686	3.659176
97	1	0	3.271529	-1.963827	4.149438
98	1	0	1.876118	-0.893398	4.441495
99	1	0	1.805521	-2.061259	3.125850
100	5	0	-0.897537	-1.060311	2.788920
101	9	0	-2.206544	-0.785131	2.347543
102	9	0	-0.662929	-0.521948	4.036742
103	9	0	0.006947	-0.426504	1.843060
104	9	0	-0.651874	-2.427818	2.741037

$TS_{2\text{-}3}$, major product

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4008.482507

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.185351	2.390700	0.570334
2	6	0	2.157807	3.265658	0.414127
3	1	0	4.222920	2.536867	0.851595

4	1	0	2.098933	4.342169	0.537089
5	6	0	1.365241	1.189559	-0.069580
6	6	0	-0.247331	3.080475	-0.174918
7	6	0	-1.085335	3.229893	0.944071
8	6	0	-0.629585	3.442998	-1.478087
9	6	0	-2.336353	3.821121	0.730758
10	6	0	-1.900592	4.006945	-1.642148
11	6	0	-2.739758	4.206101	-0.546034
12	1	0	-3.014130	3.955877	1.575306
13	1	0	-2.239875	4.292649	-2.639331
14	6	0	3.496245	-0.050417	0.342452
15	6	0	4.194980	-0.436607	-0.815504
16	6	0	3.605149	-0.729631	1.572257
17	6	0	5.059443	-1.534577	-0.711936
18	6	0	4.488619	-1.815676	1.623619
19	6	0	5.213658	-2.208750	0.498696
20	1	0	5.613922	-1.867949	-1.591327
21	1	0	4.598636	-2.369530	2.556632
22	6	0	2.799687	-0.308223	2.793571
23	1	0	1.887856	0.182177	2.429004
24	6	0	3.978485	0.258763	-2.151052
25	1	0	3.406597	1.178508	-1.961457
26	6	0	0.265751	3.159558	-2.675693
27	1	0	1.292026	3.025625	-2.300801
28	6	0	-0.675257	2.738513	2.324278
29	1	0	0.150731	2.027409	2.190193
30	29	0	0.005326	-0.213356	-0.479005
31	7	0	-1.796877	-1.155723	-1.365176
32	6	0	-2.560453	-0.294440	-0.633570
33	8	0	-1.940968	0.698538	-0.210596
34	6	0	-4.016690	-0.454049	-0.438209
35	6	0	-4.771936	-1.358955	-1.199872
36	6	0	-4.646408	0.341686	0.531672
37	6	0	-6.145892	-1.471444	-0.987550
38	1	0	-4.283582	-1.967538	-1.962199
39	6	0	-6.016773	0.217800	0.747740
40	1	0	-4.038577	1.031840	1.115651
41	6	0	-6.767894	-0.686817	-0.011321
42	1	0	-6.733382	-2.173717	-1.583181
43	1	0	-6.503353	0.824401	1.514726
44	1	0	-7.843011	-0.781692	0.159779
45	6	0	-1.633528	-2.468943	-1.270618
46	6	0	-0.621661	-3.021466	-2.175644
47	6	0	-2.159369	-3.289409	-0.219657
48	6	0	-0.296508	-4.399261	-2.045498
49	6	0	-1.756951	-4.592176	-0.101833
50	1	0	-2.815969	-2.835768	0.519800
51	6	0	-0.821686	-5.154174	-1.023168
52	1	0	0.412357	-4.838062	-2.751020
53	1	0	-2.129223	-5.199288	0.725184
54	1	0	-0.531352	-6.202131	-0.914877
55	8	0	0.734545	-1.968313	-1.000382
56	6	0	1.503984	-2.711456	-0.101078
57	1	0	1.372189	-2.336880	0.922552
58	1	0	1.137236	-3.757281	-0.083539
59	1	0	2.569790	-2.729602	-0.382639
60	6	0	-0.289229	-2.307443	-3.451259
61	1	0	0.689698	-2.630181	-3.830321
62	1	0	-1.049857	-2.547309	-4.214669
63	1	0	-0.284532	-1.221684	-3.313376
64	7	0	1.059143	2.511575	0.027432
65	7	0	2.677241	1.130228	0.278303
66	1	0	-3.726138	4.652982	-0.692852
67	1	0	5.895432	-3.060328	0.563042
68	6	0	-0.164669	3.897757	3.194616

69	1	0	-0.958127	4.645542	3.358133
70	1	0	0.158176	3.525321	4.179806
71	1	0	0.689896	4.413798	2.729495
72	6	0	-1.797176	1.962249	3.024011
73	1	0	-1.412325	1.475821	3.931165
74	1	0	-2.630225	2.622485	3.317432
75	1	0	-2.180720	1.164634	2.376887
76	6	0	0.300572	4.310963	-3.687733
77	1	0	-0.673833	4.452368	-4.181350
78	1	0	0.575051	5.262104	-3.205803
79	1	0	1.037803	4.101192	-4.478823
80	6	0	-0.148899	1.839428	-3.346616
81	1	0	-0.126095	1.007663	-2.627648
82	1	0	-1.176010	1.904127	-3.739758
83	1	0	0.527481	1.590681	-4.180204
84	6	0	5.293830	0.673124	-2.822170
85	1	0	5.907102	-0.200890	-3.093275
86	1	0	5.090539	1.230937	-3.750148
87	1	0	5.897739	1.315275	-2.162038
88	6	0	3.118699	-0.625022	-3.069597
89	1	0	2.195125	-0.933699	-2.561267
90	1	0	2.856062	-0.085802	-3.994419
91	1	0	3.665124	-1.539452	-3.354788
92	6	0	3.583078	0.700439	3.650826
93	1	0	2.977211	1.014823	4.515270
94	1	0	4.513375	0.249114	4.033513
95	1	0	3.854928	1.603649	3.085056
96	6	0	2.335132	-1.493405	3.648556
97	1	0	3.171793	-1.959356	4.195002
98	1	0	1.594611	-1.148912	4.383393
99	1	0	1.835885	-2.262883	3.044868
100	5	0	-1.037787	-1.484931	2.548870
101	9	0	-2.353016	-1.319814	2.072280
102	9	0	-0.927979	-1.092008	3.869679
103	9	0	-0.186938	-0.628624	1.749007
104	9	0	-0.613317	-2.797422	2.356121

QI, major product

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4008.512938

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.788004	1.828700	0.111036
2	6	0	2.943821	2.893052	0.062574
3	1	0	4.864502	1.765940	0.233530
4	1	0	3.124060	3.960815	0.134542
5	6	0	1.683280	1.015387	-0.180541
6	6	0	0.471554	3.174802	-0.118968
7	6	0	-0.200754	3.381871	1.100328
8	6	0	0.025420	3.703345	-1.343417
9	6	0	-1.316166	4.226985	1.076603
10	6	0	-1.105357	4.528676	-1.315331
11	6	0	-1.756146	4.803112	-0.112921
12	1	0	-1.867327	4.409113	1.999518
13	1	0	-1.486878	4.955235	-2.244535
14	6	0	3.516246	-0.644191	0.046920
15	6	0	4.020323	-1.237438	-1.126175
16	6	0	3.517552	-1.290255	1.300105
17	6	0	4.577413	-2.517826	-1.013330

18	6	0	4.106314	-2.561235	1.361411
19	6	0	4.634157	-3.164986	0.221052
20	1	0	4.973722	-3.014584	-1.899841
21	1	0	4.128779	-3.093516	2.312672
22	6	0	2.879416	-0.654358	2.528115
23	1	0	2.058000	-0.020942	2.169692
24	6	0	3.897571	-0.536631	-2.472163
25	1	0	3.895791	0.547521	-2.279894
26	6	0	0.679230	3.301619	-2.657490
27	1	0	1.706276	2.973484	-2.435417
28	6	0	0.234899	2.679277	2.378971
29	1	0	0.720973	1.741760	2.078204
30	29	0	0.092877	-0.069447	-0.293147
31	7	0	-1.774500	-0.702674	-0.686641
32	6	0	-2.653538	0.274860	-0.179293
33	8	0	-2.183508	1.282068	0.307792
34	6	0	-4.124236	0.114178	-0.377375
35	6	0	-4.661067	-0.407602	-1.563081
36	6	0	-4.978044	0.551427	0.645056
37	6	0	-6.044766	-0.494194	-1.723485
38	1	0	-3.994753	-0.731604	-2.364775
39	6	0	-6.359535	0.441357	0.489854
40	1	0	-4.536608	0.943416	1.561985
41	6	0	-6.894714	-0.077688	-0.694442
42	1	0	-6.461719	-0.889101	-2.652904
43	1	0	-7.023923	0.761830	1.295670
44	1	0	-7.977778	-0.156652	-0.815966
45	6	0	-1.997894	-1.989058	-0.727538
46	6	0	-0.996113	-2.768180	-1.612461
47	6	0	-3.040808	-2.696429	-0.035184
48	6	0	-1.253818	-4.249256	-1.659586
49	6	0	-3.173702	-4.042260	-0.186528
50	1	0	-3.653066	-2.151533	0.677881
51	6	0	-2.291581	-4.827511	-1.027225
52	1	0	-0.545802	-4.834941	-2.251839
53	1	0	-3.947224	-4.564071	0.382373
54	1	0	-2.459621	-5.904255	-1.102660
55	8	0	0.336015	-2.489301	-1.191440
56	6	0	0.772004	-3.186570	-0.018766
57	1	0	1.729652	-2.738502	0.256892
58	1	0	0.063562	-3.070028	0.813452
59	1	0	0.930449	-4.256163	-0.230027
60	6	0	-1.113900	-2.208936	-3.040658
61	1	0	-0.383031	-2.708307	-3.691727
62	1	0	-2.125626	-2.373176	-3.439075
63	1	0	-0.906893	-1.130458	-3.018933
64	7	0	1.667329	2.373599	-0.110931
65	7	0	2.996659	0.692998	-0.033279
66	1	0	-2.635000	5.452565	-0.108599
67	1	0	5.081778	-4.159355	0.291703
68	6	0	1.260252	3.515386	3.161327
69	1	0	0.817482	4.471256	3.486634
70	1	0	1.591196	2.971036	4.060246
71	1	0	2.152308	3.744859	2.559022
72	6	0	-0.945946	2.272465	3.266890
73	1	0	-0.602728	1.590958	4.057677
74	1	0	-1.416794	3.145190	3.749332
75	1	0	-1.703219	1.733388	2.684082
76	6	0	0.777047	4.449033	-3.668715
77	1	0	-0.215723	4.771257	-4.020505
78	1	0	1.281848	5.326482	-3.235422
79	1	0	1.346379	4.128354	-4.555495
80	6	0	-0.064740	2.092210	-3.252064
81	1	0	-0.092376	1.260326	-2.531969
82	1	0	-1.106004	2.358572	-3.495394

83	1	0	0.428098	1.738498	-4.172233
84	6	0	5.066981	-0.826530	-3.419114
85	1	0	5.070476	-1.874902	-3.757443
86	1	0	4.987910	-0.197997	-4.319844
87	1	0	6.038121	-0.621437	-2.942234
88	6	0	2.550365	-0.883596	-3.128802
89	1	0	1.710235	-0.633547	-2.468528
90	1	0	2.429260	-0.336769	-4.078067
91	1	0	2.487931	-1.963365	-3.336873
92	6	0	3.878289	0.239203	3.281570
93	1	0	3.384674	0.716363	4.142827
94	1	0	4.726178	-0.354895	3.660631
95	1	0	4.282451	1.037772	2.642347
96	6	0	2.243323	-1.680842	3.471644
97	1	0	3.002656	-2.267141	4.015134
98	1	0	1.613382	-1.167495	4.210764
99	1	0	1.583213	-2.371192	2.930110
100	5	0	-1.251069	-1.303451	2.700567
101	9	0	-2.520196	-0.827076	2.329821
102	9	0	-0.942702	-0.964693	4.002162
103	9	0	-0.268274	-0.692515	1.827315
104	9	0	-1.186339	-2.685349	2.488928

IM2, minor product

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4008.487850

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.446372	-2.030516	-0.099662
2	6	0	-2.501727	-2.984291	-0.314532
3	1	0	-4.520841	-2.093265	0.035919
4	1	0	-2.567626	-4.063192	-0.407428
5	6	0	-1.459546	-0.981560	-0.283326
6	6	0	-0.037718	-2.987859	-0.665757
7	6	0	0.673786	-3.484242	0.439215
8	6	0	0.422721	-3.074840	-1.990674
9	6	0	1.885335	-4.133396	0.174284
10	6	0	1.651149	-3.713477	-2.198609
11	6	0	2.369631	-4.244439	-1.127683
12	1	0	2.470619	-4.531956	1.004272
13	1	0	2.053419	-3.794257	-3.209821
14	6	0	-3.507620	0.430201	0.081269
15	6	0	-3.946358	1.094757	-1.078225
16	6	0	-3.789847	0.876834	1.383645
17	6	0	-4.721138	2.245755	-0.901886
18	6	0	-4.580468	2.029671	1.504314
19	6	0	-5.042650	2.704153	0.376900
20	1	0	-5.076529	2.793167	-1.777111
21	1	0	-4.821137	2.408554	2.498541
22	6	0	-3.273808	0.150549	2.617279
23	1	0	-2.424840	-0.471105	2.306338
24	6	0	-3.609475	0.591247	-2.473603
25	1	0	-2.854186	-0.200155	-2.371151
26	6	0	-0.340616	-2.443441	-3.147669
27	1	0	-1.381726	-2.294894	-2.821687
28	6	0	0.173703	-3.295318	1.863246
29	1	0	-0.549176	-2.468125	1.853243
30	29	0	0.028405	0.318110	-0.298759
31	7	0	1.703771	1.276630	-0.656865

32	6	0	2.405112	0.213643	-0.320115
33	8	0	1.656314	-0.811235	-0.118740
34	6	0	3.869129	0.100864	-0.210301
35	6	0	4.728214	0.896369	-0.983753
36	6	0	4.394090	-0.847251	0.681085
37	6	0	6.109121	0.744952	-0.860488
38	1	0	4.314831	1.627525	-1.680154
39	6	0	5.775595	-0.982557	0.809090
40	1	0	3.706103	-1.447389	1.275421
41	6	0	6.633137	-0.189752	0.039015
42	1	0	6.779563	1.359820	-1.465085
43	1	0	6.186733	-1.707030	1.515539
44	1	0	7.715596	-0.299220	0.140815
45	6	0	1.940219	2.629626	-0.857269
46	6	0	2.618133	3.462517	0.073845
47	6	0	1.379279	3.179772	-2.031972
48	6	0	2.724078	4.824556	-0.245375
49	6	0	1.496611	4.534279	-2.311073
50	1	0	0.846002	2.507338	-2.703306
51	6	0	2.174826	5.363314	-1.409193
52	1	0	3.243914	5.480474	0.457579
53	1	0	1.059366	4.946312	-3.223171
54	1	0	2.270368	6.433023	-1.610211
55	8	0	-1.042992	1.725654	-0.786987
56	6	0	-1.117648	2.698108	0.210928
57	1	0	-0.133801	2.986254	0.624818
58	1	0	-1.543666	3.603476	-0.266333
59	1	0	-1.776277	2.407456	1.043635
60	6	0	3.227300	2.940054	1.341384
61	1	0	3.254252	3.730300	2.104773
62	1	0	2.680354	2.088217	1.757166
63	1	0	4.265198	2.610174	1.164378
64	7	0	-1.290119	-2.317786	-0.422970
65	7	0	-2.786032	-0.808821	-0.081156
66	1	0	3.325993	-4.740365	-1.310515
67	1	0	-5.652306	3.603461	0.493646
68	6	0	-0.549439	-4.556023	2.363905
69	1	0	0.137601	-5.417810	2.388691
70	1	0	-0.933618	-4.398816	3.384128
71	1	0	-1.399946	-4.826976	1.718781
72	6	0	1.289132	-2.870224	2.824755
73	1	0	0.857486	-2.577639	3.792586
74	1	0	2.010106	-3.684715	3.004428
75	1	0	1.819405	-1.991332	2.438816
76	6	0	-0.385146	-3.341085	-4.390729
77	1	0	0.611210	-3.462339	-4.844036
78	1	0	-0.769551	-4.343947	-4.148975
79	1	0	-1.039389	-2.897379	-5.157599
80	6	0	0.231370	-1.056578	-3.489328
81	1	0	0.179447	-0.373502	-2.629928
82	1	0	1.289173	-1.130156	-3.787489
83	1	0	-0.331607	-0.594486	-4.315902
84	6	0	-4.844903	-0.033794	-3.140371
85	1	0	-5.642954	0.713970	-3.275978
86	1	0	-4.589620	-0.439187	-4.132836
87	1	0	-5.257500	-0.854551	-2.532654
88	6	0	-2.979760	1.683396	-3.348257
89	1	0	-2.094883	2.099088	-2.846593
90	1	0	-2.672160	1.261170	-4.318853
91	1	0	-3.688215	2.501257	-3.556170
92	6	0	-4.357702	-0.770596	3.201068
93	1	0	-3.967860	-1.312415	4.077195
94	1	0	-5.236346	-0.188783	3.524836
95	1	0	-4.703298	-1.516553	2.468441
96	6	0	-2.732291	1.109686	3.684785

97	1	0	-3.537279	1.696793	4.156323
98	1	0	-2.218801	0.537872	4.470065
99	1	0	-1.987798	1.798978	3.264868
100	5	0	0.687413	0.658889	2.988093
101	9	0	2.000243	0.303001	2.634605
102	9	0	0.308990	0.065477	4.174985
103	9	0	-0.185569	0.160800	1.935425
104	9	0	0.548653	2.042204	3.008657

$TS_{2\text{-}3}$, minor product

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4008.477298

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.259193	2.404410	0.244392
2	6	0	2.214792	3.268178	0.141879
3	1	0	4.318248	2.567426	0.414693
4	1	0	2.161210	4.349812	0.209468
5	6	0	1.395303	1.168905	-0.147405
6	6	0	-0.235816	3.035448	-0.233998
7	6	0	-0.985534	3.266198	0.932724
8	6	0	-0.729312	3.276350	-1.527968
9	6	0	-2.265915	3.808921	0.772629
10	6	0	-2.024927	3.796641	-1.634885
11	6	0	-2.780549	4.070846	-0.495443
12	1	0	-2.878685	4.001006	1.654786
13	1	0	-2.450089	3.986514	-2.622159
14	6	0	3.567680	-0.043584	0.081654
15	6	0	4.133947	-0.464962	-1.134949
16	6	0	3.823004	-0.679762	1.312082
17	6	0	5.022381	-1.547837	-1.092322
18	6	0	4.726450	-1.750527	1.301129
19	6	0	5.327106	-2.173980	0.115584
20	1	0	5.477455	-1.906358	-2.017906
21	1	0	4.950116	-2.269176	2.234205
22	6	0	3.145416	-0.231795	2.598960
23	1	0	2.203029	0.255606	2.319100
24	6	0	3.769197	0.182610	-2.462481
25	1	0	3.134371	1.054038	-2.248704
26	6	0	0.074141	2.919114	-2.770463
27	1	0	1.122704	2.784979	-2.464430
28	6	0	-0.450277	2.908265	2.310773
29	1	0	0.371739	2.193719	2.169282
30	29	0	0.005665	-0.254381	-0.352202
31	7	0	-1.769689	-1.224075	-1.159356
32	6	0	-2.533613	-0.321191	-0.503502
33	8	0	-1.890804	0.644448	-0.038847
34	6	0	-4.009661	-0.353719	-0.454626
35	6	0	-4.759866	-1.066982	-1.400550
36	6	0	-4.655177	0.378609	0.552835
37	6	0	-6.153246	-1.052809	-1.334907
38	1	0	-4.248547	-1.624611	-2.187668
39	6	0	-6.047101	0.374053	0.624339
40	1	0	-4.046370	0.919942	1.277174
41	6	0	-6.796622	-0.337916	-0.319085
42	1	0	-6.739703	-1.601798	-2.075092
43	1	0	-6.552277	0.926088	1.420042
44	1	0	-7.887889	-0.335602	-0.262670
45	6	0	-1.607567	-2.544567	-1.215745

46	6	0	-2.152215	-3.549080	-0.331102
47	6	0	-0.552197	-2.918049	-2.146641
48	6	0	-1.657783	-4.833365	-0.461471
49	6	0	-0.147099	-4.260717	-2.283283
50	1	0	-0.307864	-2.186430	-2.914192
51	6	0	-0.667234	-5.196227	-1.415425
52	1	0	-2.046423	-5.606747	0.204997
53	1	0	0.597278	-4.531436	-3.033871
54	1	0	-0.341298	-6.238044	-1.466862
55	8	0	0.801405	-1.926598	-0.954677
56	6	0	1.560760	-2.723932	-0.087562
57	1	0	1.427840	-2.392355	0.951672
58	1	0	1.179461	-3.763469	-0.123924
59	1	0	2.626180	-2.738628	-0.365588
60	6	0	-3.210929	-3.243646	0.683566
61	1	0	-3.294689	-4.073939	1.397424
62	1	0	-2.978986	-2.339050	1.258567
63	1	0	-4.192137	-3.099378	0.204319
64	7	0	1.089413	2.491960	-0.094176
65	7	0	2.734480	1.128796	0.070417
66	1	0	-3.788907	4.479014	-0.599103
67	1	0	6.026962	-3.013055	0.131230
68	6	0	0.115293	4.148092	3.021819
69	1	0	-0.673052	4.901944	3.182014
70	1	0	0.526408	3.873328	4.006263
71	1	0	0.919135	4.624871	2.439237
72	6	0	-1.495925	2.192521	3.173970
73	1	0	-1.021719	1.788984	4.081054
74	1	0	-2.301361	2.875378	3.491566
75	1	0	-1.932675	1.342087	2.636928
76	6	0	0.052327	4.026751	-3.831381
77	1	0	-0.955124	4.170135	-4.252838
78	1	0	0.381792	4.990363	-3.412833
79	1	0	0.721527	3.768361	-4.667388
80	6	0	-0.404368	1.578488	-3.352454
81	1	0	-0.330752	0.771508	-2.609324
82	1	0	-1.458651	1.640029	-3.666660
83	1	0	0.201171	1.292890	-4.227761
84	6	0	5.003297	0.693560	-3.217615
85	1	0	5.677589	-0.131096	-3.498866
86	1	0	4.701609	1.204542	-4.145897
87	1	0	5.581132	1.405484	-2.607489
88	6	0	2.930857	-0.783566	-3.315317
89	1	0	2.068599	-1.150480	-2.740167
90	1	0	2.571005	-0.280834	-4.227855
91	1	0	3.529271	-1.656078	-3.625643
92	6	0	4.012275	0.789398	3.354183
93	1	0	3.498692	1.120748	4.270494
94	1	0	4.977550	0.344295	3.647061
95	1	0	4.223879	1.681502	2.745815
96	6	0	2.765336	-1.403464	3.512376
97	1	0	3.649649	-1.859981	3.986988
98	1	0	2.089674	-1.054022	4.304752
99	1	0	2.222109	-2.184327	2.962822
100	5	0	-0.793718	-1.322063	2.706078
101	9	0	-2.125148	-0.926812	2.481233
102	9	0	-0.441054	-1.163809	4.030276
103	9	0	0.051276	-0.464513	1.900555
104	9	0	-0.598966	-2.627534	2.253549

QI, minor product

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4008.513274

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.906991	2.935931	-0.523067
2	6	0	1.741344	3.617811	-0.354665
3	1	0	3.921966	3.279458	-0.696625
4	1	0	1.523214	4.681107	-0.343432
5	6	0	1.259683	1.397524	-0.213074
6	6	0	-0.627060	2.919476	0.124858
7	6	0	-1.004933	3.070381	1.471946
8	6	0	-1.543438	2.955485	-0.942531
9	6	0	-2.365667	3.273955	1.733984
10	6	0	-2.892474	3.153858	-0.625989
11	6	0	-3.296720	3.317541	0.698471
12	1	0	-2.702458	3.376460	2.766518
13	1	0	-3.639035	3.166306	-1.422442
14	6	0	3.535027	0.503937	-0.511815
15	6	0	3.949678	0.080421	-1.788952
16	6	0	3.979844	-0.097109	0.685297
17	6	0	4.859994	-0.982772	-1.852518
18	6	0	4.881836	-1.162605	0.562813
19	6	0	5.320795	-1.595693	-0.688430
20	1	0	5.203621	-1.342877	-2.823139
21	1	0	5.238358	-1.666534	1.460575
22	6	0	3.511513	0.400066	2.047663
23	1	0	2.441524	0.628837	1.950204
24	6	0	3.372441	0.705429	-3.052696
25	1	0	3.074385	1.735978	-2.807911
26	6	0	-1.100609	2.742494	-2.383301
27	1	0	-0.001375	2.764858	-2.401530
28	6	0	0.009134	2.964241	2.602929
29	1	0	1.011050	3.077183	2.162569
30	29	0	0.248458	-0.225443	-0.004221
31	7	0	-1.570106	-1.145341	-0.053250
32	6	0	-2.559178	-0.437254	0.654476
33	8	0	-2.330220	0.101122	1.714477
34	6	0	-3.867482	-0.244509	-0.057281
35	6	0	-4.090137	-0.632938	-1.385401
36	6	0	-4.898003	0.386783	0.656250
37	6	0	-5.324947	-0.391804	-1.991673
38	1	0	-3.294349	-1.107309	-1.957381
39	6	0	-6.132444	0.619803	0.054613
40	1	0	-4.698216	0.687065	1.685248
41	6	0	-6.347600	0.233978	-1.273862
42	1	0	-5.487546	-0.691070	-3.029641
43	1	0	-6.931610	1.105944	0.619204
44	1	0	-7.313911	0.420355	-1.748725
45	6	0	-1.586482	-2.386995	-0.422735
46	6	0	-2.479147	-3.431468	0.073025
47	6	0	-0.574469	-2.719924	-1.536527
48	6	0	-2.375382	-4.674208	-0.480341
49	6	0	-0.494581	-4.154348	-1.934900
50	1	0	-1.013698	-2.199809	-2.416222
51	6	0	-1.401344	-5.041182	-1.486550
52	1	0	-3.012055	-5.469292	-0.083293
53	1	0	0.273580	-4.433222	-2.658366
54	1	0	-1.384125	-6.075403	-1.837931
55	8	0	0.666152	-2.070282	-1.321541
56	6	0	1.789111	-2.866294	-0.922424
57	1	0	2.490210	-2.180475	-0.437667
58	1	0	1.488702	-3.634906	-0.201357
59	1	0	2.275124	-3.313975	-1.804494

60	6	0	-3.331930	-3.187603	1.286090
61	1	0	-3.753523	-4.135777	1.647071
62	1	0	-2.710584	-2.757180	2.087028
63	1	0	-4.166776	-2.500088	1.088914
64	7	0	0.754657	2.658644	-0.164238
65	7	0	2.590380	1.584414	-0.428466
66	1	0	-4.355096	3.461868	0.925105
67	1	0	6.024014	-2.429337	-0.756008
68	6	0	-0.153642	4.088393	3.634930
69	1	0	-1.101461	3.998850	4.188926
70	1	0	0.659808	4.041870	4.375909
71	1	0	-0.131241	5.082864	3.161440
72	6	0	-0.038007	1.580649	3.272783
73	1	0	0.739117	1.512369	4.051016
74	1	0	-1.016467	1.397224	3.740093
75	1	0	0.120496	0.764827	2.556896
76	6	0	-1.595914	3.857721	-3.313489
77	1	0	-2.694981	3.866390	-3.387819
78	1	0	-1.276623	4.849194	-2.956280
79	1	0	-1.198196	3.714824	-4.331008
80	6	0	-1.531124	1.356567	-2.886571
81	1	0	-1.151893	0.570122	-2.217681
82	1	0	-2.628450	1.273351	-2.919540
83	1	0	-1.140110	1.171030	-3.899886
84	6	0	4.381819	0.791498	-4.202825
85	1	0	4.647727	-0.204449	-4.591180
86	1	0	3.950989	1.359849	-5.041983
87	1	0	5.311950	1.291798	-3.891232
88	6	0	2.098533	-0.040491	-3.484983
89	1	0	1.362188	-0.083053	-2.672483
90	1	0	1.637594	0.453024	-4.356172
91	1	0	2.335078	-1.080083	-3.764010
92	6	0	4.248851	1.692139	2.443734
93	1	0	3.865206	2.066210	3.406273
94	1	0	5.328407	1.501854	2.560638
95	1	0	4.125407	2.493596	1.702179
96	6	0	3.636197	-0.641124	3.161971
97	1	0	4.690167	-0.855622	3.405628
98	1	0	3.166259	-0.249462	4.077190
99	1	0	3.119797	-1.575985	2.913122
100	5	0	0.407858	-2.583484	2.362654
101	9	0	-0.719639	-2.139882	3.031923
102	9	0	1.376187	-3.080140	3.210236
103	9	0	0.983799	-1.456562	1.640233
104	9	0	0.048636	-3.549059	1.397122

IM1

charge = 0, mult = 2

Sum of electronic and thermal Free Energies= -3893.520248

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.307047	1.869467	-0.443317
2	6	0	2.380225	2.760990	-0.000792
3	1	0	4.353580	1.989181	-0.700376
4	1	0	2.443710	3.825051	0.200932
5	6	0	1.357315	0.754006	-0.181530
6	6	0	-0.088109	2.671368	0.393767
7	6	0	-0.774755	3.190729	-0.720077
8	6	0	-0.585450	2.735601	1.709603

9	6	0	-2.050497	3.723136	-0.497152
10	6	0	-1.861282	3.287283	1.876869
11	6	0	-2.591637	3.757865	0.785609
12	1	0	-2.629966	4.107218	-1.338106
13	1	0	-2.291623	3.343220	2.877289
14	6	0	3.274636	-0.554323	-1.059131
15	6	0	4.266590	-1.197957	-0.290936
16	6	0	2.861742	-1.028611	-2.321287
17	6	0	4.863937	-2.339262	-0.838130
18	6	0	3.482903	-2.185371	-2.811812
19	6	0	4.477688	-2.831483	-2.083388
20	1	0	5.631943	-2.862764	-0.266869
21	1	0	3.182410	-2.581257	-3.783812
22	6	0	1.800173	-0.340817	-3.169094
23	1	0	1.403931	0.510078	-2.601750
24	6	0	4.689677	-0.698852	1.081710
25	1	0	3.917154	-0.008647	1.442365
26	6	0	0.270822	2.317006	2.892997
27	1	0	0.935959	1.511989	2.563361
28	6	0	-0.149573	3.225634	-2.110001
29	1	0	0.891044	2.885248	-2.022754
30	29	0	0.188664	-0.841556	0.004664
31	6	0	-1.891708	-2.033613	-0.341278
32	8	0	-0.741950	-2.571942	-0.149572
33	7	0	-1.857188	-0.739636	-0.603609
34	6	0	-3.101978	-2.886304	-0.202148
35	6	0	-4.319140	-2.615765	-0.848880
36	6	0	-2.992898	-4.021940	0.619423
37	6	0	-5.410155	-3.466329	-0.666149
38	1	0	-4.415328	-1.749293	-1.500213
39	6	0	-4.090194	-4.861023	0.808082
40	1	0	-2.037532	-4.222879	1.105826
41	6	0	-5.301308	-4.584364	0.166033
42	1	0	-6.351958	-3.253012	-1.176896
43	1	0	-4.000257	-5.735030	1.457230
44	1	0	-6.161255	-5.242708	0.312025
45	6	0	-2.965423	0.125946	-0.598708
46	6	0	-3.423603	0.646940	-1.819678
47	6	0	-3.635063	0.458108	0.602851
48	6	0	-4.538411	1.480548	-1.873445
49	1	0	-2.904706	0.350647	-2.730655
50	6	0	-4.753158	1.298647	0.523923
51	6	0	-5.209030	1.809389	-0.692443
52	1	0	-4.887578	1.864153	-2.835230
53	1	0	-5.276636	1.557591	1.448126
54	1	0	-6.084998	2.461927	-0.717720
55	6	0	-3.181248	-0.102377	1.919405
56	1	0	-3.642671	0.439234	2.756945
57	1	0	-3.458954	-1.165823	2.014026
58	1	0	-2.091264	-0.056290	2.028415
59	7	0	1.192201	2.056882	0.147237
60	7	0	2.662125	0.644606	-0.543571
61	1	0	4.950405	-3.731000	-2.484720
62	1	0	-3.594189	4.161543	0.937677
63	6	0	2.401821	0.227018	-4.463000
64	1	0	3.222642	0.928439	-4.246429
65	1	0	2.804614	-0.572093	-5.105488
66	1	0	1.633429	0.765796	-5.040462
67	6	0	0.618508	-1.278483	-3.458376
68	1	0	-0.181389	-0.738183	-3.987804
69	1	0	0.923903	-2.127543	-4.089868
70	1	0	0.195514	-1.691935	-2.530877
71	6	0	-0.841626	2.273631	-3.090070
72	1	0	-1.885158	2.572746	-3.268141
73	1	0	-0.315760	2.272467	-4.058237

74	1	0	-0.847428	1.249021	-2.696887
75	6	0	-0.099313	4.658867	-2.659892
76	1	0	-1.109809	5.064916	-2.824657
77	1	0	0.423351	5.335983	-1.966445
78	1	0	0.429388	4.681179	-3.626237
79	6	0	1.153446	3.496557	3.341008
80	1	0	1.815215	3.184611	4.164153
81	1	0	1.789040	3.870016	2.524217
82	1	0	0.535533	4.338235	3.695038
83	6	0	-0.525058	1.769827	4.080317
84	1	0	0.172164	1.360498	4.826319
85	1	0	-1.122140	2.552635	4.576857
86	1	0	-1.193062	0.955820	3.773773
87	6	0	6.027496	0.056327	1.004672
88	1	0	6.836624	-0.611742	0.667034
89	1	0	5.991003	0.904466	0.303591
90	1	0	6.305145	0.449135	1.995653
91	6	0	4.774164	-1.832263	2.114051
92	1	0	5.629919	-2.499153	1.919589
93	1	0	4.905181	-1.407378	3.120359
94	1	0	3.856626	-2.433432	2.120356
95	5	0	1.281928	-1.329440	2.524391
96	9	0	1.288843	-2.400941	3.359320
97	9	0	1.693048	-1.740312	1.181246
98	9	0	2.120554	-0.301937	2.931881
99	9	0	-0.034276	-0.814868	2.319866

MeO radical

charge = 0, mult =2

Sum of electronic and thermal Free Energies= -114.952190

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.296422	-0.093548	0.026249
2	1	0	0.078329	-1.148269	0.030012
3	1	0	0.088089	0.355097	-0.915995
4	1	0	-1.405458	-0.173200	-0.001151
5	8	0	0.194425	0.472048	1.154824

IM2, R_a, distal, re

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4639.916753

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.433355	-2.557359	0.456118
2	6	0	-2.504285	-1.444186	0.553159
3	1	0	-2.818830	-1.328229	1.601843
4	6	0	-0.406116	-0.463199	0.134719
5	6	0	-2.361353	1.022507	-0.053346
6	6	0	-2.557494	1.446423	-1.385290
7	6	0	-2.835191	1.776587	1.038281
8	6	0	-3.256647	2.640929	-1.594375
9	6	0	-3.545543	2.951347	0.767829
10	6	0	-3.767970	3.400234	-0.538226

11	1	0	-3.410142	2.993895	-2.616553
12	1	0	-3.907273	3.546600	1.608814
13	6	0	1.053522	-2.438132	0.077722
14	6	0	1.215081	-3.188415	-1.100821
15	6	0	2.072430	-2.390851	1.029491
16	6	0	2.416376	-3.877112	-1.312919
17	6	0	3.272769	-3.062444	0.792175
18	6	0	3.447087	-3.807533	-0.375088
19	1	0	2.544702	-4.457155	-2.230058
20	1	0	4.071200	-3.001642	1.534192
21	6	0	-2.506715	1.408875	2.475773
22	1	0	-1.969345	0.454719	2.474352
23	6	0	-1.985960	0.677893	-2.566434
24	1	0	-1.760742	-0.339086	-2.231510
25	29	0	1.003418	0.905796	0.079892
26	7	0	3.706258	1.900688	-0.090768
27	6	0	3.643554	0.703598	-0.692775
28	8	0	2.561682	0.183502	-1.057667
29	6	0	4.913545	-0.054189	-0.832902
30	6	0	6.081738	0.345027	-0.165883
31	6	0	4.936074	-1.179012	-1.669976
32	6	0	7.261700	-0.379379	-0.333863
33	1	0	6.043416	1.214087	0.492360
34	6	0	6.120567	-1.892595	-1.846108
35	1	0	4.012470	-1.479727	-2.164647
36	6	0	7.283381	-1.496417	-1.176493
37	1	0	8.167514	-0.075894	0.196013
38	1	0	6.137722	-2.766192	-2.502182
39	1	0	8.209695	-2.060881	-1.309597
40	6	0	3.156971	3.068115	-0.324790
41	6	0	2.819521	3.551442	-1.662948
42	6	0	2.965440	3.956924	0.823013
43	6	0	2.418673	4.861413	-1.804777
44	6	0	2.574097	5.275793	0.596726
45	6	0	2.286557	5.722317	-0.688741
46	1	0	2.188181	5.242631	-2.802247
47	1	0	2.460706	5.948804	1.448788
48	1	0	1.971117	6.756368	-0.847513
49	8	0	0.773790	2.779712	0.309916
50	6	0	-0.129823	3.661336	-0.223128
51	1	0	-1.051123	3.699600	0.387180
52	1	0	0.278759	4.699683	-0.192091
53	1	0	-0.396091	3.451417	-1.273803
54	6	0	2.962833	2.654147	-2.853382
55	1	0	2.819334	3.216696	-3.785714
56	1	0	3.957693	2.180992	-2.881481
57	1	0	2.231844	1.833182	-2.816810
58	7	0	-1.718568	-0.233164	0.184946
59	7	0	-0.187816	-1.774393	0.308402
60	1	0	4.388459	-4.329129	-0.559126
61	6	0	-2.963779	0.570047	-3.741935
62	1	0	-3.115880	1.539557	-4.243632
63	1	0	-2.564172	-0.127624	-4.495029
64	1	0	-3.945258	0.197418	-3.415068
65	6	0	-0.645660	1.273666	-3.024320
66	1	0	-0.196897	0.640056	-3.804125
67	1	0	-0.774431	2.292913	-3.425205
68	1	0	0.066434	1.319597	-2.188446
69	6	0	-3.762016	1.248944	3.342552
70	1	0	-4.320277	2.194974	3.434030
71	1	0	-4.451789	0.497873	2.924900
72	1	0	-3.484570	0.928037	4.358711
73	6	0	-1.529867	2.434892	3.073392
74	1	0	-0.629008	2.522664	2.451786
75	1	0	-1.999429	3.429746	3.157147

76	1	0	-1.199899	2.115970	4.071897
77	5	0	1.461658	0.260971	3.259852
78	9	0	2.145137	-0.788017	3.856057
79	9	0	0.134497	-0.137181	2.982925
80	9	0	2.093054	0.538820	1.987777
81	9	0	1.474576	1.413124	4.021735
82	6	0	-4.490794	4.709426	-0.805128
83	1	0	-4.628657	4.783609	-1.897553
84	6	0	-5.881445	4.749738	-0.157470
85	1	0	-5.813236	4.711497	0.941625
86	1	0	-6.409862	5.679258	-0.424021
87	1	0	-6.496984	3.897548	-0.484341
88	6	0	-3.632557	5.906176	-0.364209
89	1	0	-4.128021	6.859823	-0.609093
90	1	0	-3.458208	5.886247	0.723870
91	1	0	-2.648916	5.891787	-0.859016
92	1	0	-1.600347	-3.141060	-0.459659
93	6	0	-3.732959	-1.655835	-0.298476
94	6	0	-4.995305	-1.351440	0.224893
95	6	0	-3.642511	-2.129574	-1.615688
96	6	0	-6.148118	-1.517737	-0.546375
97	1	0	-5.072642	-0.976600	1.247817
98	6	0	-4.792776	-2.301313	-2.386690
99	1	0	-2.667260	-2.340241	-2.056079
100	6	0	-6.049683	-1.996538	-1.854859
101	1	0	-7.125041	-1.274093	-0.122477
102	1	0	-4.705058	-2.665076	-3.413305
103	1	0	-6.949414	-2.129502	-2.460349
104	6	0	-1.409180	-3.516362	1.619733
105	6	0	-1.963935	-4.793261	1.469432
106	6	0	-0.861982	-3.140844	2.855023
107	6	0	-1.978165	-5.691001	2.540244
108	1	0	-2.392191	-5.083405	0.506000
109	6	0	-0.869008	-4.042917	3.920633
110	1	0	-0.422490	-2.149569	2.980193
111	6	0	-1.426617	-5.316737	3.768283
112	1	0	-2.415911	-6.684252	2.413608
113	1	0	-0.429082	-3.745068	4.875174
114	1	0	-1.428216	-6.018846	4.605686
115	1	0	1.934451	-1.838684	1.954389
116	6	0	0.144088	-3.185418	-2.157571
117	8	0	-0.231387	-2.136374	-2.672608
118	7	0	-0.377418	-4.401428	-2.520031
119	6	0	-1.311927	-4.463160	-3.629501
120	1	0	-1.029114	-5.277455	-4.317248
121	1	0	-2.340212	-4.653734	-3.273698
122	1	0	-1.294188	-3.506029	-4.162417
123	6	0	-0.173394	-5.642001	-1.792747
124	1	0	-1.149521	-6.115301	-1.592942
125	1	0	0.438604	-6.357132	-2.370488
126	1	0	0.315465	-5.455609	-0.830994
127	6	0	3.262507	3.453394	2.189877
128	1	0	2.479225	2.755789	2.522164
129	1	0	4.194366	2.868509	2.194876
130	1	0	3.327420	4.278011	2.912535

$TS_{2\text{-}3}$, R_a, distal, re

cherge = 0, mult =1

Sum of electronic and thermal Free Energies= -4639.915106

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.426532	-2.570512	0.410896
2	6	0	-2.503118	-1.466085	0.528025
3	1	0	-2.821392	-1.375015	1.578357
4	6	0	-0.404657	-0.460949	0.148296
5	6	0	-2.368456	1.009476	-0.034328
6	6	0	-2.559211	1.448986	-1.362093
7	6	0	-2.845390	1.750737	1.064754
8	6	0	-3.258112	2.645757	-1.559410
9	6	0	-3.555825	2.928369	0.806069
10	6	0	-3.773646	3.392187	-0.495810
11	1	0	-3.408301	3.011161	-2.577642
12	1	0	-3.919466	3.514467	1.652632
13	6	0	1.058710	-2.434863	0.049496
14	6	0	1.228232	-3.155358	-1.146707
15	6	0	2.071995	-2.415103	1.008380
16	6	0	2.432210	-3.835721	-1.370867
17	6	0	3.274909	-3.078039	0.760276
18	6	0	3.458072	-3.789711	-0.426383
19	1	0	2.565272	-4.392392	-2.301747
20	1	0	4.067673	-3.038172	1.509808
21	6	0	-2.512285	1.368631	2.497381
22	1	0	-1.983952	0.409417	2.485272
23	6	0	-1.987364	0.689280	-2.549158
24	1	0	-1.781722	-0.335122	-2.225197
25	29	0	1.001250	0.917111	0.169359
26	7	0	3.655891	1.930135	-0.047261
27	6	0	3.657844	0.725460	-0.656659
28	8	0	2.597547	0.182552	-1.026966
29	6	0	4.956993	0.017984	-0.771903
30	6	0	6.100826	0.475929	-0.100447
31	6	0	5.030736	-1.122002	-1.585223
32	6	0	7.309841	-0.204814	-0.242613
33	1	0	6.021290	1.353717	0.542621
34	6	0	6.243448	-1.792829	-1.733849
35	1	0	4.124571	-1.466894	-2.083137
36	6	0	7.382875	-1.337234	-1.061379
37	1	0	8.197668	0.143810	0.289832
38	1	0	6.301637	-2.678828	-2.370584
39	1	0	8.331518	-1.868200	-1.173179
40	6	0	3.099832	3.067294	-0.355862
41	6	0	2.854461	3.526315	-1.726348
42	6	0	2.713997	3.941829	0.763371
43	6	0	2.455946	4.826734	-1.909977
44	6	0	2.380580	5.285145	0.485241
45	6	0	2.239618	5.715109	-0.815078
46	1	0	2.308884	5.198295	-2.926971
47	1	0	2.192463	5.963952	1.319050
48	1	0	1.959452	6.750749	-1.022378
49	8	0	0.836553	2.850996	0.400123
50	6	0	-0.129247	3.626054	-0.222725
51	1	0	-1.101500	3.482284	0.276685
52	1	0	0.103195	4.705301	-0.124675
53	1	0	-0.239371	3.406207	-1.297161
54	6	0	3.100234	2.613530	-2.889579
55	1	0	3.023151	3.162398	-3.837873
56	1	0	4.100089	2.153674	-2.836246
57	1	0	2.376363	1.784968	-2.897995
58	7	0	-1.721121	-0.244931	0.190348
59	7	0	-0.184154	-1.778026	0.291235
60	1	0	4.401049	-4.305643	-0.618899
61	6	0	-2.957836	0.611495	-3.733134
62	1	0	-3.088738	1.588721	-4.225926
63	1	0	-2.564576	-0.085155	-4.490465

64	1	0	-3.948382	0.252678	-3.418031
65	6	0	-0.632587	1.264416	-2.991969
66	1	0	-0.201718	0.638486	-3.787764
67	1	0	-0.737509	2.295729	-3.368390
68	1	0	0.082684	1.268938	-2.157339
69	6	0	-3.763135	1.212938	3.371068
70	1	0	-4.312336	2.163058	3.474633
71	1	0	-4.462079	0.471294	2.951687
72	1	0	-3.481648	0.880919	4.382498
73	6	0	-1.522455	2.381760	3.096559
74	1	0	-0.623321	2.467716	2.471765
75	1	0	-1.982743	3.380289	3.188435
76	1	0	-1.190524	2.053003	4.091250
77	5	0	1.449785	0.163053	3.323937
78	9	0	2.110008	-0.916389	3.892204
79	9	0	0.115909	-0.197159	3.033056
80	9	0	2.092093	0.454173	2.054046
81	9	0	1.492100	1.295337	4.108014
82	6	0	-4.497211	4.703642	-0.749468
83	1	0	-4.622337	4.795661	-1.842056
84	6	0	-5.895697	4.727689	-0.117907
85	1	0	-5.840223	4.668942	0.981015
86	1	0	-6.424110	5.660322	-0.373435
87	1	0	-6.504348	3.879744	-0.467893
88	6	0	-3.649066	5.895912	-0.278138
89	1	0	-4.144717	6.851694	-0.514146
90	1	0	-3.488739	5.859172	0.811636
91	1	0	-2.658887	5.892715	-0.759972
92	1	0	-1.584765	-3.134287	-0.518771
93	6	0	-3.730442	-1.660895	-0.330148
94	6	0	-4.990483	-1.341245	0.190061
95	6	0	-3.642401	-2.126752	-1.650200
96	6	0	-6.142496	-1.484205	-0.586880
97	1	0	-5.066129	-0.971701	1.215069
98	6	0	-4.791926	-2.275458	-2.427173
99	1	0	-2.669076	-2.348576	-2.088901
100	6	0	-6.046155	-1.955139	-1.898433
101	1	0	-7.117269	-1.228453	-0.165136
102	1	0	-4.705413	-2.633271	-3.455983
103	1	0	-6.945308	-2.069917	-2.508494
104	6	0	-1.404906	-3.555949	1.552600
105	6	0	-1.951807	-4.832061	1.370702
106	6	0	-0.867191	-3.205306	2.799274
107	6	0	-1.966919	-5.753758	2.421017
108	1	0	-2.373343	-5.102726	0.398685
109	6	0	-0.874832	-4.131058	3.844343
110	1	0	-0.434844	-2.214434	2.949761
111	6	0	-1.424147	-5.404304	3.660229
112	1	0	-2.398490	-6.746273	2.269641
113	1	0	-0.441671	-3.852005	4.807618
114	1	0	-1.426259	-6.125169	4.481559
115	1	0	1.926994	-1.890959	1.948054
116	6	0	0.162322	-3.135902	-2.208347
117	8	0	-0.213715	-2.079998	-2.707892
118	7	0	-0.353388	-4.347681	-2.594353
119	6	0	-1.280745	-4.393941	-3.710346
120	1	0	-0.985457	-5.188840	-4.415510
121	1	0	-2.308751	-4.604292	-3.365037
122	1	0	-1.270514	-3.424419	-4.220576
123	6	0	-0.146862	-5.600411	-1.889056
124	1	0	-1.121473	-6.083136	-1.705210
125	1	0	0.473557	-6.301058	-2.475565
126	1	0	0.333900	-5.429335	-0.920430
127	6	0	2.982876	3.496402	2.158032
128	1	0	2.549143	2.512086	2.359788

129	1	0	4.072263	3.397316	2.307043
130	1	0	2.588294	4.218615	2.884616

QI, R_a, distal, re

charge = 0, mult =1

Sum of electronic and thermal Free Energies= -4639.960511

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.333781	-1.937275	0.051705
2	6	0	1.124045	-2.663403	-0.604363
3	1	0	0.941641	-3.622675	-0.105439
4	6	0	0.445339	-0.528290	0.138656
5	6	0	-1.364949	-2.105953	-0.388555
6	6	0	-2.177840	-1.636251	-1.443561
7	6	0	-1.899072	-2.948693	0.613022
8	6	0	-3.525416	-2.013076	-1.451418
9	6	0	-3.249840	-3.309536	0.540428
10	6	0	-4.085562	-2.842296	-0.476547
11	1	0	-4.166573	-1.643748	-2.255241
12	1	0	-3.655897	-3.955975	1.319268
13	6	0	2.590293	0.468731	0.789657
14	6	0	3.649145	0.992032	0.030538
15	6	0	2.354183	0.944617	2.080583
16	6	0	4.472952	1.974435	0.592762
17	6	0	3.161788	1.943048	2.621738
18	6	0	4.231941	2.449545	1.882793
19	1	0	5.289807	2.388952	-0.002354
20	1	0	2.935184	2.309882	3.624153
21	6	0	-1.060639	-3.472754	1.768186
22	1	0	-0.082238	-2.987375	1.715372
23	6	0	-1.664634	-0.764093	-2.577277
24	1	0	-0.664462	-0.403137	-2.305013
25	29	0	-0.617406	1.028944	0.451267
26	7	0	-1.134959	2.725207	-0.525253
27	6	0	-0.082444	3.066609	-1.412392
28	8	0	-0.134634	2.750868	-2.584577
29	6	0	1.074976	3.769992	-0.799898
30	6	0	1.081701	4.167299	0.546562
31	6	0	2.155554	4.095758	-1.634690
32	6	0	2.144725	4.925701	1.037344
33	1	0	0.276548	3.861169	1.214255
34	6	0	3.214693	4.850103	-1.136724
35	1	0	2.138616	3.740148	-2.664699
36	6	0	3.203653	5.276767	0.196169
37	1	0	2.151626	5.228022	2.086509
38	1	0	4.054424	5.106870	-1.787013
39	1	0	4.034691	5.870472	0.585604
40	6	0	-2.358585	3.121544	-0.572160
41	6	0	-2.872171	4.216463	-1.412506
42	6	0	-3.346984	2.431789	0.382720
43	6	0	-4.210653	4.245729	-1.656145
44	6	0	-4.745613	2.392212	-0.184185
45	6	0	-5.145289	3.274302	-1.114182
46	1	0	-4.604675	5.025205	-2.314679
47	1	0	-5.444775	1.684734	0.265220
48	1	0	-6.179744	3.290577	-1.464449
49	8	0	-2.841901	1.115959	0.600257
50	6	0	-3.453262	0.305225	1.601418
51	1	0	-2.983566	-0.679092	1.506637

52	1	0	-3.265541	0.699893	2.608440
53	1	0	-4.533313	0.190924	1.420396
54	6	0	-1.941004	5.227226	-2.023819
55	1	0	-2.506188	6.109288	-2.356061
56	1	0	-1.176891	5.557754	-1.304122
57	1	0	-1.405776	4.810661	-2.889761
58	7	0	0.016153	-1.725340	-0.295887
59	7	0	1.786552	-0.582628	0.258612
60	1	0	4.870359	3.231185	2.300167
61	6	0	-1.547391	-1.585515	-3.871300
62	1	0	-2.544706	-1.907385	-4.214058
63	1	0	-1.092014	-0.980429	-4.670595
64	1	0	-0.933717	-2.484384	-3.731620
65	6	0	-2.554149	0.467955	-2.804587
66	1	0	-2.020435	1.216903	-3.405195
67	1	0	-3.488708	0.202093	-3.324674
68	1	0	-2.822614	0.927064	-1.847460
69	6	0	-0.832490	-4.987678	1.648378
70	1	0	-1.776786	-5.543859	1.765410
71	1	0	-0.412212	-5.260022	0.666896
72	1	0	-0.134405	-5.334672	2.426735
73	6	0	-1.647441	-3.102356	3.137256
74	1	0	-1.736412	-2.013380	3.246110
75	1	0	-2.635467	-3.563313	3.297364
76	1	0	-0.981399	-3.461442	3.938399
77	5	0	-0.642927	1.271536	3.614531
78	9	0	0.391767	1.597076	4.468021
79	9	0	-0.526406	-0.070936	3.180892
80	9	0	-0.529455	2.091826	2.421186
81	9	0	-1.892278	1.492799	4.169990
82	6	0	-5.575972	-3.140867	-0.513924
83	1	0	-5.870200	-3.149706	-1.578195
84	6	0	-5.952808	-4.499549	0.083543
85	1	0	-5.780772	-4.526046	1.171595
86	1	0	-7.021528	-4.708838	-0.080364
87	1	0	-5.369540	-5.315518	-0.370291
88	6	0	-6.357760	-2.003804	0.167787
89	1	0	-7.444950	-2.169540	0.094224
90	1	0	-6.093206	-1.941068	1.236022
91	1	0	-6.125177	-1.031485	-0.293448
92	1	0	3.166592	-1.906285	-0.662400
93	6	0	1.293616	-2.909832	-2.086037
94	6	0	1.081066	-4.189237	-2.611268
95	6	0	1.682622	-1.871250	-2.946331
96	6	0	1.260421	-4.437006	-3.976122
97	1	0	0.771528	-4.999019	-1.945196
98	6	0	1.868780	-2.120471	-4.305740
99	1	0	1.833207	-0.857830	-2.569801
100	6	0	1.660150	-3.402876	-4.825297
101	1	0	1.087709	-5.439643	-4.374416
102	1	0	2.167056	-1.301021	-4.963678
103	1	0	1.800797	-3.593157	-5.892014
104	6	0	2.807983	-2.582857	1.336532
105	6	0	3.870841	-3.494186	1.291337
106	6	0	2.167903	-2.341112	2.560903
107	6	0	4.283699	-4.165546	2.444919
108	1	0	4.376698	-3.683032	0.340176
109	6	0	2.581237	-3.010597	3.714506
110	1	0	1.346655	-1.627109	2.627054
111	6	0	3.637090	-3.925509	3.660381
112	1	0	5.114122	-4.874025	2.395010
113	1	0	2.074910	-2.807104	4.660757
114	1	0	3.960226	-4.445226	4.565487
115	1	0	1.537396	0.532707	2.662295
116	6	0	3.806340	0.613600	-1.417112

117	8	0	2.997954	1.016907	-2.245841
118	7	0	4.877092	-0.171831	-1.752771
119	6	0	5.110484	-0.491624	-3.149610
120	1	0	6.150154	-0.249169	-3.427621
121	1	0	4.936346	-1.564182	-3.342912
122	1	0	4.417195	0.094463	-3.762940
123	6	0	5.793502	-0.764067	-0.797685
124	1	0	5.865472	-1.851932	-0.969539
125	1	0	6.807895	-0.338480	-0.897956
126	1	0	5.445325	-0.600520	0.227931
127	6	0	-3.376199	3.259509	1.692119
128	1	0	-2.402758	3.173162	2.189757
129	1	0	-3.598656	4.311269	1.464004
130	1	0	-4.153338	2.879958	2.369082

IM2, R_a, distal, si

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4639.923188

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.398080	-1.766090	0.453849
2	6	0	-2.972403	-0.331246	0.325895
3	1	0	-3.368416	-0.011947	1.298129
4	6	0	-0.640584	-0.250592	0.155032
5	6	0	-1.812545	1.877411	-0.276400
6	6	0	-1.470064	2.298167	-1.577804
7	6	0	-2.208861	2.802343	0.714239
8	6	0	-1.522963	3.669435	-1.858379
9	6	0	-2.261499	4.153753	0.367054
10	6	0	-1.912885	4.612521	-0.908011
11	1	0	-1.245343	4.013844	-2.857548
12	1	0	-2.560999	4.874887	1.130009
13	6	0	-0.065084	-2.660452	0.297710
14	6	0	-0.092570	-3.425429	-0.881023
15	6	0	0.747199	-3.034440	1.366676
16	6	0	0.737743	-4.547205	-0.985145
17	6	0	1.581680	-4.147504	1.241894
18	6	0	1.582981	-4.902584	0.067599
19	1	0	0.727160	-5.135316	-1.905790
20	1	0	2.226439	-4.425631	2.078212
21	6	0	-2.559368	2.393373	2.138532
22	1	0	-2.263336	1.347811	2.274762
23	6	0	-1.018413	1.346399	-2.675009
24	1	0	-1.144779	0.318819	-2.323392
25	29	0	1.245300	0.361883	0.052788
26	7	0	3.182100	0.586917	-0.373646
27	6	0	3.204300	-0.639764	-0.853113
28	8	0	2.041060	-1.187513	-0.886672
29	6	0	4.381178	-1.383812	-1.348797
30	6	0	5.554042	-0.737642	-1.771926
31	6	0	4.291488	-2.783945	-1.409367
32	6	0	6.630322	-1.491505	-2.239190
33	1	0	5.622807	0.349562	-1.738601
34	6	0	5.374812	-3.531416	-1.869194
35	1	0	3.369050	-3.264019	-1.083069
36	6	0	6.545155	-2.887157	-2.283129
37	1	0	7.541062	-0.987655	-2.570284
38	1	0	5.307128	-4.621203	-1.905355
39	1	0	7.393822	-3.473557	-2.643596

40	6	0	4.205119	1.399288	0.112940
41	6	0	4.342846	2.689004	-0.462438
42	6	0	5.038639	0.972971	1.179936
43	6	0	5.357487	3.524269	0.008285
44	6	0	6.039550	1.848778	1.616524
45	6	0	6.204873	3.107959	1.038724
46	1	0	5.478657	4.516447	-0.433289
47	1	0	6.690481	1.536729	2.436701
48	1	0	6.989341	3.775554	1.403026
49	8	0	0.815848	2.091074	0.496348
50	6	0	1.495381	2.671427	1.557342
51	1	0	2.594143	2.543526	1.513461
52	1	0	1.316402	3.764119	1.464727
53	1	0	1.140767	2.341288	2.544155
54	6	0	3.398724	3.127270	-1.546457
55	1	0	3.641663	4.139845	-1.897597
56	1	0	3.433917	2.440453	-2.407111
57	1	0	2.360620	3.112240	-1.181867
58	7	0	-1.747207	0.476361	0.046341
59	7	0	-0.937867	-1.530727	0.404204
60	1	0	2.235767	-5.773454	-0.028238
61	6	0	-1.855275	1.500564	-3.953492
62	1	0	-1.655006	2.459693	-4.457815
63	1	0	-1.606676	0.695360	-4.663545
64	1	0	-2.932151	1.452095	-3.739560
65	6	0	0.474422	1.505653	-2.993489
66	1	0	0.795788	0.732166	-3.707823
67	1	0	0.691817	2.495890	-3.426134
68	1	0	1.088019	1.408238	-2.090177
69	6	0	-4.069547	2.531124	2.391867
70	1	0	-4.376306	3.589287	2.358015
71	1	0	-4.664128	2.001081	1.634922
72	1	0	-4.336234	2.134829	3.384811
73	6	0	-1.772645	3.183941	3.192225
74	1	0	-0.693803	3.097965	3.026174
75	1	0	-2.045785	4.251654	3.192998
76	1	0	-1.985561	2.782451	4.194796
77	5	0	0.884078	-0.115303	3.416468
78	9	0	0.723837	-1.361265	4.020529
79	9	0	-0.368266	0.360904	2.983185
80	9	0	1.694153	-0.300632	2.224299
81	9	0	1.503596	0.791570	4.242921
82	6	0	-1.928920	6.094487	-1.240144
83	1	0	-1.667322	6.187347	-2.308314
84	6	0	-3.321029	6.712669	-1.047822
85	1	0	-3.633962	6.670834	0.008022
86	1	0	-3.325352	7.771477	-1.353667
87	1	0	-4.078660	6.179065	-1.642265
88	6	0	-0.863455	6.853428	-0.433843
89	1	0	-0.834309	7.917087	-0.721558
90	1	0	-1.075189	6.803387	0.646575
91	1	0	0.136862	6.423469	-0.596972
92	1	0	-2.687951	-2.345804	-0.434444
93	6	0	-4.066715	-0.229260	-0.707804
94	6	0	-5.365797	0.118841	-0.319269
95	6	0	-3.825947	-0.563867	-2.048570
96	6	0	-6.405612	0.154362	-1.252679
97	1	0	-5.568638	0.353629	0.727243
98	6	0	-4.862025	-0.525054	-2.982191
99	1	0	-2.824514	-0.856618	-2.365368
100	6	0	-6.154707	-0.162710	-2.588969
101	1	0	-7.413045	0.429701	-0.932322
102	1	0	-4.656132	-0.774933	-4.025731
103	1	0	-6.963772	-0.130864	-3.322577
104	6	0	-2.841327	-2.521644	1.679865

105	6	0	-3.821801	-3.514285	1.560541
106	6	0	-2.300425	-2.229025	2.939567
107	6	0	-4.266354	-4.208098	2.689208
108	1	0	-4.240385	-3.743068	0.576471
109	6	0	-2.736154	-2.933032	4.063106
110	1	0	-1.528493	-1.466886	3.045436
111	6	0	-3.720454	-3.919616	3.942913
112	1	0	-5.033930	-4.979208	2.587813
113	1	0	-2.291305	-2.708641	5.035053
114	1	0	-4.058253	-4.468144	4.825624
115	1	0	0.733576	-2.459719	2.289026
116	6	0	-0.928268	-2.998071	-2.056918
117	8	0	-0.756302	-1.904213	-2.585552
118	7	0	-1.863956	-3.889888	-2.511687
119	6	0	-2.588556	-3.591390	-3.734694
120	1	0	-2.589334	-4.474195	-4.395369
121	1	0	-3.635291	-3.315946	-3.518696
122	1	0	-2.100183	-2.751648	-4.241467
123	6	0	-2.300119	-5.072576	-1.790629
124	1	0	-3.400408	-5.067494	-1.707843
125	1	0	-2.003591	-5.999292	-2.312788
126	1	0	-1.882200	-5.090324	-0.778683
127	6	0	4.854883	-0.368753	1.832558
128	1	0	3.794844	-0.562131	2.045589
129	1	0	5.224013	-1.183811	1.188448
130	1	0	5.412040	-0.414683	2.778488

$TS_{2\text{-}3}$, R_a, distal, si

charge = 0, mult =1

Sum of electronic and thermal Free Energies= -4639.914263

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.899205	-2.202270	0.596608
2	6	0	-2.787098	-0.943864	0.418860
3	1	0	-3.224028	-0.671698	1.385719
4	6	0	-0.535723	-0.368273	0.032003
5	6	0	-2.187780	1.448848	-0.249606
6	6	0	-2.028681	1.953081	-1.558386
7	6	0	-2.739682	2.249844	0.779581
8	6	0	-2.403868	3.280128	-1.802323
9	6	0	-3.134981	3.551435	0.459885
10	6	0	-2.960657	4.094633	-0.816534
11	1	0	-2.264642	3.689880	-2.805592
12	1	0	-3.560616	4.173200	1.249375
13	6	0	0.538174	-2.593471	0.270184
14	6	0	0.628042	-3.387575	-0.884440
15	6	0	1.428593	-2.772095	1.328383
16	6	0	1.645835	-4.343789	-0.977261
17	6	0	2.443811	-3.724464	1.218107
18	6	0	2.555459	-4.509500	0.068302
19	1	0	1.726818	-4.953682	-1.880023
20	1	0	3.146786	-3.852209	2.043988
21	6	0	-2.928830	1.765816	2.214548
22	1	0	-2.365255	0.833812	2.337212
23	6	0	-1.483640	1.130800	-2.717210
24	1	0	-1.305363	0.108778	-2.368950
25	29	0	1.207279	0.544333	-0.364098
26	7	0	3.150905	1.109333	-0.886548
27	6	0	3.464397	-0.173717	-1.022057

28	8	0	2.454340	-0.943892	-1.044736
29	6	0	4.833464	-0.694567	-1.226233
30	6	0	5.911452	0.160955	-1.501798
31	6	0	5.038907	-2.080497	-1.155890
32	6	0	7.187567	-0.367917	-1.692658
33	1	0	5.746333	1.237499	-1.567413
34	6	0	6.318240	-2.603478	-1.339733
35	1	0	4.185267	-2.723737	-0.944263
36	6	0	7.393195	-1.749329	-1.607512
37	1	0	8.025709	0.298409	-1.908482
38	1	0	6.479858	-3.681971	-1.273618
39	1	0	8.395120	-2.160674	-1.752353
40	6	0	3.599545	2.193582	-0.203286
41	6	0	3.195679	3.468308	-0.733043
42	6	0	4.205992	2.102127	1.095930
43	6	0	3.363095	4.609538	0.059205
44	6	0	4.323485	3.269030	1.838069
45	6	0	3.891311	4.510425	1.339656
46	1	0	3.053943	5.580354	-0.335626
47	1	0	4.738942	3.210428	2.846045
48	1	0	3.985796	5.402452	1.963551
49	8	0	0.957999	2.380050	-0.114335
50	6	0	0.410069	2.988382	1.000014
51	1	0	1.210701	3.433301	1.626204
52	1	0	-0.324455	3.764624	0.718393
53	1	0	-0.094650	2.261256	1.652129
54	6	0	2.724697	3.607740	-2.153073
55	1	0	3.460647	4.186989	-2.736896
56	1	0	2.595221	2.631255	-2.630600
57	1	0	1.765789	4.142503	-2.195371
58	7	0	-1.788852	0.098535	0.039117
59	7	0	-0.541985	-1.663009	0.374141
60	1	0	3.350134	-5.254781	-0.015148
61	6	0	-2.489921	1.058782	-3.876254
62	1	0	-2.600744	2.035478	-4.374373
63	1	0	-2.140801	0.338333	-4.633755
64	1	0	-3.484092	0.742269	-3.532037
65	6	0	-0.132138	1.658770	-3.214376
66	1	0	0.294476	0.970504	-3.960545
67	1	0	-0.233507	2.652804	-3.680597
68	1	0	0.575507	1.764868	-2.385234
69	6	0	-4.418033	1.503884	2.500068
70	1	0	-4.982800	2.450253	2.505323
71	1	0	-4.878653	0.862230	1.737023
72	1	0	-4.549625	1.026534	3.484264
73	6	0	-2.366133	2.731307	3.268781
74	1	0	-1.293206	2.906665	3.130542
75	1	0	-2.888748	3.701007	3.259202
76	1	0	-2.496551	2.294451	4.270831
77	5	0	1.267150	0.355139	3.117767
78	9	0	1.473764	-0.803187	3.862826
79	9	0	-0.125912	0.549318	2.945766
80	9	0	1.825631	0.141946	1.804900
81	9	0	1.860273	1.463381	3.677578
82	6	0	-3.328921	5.537847	-1.113373
83	1	0	-3.167802	5.694661	-2.193828
84	6	0	-4.805960	5.831813	-0.816636
85	1	0	-5.028734	5.718636	0.256669
86	1	0	-5.063867	6.864774	-1.101060
87	1	0	-5.467129	5.146852	-1.369609
88	6	0	-2.402780	6.506220	-0.360721
89	1	0	-2.627103	7.552568	-0.624886
90	1	0	-2.523889	6.400930	0.729680
91	1	0	-1.346087	6.308200	-0.597842
92	1	0	-2.125811	-2.919126	-0.206880

93	6	0	-3.903218	-1.159341	-0.575725
94	6	0	-5.235137	-1.155223	-0.143681
95	6	0	-3.626366	-1.462832	-1.916516
96	6	0	-6.277252	-1.425430	-1.035131
97	1	0	-5.459696	-0.950712	0.904787
98	6	0	-4.666097	-1.727735	-2.808758
99	1	0	-2.593827	-1.491288	-2.266065
100	6	0	-5.995133	-1.706904	-2.373187
101	1	0	-7.310627	-1.415717	-0.680857
102	1	0	-4.435881	-1.944844	-3.854439
103	1	0	-6.807055	-1.911980	-3.074974
104	6	0	-2.051614	-2.906737	1.920775
105	6	0	-2.745667	-4.120674	1.984366
106	6	0	-1.521025	-2.349908	3.093108
107	6	0	-2.917153	-4.774263	3.207947
108	1	0	-3.153704	-4.556707	1.068056
109	6	0	-1.682263	-3.010352	4.311768
110	1	0	-0.964657	-1.412404	3.057603
111	6	0	-2.382441	-4.219964	4.373816
112	1	0	-3.461684	-5.720790	3.248726
113	1	0	-1.245332	-2.575414	5.213348
114	1	0	-2.505610	-4.734157	5.330168
115	1	0	1.341147	-2.162900	2.224922
116	6	0	-0.302388	-3.151526	-2.043387
117	8	0	-0.355805	-2.056889	-2.595890
118	7	0	-1.062183	-4.215826	-2.455235
119	6	0	-1.847347	-4.098198	-3.671006
120	1	0	-1.656994	-4.963917	-4.327515
121	1	0	-2.926264	-4.064229	-3.443173
122	1	0	-1.564544	-3.174340	-4.187757
123	6	0	-1.253660	-5.439254	-1.697522
124	1	0	-2.333765	-5.631606	-1.576792
125	1	0	-0.809863	-6.309831	-2.212049
126	1	0	-0.806733	-5.356405	-0.701303
127	6	0	4.693715	0.801956	1.668226
128	1	0	3.999689	-0.021800	1.469184
129	1	0	5.677858	0.529962	1.252429
130	1	0	4.786961	0.885726	2.759038

QI, R_a, distal, si

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4639.954964

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.621392	0.970020	0.667374
2	6	0	-1.845028	2.178813	0.091682
3	1	0	-1.792328	2.979288	0.836476
4	6	0	-0.503024	0.245620	-0.060200
5	6	0	0.647352	2.406830	-0.333047
6	6	0	1.234525	2.454315	-1.614204
7	6	0	1.164126	3.183100	0.733003
8	6	0	2.345615	3.287835	-1.802465
9	6	0	2.261460	4.010555	0.478458
10	6	0	2.871885	4.076285	-0.778743
11	1	0	2.816023	3.326458	-2.788001
12	1	0	2.665858	4.603128	1.300957
13	6	0	-2.096519	-1.503197	0.576126
14	6	0	-3.365114	-2.018007	0.251739
15	6	0	-1.184571	-2.312264	1.267473

16	6	0	-3.676284	-3.340307	0.598042
17	6	0	-1.497896	-3.632063	1.582136
18	6	0	-2.748274	-4.153824	1.246013
19	1	0	-4.660365	-3.734892	0.333603
20	1	0	-0.753078	-4.239030	2.097852
21	6	0	0.580620	3.139846	2.137709
22	1	0	-0.112458	2.293449	2.182523
23	6	0	0.729398	1.639741	-2.795153
24	1	0	-0.123558	1.038547	-2.455468
25	29	0	1.045874	-0.887443	-0.204303
26	7	0	1.835829	-2.678933	-0.836071
27	6	0	0.825172	-3.674257	-0.954164
28	8	0	0.805003	-4.653021	-0.235165
29	6	0	-0.272366	-3.354969	-1.906645
30	6	0	-0.242743	-2.227226	-2.742616
31	6	0	-1.393563	-4.197726	-1.925477
32	6	0	-1.333836	-1.925208	-3.553094
33	1	0	0.627125	-1.576618	-2.732946
34	6	0	-2.483663	-3.893796	-2.737583
35	1	0	-1.398905	-5.067925	-1.269400
36	6	0	-2.462267	-2.750321	-3.540883
37	1	0	-1.315292	-1.028980	-4.177369
38	1	0	-3.366583	-4.536606	-2.725970
39	1	0	-3.333884	-2.490468	-4.143941
40	6	0	3.073730	-2.923881	-0.571276
41	6	0	3.986454	-1.737907	-0.256050
42	6	0	3.748025	-4.235999	-0.594404
43	6	0	4.860980	-2.057077	0.938485
44	6	0	4.781628	-4.388676	0.278402
45	6	0	5.255093	-3.323058	1.148260
46	1	0	5.211303	-1.234428	1.559934
47	1	0	5.263954	-5.368360	0.350780
48	1	0	5.943155	-3.568646	1.959443
49	8	0	3.182477	-0.580125	-0.103649
50	6	0	3.772893	0.593021	0.453322
51	1	0	3.901144	0.483504	1.537231
52	1	0	4.731901	0.825692	-0.037486
53	1	0	3.070144	1.406248	0.257930
54	6	0	4.897850	-1.527686	-1.500854
55	1	0	5.510182	-2.415820	-1.701331
56	1	0	4.266721	-1.310848	-2.375082
57	1	0	5.567633	-0.674484	-1.328025
58	7	0	-0.498233	1.585573	-0.093341
59	7	0	-1.752863	-0.159519	0.265654
60	1	0	-3.002808	-5.186828	1.492679
61	6	0	0.232114	2.548176	-3.928023
62	1	0	1.058112	3.131946	-4.365780
63	1	0	-0.217218	1.946549	-4.734312
64	1	0	-0.529251	3.252413	-3.567766
65	6	0	1.812557	0.670544	-3.292884
66	1	0	1.426320	0.040648	-4.109619
67	1	0	2.689421	1.212570	-3.681205
68	1	0	2.157414	0.018625	-2.476952
69	6	0	-0.199146	4.426912	2.456546
70	1	0	0.477405	5.296005	2.500625
71	1	0	-0.966248	4.651647	1.699066
72	1	0	-0.703245	4.338385	3.431756
73	6	0	1.645793	2.881586	3.212971
74	1	0	2.206342	1.963144	3.004583
75	1	0	2.348835	3.725588	3.304181
76	1	0	1.156581	2.753248	4.191421
77	5	0	1.865320	-0.981233	2.956588
78	9	0	1.056044	-1.185398	4.060066
79	9	0	1.273287	0.042171	2.143815
80	9	0	1.929630	-2.145425	2.155892

81	9	0	3.152169	-0.570168	3.309601
82	6	0	4.100199	4.938519	-1.012880
83	1	0	4.322185	4.895058	-2.093068
84	6	0	3.856956	6.409122	-0.647298
85	1	0	3.660034	6.527126	0.430389
86	1	0	4.738922	7.022832	-0.891296
87	1	0	2.992063	6.817169	-1.192700
88	6	0	5.317385	4.370327	-0.265792
89	1	0	6.222664	4.962096	-0.477437
90	1	0	5.152988	4.383041	0.823886
91	1	0	5.511537	3.327459	-0.560892
92	1	0	-3.601736	0.907611	0.183367
93	6	0	-2.379181	2.749100	-1.203891
94	6	0	-2.356487	4.134141	-1.409578
95	6	0	-2.865392	1.913389	-2.221253
96	6	0	-2.822810	4.684077	-2.607291
97	1	0	-1.968295	4.787970	-0.624590
98	6	0	-3.337234	2.464071	-3.413790
99	1	0	-2.899049	0.830928	-2.086080
100	6	0	-3.318838	3.848714	-3.611113
101	1	0	-2.799883	5.766497	-2.754106
102	1	0	-3.723335	1.802367	-4.192792
103	1	0	-3.687687	4.275608	-4.546891
104	6	0	-2.803702	1.030345	2.171067
105	6	0	-3.969855	1.599295	2.699716
106	6	0	-1.806606	0.576881	3.045974
107	6	0	-4.137766	1.717476	4.081758
108	1	0	-4.751308	1.955362	2.021883
109	6	0	-1.976147	0.688061	4.427693
110	1	0	-0.883304	0.137469	2.672698
111	6	0	-3.140461	1.259369	4.949182
112	1	0	-5.051488	2.163325	4.482715
113	1	0	-1.183714	0.315247	5.080263
114	1	0	-3.274644	1.344604	6.030310
115	1	0	-0.225904	-1.908883	1.584150
116	6	0	-4.366449	-1.234484	-0.550753
117	8	0	-4.134494	-0.921577	-1.714733
118	7	0	-5.545049	-0.916421	0.070919
119	6	0	-6.589073	-0.257556	-0.692252
120	1	0	-7.525839	-0.839421	-0.648015
121	1	0	-6.791494	0.749779	-0.287740
122	1	0	-6.259554	-0.166304	-1.733069
123	6	0	-5.835361	-1.158520	1.473590
124	1	0	-6.263729	-0.248448	1.922833
125	1	0	-6.563581	-1.979589	1.600160
126	1	0	-4.922730	-1.406478	2.024515
127	6	0	3.291944	-5.357650	-1.488048
128	1	0	2.502215	-5.956496	-1.012788
129	1	0	2.877358	-4.974021	-2.433371
130	1	0	4.141908	-6.013402	-1.727110

IM2, R_a, proximal, re

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4639.909811

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.481127	-0.892041	-0.522472
2	6	0	3.355805	0.566246	0.003123
3	1	0	3.740902	1.262106	-0.747874

4	6	0	1.246259	-0.438066	-0.067777
5	6	0	1.213302	2.011200	0.092794
6	6	0	0.618887	2.467321	1.290340
7	6	0	1.133683	2.754258	-1.100985
8	6	0	-0.155581	3.626896	1.217889
9	6	0	0.346833	3.907571	-1.107011
10	6	0	-0.350154	4.333273	0.024700
11	1	0	-0.643447	3.984941	2.126501
12	1	0	0.240242	4.448163	-2.043712
13	6	0	1.903181	-2.835607	-0.097289
14	6	0	1.336607	-3.380699	1.069257
15	6	0	2.296811	-3.695090	-1.132052
16	6	0	1.129968	-4.763862	1.159027
17	6	0	2.098152	-5.069351	-1.024631
18	6	0	1.502861	-5.610242	0.118225
19	1	0	0.669618	-5.172353	2.061580
20	1	0	2.397030	-5.719798	-1.849419
21	6	0	1.922723	2.373211	-2.345525
22	1	0	2.276178	1.345757	-2.216342
23	6	0	0.877827	1.826478	2.649184
24	1	0	1.289262	0.822746	2.475510
25	29	0	-0.698313	-0.752107	-0.330472
26	7	0	-2.607879	-1.209987	-0.011091
27	6	0	-2.678430	-0.224031	0.855585
28	8	0	-1.550715	0.369386	1.024449
29	6	0	-3.852159	0.207659	1.636691
30	6	0	-4.797694	-0.710316	2.114590
31	6	0	-3.991648	1.577085	1.907204
32	6	0	-5.882654	-0.255515	2.864690
33	1	0	-4.680751	-1.773629	1.899008
34	6	0	-5.085599	2.025066	2.646158
35	1	0	-3.255578	2.268022	1.497442
36	6	0	-6.029294	1.110977	3.127212
37	1	0	-6.619195	-0.968239	3.242781
38	1	0	-5.207013	3.093052	2.841425
39	1	0	-6.885790	1.464643	3.706559
40	6	0	-3.541301	-2.048742	-0.615822
41	6	0	-4.724189	-1.571844	-1.245549
42	6	0	-3.236630	-3.441622	-0.598771
43	6	0	-5.562209	-2.514292	-1.859755
44	6	0	-4.106534	-4.331608	-1.226180
45	6	0	-5.262990	-3.873376	-1.863999
46	1	0	-6.471572	-2.156434	-2.349119
47	1	0	-3.874571	-5.399551	-1.212469
48	1	0	-5.932047	-4.580263	-2.360913
49	8	0	-0.232862	-1.916421	-1.690709
50	6	0	-1.005636	-1.786464	-2.846504
51	1	0	-0.623768	-1.007274	-3.530090
52	1	0	-0.986247	-2.768395	-3.362537
53	1	0	-2.068764	-1.555916	-2.650378
54	6	0	-5.153583	-0.133307	-1.233783
55	1	0	-5.907951	0.024534	-0.443864
56	1	0	-4.334242	0.565592	-1.062285
57	1	0	-5.612993	0.130755	-2.196656
58	7	0	1.870403	0.725126	0.055354
59	7	0	2.148981	-1.436224	-0.186379
60	1	0	1.330880	-6.685639	0.197511
61	6	0	1.933500	2.656256	3.401996
62	1	0	1.531772	3.653912	3.642151
63	1	0	2.213803	2.166669	4.348332
64	1	0	2.845541	2.798551	2.808489
65	6	0	-0.368200	1.658005	3.527130
66	1	0	-0.085119	1.197512	4.487678
67	1	0	-0.833999	2.627435	3.764607
68	1	0	-1.111211	1.025224	3.031380

69	6	0	3.161886	3.278715	-2.469514
70	1	0	2.863337	4.317947	-2.680983
71	1	0	3.754872	3.297930	-1.540514
72	1	0	3.814070	2.935909	-3.289060
73	6	0	1.123690	2.371862	-3.652045
74	1	0	0.278620	1.679344	-3.587514
75	1	0	0.715033	3.364374	-3.891310
76	1	0	1.783165	2.067631	-4.481108
77	5	0	-2.192436	1.710987	-2.210844
78	9	0	-2.866303	2.054630	-1.022801
79	9	0	-1.012623	0.960311	-1.836296
80	9	0	-1.815322	2.857669	-2.892028
81	9	0	-2.974388	0.879448	-3.004005
82	6	0	-1.326604	5.502467	-0.007221
83	1	0	-0.995098	6.223047	0.764713
84	6	0	-1.366161	6.229646	-1.353113
85	1	0	-1.711670	5.548781	-2.146688
86	1	0	-2.064744	7.079427	-1.306181
87	1	0	-0.378287	6.622875	-1.639961
88	6	0	-2.740538	5.022923	0.371731
89	1	0	-3.451576	5.864812	0.352909
90	1	0	-3.078628	4.247622	-0.330592
91	1	0	-2.762125	4.589982	1.383759
92	1	0	4.258248	-1.438311	0.028877
93	6	0	4.062571	0.833292	1.307231
94	6	0	4.977575	1.888786	1.391588
95	6	0	3.852579	0.021355	2.430885
96	6	0	5.671604	2.136888	2.579623
97	1	0	5.143169	2.526029	0.519533
98	6	0	4.542058	0.268892	3.617150
99	1	0	3.133289	-0.795811	2.378858
100	6	0	5.454231	1.327051	3.695303
101	1	0	6.378702	2.967633	2.632982
102	1	0	4.366150	-0.361235	4.492133
103	1	0	5.990359	1.520436	4.627117
104	6	0	3.773903	-0.917976	-2.011276
105	6	0	5.103074	-0.825030	-2.442451
106	6	0	2.739912	-0.928527	-2.958185
107	6	0	5.399001	-0.730055	-3.804308
108	1	0	5.912752	-0.819370	-1.706899
109	6	0	3.038493	-0.835933	-4.319490
110	1	0	1.702612	-1.030906	-2.631553
111	6	0	4.365501	-0.731483	-4.745954
112	1	0	6.439012	-0.657604	-4.131087
113	1	0	2.224352	-0.840839	-5.047294
114	1	0	4.595211	-0.656288	-5.811306
115	1	0	2.735590	-3.279085	-2.035440
116	6	0	0.861623	-2.507073	2.197413
117	8	0	-0.159151	-1.838818	2.068175
118	7	0	1.591058	-2.512666	3.352438
119	6	0	1.116550	-1.737640	4.487858
120	1	0	0.941577	-2.394738	5.356490
121	1	0	1.860785	-0.974640	4.769869
122	1	0	0.183020	-1.238082	4.208817
123	6	0	2.796897	-3.291839	3.565190
124	1	0	3.578357	-2.656205	4.011808
125	1	0	2.612058	-4.136839	4.252054
126	1	0	3.175371	-3.688832	2.617474
127	6	0	-1.995716	-3.936232	0.087520
128	1	0	-1.998088	-5.033047	0.161188
129	1	0	-1.101004	-3.621056	-0.468385
130	1	0	-1.895603	-3.505376	1.094776

$TS_{2\text{-}3}$, R_a, proximal, re

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4639.899121

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.560871	-0.539828	-0.364331
2	6	0	3.241674	0.969233	-0.152626
3	1	0	3.522515	1.534666	-1.047664
4	6	0	1.247668	-0.278934	0.024072
5	6	0	0.936525	2.129377	-0.182669
6	6	0	0.304117	2.678283	0.954346
7	6	0	0.719386	2.656498	-1.469913
8	6	0	-0.632160	3.692115	0.741982
9	6	0	-0.223414	3.675982	-1.617360
10	6	0	-0.949151	4.173405	-0.534055
11	1	0	-1.150902	4.111755	1.606101
12	1	0	-0.428163	4.042613	-2.619903
13	6	0	2.174658	-2.556204	0.289531
14	6	0	1.733518	-2.970657	1.560889
15	6	0	2.599591	-3.519904	-0.634766
16	6	0	1.702130	-4.335542	1.870770
17	6	0	2.571011	-4.875784	-0.310928
18	6	0	2.117536	-5.289844	0.943304
19	1	0	1.344352	-4.647356	2.854915
20	1	0	2.897513	-5.611310	-1.049269
21	6	0	1.513152	2.186602	-2.680728
22	1	0	2.054751	1.280242	-2.393365
23	6	0	0.673822	2.289413	2.380774
24	1	0	1.239675	1.348963	2.335114
25	29	0	-0.685121	-0.821375	0.074991
26	7	0	-2.664494	-1.607109	0.593467
27	6	0	-2.969192	-0.393221	1.100287
28	8	0	-2.011138	0.407075	1.156286
29	6	0	-4.278176	-0.056329	1.701777
30	6	0	-5.121762	-1.046525	2.223299
31	6	0	-4.651087	1.294172	1.761202
32	6	0	-6.339213	-0.686251	2.802156
33	1	0	-4.816333	-2.093867	2.177881
34	6	0	-5.876802	1.646418	2.323913
35	1	0	-3.983192	2.038504	1.328020
36	6	0	-6.719488	0.659241	2.847548
37	1	0	-6.994961	-1.455462	3.216754
38	1	0	-6.179889	2.695646	2.350707
39	1	0	-7.677899	0.939236	3.291798
40	6	0	-3.101952	-2.454913	-0.330409
41	6	0	-4.140607	-2.216665	-1.309510
42	6	0	-2.255340	-3.655173	-0.444512
43	6	0	-4.240149	-3.100387	-2.364140
44	6	0	-2.469816	-4.540766	-1.530462
45	6	0	-3.402299	-4.240280	-2.494693
46	1	0	-5.001463	-2.916659	-3.125165
47	1	0	-1.863473	-5.446700	-1.596568
48	1	0	-3.540320	-4.904135	-3.351976
49	8	0	-0.679368	-2.426467	-1.028485
50	6	0	-0.355178	-2.367521	-2.382048
51	1	0	0.628655	-2.829045	-2.599899
52	1	0	-1.116792	-2.921155	-2.967016
53	1	0	-0.385107	-1.329455	-2.751434
54	6	0	-5.120572	-1.091094	-1.178041
55	1	0	-5.835159	-1.292115	-0.363484
56	1	0	-4.630995	-0.134120	-0.970361

57	1	0	-5.681028	-0.972797	-2.114168
58	7	0	1.756011	0.949297	-0.055419
59	7	0	2.266784	-1.171558	-0.022486
60	1	0	2.085754	-6.351203	1.198446
61	6	0	1.590517	3.372455	2.976722
62	1	0	1.039171	4.320641	3.083680
63	1	0	1.950377	3.075436	3.974948
64	1	0	2.465139	3.564754	2.341937
65	6	0	-0.524931	2.053205	3.307281
66	1	0	-0.168329	1.780933	4.314039
67	1	0	-1.133859	2.964073	3.421409
68	1	0	-1.170737	1.256100	2.924036
69	6	0	2.563807	3.245259	-3.058620
70	1	0	2.077058	4.168213	-3.412000
71	1	0	3.194366	3.520981	-2.197551
72	1	0	3.219813	2.875577	-3.863623
73	6	0	0.666771	1.796596	-3.896372
74	1	0	-0.048551	1.009799	-3.634405
75	1	0	0.081027	2.642088	-4.284198
76	1	0	1.327039	1.439383	-4.704272
77	5	0	-2.554556	1.049023	-2.315684
78	9	0	-3.362450	1.452604	-1.232825
79	9	0	-1.332195	0.513494	-1.772633
80	9	0	-2.271505	2.144142	-3.122526
81	9	0	-3.170468	0.035216	-3.042480
82	6	0	-2.083125	5.177664	-0.698531
83	1	0	-1.842537	6.046538	-0.056414
84	6	0	-2.253510	5.678398	-2.134524
85	1	0	-2.514390	4.842820	-2.802529
86	1	0	-3.065067	6.420960	-2.184981
87	1	0	-1.337741	6.155770	-2.517316
88	6	0	-3.405796	4.570150	-0.194285
89	1	0	-4.229141	5.295175	-0.302209
90	1	0	-3.646632	3.661427	-0.764352
91	1	0	-3.341892	4.291731	0.868990
92	1	0	4.332193	-0.871272	0.344571
93	6	0	3.935962	1.593207	1.032578
94	6	0	4.664862	2.776124	0.870507
95	6	0	3.890278	0.989236	2.296670
96	6	0	5.339017	3.350730	1.952626
97	1	0	4.701399	3.253284	-0.111803
98	6	0	4.562191	1.559091	3.376911
99	1	0	3.307394	0.078328	2.433708
100	6	0	5.290255	2.742111	3.207733
101	1	0	5.900579	4.277166	1.813176
102	1	0	4.515074	1.086297	4.360924
103	1	0	5.813276	3.189728	4.055814
104	6	0	4.025165	-0.825589	-1.777555
105	6	0	5.396012	-0.891043	-2.052190
106	6	0	3.110311	-0.941330	-2.833748
107	6	0	5.849827	-1.059850	-3.363437
108	1	0	6.115112	-0.806505	-1.232693
109	6	0	3.561894	-1.109842	-4.143475
110	1	0	2.039703	-0.916155	-2.632135
111	6	0	4.933311	-1.166713	-4.412557
112	1	0	6.922439	-1.111124	-3.564755
113	1	0	2.836523	-1.196881	-4.955437
114	1	0	5.286076	-1.298973	-5.437940
115	1	0	2.945177	-3.201832	-1.615783
116	6	0	1.213334	-1.992663	2.583215
117	8	0	0.082535	-1.528471	2.475543
118	7	0	2.035706	-1.683375	3.629738
119	6	0	1.538742	-0.811585	4.682381
120	1	0	1.520643	-1.344593	5.648319
121	1	0	2.185598	0.075049	4.783006

122	1	0	0.526171	-0.486727	4.422461
123	6	0	3.353984	-2.253883	3.838592
124	1	0	4.068658	-1.457894	4.102387
125	1	0	3.345502	-2.990407	4.661918
126	1	0	3.710606	-2.750843	2.930234
127	6	0	-1.529544	-4.156521	0.768081
128	1	0	-0.693899	-4.802257	0.471376
129	1	0	-1.150028	-3.333410	1.381557
130	1	0	-2.226072	-4.752577	1.384509

QI, R_a, proximal, re

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4639.934837

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.601499	-0.745357	-0.122894
2	6	0	3.386735	0.757347	0.244938
3	1	0	3.850625	1.391439	-0.521539
4	6	0	1.280441	-0.279963	-0.027702
5	6	0	1.167134	2.115830	0.169628
6	6	0	0.403963	2.434612	1.313242
7	6	0	1.069226	2.874091	-1.010622
8	6	0	-0.518653	3.476455	1.209147
9	6	0	0.114855	3.894336	-1.062055
10	6	0	-0.716765	4.189311	0.019479
11	1	0	-1.135947	3.718328	2.076938
12	1	0	-0.011229	4.431489	-1.999598
13	6	0	1.867406	-2.631230	-0.328648
14	6	0	1.147786	-3.323941	0.662435
15	6	0	2.199026	-3.292989	-1.519045
16	6	0	0.746258	-4.645007	0.431461
17	6	0	1.819978	-4.619158	-1.724902
18	6	0	1.086093	-5.299295	-0.751422
19	1	0	0.161536	-5.159887	1.196882
20	1	0	2.084751	-5.113532	-2.662144
21	6	0	1.933048	2.599803	-2.234039
22	1	0	2.719477	1.895835	-1.938487
23	6	0	0.586956	1.718467	2.644863
24	1	0	1.318362	0.916842	2.491869
25	29	0	-0.629421	-0.427279	-0.253183
26	7	0	-2.619566	-0.679015	0.005047
27	6	0	-3.128460	0.208804	0.984519
28	8	0	-2.979902	1.406319	0.911041
29	6	0	-3.730702	-0.439553	2.194037
30	6	0	-3.613436	-1.809002	2.465839
31	6	0	-4.415005	0.390634	3.096684
32	6	0	-4.186410	-2.342976	3.621956
33	1	0	-3.042161	-2.444355	1.795124
34	6	0	-4.994415	-0.146279	4.243972
35	1	0	-4.483031	1.455882	2.870709
36	6	0	-4.881276	-1.516562	4.508691
37	1	0	-4.081799	-3.409604	3.834255
38	1	0	-5.534852	0.502626	4.937276
39	1	0	-5.332143	-1.937972	5.410718
40	6	0	-3.255120	-1.299305	-0.935416
41	6	0	-4.654172	-1.091269	-1.315103
42	6	0	-2.450167	-2.431534	-1.631016
43	6	0	-5.120581	-1.743474	-2.417630
44	6	0	-3.061159	-2.932007	-2.903141

45	6	0	-4.330609	-2.642290	-3.229858
46	1	0	-6.145222	-1.539906	-2.739443
47	1	0	-2.458863	-3.618170	-3.501125
48	1	0	-4.786505	-3.071960	-4.124647
49	8	0	-1.076948	-2.060596	-1.780402
50	6	0	-0.608000	-1.655458	-3.066882
51	1	0	-0.430293	-2.530734	-3.713069
52	1	0	-1.296055	-0.944585	-3.540493
53	1	0	0.355089	-1.162089	-2.886260
54	6	0	-5.510449	-0.078593	-0.609149
55	1	0	-5.650136	-0.319115	0.454472
56	1	0	-5.046677	0.914571	-0.687323
57	1	0	-6.502659	-0.034686	-1.079193
58	7	0	1.913348	0.883507	0.148288
59	7	0	2.210023	-1.260364	-0.137052
60	1	0	0.773476	-6.332988	-0.914614
61	6	0	1.183670	2.679947	3.683914
62	1	0	0.481454	3.495720	3.919528
63	1	0	1.409226	2.147188	4.622030
64	1	0	2.117162	3.131386	3.317326
65	6	0	-0.693701	1.054316	3.161749
66	1	0	-0.538755	0.665783	4.181333
67	1	0	-1.541474	1.752801	3.192072
68	1	0	-0.976602	0.208199	2.523040
69	6	0	2.651099	3.870196	-2.712883
70	1	0	1.938239	4.615538	-3.097735
71	1	0	3.220686	4.342333	-1.896313
72	1	0	3.351486	3.630428	-3.529471
73	6	0	1.150384	1.937958	-3.374619
74	1	0	0.686017	1.003038	-3.038427
75	1	0	0.322264	2.570763	-3.720789
76	1	0	1.821295	1.727742	-4.224898
77	5	0	-2.420585	1.552389	-2.670790
78	9	0	-3.506122	1.937168	-1.887114
79	9	0	-1.348362	1.096592	-1.820790
80	9	0	-1.955904	2.620294	-3.430526
81	9	0	-2.792243	0.464657	-3.483311
82	6	0	-1.831911	5.223761	-0.063892
83	1	0	-1.654694	5.947080	0.755402
84	6	0	-1.849862	5.998305	-1.383924
85	1	0	-2.051947	5.318836	-2.227251
86	1	0	-2.647508	6.757156	-1.366741
87	1	0	-0.896868	6.516486	-1.575913
88	6	0	-3.201357	4.562844	0.175932
89	1	0	-3.998040	5.325012	0.159115
90	1	0	-3.404087	3.810822	-0.599702
91	1	0	-3.241239	4.041821	1.142547
92	1	0	4.170199	-1.255460	0.667301
93	6	0	3.932344	1.187345	1.586265
94	6	0	4.613754	2.403158	1.704068
95	6	0	3.741342	0.402397	2.731115
96	6	0	5.107003	2.824982	2.942776
97	1	0	4.755602	3.026980	0.817923
98	6	0	4.232847	0.817985	3.967804
99	1	0	3.178693	-0.527125	2.648894
100	6	0	4.920757	2.031536	4.076233
101	1	0	5.636117	3.777401	3.020953
102	1	0	4.074136	0.199343	4.854505
103	1	0	5.303861	2.359771	5.045082
104	6	0	4.333814	-0.916460	-1.435970
105	6	0	5.633072	-1.431517	-1.456710
106	6	0	3.736339	-0.522828	-2.643537
107	6	0	6.331611	-1.551059	-2.663141
108	1	0	6.103891	-1.743894	-0.520671
109	6	0	4.429741	-0.640978	-3.847079

110	1	0	2.715627	-0.139749	-2.645843
111	6	0	5.731931	-1.155549	-3.860083
112	1	0	7.345798	-1.957253	-2.665618
113	1	0	3.950273	-0.331726	-4.778642
114	1	0	6.274986	-1.249239	-4.803311
115	1	0	2.734159	-2.756912	-2.298353
116	6	0	0.704570	-2.686520	1.954401
117	8	0	-0.467673	-2.366871	2.105199
118	7	0	1.647850	-2.528691	2.935820
119	6	0	1.230260	-1.983429	4.217444
120	1	0	1.179745	-2.776599	4.984703
121	1	0	1.944935	-1.216734	4.555130
122	1	0	0.239746	-1.532227	4.103868
123	6	0	2.941230	-3.188208	2.917023
124	1	0	3.728981	-2.497508	3.257697
125	1	0	2.947061	-4.065235	3.590059
126	1	0	3.189310	-3.528005	1.905834
127	6	0	-2.434970	-3.603006	-0.622764
128	1	0	-1.925542	-4.464364	-1.075645
129	1	0	-1.872144	-3.283606	0.265525
130	1	0	-3.457353	-3.889309	-0.337275

IM2, R_a, proximal, si

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4639.907897

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.108920	-1.924898	0.088987
2	6	0	-3.327610	-0.417847	-0.128397
3	1	0	-3.786695	0.010933	0.765223
4	6	0	-1.035980	-0.906011	-0.285713
5	6	0	-1.717962	1.497015	0.045423
6	6	0	-1.359687	2.339058	-1.025697
7	6	0	-2.038998	2.015435	1.319857
8	6	0	-1.396366	3.717399	-0.795629
9	6	0	-2.034751	3.400018	1.487873
10	6	0	-1.723479	4.270927	0.441998
11	1	0	-1.108078	4.392918	-1.602345
12	1	0	-2.238031	3.802476	2.480175
13	6	0	-1.184719	-3.371805	-0.625848
14	6	0	-0.120328	-3.571754	-1.526138
15	6	0	-1.780408	-4.498947	-0.031191
16	6	0	0.371097	-4.867250	-1.740251
17	6	0	-1.308304	-5.783416	-0.290705
18	6	0	-0.218066	-5.976948	-1.140597
19	1	0	1.229421	-4.989952	-2.403790
20	1	0	-1.790721	-6.635217	0.193588
21	6	0	-2.353885	1.129945	2.517934
22	1	0	-2.245103	0.086712	2.205719
23	6	0	-0.882190	1.836822	-2.383208
24	1	0	-0.558035	0.796882	-2.249537
25	29	0	0.954019	-0.768804	0.129867
26	7	0	2.883319	-0.392354	0.379815
27	6	0	2.837145	0.481214	-0.606049
28	8	0	1.673268	0.564778	-1.141764
29	6	0	3.951226	1.326406	-1.065555
30	6	0	4.970176	1.717818	-0.184579
31	6	0	3.972684	1.752559	-2.401615
32	6	0	6.016411	2.511503	-0.651248

33	1	0	4.909297	1.437049	0.865204
34	6	0	5.026261	2.539858	-2.864061
35	1	0	3.161152	1.458972	-3.067004
36	6	0	6.050978	2.916396	-1.989949
37	1	0	6.803668	2.827438	0.036643
38	1	0	5.046560	2.865518	-3.906533
39	1	0	6.874421	3.537784	-2.350503
40	6	0	3.903966	-1.110174	0.969443
41	6	0	3.917848	-1.185465	2.396013
42	6	0	4.882299	-1.796860	0.187007
43	6	0	4.938652	-1.911756	3.009426
44	6	0	5.883461	-2.503512	0.860572
45	6	0	5.916497	-2.564285	2.254059
46	1	0	4.965446	-1.965558	4.100221
47	1	0	6.645436	-3.023439	0.274913
48	1	0	6.705075	-3.130862	2.755492
49	8	0	0.668087	-2.111194	1.379211
50	6	0	1.521409	-3.205791	1.426516
51	1	0	2.446073	-3.073205	0.828660
52	1	0	1.858471	-3.381530	2.466685
53	1	0	1.025608	-4.119188	1.045608
54	6	0	2.866415	-0.491749	3.204877
55	1	0	3.036841	-0.648081	4.279166
56	1	0	2.860797	0.584850	2.982855
57	1	0	1.864173	-0.858258	2.937260
58	7	0	-1.910840	0.081692	-0.163108
59	7	0	-1.707912	-2.088585	-0.351445
60	1	0	0.169559	-6.979082	-1.333471
61	6	0	-1.983608	1.865902	-3.452611
62	1	0	-2.393049	2.882733	-3.562607
63	1	0	-1.576027	1.566423	-4.433125
64	1	0	-2.816678	1.197054	-3.213391
65	6	0	0.338633	2.637191	-2.866550
66	1	0	0.814560	2.123658	-3.716628
67	1	0	0.042983	3.636470	-3.223978
68	1	0	1.072597	2.752095	-2.061208
69	6	0	-3.797665	1.321537	3.011597
70	1	0	-3.938097	2.328611	3.435439
71	1	0	-4.540615	1.204127	2.205540
72	1	0	-4.035140	0.585582	3.795987
73	6	0	-1.360226	1.320470	3.673201
74	1	0	-0.335311	1.144573	3.330924
75	1	0	-1.400521	2.342424	4.079402
76	1	0	-1.604516	0.617696	4.486922
77	5	0	1.485219	2.558986	1.532985
78	9	0	2.835464	2.359988	1.871943
79	9	0	0.840139	3.304814	2.510286
80	9	0	0.854190	1.258398	1.463869
81	9	0	1.402260	3.166482	0.280858
82	6	0	-1.592960	5.768077	0.652965
83	1	0	-1.751485	6.243885	-0.331510
84	6	0	-2.631079	6.345694	1.620422
85	1	0	-2.468673	5.984430	2.648458
86	1	0	-2.558645	7.444505	1.649987
87	1	0	-3.658009	6.077041	1.324836
88	6	0	-0.159587	6.095912	1.109658
89	1	0	-0.023368	7.185508	1.211809
90	1	0	0.057574	5.612087	2.073187
91	1	0	0.580440	5.704032	0.397731
92	1	0	-3.767048	-2.527035	-0.549980
93	6	0	-4.153141	0.018858	-1.314914
94	6	0	-4.717534	1.303850	-1.290059
95	6	0	-4.377962	-0.798695	-2.429745
96	6	0	-5.480108	1.764131	-2.363860
97	1	0	-4.541828	1.950671	-0.428243

98	6	0	-5.144546	-0.340160	-3.504279
99	1	0	-3.955343	-1.803160	-2.469361
100	6	0	-5.695092	0.943561	-3.474801
101	1	0	-5.905989	2.769351	-2.333350
102	1	0	-5.311810	-0.988999	-4.367180
103	1	0	-6.292912	1.302825	-4.315490
104	6	0	-3.346875	-2.291669	1.546092
105	6	0	-4.667344	-2.489044	1.971470
106	6	0	-2.303705	-2.339015	2.479327
107	6	0	-4.948723	-2.717307	3.319924
108	1	0	-5.483686	-2.453259	1.243846
109	6	0	-2.589986	-2.568291	3.827957
110	1	0	-1.266006	-2.204025	2.159374
111	6	0	-3.908156	-2.752682	4.253296
112	1	0	-5.981837	-2.866581	3.642348
113	1	0	-1.770509	-2.596844	4.549635
114	1	0	-4.125720	-2.927697	5.309508
115	1	0	-2.603376	-4.371687	0.667425
116	6	0	0.635920	-2.484427	-2.238007
117	8	0	1.804733	-2.276486	-1.909940
118	7	0	0.041289	-1.819052	-3.257832
119	6	0	0.836237	-0.847182	-3.997255
120	1	0	1.428498	-1.340778	-4.787880
121	1	0	0.163836	-0.114835	-4.460861
122	1	0	1.510443	-0.331279	-3.306409
123	6	0	-1.278687	-2.116436	-3.778251
124	1	0	-1.920540	-1.223371	-3.729882
125	1	0	-1.213701	-2.439683	-4.831757
126	1	0	-1.744617	-2.922646	-3.201237
127	6	0	4.884509	-1.755159	-1.314908
128	1	0	3.869053	-1.787446	-1.726759
129	1	0	5.368968	-0.834969	-1.680746
130	1	0	5.450808	-2.608219	-1.716077

$TS_{2\text{-}3}$, R_a, proximal, si

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4639.898189

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.192372	-1.711287	-0.137206
2	6	0	3.346037	-0.201709	0.075628
3	1	0	3.795535	0.254410	-0.809839
4	6	0	1.080170	-0.810715	0.325784
5	6	0	1.631110	1.617334	-0.062255
6	6	0	1.169367	2.413831	1.005320
7	6	0	1.950012	2.185674	-1.315253
8	6	0	1.118741	3.795457	0.798964
9	6	0	1.871966	3.571380	-1.457721
10	6	0	1.467041	4.398776	-0.409402
11	1	0	0.753746	4.432945	1.605219
12	1	0	2.083965	4.006026	-2.434716
13	6	0	1.461656	-3.246309	0.804408
14	6	0	0.414155	-3.502318	1.712215
15	6	0	2.192746	-4.341585	0.300675
16	6	0	0.092459	-4.829097	2.034266
17	6	0	1.878910	-5.649004	0.659655
18	6	0	0.815771	-5.904665	1.527258
19	1	0	-0.749961	-5.003409	2.706907
20	1	0	2.463730	-6.471322	0.241654

21	6	0	2.295192	1.343171	-2.535064
22	1	0	2.267447	0.290637	-2.238653
23	6	0	0.689029	1.862855	2.343322
24	1	0	0.426440	0.807317	2.191600
25	29	0	-0.894736	-0.699854	-0.101632
26	7	0	-3.049765	-0.316116	-0.531074
27	6	0	-3.128409	0.367567	0.620829
28	8	0	-2.084819	0.406658	1.308936
29	6	0	-4.333910	1.146987	0.972015
30	6	0	-5.318465	1.428070	0.013974
31	6	0	-4.470262	1.624046	2.283502
32	6	0	-6.446843	2.161803	0.377708
33	1	0	-5.166343	1.111585	-1.017451
34	6	0	-5.604489	2.349257	2.644189
35	1	0	-3.677741	1.419379	3.004057
36	6	0	-6.594866	2.615867	1.692371
37	1	0	-7.207508	2.394628	-0.370719
38	1	0	-5.715219	2.715917	3.667267
39	1	0	-7.480092	3.191653	1.973614
40	6	0	-3.545970	-1.378531	-1.118838
41	6	0	-3.073079	-1.612500	-2.488634
42	6	0	-4.325105	-2.397612	-0.434610
43	6	0	-3.485054	-2.797242	-3.141271
44	6	0	-4.644601	-3.541369	-1.128968
45	6	0	-4.227149	-3.746332	-2.474278
46	1	0	-3.182317	-2.957055	-4.177961
47	1	0	-5.230237	-4.318573	-0.632130
48	1	0	-4.520968	-4.667418	-2.984078
49	8	0	-1.202842	-2.104423	-1.472817
50	6	0	-1.063595	-3.463591	-1.212126
51	1	0	-1.415397	-3.738778	-0.204289
52	1	0	-1.672521	-4.037153	-1.942115
53	1	0	-0.022228	-3.809559	-1.347823
54	6	0	-2.484180	-0.492606	-3.281406
55	1	0	-1.982687	-0.882360	-4.177896
56	1	0	-3.282236	0.201551	-3.592696
57	1	0	-1.787841	0.102329	-2.686294
58	7	0	1.907027	0.213855	0.119748
59	7	0	1.846149	-1.945492	0.419069
60	1	0	0.552838	-6.927206	1.804819
61	6	0	1.775869	1.944406	3.425488
62	1	0	2.110325	2.985592	3.559090
63	1	0	1.384436	1.596195	4.396115
64	1	0	2.657495	1.343751	3.177573
65	6	0	-0.582977	2.585873	2.818056
66	1	0	-1.037552	2.038579	3.657298
67	1	0	-0.350482	3.598517	3.184699
68	1	0	-1.316161	2.664343	2.007631
69	6	0	3.702952	1.636741	-3.075259
70	1	0	3.772405	2.664555	-3.465480
71	1	0	4.479377	1.531005	-2.299521
72	1	0	3.951688	0.945063	-3.895839
73	6	0	1.240426	1.489026	-3.642250
74	1	0	0.240304	1.276347	-3.249615
75	1	0	1.217733	2.511691	-4.048166
76	1	0	1.467988	0.794465	-4.467857
77	5	0	-1.711507	2.579225	-1.423349
78	9	0	-2.976305	2.231288	-1.901506
79	9	0	-1.036905	3.372092	-2.341986
80	9	0	-0.935590	1.354903	-1.248914
81	9	0	-1.817457	3.196068	-0.177564
82	6	0	1.265096	5.893407	-0.582874
83	1	0	1.411302	6.350076	0.412668
84	6	0	2.266868	6.543079	-1.542369
85	1	0	2.110245	6.203229	-2.578673

86	1	0	2.145215	7.637916	-1.540777
87	1	0	3.307732	6.312761	-1.263687
88	6	0	-0.185039	6.172393	-1.018144
89	1	0	-0.371927	7.257868	-1.074141
90	1	0	-0.385482	5.719661	-1.999938
91	1	0	-0.902289	5.717806	-0.320138
92	1	0	3.944219	-2.273348	0.429732
93	6	0	4.126002	0.256656	1.286172
94	6	0	4.633435	1.564688	1.294815
95	6	0	4.342963	-0.562763	2.401572
96	6	0	5.337213	2.044794	2.400097
97	1	0	4.457775	2.213859	0.434569
98	6	0	5.051067	-0.084529	3.506933
99	1	0	3.954457	-1.581719	2.419039
100	6	0	5.548086	1.221334	3.509584
101	1	0	5.719344	3.067958	2.395606
102	1	0	5.212638	-0.734514	4.370129
103	1	0	6.099212	1.596317	4.374992
104	6	0	3.285375	-2.076473	-1.611625
105	6	0	4.553893	-2.268988	-2.174959
106	6	0	2.153083	-2.137795	-2.435069
107	6	0	4.694257	-2.508930	-3.543457
108	1	0	5.441856	-2.221530	-1.537724
109	6	0	2.295685	-2.377691	-3.803953
110	1	0	1.151008	-1.985087	-2.030153
111	6	0	3.562787	-2.560883	-4.363089
112	1	0	5.689226	-2.654831	-3.970430
113	1	0	1.403736	-2.413196	-4.433253
114	1	0	3.669840	-2.745705	-5.434421
115	1	0	2.994656	-4.174616	-0.414539
116	6	0	-0.501930	-2.478994	2.334412
117	8	0	-1.676468	-2.440946	1.968776
118	7	0	-0.026017	-1.717984	3.350317
119	6	0	-0.956725	-0.841128	4.048216
120	1	0	-1.501333	-1.392286	4.835775
121	1	0	-0.394116	-0.022824	4.514294
122	1	0	-1.672021	-0.423835	3.332132
123	6	0	1.305438	-1.839480	3.911810
124	1	0	1.850572	-0.887120	3.830503
125	1	0	1.248096	-2.116249	4.978999
126	1	0	1.871553	-2.617251	3.388250
127	6	0	-4.734785	-2.198661	0.993370
128	1	0	-3.846929	-2.043376	1.624913
129	1	0	-5.391662	-1.323134	1.108727
130	1	0	-5.271201	-3.082255	1.366191

QI, R_a, proximal, si

charge = 0, mult =1

Sum of electronic and thermal Free Energies= -4639.932712

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.763142	-2.340536	-0.388544
2	6	0	3.389852	-0.950359	-0.228604
3	1	0	3.841156	-0.629114	-1.171448
4	6	0	1.124378	-0.885420	0.420339
5	6	0	2.200659	1.277233	-0.178739
6	6	0	2.125318	2.152063	0.924502
7	6	0	2.373640	1.769268	-1.491635
8	6	0	2.259290	3.520839	0.677338

9	6	0	2.496258	3.147572	-1.672010
10	6	0	2.436062	4.043687	-0.603531
11	1	0	2.184454	4.216880	1.515515
12	1	0	2.588399	3.530205	-2.688407
13	6	0	0.810737	-3.356460	0.793570
14	6	0	-0.243532	-3.373410	1.734724
15	6	0	1.193845	-4.587315	0.214503
16	6	0	-0.899840	-4.586467	2.005963
17	6	0	0.551090	-5.780609	0.525960
18	6	0	-0.514531	-5.789465	1.425680
19	1	0	-1.741314	-4.559637	2.700431
20	1	0	0.881840	-6.703475	0.044415
21	6	0	2.391528	0.864079	-2.715145
22	1	0	2.209405	-0.160127	-2.379429
23	6	0	1.863485	1.698976	2.353941
24	1	0	1.620093	0.628249	2.331300
25	29	0	-0.557526	-0.000068	0.615490
26	7	0	-3.309016	0.069991	-0.239970
27	6	0	-3.159404	0.936479	0.759796
28	8	0	-2.121112	0.904223	1.458803
29	6	0	-4.148189	2.027769	0.934508
30	6	0	-5.394573	2.013952	0.292665
31	6	0	-3.794294	3.109823	1.752446
32	6	0	-6.292933	3.061196	0.491689
33	1	0	-5.658168	1.190908	-0.373221
34	6	0	-4.693080	4.156610	1.946284
35	1	0	-2.801735	3.120668	2.201147
36	6	0	-5.944051	4.132155	1.320871
37	1	0	-7.263445	3.048844	-0.009401
38	1	0	-4.413426	5.003488	2.576962
39	1	0	-6.645391	4.956914	1.469643
40	6	0	-3.905914	-0.952835	-0.692924
41	6	0	-3.439037	-1.436280	-2.091497
42	6	0	-4.936753	-1.698885	0.047357
43	6	0	-4.431485	-2.368940	-2.738104
44	6	0	-5.678139	-2.599395	-0.650976
45	6	0	-5.461102	-2.903222	-2.059216
46	1	0	-4.235268	-2.631844	-3.780782
47	1	0	-6.481260	-3.131714	-0.132714
48	1	0	-6.148161	-3.599870	-2.546448
49	8	0	-2.188150	-2.130626	-1.935006
50	6	0	-2.186990	-3.243434	-1.054698
51	1	0	-2.323229	-2.932355	-0.006820
52	1	0	-2.964457	-3.980780	-1.318507
53	1	0	-1.205007	-3.722076	-1.155952
54	6	0	-3.133726	-0.241308	-2.988804
55	1	0	-2.728433	-0.606153	-3.943739
56	1	0	-4.044826	0.342193	-3.184047
57	1	0	-2.400935	0.410384	-2.497650
58	7	0	2.162386	-0.147855	0.011303
59	7	0	1.529382	-2.199988	0.415402
60	1	0	-1.038692	-6.715427	1.669532
61	6	0	3.099201	1.875138	3.246768
62	1	0	3.384059	2.937153	3.319868
63	1	0	2.894575	1.513613	4.268523
64	1	0	3.962296	1.322159	2.855110
65	6	0	0.645165	2.430826	2.940056
66	1	0	0.409711	2.045533	3.943447
67	1	0	0.843730	3.508305	3.044727
68	1	0	-0.236502	2.320345	2.294803
69	6	0	3.757035	0.886899	-3.419872
70	1	0	3.969416	1.882149	-3.841977
71	1	0	4.584162	0.643147	-2.732360
72	1	0	3.777131	0.156624	-4.244510
73	6	0	1.257047	1.181653	-3.699478

74	1	0	0.285918	1.126602	-3.195439
75	1	0	1.351456	2.194775	-4.118730
76	1	0	1.278699	0.459983	-4.532458
77	5	0	-1.149849	2.719923	-1.174883
78	9	0	-2.523512	2.740115	-1.392302
79	9	0	-0.469121	3.355195	-2.201420
80	9	0	-0.736188	1.315198	-1.159373
81	9	0	-0.831723	3.259746	0.072461
82	6	0	2.422973	5.547758	-0.807353
83	1	0	2.811270	5.998768	0.123664
84	6	0	3.313831	6.022351	-1.959569
85	1	0	2.923512	5.688242	-2.934135
86	1	0	3.350972	7.122945	-1.987598
87	1	0	4.344600	5.646279	-1.859745
88	6	0	0.970856	6.025276	-0.992492
89	1	0	0.929586	7.124154	-1.076217
90	1	0	0.531424	5.576545	-1.895221
91	1	0	0.339074	5.703904	-0.152145
92	1	0	3.416799	-3.114339	0.033080
93	6	0	4.406739	-0.771782	0.875876
94	6	0	5.384316	0.222456	0.734765
95	6	0	4.383939	-1.540054	2.048179
96	6	0	6.324987	0.443316	1.743156
97	1	0	5.397935	0.835196	-0.169468
98	6	0	5.323267	-1.320396	3.057803
99	1	0	3.627551	-2.314681	2.177898
100	6	0	6.297183	-0.328822	2.907315
101	1	0	7.078822	1.224121	1.620331
102	1	0	5.295190	-1.926862	3.966194
103	1	0	7.031414	-0.157108	3.697672
104	6	0	2.447677	-2.651098	-1.846531
105	6	0	3.466644	-3.136365	-2.676208
106	6	0	1.183006	-2.399502	-2.394456
107	6	0	3.227815	-3.360291	-4.034353
108	1	0	4.458370	-3.334088	-2.258701
109	6	0	0.941268	-2.630547	-3.749530
110	1	0	0.370883	-2.005138	-1.783739
111	6	0	1.962710	-3.108024	-4.574556
112	1	0	4.031804	-3.735463	-4.671966
113	1	0	-0.055712	-2.427218	-4.145099
114	1	0	1.775570	-3.285037	-5.636215
115	1	0	1.987008	-4.615877	-0.526615
116	6	0	-0.871804	-2.214050	2.468749
117	8	0	-2.063284	-1.979336	2.267592
118	7	0	-0.166027	-1.575498	3.435560
119	6	0	-0.858362	-0.552424	4.208918
120	1	0	-1.504968	-1.008746	4.978976
121	1	0	-0.113424	0.084033	4.701663
122	1	0	-1.480469	0.062129	3.547308
123	6	0	1.185246	-1.917340	3.828323
124	1	0	1.886862	-1.097174	3.604667
125	1	0	1.227460	-2.122658	4.911379
126	1	0	1.517957	-2.817955	3.300451
127	6	0	-5.143565	-1.407637	1.504487
128	1	0	-4.192459	-1.503161	2.049072
129	1	0	-5.514816	-0.382861	1.662963
130	1	0	-5.876096	-2.103310	1.937640

IM2, S_a, distal, re

charge = 0, mult =1

Sum of electronic and thermal Free Energies= -4639.930680

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.026856	2.220830	0.672657
2	6	0	-2.829169	0.908040	0.567127
3	1	0	-3.451657	0.928689	-0.338341
4	6	0	-0.588554	0.477040	0.064614
5	6	0	-2.173805	-1.435127	-0.043512
6	6	0	-2.267341	-2.430976	0.944442
7	6	0	-2.570638	-1.678981	-1.379119
8	6	0	-2.786824	-3.679499	0.566363
9	6	0	-3.069810	-2.942454	-1.696456
10	6	0	-3.191977	-3.957005	-0.737534
11	1	0	-2.862251	-4.465699	1.320828
12	1	0	-3.366259	-3.144322	-2.727875
13	6	0	0.363683	2.763432	0.148410
14	6	0	0.960134	3.117540	-1.070342
15	6	0	0.782066	3.353432	1.342182
16	6	0	2.002472	4.053046	-1.069558
17	6	0	1.815219	4.288279	1.326915
18	6	0	2.431182	4.635869	0.122240
19	1	0	2.491940	4.309419	-2.011773
20	1	0	2.160693	4.722685	2.267320
21	6	0	-2.467909	-0.628214	-2.478016
22	1	0	-1.933919	0.240675	-2.071608
23	6	0	-1.794178	-2.232821	2.374443
24	1	0	-1.486885	-1.187060	2.487193
25	29	0	1.157932	-0.316515	-0.403410
26	7	0	3.064578	-0.809600	-0.575673
27	6	0	3.403224	0.247280	0.138997
28	8	0	2.419644	1.038455	0.340114
29	6	0	4.739323	0.571003	0.672723
30	6	0	5.914497	0.145535	0.034280
31	6	0	4.803843	1.332218	1.851346
32	6	0	7.154624	0.484231	0.574684
33	1	0	5.855478	-0.444249	-0.881628
34	6	0	6.049690	1.655508	2.389738
35	1	0	3.872235	1.618879	2.341899
36	6	0	7.222534	1.236168	1.753176
37	1	0	8.071685	0.159104	0.078077
38	1	0	6.105798	2.231828	3.316067
39	1	0	8.196061	1.492337	2.178728
40	6	0	3.683888	-2.033021	-0.794205
41	6	0	4.106374	-2.863580	0.276622
42	6	0	3.791866	-2.451692	-2.146452
43	6	0	4.690651	-4.095262	-0.047462
44	6	0	4.377222	-3.688767	-2.415247
45	6	0	4.829362	-4.505674	-1.373231
46	1	0	5.025419	-4.748307	0.762294
47	1	0	4.474806	-4.020292	-3.452056
48	1	0	5.280087	-5.475431	-1.597990
49	8	0	0.433463	-1.704078	-1.371448
50	6	0	0.591540	-3.008838	-0.925983
51	1	0	-0.203758	-3.327429	-0.233093
52	1	0	0.555566	-3.667404	-1.818254
53	1	0	1.575162	-3.208862	-0.457197
54	6	0	3.927948	-2.453869	1.712309
55	1	0	3.962051	-3.333556	2.370412
56	1	0	4.730663	-1.769481	2.033095
57	1	0	2.977450	-1.928871	1.882038
58	7	0	-1.757644	-0.104626	0.310492
59	7	0	-0.694064	1.805636	0.179491
60	1	0	3.255433	5.352454	0.111523
61	6	0	-2.914045	-2.521604	3.384109

62	1	0	-3.142522	-3.599261	3.430521
63	1	0	-2.600258	-2.204669	4.390312
64	1	0	-3.840965	-1.991140	3.130812
65	6	0	-0.565002	-3.104172	2.680347
66	1	0	-0.197299	-2.878213	3.690816
67	1	0	-0.814403	-4.176746	2.618862
68	1	0	0.256275	-2.890143	1.987350
69	6	0	-3.860420	-0.166022	-2.938208
70	1	0	-4.418913	-0.996017	-3.399301
71	1	0	-4.468612	0.213698	-2.102287
72	1	0	-3.777496	0.637659	-3.688454
73	6	0	-1.628681	-1.115119	-3.667527
74	1	0	-0.624943	-1.392672	-3.321193
75	1	0	-2.094240	-1.981110	-4.164922
76	1	0	-1.535999	-0.313812	-4.417611
77	5	0	0.917592	0.156377	3.194636
78	9	0	2.003552	1.008739	3.359736
79	9	0	-0.244895	0.934253	2.907124
80	9	0	0.689603	-0.623618	4.309141
81	9	0	1.150982	-0.696481	2.062309
82	6	0	-3.718369	-5.330685	-1.115399
83	1	0	-3.756877	-5.925688	-0.187054
84	6	0	-5.143217	-5.263889	-1.683321
85	1	0	-5.170648	-4.697219	-2.628274
86	1	0	-5.529921	-6.274700	-1.891186
87	1	0	-5.829674	-4.771245	-0.977501
88	6	0	-2.762085	-6.043341	-2.084136
89	1	0	-3.113976	-7.064069	-2.305653
90	1	0	-2.688097	-5.499133	-3.039790
91	1	0	-1.748165	-6.111967	-1.660804
92	1	0	-1.920718	2.514252	1.725240
93	6	0	-3.742213	0.620278	1.733536
94	6	0	-5.048568	0.184485	1.477011
95	6	0	-3.332709	0.809929	3.062089
96	6	0	-5.944258	-0.039962	2.525370
97	1	0	-5.366883	0.022474	0.444148
98	6	0	-4.230783	0.594438	4.107913
99	1	0	-2.301534	1.087972	3.282031
100	6	0	-5.538474	0.175453	3.844444
101	1	0	-6.960311	-0.378767	2.310062
102	1	0	-3.899003	0.739769	5.138420
103	1	0	-6.236856	0.005711	4.667444
104	6	0	-2.596909	3.371315	-0.119619
105	6	0	-2.873801	4.590979	0.506448
106	6	0	-2.854094	3.236441	-1.492257
107	6	0	-3.410899	5.657915	-0.220344
108	1	0	-2.667567	4.703432	1.573515
109	6	0	-3.398622	4.295697	-2.217469
110	1	0	-2.622996	2.297523	-1.997232
111	6	0	-3.678672	5.511049	-1.583061
112	1	0	-3.624366	6.604352	0.281708
113	1	0	-3.608603	4.172559	-3.282712
114	1	0	-4.106000	6.340834	-2.150952
115	1	0	0.344965	3.013604	2.279633
116	6	0	0.609406	2.378747	-2.328351
117	8	0	0.768988	1.157352	-2.392085
118	7	0	0.150828	3.102811	-3.387650
119	6	0	-0.082245	2.431661	-4.654244
120	1	0	-1.157229	2.439271	-4.906123
121	1	0	0.465220	2.942574	-5.464162
122	1	0	0.258211	1.393796	-4.574123
123	6	0	-0.144105	4.524279	-3.352424
124	1	0	-1.099532	4.709444	-3.865945
125	1	0	-0.244154	4.876176	-2.320913
126	1	0	0.639871	5.113746	-3.860428

127	6	0	3.263301	-1.561627	-3.236860
128	1	0	2.190284	-1.371167	-3.082455
129	1	0	3.754326	-0.575109	-3.217660
130	1	0	3.417095	-2.012994	-4.227330

$TS_{2\text{-}3}$, S_a, distal, re

charge = 0, mult =1

Sum of electronic and thermal Free Energies= -4639.916344

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.686560	2.536275	0.655988
2	6	0	-2.706860	1.371792	0.652702
3	1	0	-3.396921	1.472280	-0.198862
4	6	0	-0.577458	0.530221	0.086016
5	6	0	-2.447590	-1.054460	-0.001607
6	6	0	-2.739525	-2.040804	0.962022
7	6	0	-2.783754	-1.246099	-1.363563
8	6	0	-3.403369	-3.199657	0.532779
9	6	0	-3.453193	-2.417105	-1.728307
10	6	0	-3.777758	-3.406741	-0.794312
11	1	0	-3.628618	-3.975366	1.268065
12	1	0	-3.706855	-2.569852	-2.779419
13	6	0	0.777526	2.582705	0.205889
14	6	0	1.473824	2.830445	-0.985068
15	6	0	1.288298	3.036904	1.424629
16	6	0	2.692135	3.520219	-0.936638
17	6	0	2.496617	3.729443	1.460292
18	6	0	3.204177	3.968834	0.279673
19	1	0	3.247000	3.691114	-1.862197
20	1	0	2.903100	4.054472	2.420410
21	6	0	-2.396526	-0.263688	-2.461093
22	1	0	-1.817927	0.550235	-2.007823
23	6	0	-2.356022	-1.929209	2.429028
24	1	0	-1.818502	-0.984055	2.565330
25	29	0	1.019238	-0.508178	-0.483053
26	7	0	3.358503	-1.117845	-0.874999
27	6	0	3.618215	-0.166020	0.059643
28	8	0	2.660821	0.541325	0.397889
29	6	0	4.989451	0.120357	0.537179
30	6	0	6.120716	-0.324461	-0.161074
31	6	0	5.128826	0.858383	1.723101
32	6	0	7.394969	-0.024897	0.322312
33	1	0	5.994545	-0.895103	-1.083458
34	6	0	6.405413	1.142170	2.206454
35	1	0	4.225915	1.151919	2.260595
36	6	0	7.536834	0.707122	1.506212
37	1	0	8.279514	-0.362364	-0.222879
38	1	0	6.521228	1.699114	3.139154
39	1	0	8.535278	0.934973	1.887857
40	6	0	3.219929	-2.417382	-0.878391
41	6	0	3.437054	-3.304699	0.257541
42	6	0	2.570668	-2.946977	-2.095290
43	6	0	3.202831	-4.645745	0.073257
44	6	0	2.458898	-4.361192	-2.231360
45	6	0	2.742909	-5.181011	-1.169657
46	1	0	3.376973	-5.330278	0.906881
47	1	0	2.094862	-4.772365	-3.175076
48	1	0	2.620931	-6.262965	-1.264134
49	8	0	0.847091	-2.293286	-1.309195

50	6	0	0.031358	-3.256596	-0.702400
51	1	0	-0.988006	-3.221639	-1.118282
52	1	0	0.427517	-4.270295	-0.901466
53	1	0	-0.006933	-3.121258	0.387325
54	6	0	3.910864	-2.761425	1.571981
55	1	0	3.895309	-3.549132	2.337463
56	1	0	4.937981	-2.371228	1.503686
57	1	0	3.263885	-1.944165	1.922767
58	7	0	-1.837788	0.190431	0.378103
59	7	0	-0.456301	1.866875	0.191153
60	1	0	4.162852	4.491351	0.307535
61	6	0	-3.608012	-1.927849	3.319834
62	1	0	-4.102988	-2.913168	3.303375
63	1	0	-3.330267	-1.712205	4.362400
64	1	0	-4.342409	-1.177502	2.999770
65	6	0	-1.403898	-3.053179	2.866207
66	1	0	-1.137748	-2.915790	3.923226
67	1	0	-1.867219	-4.046302	2.743793
68	1	0	-0.463213	-3.017643	2.305840
69	6	0	-3.629657	0.354245	-3.136498
70	1	0	-4.230930	-0.411551	-3.651691
71	1	0	-4.286053	0.853853	-2.406681
72	1	0	-3.327315	1.100438	-3.889863
73	6	0	-1.462110	-0.927137	-3.484311
74	1	0	-0.571951	-1.332498	-2.984698
75	1	0	-1.970881	-1.746344	-4.017757
76	1	0	-1.132459	-0.191522	-4.233562
77	5	0	1.101100	-0.469939	3.068486
78	9	0	2.395234	0.029649	3.223653
79	9	0	0.194158	0.606082	2.839642
80	9	0	0.696445	-1.181905	4.183600
81	9	0	1.074327	-1.324188	1.920387
82	6	0	-4.465574	-4.692459	-1.219577
83	1	0	-4.667732	-5.267291	-0.299795
84	6	0	-5.811699	-4.427959	-1.907968
85	1	0	-5.676818	-3.874523	-2.851499
86	1	0	-6.320671	-5.375112	-2.149306
87	1	0	-6.477900	-3.833762	-1.263683
88	6	0	-3.541338	-5.543622	-2.104570
89	1	0	-4.015134	-6.505514	-2.359792
90	1	0	-3.308004	-5.022897	-3.047704
91	1	0	-2.587860	-5.752430	-1.595307
92	1	0	-1.530972	2.886679	1.685892
93	6	0	-3.531112	1.309612	1.915508
94	6	0	-4.927646	1.317654	1.833673
95	6	0	-2.916082	1.307017	3.177597
96	6	0	-5.708341	1.335292	2.993747
97	1	0	-5.408249	1.314893	0.851720
98	6	0	-3.695400	1.325260	4.333628
99	1	0	-1.827704	1.257323	3.254132
100	6	0	-5.091870	1.345051	4.246312
101	1	0	-6.798179	1.342689	2.916625
102	1	0	-3.207223	1.311832	5.310774
103	1	0	-5.698057	1.358728	5.155301
104	6	0	-2.057652	3.719085	-0.208060
105	6	0	-2.044316	5.013331	0.323281
106	6	0	-2.411519	3.543561	-1.554230
107	6	0	-2.392210	6.113195	-0.467629
108	1	0	-1.761287	5.159108	1.368623
109	6	0	-2.772515	4.636062	-2.341952
110	1	0	-2.405464	2.544552	-1.989110
111	6	0	-2.764308	5.926381	-1.800532
112	1	0	-2.379372	7.117281	-0.037261
113	1	0	-3.061832	4.480101	-3.384237
114	1	0	-3.047508	6.782856	-2.416977

115	1	0	0.769455	2.769789	2.343962
116	6	0	1.009242	2.234631	-2.282327
117	8	0	1.015688	1.011662	-2.444689
118	7	0	0.628405	3.095961	-3.265298
119	6	0	0.272160	2.573491	-4.571609
120	1	0	-0.801625	2.731946	-4.774379
121	1	0	0.851657	3.083828	-5.359098
122	1	0	0.485587	1.499487	-4.594888
123	6	0	0.560244	4.538944	-3.108171
124	1	0	-0.343567	4.914875	-3.608343
125	1	0	0.494865	4.812434	-2.050058
126	1	0	1.439115	5.037205	-3.554911
127	6	0	2.523360	-2.085678	-3.322458
128	1	0	2.197195	-1.066910	-3.084364
129	1	0	3.529713	-2.026085	-3.771913
130	1	0	1.838574	-2.521489	-4.063197

QI, S_a, distal, re

charge = 0, mult =1

Sum of electronic and thermal Free Energies= -4639.937864

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.464073	2.697469	0.622664
2	6	0	-2.646596	1.700546	0.447042
3	1	0	-3.245132	1.958070	-0.439628
4	6	0	-0.609186	0.551277	0.131798
5	6	0	-2.623650	-0.701512	-0.432967
6	6	0	-3.296757	-1.673710	0.340432
7	6	0	-2.603409	-0.804135	-1.848125
8	6	0	-3.990636	-2.689624	-0.335356
9	6	0	-3.298435	-1.850874	-2.459580
10	6	0	-4.012373	-2.799931	-1.723642
11	1	0	-4.517641	-3.440885	0.256383
12	1	0	-3.270766	-1.930315	-3.548094
13	6	0	1.025598	2.303991	0.636299
14	6	0	1.990857	2.433328	-0.375256
15	6	0	1.346323	2.651242	1.952210
16	6	0	3.269893	2.902005	-0.047583
17	6	0	2.617349	3.129692	2.263359
18	6	0	3.582575	3.256629	1.263152
19	1	0	4.027376	2.977991	-0.830724
20	1	0	2.862281	3.369609	3.299840
21	6	0	-1.823272	0.141583	-2.751739
22	1	0	-1.266927	0.846871	-2.123539
23	6	0	-3.277844	-1.733890	1.859271
24	1	0	-2.596365	-0.959980	2.224595
25	29	0	0.750964	-0.788824	-0.034795
26	7	0	2.666110	-1.385684	0.195620
27	6	0	3.414028	-0.481363	0.982580
28	8	0	3.004756	-0.010332	2.015813
29	6	0	4.709209	-0.040317	0.370592
30	6	0	4.954356	-0.104808	-1.007070
31	6	0	5.662519	0.539903	1.221102
32	6	0	6.147161	0.402965	-1.527849
33	1	0	4.191724	-0.507813	-1.669556
34	6	0	6.859424	1.028588	0.701665
35	1	0	5.434217	0.607256	2.286051
36	6	0	7.102602	0.964154	-0.675999
37	1	0	6.328148	0.365282	-2.604751
38	1	0	7.604545	1.469053	1.368527

39	1	0	8.037474	1.355606	-1.084750
40	6	0	2.822653	-2.661462	0.053493
41	6	0	3.617448	-3.529153	0.918051
42	6	0	2.048981	-3.247758	-1.161065
43	6	0	3.684450	-4.855260	0.603456
44	6	0	2.192634	-4.731552	-1.319150
45	6	0	2.999104	-5.456478	-0.524612
46	1	0	4.244694	-5.518808	1.267809
47	1	0	1.640902	-5.187067	-2.145141
48	1	0	3.122742	-6.529079	-0.692230
49	8	0	0.673413	-2.843690	-1.077934
50	6	0	-0.203767	-3.670493	-0.307458
51	1	0	-1.160063	-3.138729	-0.272061
52	1	0	-0.352385	-4.648142	-0.790916
53	1	0	0.170498	-3.801059	0.717597
54	6	0	4.207758	-2.990023	2.192105
55	1	0	4.647028	-3.806612	2.781542
56	1	0	5.000149	-2.250681	2.001266
57	1	0	3.430669	-2.493914	2.796231
58	7	0	-1.943634	0.414044	0.177211
59	7	0	-0.293963	1.843348	0.341277
60	1	0	4.587982	3.606849	1.504535
61	6	0	-4.676478	-1.483858	2.441830
62	1	0	-5.367635	-2.298888	2.169107
63	1	0	-4.625133	-1.440970	3.539827
64	1	0	-5.109814	-0.540640	2.084737
65	6	0	-2.727780	-3.076876	2.364809
66	1	0	-2.703145	-3.069528	3.462097
67	1	0	-3.348256	-3.924986	2.031632
68	1	0	-1.694750	-3.223810	2.032436
69	6	0	-2.756474	0.953938	-3.662385
70	1	0	-3.303710	0.300825	-4.360284
71	1	0	-3.505218	1.514794	-3.081436
72	1	0	-2.179940	1.674960	-4.265224
73	6	0	-0.773184	-0.628138	-3.565949
74	1	0	-0.119455	-1.204390	-2.899056
75	1	0	-1.248704	-1.325365	-4.274356
76	1	0	-0.146465	0.067251	-4.142089
77	5	0	0.246240	-1.136649	3.281134
78	9	0	1.417383	-1.362697	3.978529
79	9	0	0.069086	0.233866	2.966046
80	9	0	-0.864927	-1.567470	3.998201
81	9	0	0.309034	-1.861693	2.029843
82	6	0	-4.734644	-3.948510	-2.405715
83	1	0	-5.285965	-4.492528	-1.619921
84	6	0	-5.758641	-3.460048	-3.439267
85	1	0	-5.267110	-2.929837	-4.271132
86	1	0	-6.314452	-4.308376	-3.870218
87	1	0	-6.484603	-2.768881	-2.984064
88	6	0	-3.731065	-4.929739	-3.032150
89	1	0	-4.248662	-5.796743	-3.474031
90	1	0	-3.148654	-4.441648	-3.830736
91	1	0	-3.018452	-5.300353	-2.278978
92	1	0	-1.422458	3.020412	1.671845
93	6	0	-3.544319	1.702883	1.660677
94	6	0	-4.876426	2.112595	1.549746
95	6	0	-3.023930	1.373381	2.922882
96	6	0	-5.689965	2.194918	2.684866
97	1	0	-5.280684	2.371035	0.567207
98	6	0	-3.839064	1.446611	4.051383
99	1	0	-1.989478	1.032864	3.022919
100	6	0	-5.171401	1.860938	3.937127
101	1	0	-6.729932	2.515595	2.587480
102	1	0	-3.429815	1.166453	5.024559
103	1	0	-5.805925	1.916581	4.824994

104	6	0	-1.515673	3.929852	-0.250636
105	6	0	-1.345464	5.198813	0.314799
106	6	0	-1.733726	3.829580	-1.632340
107	6	0	-1.408878	6.348782	-0.478939
108	1	0	-1.166804	5.285583	1.389423
109	6	0	-1.812904	4.974194	-2.424859
110	1	0	-1.845356	2.849287	-2.091643
111	6	0	-1.652111	6.239760	-1.849689
112	1	0	-1.277366	7.332187	-0.021539
113	1	0	-1.999463	4.877906	-3.497369
114	1	0	-1.715347	7.137332	-2.469469
115	1	0	0.613075	2.478266	2.737563
116	6	0	1.715258	2.032294	-1.799584
117	8	0	1.710221	0.850457	-2.138213
118	7	0	1.526706	3.052848	-2.685448
119	6	0	1.363783	2.751311	-4.094766
120	1	0	0.359687	3.049557	-4.443464
121	1	0	2.113407	3.294746	-4.694946
122	1	0	1.491051	1.673311	-4.241464
123	6	0	1.578901	4.461171	-2.329039
124	1	0	0.847776	5.013254	-2.934555
125	1	0	1.318652	4.609322	-1.275981
126	1	0	2.581101	4.889084	-2.512037
127	6	0	2.583400	-2.566181	-2.432112
128	1	0	2.383314	-1.486974	-2.369816
129	1	0	3.664265	-2.737269	-2.537670
130	1	0	2.066426	-2.977400	-3.310500

IM2, S_a, distal, si

charge = 0, mult =1

Sum of electronic and thermal Free Energies= -4639.925879

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.126300	-2.123271	0.677751
2	6	0	2.849291	-0.755280	0.695111
3	1	0	3.584260	-0.720338	-0.120703
4	6	0	0.641672	-0.457476	-0.017290
5	6	0	2.094289	1.542367	-0.019544
6	6	0	1.938998	2.590375	0.904183
7	6	0	2.639221	1.763702	-1.303431
8	6	0	2.317861	3.875989	0.498533
9	6	0	3.003616	3.067740	-1.651212
10	6	0	2.842655	4.140530	-0.767893
11	1	0	2.185679	4.704666	1.198161
12	1	0	3.419622	3.250132	-2.644591
13	6	0	-0.124342	-2.798817	-0.230732
14	6	0	-0.708647	-2.936897	-1.501406
15	6	0	-0.462861	-3.687971	0.793335
16	6	0	-1.663841	-3.943504	-1.704602
17	6	0	-1.403510	-4.689862	0.571040
18	6	0	-2.016885	-4.814709	-0.677535
19	1	0	-2.139396	-4.032286	-2.683951
20	1	0	-1.678107	-5.359385	1.388877
21	6	0	2.881400	0.640163	-2.306644
22	1	0	2.467213	-0.286208	-1.890826
23	6	0	1.348994	2.386035	2.284858
24	1	0	1.111986	1.324408	2.396193
25	29	0	-1.178033	0.234935	-0.336576
26	7	0	-3.104064	0.570930	-0.542569

27	6	0	-3.367603	-0.527937	0.142976
28	8	0	-2.348670	-1.291002	0.264986
29	6	0	-4.663180	-0.893476	0.748127
30	6	0	-5.883294	-0.486244	0.185720
31	6	0	-4.643866	-1.661892	1.923632
32	6	0	-7.082541	-0.856112	0.793872
33	1	0	-5.892697	0.113913	-0.724882
34	6	0	-5.849094	-2.015271	2.531097
35	1	0	-3.683414	-1.927573	2.367278
36	6	0	-7.065857	-1.618595	1.967081
37	1	0	-8.033341	-0.545585	0.354685
38	1	0	-5.837150	-2.595699	3.456393
39	1	0	-8.007120	-1.898855	2.446639
40	6	0	-3.793055	1.768720	-0.699436
41	6	0	-4.061236	2.623811	0.397521
42	6	0	-4.153055	2.122562	-2.024900
43	6	0	-4.708373	3.836749	0.132143
44	6	0	-4.803393	3.339960	-2.237446
45	6	0	-5.075164	4.195561	-1.166014
46	1	0	-4.920811	4.513002	0.963860
47	1	0	-5.095646	3.621967	-3.252161
48	1	0	-5.574150	5.151046	-1.345549
49	8	0	-0.650187	1.985058	-0.489233
50	6	0	-0.672115	2.623208	-1.713485
51	1	0	-1.668686	2.636509	-2.194243
52	1	0	-0.400937	3.681944	-1.519535
53	1	0	0.074736	2.233799	-2.427534
54	6	0	-3.682928	2.233792	1.797256
55	1	0	-3.724286	3.102360	2.469001
56	1	0	-4.374834	1.471290	2.192948
57	1	0	-2.677876	1.797049	1.851894
58	7	0	1.747793	0.188565	0.336984
59	7	0	0.840565	-1.783109	0.024740
60	1	0	-2.771398	-5.585191	-0.849693
61	6	0	2.348982	2.767802	3.384852
62	1	0	2.517459	3.857492	3.413479
63	1	0	1.953396	2.458152	4.363971
64	1	0	3.321908	2.278853	3.240075
65	6	0	0.029894	3.154554	2.453115
66	1	0	-0.457095	2.840856	3.387679
67	1	0	0.204812	4.243367	2.495799
68	1	0	-0.647070	2.941176	1.617198
69	6	0	4.386633	0.417567	-2.528879
70	1	0	4.845168	1.286287	-3.027138
71	1	0	4.919758	0.267302	-1.577701
72	1	0	4.562806	-0.468120	-3.160705
73	6	0	2.158006	0.862660	-3.640907
74	1	0	1.069529	0.840908	-3.499205
75	1	0	2.435521	1.822996	-4.102096
76	1	0	2.423803	0.064971	-4.352780
77	5	0	-0.854019	-0.528435	3.237720
78	9	0	0.013584	-1.567751	2.793981
79	9	0	-1.091637	0.335810	2.122555
80	9	0	-0.214577	0.195476	4.233717
81	9	0	-2.056097	-1.071316	3.665217
82	6	0	3.204085	5.557196	-1.180591
83	1	0	3.043602	6.198578	-0.297416
84	6	0	4.680157	5.683465	-1.583124
85	1	0	4.903495	5.082999	-2.480086
86	1	0	4.935064	6.730538	-1.813701
87	1	0	5.343309	5.337768	-0.775231
88	6	0	2.274811	6.062302	-2.295143
89	1	0	2.496812	7.111548	-2.549387
90	1	0	2.394366	5.462155	-3.212103
91	1	0	1.218945	5.997889	-1.989872

92	1	0	1.907628	-2.428834	1.708424
93	6	0	3.568012	-0.423375	1.978788
94	6	0	4.887316	0.043616	1.919487
95	6	0	2.949295	-0.578598	3.228386
96	6	0	5.590919	0.337699	3.090161
97	1	0	5.367847	0.176538	0.946895
98	6	0	3.654014	-0.286005	4.396238
99	1	0	1.910164	-0.900328	3.296128
100	6	0	4.975324	0.166730	4.332585
101	1	0	6.619874	0.700098	3.030397
102	1	0	3.153437	-0.397314	5.360419
103	1	0	5.521546	0.397476	5.250445
104	6	0	2.890761	-3.207796	-0.035170
105	6	0	3.530359	-4.209423	0.702639
106	6	0	3.010075	-3.208471	-1.432578
107	6	0	4.285227	-5.193627	0.058085
108	1	0	3.435966	-4.214486	1.791259
109	6	0	3.758862	-4.192636	-2.078502
110	1	0	2.505690	-2.435927	-2.016420
111	6	0	4.400603	-5.188077	-1.333792
112	1	0	4.781175	-5.969282	0.646104
113	1	0	3.844063	-4.184175	-3.167830
114	1	0	4.987870	-5.958318	-1.839126
115	1	0	-0.036883	-3.539583	1.782792
116	6	0	-0.460016	-1.974896	-2.627673
117	8	0	-0.745613	-0.777275	-2.521783
118	7	0	0.015166	-2.496986	-3.794018
119	6	0	0.010843	-1.689196	-5.001870
120	1	0	1.037282	-1.520460	-5.365976
121	1	0	-0.556171	-2.205756	-5.794996
122	1	0	-0.454768	-0.722055	-4.787405
123	6	0	0.525763	-3.849177	-3.946029
124	1	0	1.482950	-3.814679	-4.491739
125	1	0	0.703316	-4.311948	-2.970671
126	1	0	-0.171728	-4.482596	-4.521608
127	6	0	-3.869263	1.165521	-3.152639
128	1	0	-2.824042	0.821625	-3.139932
129	1	0	-4.486447	0.255368	-3.058980
130	1	0	-4.087586	1.626296	-4.126712

$TS_{2\text{-}3}$, S_a, distal, si

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4639.918161

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.894874	-2.411272	0.394659
2	6	0	2.813627	-1.168461	0.372193
3	1	0	3.409272	-1.178816	-0.555468
4	6	0	0.610349	-0.504580	-0.101842
5	6	0	2.268053	1.285818	0.078111
6	6	0	2.277804	2.157481	1.182238
7	6	0	2.723761	1.697952	-1.192590
8	6	0	2.778755	3.452017	0.985860
9	6	0	3.211080	3.000517	-1.331507
10	6	0	3.251512	3.892036	-0.252395
11	1	0	2.785614	4.145715	1.829853
12	1	0	3.554528	3.332766	-2.313754
13	6	0	-0.537518	-2.655580	-0.279215
14	6	0	-1.250715	-2.670619	-1.489757

15	6	0	-0.985007	-3.418187	0.803066
16	6	0	-2.418373	-3.438624	-1.587927
17	6	0	-2.147648	-4.177149	0.691360
18	6	0	-2.870428	-4.187868	-0.503320
19	1	0	-2.983241	-3.430978	-2.523370
20	1	0	-2.505054	-4.734888	1.559169
21	6	0	2.664798	0.788465	-2.413614
22	1	0	2.273432	-0.186696	-2.095897
23	6	0	1.699761	1.766015	2.528633
24	1	0	1.433983	0.703907	2.483386
25	29	0	-1.071475	0.452122	-0.467006
26	7	0	-3.755491	0.921259	-0.855563
27	6	0	-3.714925	-0.087265	0.052758
28	8	0	-2.675398	-0.749455	0.167143
29	6	0	-4.928775	-0.459671	0.817323
30	6	0	-6.205861	-0.012166	0.448403
31	6	0	-4.754381	-1.261188	1.958482
32	6	0	-7.314186	-0.373774	1.214511
33	1	0	-6.322987	0.607757	-0.442843
34	6	0	-5.867688	-1.607292	2.724256
35	1	0	-3.746275	-1.566336	2.250279
36	6	0	-7.144345	-1.170851	2.352369
37	1	0	-8.312144	-0.035238	0.926149
38	1	0	-5.734619	-2.214505	3.622469
39	1	0	-8.012711	-1.447879	2.955586
40	6	0	-3.595346	2.213250	-0.827309
41	6	0	-3.235151	2.974653	0.375899
42	6	0	-3.652918	2.911740	-2.110968
43	6	0	-3.194850	4.380588	0.281158
44	6	0	-3.532676	4.277057	-2.134282
45	6	0	-3.321550	5.018728	-0.936471
46	1	0	-3.006716	4.957969	1.188370
47	1	0	-3.583924	4.807269	-3.088254
48	1	0	-3.256625	6.108235	-0.988862
49	8	0	-1.206509	2.354324	-0.333607
50	6	0	-0.476785	3.324230	-0.993182
51	1	0	-0.382294	3.134250	-2.079249
52	1	0	-0.973414	4.313047	-0.879452
53	1	0	0.528753	3.433554	-0.550871
54	6	0	-3.205924	2.314634	1.714928
55	1	0	-2.862715	3.019102	2.483385
56	1	0	-4.215780	1.968131	1.991746
57	1	0	-2.538610	1.442867	1.750751
58	7	0	1.821223	-0.064938	0.236603
59	7	0	0.630538	-1.850156	-0.135910
60	1	0	-3.792051	-4.767885	-0.587354
61	6	0	2.701339	1.961407	3.673362
62	1	0	2.894687	3.030322	3.864340
63	1	0	2.291300	1.524732	4.596957
64	1	0	3.662622	1.473700	3.461157
65	6	0	0.398974	2.542343	2.791871
66	1	0	-0.097912	2.135377	3.683748
67	1	0	0.607318	3.614754	2.951054
68	1	0	-0.288380	2.441108	1.943518
69	6	0	4.057679	0.550397	-3.014264
70	1	0	4.491195	1.482021	-3.411298
71	1	0	4.756723	0.154648	-2.260966
72	1	0	4.005395	-0.173228	-3.843975
73	6	0	1.677539	1.325968	-3.459690
74	1	0	0.657039	1.341007	-3.053687
75	1	0	1.946328	2.344390	-3.781605
76	1	0	1.674449	0.680915	-4.352471
77	5	0	-0.804598	-0.961853	3.305098
78	9	0	0.365300	-1.699823	2.931103
79	9	0	-1.061487	-0.023451	2.278281

80	9	0	-0.568833	-0.300160	4.497228
81	9	0	-1.877598	-1.853943	3.400552
82	6	0	3.741174	5.318673	-0.433366
83	1	0	3.759216	5.780440	0.568431
84	6	0	5.167149	5.378024	-0.997658
85	1	0	5.214223	4.957129	-2.015208
86	1	0	5.522144	6.419702	-1.054094
87	1	0	5.867994	4.809359	-0.367322
88	6	0	2.761576	6.127637	-1.298478
89	1	0	3.080573	7.179638	-1.378444
90	1	0	2.703407	5.715216	-2.319160
91	1	0	1.746649	6.106185	-0.872059
92	1	0	1.719776	-2.725182	1.430752
93	6	0	3.779551	-1.021532	1.522560
94	6	0	5.080705	-0.575882	1.252785
95	6	0	3.417222	-1.307970	2.846985
96	6	0	6.013581	-0.427588	2.281286
97	1	0	5.363920	-0.341626	0.223414
98	6	0	4.354438	-1.171362	3.872770
99	1	0	2.395068	-1.601797	3.087019
100	6	0	5.652798	-0.734045	3.595786
101	1	0	7.023387	-0.077418	2.054406
102	1	0	4.057978	-1.392796	4.900558
103	1	0	6.380105	-0.624587	4.403984
104	6	0	2.417215	-3.568282	-0.417027
105	6	0	2.791622	-4.758463	0.215303
106	6	0	2.565256	-3.460232	-1.807805
107	6	0	3.314068	-5.823179	-0.524815
108	1	0	2.673492	-4.847366	1.297878
109	6	0	3.088936	-4.520122	-2.548415
110	1	0	2.257341	-2.540610	-2.311100
111	6	0	3.465628	-5.705867	-1.908145
112	1	0	3.603243	-6.746780	-0.018011
113	1	0	3.207131	-4.422978	-3.630541
114	1	0	3.875997	-6.535883	-2.488115
115	1	0	-0.458325	-3.351970	1.752700
116	6	0	-0.888369	-1.785856	-2.649647
117	8	0	-1.054602	-0.561498	-2.592902
118	7	0	-0.431736	-2.395106	-3.777824
119	6	0	-0.216553	-1.612398	-4.982087
120	1	0	0.844466	-1.647122	-5.282716
121	1	0	-0.822510	-2.014621	-5.811903
122	1	0	-0.501557	-0.573314	-4.789020
123	6	0	-0.195535	-3.823902	-3.898796
124	1	0	0.759808	-3.992282	-4.419183
125	1	0	-0.133205	-4.292664	-2.912232
126	1	0	-0.995967	-4.314611	-4.480519
127	6	0	-3.809346	2.081519	-3.346560
128	1	0	-2.986701	1.349054	-3.407312
129	1	0	-4.737785	1.489573	-3.313898
130	1	0	-3.813215	2.706413	-4.250577

QI, S_a, distal, si

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4639.947926

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.236105	-0.714823	-0.620031
2	6	0	-3.108931	0.836345	-0.601752

3	1	0	-3.684062	1.252261	0.238600
4	6	0	-1.009713	-0.121862	-0.096565
5	6	0	-1.104335	2.301708	0.019935
6	6	0	-0.415752	3.058863	-0.946889
7	6	0	-1.214948	2.750388	1.356538
8	6	0	0.152954	4.275106	-0.545865
9	6	0	-0.640557	3.979399	1.696656
10	6	0	0.054677	4.754720	0.761561
11	1	0	0.703531	4.865127	-1.282960
12	1	0	-0.717975	4.325123	2.729058
13	6	0	-1.486249	-2.495917	-0.120421
14	6	0	-1.337244	-3.140677	1.120563
15	6	0	-1.207227	-3.174496	-1.308729
16	6	0	-0.849418	-4.454650	1.141946
17	6	0	-0.729336	-4.484133	-1.271205
18	6	0	-0.538050	-5.121851	-0.043563
19	1	0	-0.703714	-4.951576	2.103455
20	1	0	-0.473749	-4.983480	-2.207331
21	6	0	-1.912502	1.928601	2.431862
22	1	0	-2.119620	0.936701	2.014430
23	6	0	-0.226273	2.582499	-2.374746
24	1	0	-0.733213	1.617928	-2.476206
25	29	0	0.862545	-0.472754	0.091976
26	7	0	4.438245	-1.044369	1.216893
27	6	0	3.406671	-1.796766	0.725938
28	8	0	2.232651	-1.592928	1.064562
29	6	0	3.777308	-2.930838	-0.155318
30	6	0	5.110125	-3.351995	-0.301404
31	6	0	2.762425	-3.544647	-0.906128
32	6	0	5.421090	-4.377291	-1.192569
33	1	0	5.890879	-2.873937	0.292228
34	6	0	3.081349	-4.553793	-1.811007
35	1	0	1.737942	-3.196569	-0.809073
36	6	0	4.407376	-4.974053	-1.952325
37	1	0	6.455899	-4.710096	-1.302019
38	1	0	2.291349	-4.990032	-2.424029
39	1	0	4.656249	-5.764438	-2.664942
40	6	0	4.762783	0.182705	1.031757
41	6	0	4.050558	1.068927	-0.021161
42	6	0	5.868633	0.731488	1.825831
43	6	0	4.575481	2.480962	-0.077600
44	6	0	6.250957	2.021257	1.627485
45	6	0	5.606968	2.906144	0.670245
46	1	0	4.059916	3.135322	-0.785007
47	1	0	7.073216	2.425059	2.225004
48	1	0	5.973381	3.931621	0.581410
49	8	0	2.643371	1.117295	0.261718
50	6	0	2.297386	1.686869	1.520582
51	1	0	2.549865	1.001136	2.346660
52	1	0	2.795341	2.656825	1.673673
53	1	0	1.214339	1.844211	1.501204
54	6	0	4.231516	0.433432	-1.405432
55	1	0	3.779660	1.071449	-2.174632
56	1	0	5.303221	0.313627	-1.618840
57	1	0	3.731275	-0.538901	-1.465493
58	7	0	-1.662312	1.026652	-0.322991
59	7	0	-1.893291	-1.131292	-0.178612
60	1	0	-0.135654	-6.136651	-0.006352
61	6	0	-0.844098	3.561069	-3.381210
62	1	0	-0.315092	4.528793	-3.378309
63	1	0	-0.778356	3.148050	-4.399607
64	1	0	-1.903920	3.752233	-3.160379
65	6	0	1.255285	2.319764	-2.671783
66	1	0	1.371860	1.838439	-3.652761
67	1	0	1.842295	3.254882	-2.661408

68	1	0	1.670745	1.640401	-1.920076
69	6	0	-3.246738	2.571102	2.841601
70	1	0	-3.085757	3.554761	3.311700
71	1	0	-3.906323	2.725950	1.973280
72	1	0	-3.781274	1.935321	3.566220
73	6	0	-1.015702	1.676986	3.651165
74	1	0	-0.103075	1.141086	3.358018
75	1	0	-0.735503	2.614429	4.158143
76	1	0	-1.542057	1.041611	4.379352
77	5	0	0.895514	-1.234903	-3.180180
78	9	0	-0.421377	-0.731835	-3.031379
79	9	0	1.589436	-0.992395	-1.930501
80	9	0	1.560501	-0.571544	-4.187689
81	9	0	0.854085	-2.609707	-3.384630
82	6	0	0.758609	6.041792	1.159038
83	1	0	0.978205	6.586726	0.224821
84	6	0	-0.104083	6.956142	2.036862
85	1	0	-0.304208	6.502537	3.020930
86	1	0	0.407354	7.914964	2.217909
87	1	0	-1.073866	7.168166	1.560976
88	6	0	2.103808	5.727219	1.835820
89	1	0	2.647887	6.652553	2.086654
90	1	0	1.947271	5.161661	2.769168
91	1	0	2.745298	5.117694	1.180729
92	1	0	-3.386988	-1.060126	-1.654090
93	6	0	-3.578418	1.506853	-1.871857
94	6	0	-4.446282	2.601977	-1.801238
95	6	0	-3.157584	1.046309	-3.129479
96	6	0	-4.902365	3.226065	-2.966473
97	1	0	-4.770111	2.967884	-0.823251
98	6	0	-3.614515	1.666966	-4.291746
99	1	0	-2.442769	0.224235	-3.203652
100	6	0	-4.490731	2.754982	-4.214730
101	1	0	-5.581164	4.079418	-2.897043
102	1	0	-3.272649	1.305374	-5.264159
103	1	0	-4.844933	3.239579	-5.127739
104	6	0	-4.354115	-1.270444	0.232476
105	6	0	-5.308345	-2.123105	-0.334435
106	6	0	-4.468591	-0.933921	1.589913
107	6	0	-6.368718	-2.619358	0.430410
108	1	0	-5.222289	-2.394565	-1.389622
109	6	0	-5.532815	-1.415525	2.351582
110	1	0	-3.718427	-0.292687	2.053188
111	6	0	-6.487874	-2.259708	1.774243
112	1	0	-7.106943	-3.281057	-0.028678
113	1	0	-5.618244	-1.130998	3.403029
114	1	0	-7.321902	-2.635344	2.371881
115	1	0	-1.296557	-2.643898	-2.254156
116	6	0	-1.617163	-2.421652	2.413655
117	8	0	-1.052387	-1.372644	2.699594
118	7	0	-2.497092	-3.032462	3.271217
119	6	0	-2.674262	-2.475103	4.597266
120	1	0	-3.637664	-1.940138	4.680227
121	1	0	-2.664012	-3.280780	5.350148
122	1	0	-1.861370	-1.768555	4.798870
123	6	0	-3.399711	-4.110117	2.908840
124	1	0	-4.419250	-3.858434	3.240266
125	1	0	-3.429112	-4.244977	1.822772
126	1	0	-3.107224	-5.066079	3.378973
127	6	0	6.514084	-0.168353	2.837342
128	1	0	5.772982	-0.531922	3.566916
129	1	0	6.928211	-1.067323	2.352883
130	1	0	7.319984	0.350258	3.375186

IM2, S_a, proximal, re

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4639.921104

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.037800	0.372144	-0.693824
2	6	0	-2.311966	1.663189	-0.281680
3	1	0	-2.605871	1.946694	0.741400
4	6	0	-0.830023	-0.128990	-0.166527
5	6	0	0.060168	2.100606	0.415658
6	6	0	0.823062	2.967926	-0.385805
7	6	0	0.189715	2.087551	1.821648
8	6	0	1.699360	3.848904	0.262156
9	6	0	1.089720	2.979488	2.410667
10	6	0	1.850617	3.873524	1.649534
11	1	0	2.303538	4.527110	-0.345098
12	1	0	1.205138	2.966436	3.496575
13	6	0	-2.360313	-2.044419	-0.554678
14	6	0	-2.909053	-2.818630	0.482071
15	6	0	-2.174567	-2.584405	-1.828766
16	6	0	-3.183142	-4.172124	0.228009
17	6	0	-2.461350	-3.927641	-2.061933
18	6	0	-2.951036	-4.729638	-1.028127
19	1	0	-3.563839	-4.797827	1.037152
20	1	0	-2.274548	-4.347761	-3.052359
21	6	0	-0.547122	1.090677	2.704719
22	1	0	-1.267577	0.528128	2.101860
23	6	0	0.795843	2.938757	-1.903970
24	1	0	0.049893	2.196388	-2.210655
25	29	0	0.924623	-1.044995	-0.124703
26	7	0	2.791826	-1.633020	-0.019749
27	6	0	3.205580	-0.390286	0.067587
28	8	0	2.226038	0.442202	0.141411
29	6	0	4.590148	0.121662	0.053211
30	6	0	5.704384	-0.687019	-0.224792
31	6	0	4.764763	1.493310	0.307512
32	6	0	6.981589	-0.125669	-0.234204
33	1	0	5.573353	-1.746945	-0.441528
34	6	0	6.044332	2.045195	0.300520
35	1	0	3.882216	2.104376	0.500021
36	6	0	7.153942	1.236535	0.032057
37	1	0	7.846967	-0.754442	-0.454775
38	1	0	6.177138	3.110818	0.500699
39	1	0	8.156884	1.670234	0.024183
40	6	0	3.391019	-2.886704	0.010108
41	6	0	3.956175	-3.356386	1.222927
42	6	0	3.346924	-3.690376	-1.155718
43	6	0	4.526859	-4.632034	1.234028
44	6	0	3.927390	-4.962057	-1.090532
45	6	0	4.514142	-5.430193	0.087058
46	1	0	4.977599	-5.006535	2.156552
47	1	0	3.914191	-5.594039	-1.981849
48	1	0	4.958861	-6.427940	0.114441
49	8	0	0.224294	-2.732898	-0.135020
50	6	0	0.281562	-3.411214	1.077425
51	1	0	-0.317078	-2.928710	1.869764
52	1	0	-0.166900	-4.408333	0.890141
53	1	0	1.314543	-3.592067	1.433593
54	6	0	3.951025	-2.488629	2.452411
55	1	0	4.218625	-3.070525	3.345441
56	1	0	4.671377	-1.658385	2.364247

57	1	0	2.962827	-2.031424	2.616249
58	7	0	-0.896135	1.206053	-0.184587
59	7	0	-2.037642	-0.666608	-0.335202
60	1	0	-3.153451	-5.789584	-1.198345
61	6	0	0.403137	4.304692	-2.484263
62	1	0	1.197685	5.050183	-2.314326
63	1	0	0.251435	4.224623	-3.571466
64	1	0	-0.522041	4.691378	-2.037578
65	6	0	2.146344	2.480779	-2.478356
66	1	0	2.064977	2.369403	-3.568903
67	1	0	2.942234	3.210804	-2.254363
68	1	0	2.432767	1.507382	-2.068664
69	6	0	-1.352673	1.768799	3.820427
70	1	0	-0.704198	2.290136	4.542703
71	1	0	-2.055412	2.511704	3.409504
72	1	0	-1.934232	1.015042	4.374511
73	6	0	0.424648	0.042945	3.269279
74	1	0	0.962779	-0.463678	2.453840
75	1	0	1.179433	0.505172	3.925745
76	1	0	-0.127505	-0.720891	3.834997
77	5	0	0.234798	-0.486839	-3.487766
78	9	0	0.789242	0.300628	-4.467904
79	9	0	-1.026804	0.045664	-3.084969
80	9	0	1.084059	-0.472131	-2.323744
81	9	0	0.063444	-1.806666	-3.885482
82	6	0	2.812750	4.847434	2.309420
83	1	0	3.359632	5.356216	1.496921
84	6	0	2.054475	5.923453	3.101868
85	1	0	1.486884	5.473048	3.932603
86	1	0	2.751039	6.661864	3.531423
87	1	0	1.338250	6.457866	2.459038
88	6	0	3.848533	4.134755	3.191076
89	1	0	4.576766	4.855237	3.597347
90	1	0	3.368938	3.632491	4.046663
91	1	0	4.401007	3.369705	2.625038
92	1	0	-3.135102	0.332139	-1.788156
93	6	0	-2.590350	2.843359	-1.177856
94	6	0	-2.951554	4.064916	-0.596310
95	6	0	-2.552003	2.734795	-2.576541
96	6	0	-3.287310	5.162309	-1.393388
97	1	0	-2.974238	4.153719	0.492834
98	6	0	-2.891877	3.829659	-3.371274
99	1	0	-2.223573	1.805543	-3.043761
100	6	0	-3.265659	5.042902	-2.784652
101	1	0	-3.568815	6.108894	-0.926198
102	1	0	-2.851890	3.736449	-4.458886
103	1	0	-3.529899	5.897394	-3.412266
104	6	0	-4.404655	0.214606	-0.074669
105	6	0	-5.498641	-0.082615	-0.896904
106	6	0	-4.624933	0.431896	1.294170
107	6	0	-6.792882	-0.140079	-0.372425
108	1	0	-5.332081	-0.254180	-1.962980
109	6	0	-5.917429	0.390108	1.816921
110	1	0	-3.782088	0.631960	1.957551
111	6	0	-7.006118	0.108541	0.984990
112	1	0	-7.636166	-0.364804	-1.029437
113	1	0	-6.077206	0.581083	2.880699
114	1	0	-8.018237	0.082534	1.395890
115	1	0	-1.754977	-1.963033	-2.616305
116	6	0	-3.078030	-2.274350	1.872558
117	8	0	-2.174391	-1.649015	2.425352
118	7	0	-4.248294	-2.566132	2.520577
119	6	0	-4.362857	-2.235809	3.928171
120	1	0	-4.969440	-1.324401	4.076284
121	1	0	-4.849819	-3.064486	4.467776

122	1	0	-3.363127	-2.060692	4.340157
123	6	0	-5.472817	-3.008417	1.875395
124	1	0	-6.311991	-2.396884	2.239394
125	1	0	-5.412421	-2.874692	0.790540
126	1	0	-5.695194	-4.067372	2.095727
127	6	0	2.690793	-3.182138	-2.405772
128	1	0	1.599895	-3.120894	-2.281990
129	1	0	3.014689	-2.160199	-2.649995
130	1	0	2.906992	-3.837778	-3.260412

$TS_{2\text{-}3}$, S_a, proximal, re

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4639.913874

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.954179	0.695916	-0.656424
2	6	0	-2.130648	1.882720	-0.122105
3	1	0	-2.411369	2.093097	0.923058
4	6	0	-0.798372	-0.033716	-0.160378
5	6	0	0.295711	2.006443	0.594258
6	6	0	1.156247	2.864550	-0.113720
7	6	0	0.453300	1.788248	1.982568
8	6	0	2.161568	3.522466	0.608240
9	6	0	1.486144	2.456525	2.644508
10	6	0	2.350607	3.331017	1.976795
11	1	0	2.840390	4.189637	0.071403
12	1	0	1.622935	2.280617	3.713873
13	6	0	-2.435162	-1.789410	-0.651093
14	6	0	-3.229546	-2.535066	0.242202
15	6	0	-2.012034	-2.352755	-1.856897
16	6	0	-3.575396	-3.850027	-0.105605
17	6	0	-2.352433	-3.667418	-2.176095
18	6	0	-3.139143	-4.418766	-1.302065
19	1	0	-4.157902	-4.448960	0.596330
20	1	0	-1.994432	-4.093485	-3.115691
21	6	0	-0.413834	0.813628	2.769454
22	1	0	-1.207359	0.422761	2.124113
23	6	0	1.087195	3.057800	-1.618570
24	1	0	0.270861	2.431752	-1.997048
25	29	0	0.888581	-1.055260	-0.309472
26	7	0	2.934762	-1.813661	-0.594886
27	6	0	3.417792	-0.606862	-0.237461
28	8	0	2.570269	0.253864	0.080271
29	6	0	4.850345	-0.250600	-0.361640
30	6	0	5.811534	-1.168245	-0.810507
31	6	0	5.230552	1.057866	-0.023127
32	6	0	7.149747	-0.784250	-0.898451
33	1	0	5.505388	-2.176388	-1.095013
34	6	0	6.569137	1.436235	-0.111226
35	1	0	4.456843	1.755473	0.300520
36	6	0	7.529362	0.515493	-0.545768
37	1	0	7.899163	-1.497179	-1.249359
38	1	0	6.866179	2.453075	0.155347
39	1	0	8.578090	0.813999	-0.617314
40	6	0	2.985567	-3.046265	-0.092476
41	6	0	3.460398	-3.365443	1.234635
42	6	0	2.283210	-4.056130	-0.865642
43	6	0	3.321493	-4.663752	1.685039
44	6	0	2.195018	-5.365039	-0.348327

45	6	0	2.699435	-5.665567	0.901106
46	1	0	3.680956	-4.918224	2.685227
47	1	0	1.699307	-6.133093	-0.945580
48	1	0	2.612201	-6.679184	1.299526
49	8	0	0.568437	-2.888667	0.084894
50	6	0	-0.196113	-3.512174	1.058038
51	1	0	-0.798037	-2.781356	1.626627
52	1	0	-0.886732	-4.258334	0.624903
53	1	0	0.463372	-4.023264	1.791545
54	6	0	4.033997	-2.302549	2.129365
55	1	0	4.208391	-2.703290	3.137313
56	1	0	4.988718	-1.906572	1.752497
57	1	0	3.345957	-1.447045	2.221705
58	7	0	-0.763594	1.303419	-0.081768
59	7	0	-2.058620	-0.447981	-0.340738
60	1	0	-3.404636	-5.450941	-1.542077
61	6	0	0.796018	4.522149	-1.976799
62	1	0	1.645340	5.170602	-1.704335
63	1	0	0.634038	4.624006	-3.060730
64	1	0	-0.096170	4.901670	-1.461466
65	6	0	2.374450	2.580660	-2.309183
66	1	0	2.251510	2.633261	-3.400298
67	1	0	3.237848	3.203942	-2.022075
68	1	0	2.589755	1.538479	-2.053853
69	6	0	-1.115916	1.483576	3.958329
70	1	0	-0.399614	1.835796	4.718047
71	1	0	-1.707028	2.354451	3.631636
72	1	0	-1.797891	0.767253	4.443198
73	6	0	0.399527	-0.411467	3.213997
74	1	0	0.851376	-0.912290	2.344625
75	1	0	1.213240	-0.129159	3.901692
76	1	0	-0.254847	-1.138079	3.717618
77	5	0	0.280641	-0.171917	-3.547016
78	9	0	0.878931	0.672141	-4.447585
79	9	0	-0.946783	0.373872	-3.085034
80	9	0	1.136683	-0.327014	-2.392590
81	9	0	0.048039	-1.444150	-4.066242
82	6	0	3.469204	4.045439	2.716841
83	1	0	4.039059	4.615406	1.962743
84	6	0	2.913728	5.052025	3.735672
85	1	0	2.335014	4.539611	4.521541
86	1	0	3.729341	5.607019	4.227427
87	1	0	2.245478	5.779522	3.249843
88	6	0	4.439083	3.057693	3.382560
89	1	0	5.278630	3.592290	3.856003
90	1	0	3.934655	2.471229	4.167452
91	1	0	4.852538	2.346798	2.651234
92	1	0	-2.994789	0.745392	-1.754252
93	6	0	-2.316738	3.154291	-0.911523
94	6	0	-2.630682	4.337867	-0.233094
95	6	0	-2.237645	3.168439	-2.312766
96	6	0	-2.873480	5.520743	-0.936750
97	1	0	-2.689324	4.330141	0.858373
98	6	0	-2.483246	4.348646	-3.014437
99	1	0	-1.953518	2.264208	-2.853040
100	6	0	-2.805972	5.525752	-2.331424
101	1	0	-3.117746	6.436933	-0.393968
102	1	0	-2.410814	4.350172	-4.104435
103	1	0	-2.996273	6.447631	-2.886293
104	6	0	-4.366290	0.653802	-0.126852
105	6	0	-5.427930	0.537272	-1.033686
106	6	0	-4.657622	0.836307	1.233776
107	6	0	-6.753986	0.621576	-0.600493
108	1	0	-5.207304	0.400762	-2.095083
109	6	0	-5.979897	0.936620	1.666656

110	1	0	-3.846551	0.897540	1.960849
111	6	0	-7.032595	0.834755	0.751007
112	1	0	-7.568542	0.538081	-1.323618
113	1	0	-6.191121	1.101910	2.725783
114	1	0	-8.067016	0.922396	1.092025
115	1	0	-1.406582	-1.768462	-2.544059
116	6	0	-3.526359	-2.050276	1.635721
117	8	0	-2.631332	-1.574904	2.332876
118	7	0	-4.787544	-2.258783	2.121733
119	6	0	-5.039323	-2.030694	3.531456
120	1	0	-5.614099	-1.100939	3.686807
121	1	0	-5.621352	-2.869181	3.948756
122	1	0	-4.082002	-1.944753	4.056914
123	6	0	-5.958760	-2.526678	1.306076
124	1	0	-6.767876	-1.841807	1.600970
125	1	0	-5.744168	-2.349139	0.247387
126	1	0	-6.318517	-3.563265	1.431985
127	6	0	1.856069	-3.766290	-2.270918
128	1	0	1.478588	-2.747348	-2.403841
129	1	0	2.720406	-3.876563	-2.950066
130	1	0	1.081322	-4.475881	-2.592065

QI, S_a, proximal, re

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4639.956517

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.958612	0.916376	-0.657648
2	6	0	-2.089264	2.079681	-0.112963
3	1	0	-2.400937	2.334830	0.911992
4	6	0	-0.803091	0.116323	-0.192389
5	6	0	0.334312	2.035332	0.706223
6	6	0	1.314615	2.808812	0.054712
7	6	0	0.421975	1.752915	2.089253
8	6	0	2.386662	3.284219	0.819865
9	6	0	1.512639	2.259325	2.801587
10	6	0	2.512045	3.016604	2.185044
11	1	0	3.171906	3.857788	0.321551
12	1	0	1.595841	2.021822	3.862440
13	6	0	-2.403610	-1.563173	-0.874683
14	6	0	-3.112227	-2.460539	-0.055832
15	6	0	-1.959426	-1.960257	-2.137681
16	6	0	-3.318236	-3.769355	-0.519772
17	6	0	-2.161182	-3.267236	-2.578430
18	6	0	-2.836018	-4.178169	-1.763777
19	1	0	-3.842766	-4.481131	0.121413
20	1	0	-1.771840	-3.559834	-3.555636
21	6	0	-0.595570	0.888533	2.822397
22	1	0	-1.292269	0.458071	2.095374
23	6	0	1.274391	3.104947	-1.433687
24	1	0	0.421548	2.561870	-1.854039
25	29	0	0.769231	-0.998218	-0.220855
26	7	0	2.492127	-1.859102	0.343032
27	6	0	3.341119	-0.878136	0.929088
28	8	0	3.293285	-0.669953	2.124931
29	6	0	4.198881	-0.113934	-0.013621
30	6	0	4.307904	-0.453456	-1.370805
31	6	0	4.955765	0.950405	0.501946
32	6	0	5.170573	0.262022	-2.200664

33	1	0	3.685245	-1.240088	-1.790740
34	6	0	5.814272	1.663365	-0.329833
35	1	0	4.854127	1.199566	1.556829
36	6	0	5.924539	1.317824	-1.682255
37	1	0	5.228584	0.010628	-3.261269
38	1	0	6.397117	2.494959	0.073040
39	1	0	6.591630	1.883575	-2.337129
40	6	0	2.678141	-3.137505	0.288031
41	6	0	3.874234	-3.863954	0.731850
42	6	0	1.513833	-3.929412	-0.355582
43	6	0	3.803511	-5.224995	0.790527
44	6	0	1.535538	-5.401665	-0.051416
45	6	0	2.629055	-6.003274	0.442932
46	1	0	4.682144	-5.769642	1.147662
47	1	0	0.640589	-5.958371	-0.340418
48	1	0	2.660164	-7.085512	0.587559
49	8	0	0.280602	-3.342233	0.028172
50	6	0	-0.067660	-3.522738	1.398488
51	1	0	-0.885674	-2.828395	1.620418
52	1	0	-0.395480	-4.559364	1.585358
53	1	0	0.781412	-3.291836	2.063595
54	6	0	5.122607	-3.145800	1.168292
55	1	0	5.924281	-3.870378	1.366866
56	1	0	5.478536	-2.444215	0.400166
57	1	0	4.952538	-2.560207	2.083608
58	7	0	-0.750932	1.447876	-0.033898
59	7	0	-2.076077	-0.247631	-0.429873
60	1	0	-2.989806	-5.208666	-2.093143
61	6	0	1.079591	4.605900	-1.689393
62	1	0	1.946990	5.182676	-1.327062
63	1	0	0.975109	4.799549	-2.768065
64	1	0	0.182243	4.992723	-1.186686
65	6	0	2.521761	2.578729	-2.151055
66	1	0	2.416541	2.703083	-3.238585
67	1	0	3.434050	3.104173	-1.826567
68	1	0	2.652041	1.508458	-1.964807
69	6	0	-1.428445	1.715602	3.813106
70	1	0	-0.797887	2.148875	4.606410
71	1	0	-1.943477	2.549788	3.309700
72	1	0	-2.190568	1.081854	4.295161
73	6	0	0.069815	-0.310946	3.511304
74	1	0	0.716554	-0.850836	2.805976
75	1	0	0.698551	-0.000340	4.361017
76	1	0	-0.702352	-1.002550	3.879387
77	5	0	0.793915	-0.256458	-3.554637
78	9	0	1.634394	0.407908	-4.415080
79	9	0	-0.316319	0.546883	-3.198250
80	9	0	1.513093	-0.557303	-2.332001
81	9	0	0.346665	-1.468580	-4.078429
82	6	0	3.708397	3.546406	2.958489
83	1	0	4.528137	3.659788	2.226888
84	6	0	3.410337	4.941400	3.532019
85	1	0	2.578878	4.890718	4.254140
86	1	0	4.290407	5.353093	4.053161
87	1	0	3.119168	5.644688	2.736844
88	6	0	4.189768	2.587993	4.055244
89	1	0	5.159254	2.919151	4.460141
90	1	0	3.481241	2.554558	4.898444
91	1	0	4.295711	1.559976	3.676231
92	1	0	-3.074315	1.028333	-1.747082
93	6	0	-2.180693	3.327204	-0.957307
94	6	0	-2.540969	4.542137	-0.365060
95	6	0	-1.948786	3.280017	-2.341023
96	6	0	-2.675448	5.699172	-1.138699
97	1	0	-2.719681	4.581267	0.712668

98	6	0	-2.081199	4.434311	-3.111946
99	1	0	-1.630900	2.346914	-2.811283
100	6	0	-2.448347	5.645473	-2.515040
101	1	0	-2.957477	6.641908	-0.663891
102	1	0	-1.886354	4.389212	-4.185892
103	1	0	-2.549934	6.547667	-3.123028
104	6	0	-4.336637	0.846633	-0.044395
105	6	0	-5.462479	0.838668	-0.877350
106	6	0	-4.523141	0.867661	1.346135
107	6	0	-6.752204	0.867833	-0.338909
108	1	0	-5.323474	0.827232	-1.961265
109	6	0	-5.808583	0.908552	1.885532
110	1	0	-3.659371	0.843369	2.011122
111	6	0	-6.927814	0.912076	1.045621
112	1	0	-7.619214	0.869061	-1.003611
113	1	0	-5.937796	0.945683	2.969655
114	1	0	-7.933432	0.951990	1.471281
115	1	0	-1.431017	-1.243953	-2.761742
116	6	0	-3.503282	-2.122034	1.357788
117	8	0	-2.666775	-1.705994	2.157038
118	7	0	-4.790810	-2.394434	1.728086
119	6	0	-5.150232	-2.327390	3.131236
120	1	0	-5.821368	-1.474204	3.326238
121	1	0	-5.671623	-3.252281	3.431439
122	1	0	-4.238600	-2.205032	3.726265
123	6	0	-5.890627	-2.602130	0.803487
124	1	0	-6.718071	-1.924615	1.066053
125	1	0	-5.583765	-2.373067	-0.221862
126	1	0	-6.264358	-3.640792	0.841397
127	6	0	1.614756	-3.771580	-1.885396
128	1	0	1.498096	-2.717471	-2.168577
129	1	0	2.586622	-4.138784	-2.244803
130	1	0	0.810225	-4.347037	-2.362537

IM2, S_a, proximal, si

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4639.927603

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.105718	0.336466	0.373902
2	6	0	-2.233157	1.595845	0.512476
3	1	0	-2.218216	1.911861	1.566860
4	6	0	-0.853538	-0.283285	0.245604
5	6	0	0.297575	1.872021	0.137536
6	6	0	0.766032	2.245780	-1.136072
7	6	0	0.918276	2.317471	1.328477
8	6	0	1.908957	3.055924	-1.192595
9	6	0	2.040638	3.139319	1.205193
10	6	0	2.556929	3.512019	-0.044355
11	1	0	2.296901	3.349002	-2.170901
12	1	0	2.532394	3.497632	2.111524
13	6	0	-2.477859	-2.124959	0.409404
14	6	0	-1.804895	-3.093382	1.175228
15	6	0	-3.548363	-2.506248	-0.408523
16	6	0	-2.167793	-4.440831	1.056370
17	6	0	-3.914152	-3.847652	-0.497485
18	6	0	-3.220566	-4.821740	0.224605
19	1	0	-1.620581	-5.189723	1.633731
20	1	0	-4.732177	-4.125724	-1.164445

21	6	0	0.382681	1.961920	2.714518
22	1	0	-0.286183	1.095049	2.597876
23	6	0	0.067387	1.826745	-2.419927
24	1	0	-0.831994	1.262388	-2.155391
25	29	0	0.852042	-1.241379	-0.020884
26	7	0	2.758276	-1.784110	-0.209604
27	6	0	3.125726	-0.984911	0.773791
28	8	0	2.140769	-0.440126	1.381050
29	6	0	4.520568	-0.745090	1.201520
30	6	0	5.547547	-1.645398	0.875167
31	6	0	4.811921	0.410146	1.942327
32	6	0	6.855010	-1.385641	1.284042
33	1	0	5.317602	-2.546457	0.305104
34	6	0	6.122719	0.668972	2.341836
35	1	0	4.004561	1.103546	2.175558
36	6	0	7.144683	-0.227373	2.014021
37	1	0	7.652436	-2.088365	1.032690
38	1	0	6.350107	1.576612	2.905187
39	1	0	8.171242	-0.023510	2.327705
40	6	0	3.288442	-2.166419	-1.418315
41	6	0	3.054947	-3.513438	-1.818781
42	6	0	3.925118	-1.236209	-2.289488
43	6	0	3.513868	-3.923138	-3.072029
44	6	0	4.363099	-1.698588	-3.530790
45	6	0	4.163581	-3.026669	-3.922079
46	1	0	3.350271	-4.955994	-3.388158
47	1	0	4.854894	-1.000674	-4.212692
48	1	0	4.507321	-3.359203	-4.904390
49	8	0	0.566566	-1.961010	-1.696021
50	6	0	-0.644857	-2.327118	-2.270866
51	1	0	-0.411337	-2.596121	-3.322591
52	1	0	-1.097406	-3.215640	-1.794178
53	1	0	-1.381421	-1.512610	-2.331630
54	6	0	2.355384	-4.454775	-0.883011
55	1	0	2.295697	-5.465720	-1.309664
56	1	0	2.873354	-4.507454	0.088103
57	1	0	1.341031	-4.090220	-0.666791
58	7	0	-0.869396	1.044395	0.225600
59	7	0	-2.086965	-0.758172	0.458588
60	1	0	-3.496902	-5.874973	0.141245
61	6	0	-0.397435	3.046524	-3.228742
62	1	0	0.455994	3.608935	-3.643757
63	1	0	-1.024859	2.711089	-4.068263
64	1	0	-0.994302	3.733942	-2.616193
65	6	0	0.940137	0.903506	-3.282246
66	1	0	0.371715	0.593563	-4.172702
67	1	0	1.854052	1.415240	-3.626891
68	1	0	1.223623	-0.009172	-2.742485
69	6	0	-0.431776	3.121123	3.318321
70	1	0	0.204144	4.011499	3.448572
71	1	0	-1.285115	3.414931	2.692856
72	1	0	-0.825155	2.840627	4.308670
73	6	0	1.480355	1.544069	3.702989
74	1	0	2.058506	0.702033	3.307186
75	1	0	2.166299	2.377311	3.924083
76	1	0	1.026466	1.243572	4.660821
77	5	0	-3.831733	-0.368088	-3.202737
78	9	0	-3.672698	-1.732625	-3.407917
79	9	0	-4.140170	0.320496	-4.350214
80	9	0	-2.627640	0.150878	-2.628151
81	9	0	-4.861642	-0.168374	-2.217379
82	6	0	3.787799	4.396529	-0.151079
83	1	0	3.986158	4.537435	-1.227050
84	6	0	3.542108	5.783332	0.461015
85	1	0	3.350399	5.712067	1.544147

86	1	0	4.419322	6.435146	0.319912
87	1	0	2.671423	6.272882	-0.001539
88	6	0	5.024295	3.724708	0.462609
89	1	0	5.923937	4.341298	0.305789
90	1	0	4.902942	3.585220	1.549004
91	1	0	5.203843	2.733546	0.020188
92	1	0	-3.530519	0.279934	-0.630032
93	6	0	-2.623381	2.801841	-0.318513
94	6	0	-2.025810	4.039836	-0.024459
95	6	0	-3.573227	2.743043	-1.346911
96	6	0	-2.360426	5.187498	-0.742707
97	1	0	-1.278850	4.109768	0.765526
98	6	0	-3.909171	3.894176	-2.064921
99	1	0	-4.060926	1.809946	-1.615402
100	6	0	-3.307444	5.117844	-1.768543
101	1	0	-1.877626	6.137158	-0.500593
102	1	0	-4.644330	3.818165	-2.868791
103	1	0	-3.571087	6.013643	-2.335944
104	6	0	-4.199963	0.212817	1.399985
105	6	0	-5.525022	0.050637	0.976030
106	6	0	-3.916624	0.259862	2.771771
107	6	0	-6.552826	-0.060680	1.916809
108	1	0	-5.735844	0.008795	-0.094561
109	6	0	-4.942204	0.145356	3.710735
110	1	0	-2.883093	0.380674	3.106161
111	6	0	-6.264821	-0.015054	3.283126
112	1	0	-7.584010	-0.185336	1.578384
113	1	0	-4.712901	0.183932	4.778745
114	1	0	-7.069758	-0.102348	4.016884
115	1	0	-4.072952	-1.771326	-1.013707
116	6	0	-0.649555	-2.739570	2.066998
117	8	0	0.505267	-2.808438	1.630055
118	7	0	-0.913719	-2.346183	3.336304
119	6	0	0.198578	-1.963478	4.193469
120	1	0	-0.094030	-1.094142	4.801406
121	1	0	0.481768	-2.786611	4.873029
122	1	0	1.058568	-1.701786	3.567183
123	6	0	-2.214545	-2.476741	3.970404
124	1	0	-2.434867	-1.573880	4.558170
125	1	0	-3.002115	-2.597901	3.219911
126	1	0	-2.232914	-3.344661	4.653702
127	6	0	4.125371	0.200968	-1.896164
128	1	0	3.256395	0.611551	-1.364244
129	1	0	4.997215	0.320492	-1.232453
130	1	0	4.293859	0.823728	-2.785145

$TS_{2\text{-}3}$, S_a, proximal, si

charge = 0, mult = 1

Sum of electronic and thermal Free Energies= -4639.925203

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.088742	0.450936	0.408795
2	6	0	-2.215222	1.716985	0.510573
3	1	0	-2.218986	2.082488	1.550333
4	6	0	-0.829320	-0.174435	0.326139
5	6	0	0.328123	1.955419	0.154121
6	6	0	0.803342	2.289297	-1.127528
7	6	0	0.986173	2.378186	1.329811
8	6	0	1.984845	3.038130	-1.207838

9	6	0	2.148003	3.141158	1.187625
10	6	0	2.668739	3.472888	-0.070449
11	1	0	2.377791	3.298613	-2.193572
12	1	0	2.671335	3.474933	2.085775
13	6	0	-2.423245	-2.006556	0.503588
14	6	0	-1.730743	-2.940949	1.296935
15	6	0	-3.445092	-2.441680	-0.348000
16	6	0	-2.011726	-4.305657	1.160099
17	6	0	-3.734219	-3.801424	-0.451802
18	6	0	-3.008639	-4.740167	0.285533
19	1	0	-1.452901	-5.025774	1.762698
20	1	0	-4.513908	-4.120851	-1.145731
21	6	0	0.457496	2.039770	2.720594
22	1	0	-0.266157	1.218075	2.607233
23	6	0	0.078664	1.855888	-2.390029
24	1	0	-0.881286	1.420588	-2.099405
25	29	0	0.831510	-1.232235	0.117025
26	7	0	2.832244	-1.947598	-0.126623
27	6	0	3.301614	-1.005281	0.709191
28	8	0	2.433355	-0.290430	1.260193
29	6	0	4.736514	-0.895336	1.065615
30	6	0	5.672120	-1.865350	0.673889
31	6	0	5.152074	0.214401	1.816421
32	6	0	7.014946	-1.716507	1.019809
33	1	0	5.342334	-2.734334	0.102300
34	6	0	6.496642	0.363628	2.153300
35	1	0	4.407290	0.954310	2.110325
36	6	0	7.428973	-0.600343	1.755298
37	1	0	7.742220	-2.472919	0.716649
38	1	0	6.820974	1.236132	2.724813
39	1	0	8.482366	-0.483271	2.020793
40	6	0	3.003934	-2.275683	-1.407052
41	6	0	2.261995	-3.465990	-1.813536
42	6	0	3.581345	-1.408180	-2.405802
43	6	0	2.259150	-3.816995	-3.191112
44	6	0	3.502447	-1.799792	-3.726103
45	6	0	2.851789	-2.999053	-4.122370
46	1	0	1.755497	-4.736104	-3.497256
47	1	0	3.929745	-1.152092	-4.495267
48	1	0	2.822534	-3.262275	-5.182224
49	8	0	0.587679	-2.266436	-1.495945
50	6	0	-0.551992	-2.547237	-2.255794
51	1	0	-0.265166	-2.674095	-3.316423
52	1	0	-1.076252	-3.454935	-1.906754
53	1	0	-1.249525	-1.696892	-2.241231
54	6	0	1.872989	-4.494725	-0.790725
55	1	0	1.019603	-5.085346	-1.153888
56	1	0	2.715115	-5.189337	-0.622618
57	1	0	1.605790	-4.032241	0.165991
58	7	0	-0.853210	1.152375	0.261588
59	7	0	-2.072772	-0.631558	0.554329
60	1	0	-3.221818	-5.806777	0.187141
61	6	0	-0.229717	3.039631	-3.315142
62	1	0	0.685173	3.462542	-3.763576
63	1	0	-0.883612	2.703580	-4.134368
64	1	0	-0.751086	3.842384	-2.776034
65	6	0	0.847345	0.754719	-3.132592
66	1	0	0.255737	0.403606	-3.991709
67	1	0	1.817006	1.121763	-3.508600
68	1	0	1.034187	-0.114590	-2.488379
69	6	0	-0.278781	3.238826	3.343739
70	1	0	0.408357	4.090471	3.473775
71	1	0	-1.117880	3.583340	2.723092
72	1	0	-0.681337	2.975506	4.335381
73	6	0	1.550049	1.538694	3.675699

74	1	0	2.081463	0.683079	3.241662
75	1	0	2.283561	2.329266	3.901954
76	1	0	1.101066	1.234942	4.634840
77	5	0	-3.610435	-0.432120	-3.170615
78	9	0	-3.527634	-1.791947	-3.434086
79	9	0	-3.755353	0.334650	-4.303575
80	9	0	-2.425049	-0.033034	-2.469252
81	9	0	-4.704789	-0.194127	-2.272809
82	6	0	3.949433	4.280595	-0.201840
83	1	0	4.123497	4.428251	-1.281259
84	6	0	3.817360	5.668929	0.440306
85	1	0	3.658073	5.591470	1.528181
86	1	0	4.730757	6.264111	0.279288
87	1	0	2.966075	6.223135	0.016217
88	6	0	5.157689	3.517261	0.359870
89	1	0	6.091675	4.075944	0.186399
90	1	0	5.059025	3.363609	1.446702
91	1	0	5.257593	2.525527	-0.106312
92	1	0	-3.497843	0.358811	-0.598949
93	6	0	-2.578559	2.883806	-0.385410
94	6	0	-2.022323	4.140889	-0.096011
95	6	0	-3.436363	2.765954	-1.486943
96	6	0	-2.308790	5.252593	-0.888511
97	1	0	-1.347524	4.251617	0.753611
98	6	0	-3.723951	3.880047	-2.280117
99	1	0	-3.888615	1.814336	-1.753598
100	6	0	-3.164511	5.124631	-1.986465
101	1	0	-1.861431	6.219777	-0.647338
102	1	0	-4.386231	3.757793	-3.139725
103	1	0	-3.390145	5.991762	-2.611936
104	6	0	-4.204427	0.364263	1.415196
105	6	0	-5.519955	0.195610	0.965186
106	6	0	-3.953323	0.449129	2.791488
107	6	0	-6.571371	0.117457	1.883087
108	1	0	-5.704636	0.121993	-0.108961
109	6	0	-5.002693	0.370719	3.707872
110	1	0	-2.926352	0.570413	3.146094
111	6	0	-6.315918	0.204734	3.253857
112	1	0	-7.594823	-0.013080	1.523863
113	1	0	-4.799464	0.441773	4.779593
114	1	0	-7.138746	0.145148	3.970378
115	1	0	-3.991559	-1.730712	-0.962790
116	6	0	-0.687795	-2.519297	2.295004
117	8	0	0.510464	-2.480515	1.984698
118	7	0	-1.111896	-2.193255	3.541002
119	6	0	-0.134756	-1.765843	4.529734
120	1	0	-0.514259	-0.880357	5.063385
121	1	0	0.055841	-2.563146	5.269483
122	1	0	0.802527	-1.516689	4.021250
123	6	0	-2.466099	-2.408855	4.023817
124	1	0	-2.793690	-1.537998	4.609363
125	1	0	-3.161850	-2.539506	3.189584
126	1	0	-2.512968	-3.300454	4.674383
127	6	0	4.189508	-0.085655	-2.030372
128	1	0	3.507969	0.506432	-1.398990
129	1	0	5.131939	-0.200369	-1.474462
130	1	0	4.397027	0.506406	-2.931841

QI, S_a, proximal, si

charge = 0, mult = 1

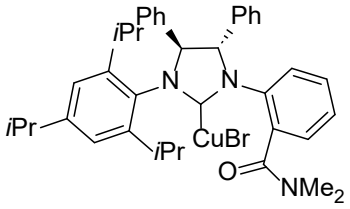
Sum of electronic and thermal Free Energies= -4639.946190

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.260610	0.130311	0.405545
2	6	0	-2.554201	1.489243	0.524648
3	1	0	-2.683905	1.879299	1.547668
4	6	0	-0.952635	-0.235447	0.564848
5	6	0	-0.035141	1.989399	0.242257
6	6	0	0.427437	2.292613	-1.052989
7	6	0	0.576665	2.530998	1.395079
8	6	0	1.554819	3.118300	-1.165320
9	6	0	1.678875	3.369617	1.218472
10	6	0	2.197578	3.657057	-0.049206
11	1	0	1.940884	3.348134	-2.161661
12	1	0	2.173049	3.781250	2.099024
13	6	0	-2.366588	-2.209882	0.755905
14	6	0	-1.514243	-3.085476	1.464134
15	6	0	-3.409842	-2.750125	-0.011479
16	6	0	-1.714876	-4.470177	1.369667
17	6	0	-3.609117	-4.127126	-0.070870
18	6	0	-2.766360	-4.997721	0.624142
19	1	0	-1.022769	-5.132268	1.894602
20	1	0	-4.417173	-4.517248	-0.693058
21	6	0	0.083633	2.210112	2.802400
22	1	0	-0.438464	1.242091	2.748379
23	6	0	-0.249709	1.761828	-2.305438
24	1	0	-1.163025	1.242183	-2.005601
25	29	0	0.733440	-1.157745	0.240510
26	7	0	2.767216	-1.181523	-0.088995
27	6	0	3.441596	-0.423895	0.859866
28	8	0	2.839966	0.382023	1.551494
29	6	0	4.886485	-0.729904	1.099469
30	6	0	5.516569	-1.884437	0.612963
31	6	0	5.624141	0.193334	1.858466
32	6	0	6.872872	-2.100670	0.862915
33	1	0	4.943175	-2.623571	0.056572
34	6	0	6.980566	-0.018709	2.096388
35	1	0	5.112484	1.078150	2.239418
36	6	0	7.608278	-1.165871	1.597018
37	1	0	7.356356	-3.005249	0.487254
38	1	0	7.552809	0.710759	2.674103
39	1	0	8.671096	-1.334094	1.786459
40	6	0	3.013073	-1.380264	-1.351671
41	6	0	2.258321	-2.602496	-1.933059
42	6	0	3.841816	-0.549641	-2.206923
43	6	0	2.409141	-2.764567	-3.416542
44	6	0	3.937814	-0.884849	-3.529670
45	6	0	3.237263	-1.990228	-4.140131
46	1	0	1.828967	-3.559399	-3.888510
47	1	0	4.526873	-0.236042	-4.183803
48	1	0	3.347712	-2.145968	-5.215308
49	8	0	0.887277	-2.364685	-1.590895
50	6	0	-0.083418	-3.392554	-1.806002
51	1	0	-0.002122	-3.819639	-2.816078
52	1	0	0.005070	-4.180020	-1.043126
53	1	0	-1.053489	-2.892387	-1.738177
54	6	0	2.793315	-3.862548	-1.223112
55	1	0	2.295645	-4.761978	-1.611392
56	1	0	3.873179	-3.972851	-1.399842
57	1	0	2.594562	-3.771654	-0.145215
58	7	0	-1.128362	1.073831	0.391002
59	7	0	-2.166476	-0.807157	0.781376
60	1	0	-2.915910	-6.078187	0.571823
61	6	0	-0.654392	2.894174	-3.257903

62	1	0	0.223630	3.355297	-3.741310
63	1	0	-1.303833	2.484169	-4.045363
64	1	0	-1.209101	3.683826	-2.733050
65	6	0	0.605589	0.718075	-3.031832
66	1	0	0.055036	0.346128	-3.907791
67	1	0	1.568612	1.140188	-3.365420
68	1	0	0.798907	-0.146579	-2.386684
69	6	0	-0.914926	3.264319	3.312089
70	1	0	-0.436407	4.256015	3.356580
71	1	0	-1.799996	3.352688	2.668710
72	1	0	-1.263356	3.011480	4.326913
73	6	0	1.225085	2.057608	3.818001
74	1	0	2.006967	1.387422	3.441563
75	1	0	1.687609	3.030258	4.050396
76	1	0	0.833473	1.659024	4.767552
77	5	0	-2.849375	-1.054159	-3.087015
78	9	0	-2.755561	-2.331121	-3.614907
79	9	0	-2.592488	-0.064016	-4.027732
80	9	0	-1.910537	-0.928459	-2.020995
81	9	0	-4.148600	-0.852010	-2.523624
82	6	0	3.431648	4.530046	-0.205363
83	1	0	3.691903	4.528642	-1.277965
84	6	0	3.145219	5.983478	0.200701
85	1	0	2.879975	6.048970	1.268569
86	1	0	4.028145	6.621952	0.033999
87	1	0	2.305440	6.397777	-0.377838
88	6	0	4.634706	3.964232	0.564950
89	1	0	5.537845	4.567788	0.379068
90	1	0	4.450275	3.967608	1.651296
91	1	0	4.847799	2.926045	0.270146
92	1	0	-3.483707	-0.070810	-0.645266
93	6	0	-3.003534	2.566720	-0.440319
94	6	0	-2.743079	3.907179	-0.115987
95	6	0	-3.668025	2.282533	-1.641779
96	6	0	-3.141971	4.942281	-0.962643
97	1	0	-2.215445	4.146069	0.808456
98	6	0	-4.072912	3.319279	-2.486113
99	1	0	-3.866483	1.258747	-1.953700
100	6	0	-3.817103	4.649993	-2.150824
101	1	0	-2.926695	5.978490	-0.691064
102	1	0	-4.581920	3.072153	-3.420134
103	1	0	-4.133921	5.456809	-2.816218
104	6	0	-4.528476	0.010567	1.209065
105	6	0	-5.738006	-0.209677	0.537307
106	6	0	-4.537223	0.143197	2.603791
107	6	0	-6.935967	-0.301279	1.250410
108	1	0	-5.727740	-0.314061	-0.550245
109	6	0	-5.732047	0.045872	3.318666
110	1	0	-3.601120	0.325733	3.133911
111	6	0	-6.935736	-0.177398	2.642003
112	1	0	-7.872932	-0.473034	0.715387
113	1	0	-5.726355	0.148331	4.406728
114	1	0	-7.872079	-0.252436	3.200233
115	1	0	-4.030610	-2.100455	-0.621724
116	6	0	-0.276980	-2.646280	2.198017
117	8	0	0.838839	-2.951045	1.740846
118	7	0	-0.380816	-1.953153	3.352654
119	6	0	0.864736	-1.488804	3.953067
120	1	0	0.630752	-0.884649	4.837669
121	1	0	1.501335	-2.337468	4.246441
122	1	0	1.427792	-0.875417	3.234400
123	6	0	-1.630456	-1.590551	3.988757
124	1	0	-1.748062	-0.494709	4.015705
125	1	0	-2.475464	-2.017207	3.438111
126	1	0	-1.659468	-1.966457	5.025168

127	6	0	4.440176	0.731155	-1.692061
128	1	0	3.697102	1.297145	-1.109791
129	1	0	5.313072	0.562425	-1.046006
130	1	0	4.757171	1.364632	-2.531795

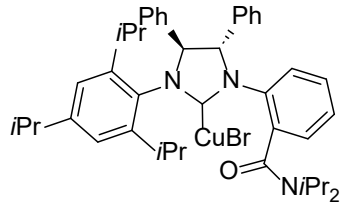
12. Analytical data of chiral NHC ligands L1-5



L1

((4*S*,5*S*)-1-(2-(dimethylcarbamoyl)phenyl)-4,5-diphenyl-3-(2,4,6-triisopropylphenyl)imidazolidin-2-ylidene)copper bromide (**L1**CuBr)

Colorless solid. 25.0 mg (0.035 mmol, 9% yield in 4 steps). Mp : 235.2 °C. R_f = 0.46 [hexane/EtOAc = 1:1 (v/v)]. $[\alpha]^{24.0}_D$ = -46.2 (*c* = 0.08, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ. 7.42-7.19 (m, 14H), 7.38-7.20 (m, 12H), 7.04 (d, *J* = 2.3 Hz, 1H), 6.76 (d, *J* = 1.8 Hz, 1H), 5.07 (d, *J* = 11 Hz, 1H), 3.33 (sept, *J* = 6.9 Hz, 1H), 3.27 (s, 3H), 3.11 (s, 3H), 2.84 (sept, *J* = 6.9 Hz, 1H), 2.71 (sept, *J* = 6.9 Hz, 1H),1.49-1.43 (m, 6H), 1.22 (d, *J* = 6.9 Hz, 6H), 1.21 (d, *J* = 6.9 Hz, 3H), 0.25 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ. 199.8, 169.1, 150.0, 147.3, 145.7, 138.3, 137.0, 134.7, 131.1, 130.3, 130.0, 129.6, 139.3, 129.2, 128.9, 128.7, 128.5, 128.2, 127.8, 127.6, 122.4, 122.3, 79.3, 75.1, 60.5, 40.9, 35.2, 34.1, 29.0, 28.4, 27.2, 26.0, 24.1, 24.0, 23.9, 22.6. IR (neat) 2852, 1631, 1593, 1570, 1543, 1487, 1472, 1419, 1389, 1307, 1233, 1177, 1121, 1093, 1034. HRMS (FD) calcd. for $C_{37}H_{42}N_2OCuBr$: 672.1776, found: 672.1776.

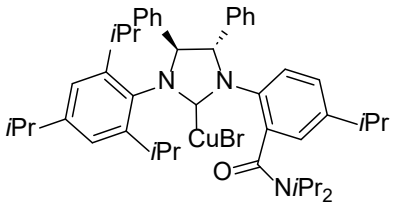


L2

((4*S*,5*S*)-1-(2-(diisopropylcarbamoyl)phenyl)-4,5-diphenyl-3-(2,4,6-triisopropylphenyl)imidazolidin-2-ylidene)copper bromide (**L2**CuBr)

Colorless solid. 0.153 g (0.199 mmol, 26% yield in 4 steps). Mp : 259.0 °C. R_f = 0.40 [hexane/EtOAc = 3:1 (v/v)]. $[\alpha]^{24.2}_D$ = -129.2 (*c* = 0.25, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ. 7.43 (d, *J* = 7.3 Hz, 2H), 7.35-7.17 (m, 1H), 7.12 (d, *J* = 7.8 Hz, 1H), 7.07 (d, *J* = 1.4 Hz, 1H), 6.76 (d, *J* = 1.8 Hz, 1H), 5.15 (d, *J* = 10 Hz, 1H), 3.84 (sept, *J* = 6.9 Hz, 1H), 3.65 (sept, *J* = 6.9 Hz, 1H), 3.42 (sept, *J* = 6.9 Hz, 1H), 2.85 (sept, *J* = 6.9 Hz, 1H), 2.69 (sept, *J* = 6.9 Hz, 1H), 1.86 (d, *J* = 6.9 Hz, 3H), 1.66 (d, *J* = 6.9 Hz, 3H), 1.52 (d, *J* = 6.9 Hz, 6H), 1.30 (d,

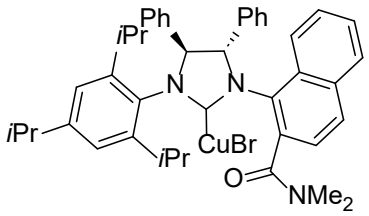
J = 6.9 Hz, 3H), 1.23 (d, *J* = 6.9 Hz, 6H), 1.15 (d, *J* = 6.9 Hz, 3H), 1.11 (d, *J* = 6.9 Hz, 3H), 0.14 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ. 199.3, 169.0, 149.8, 147.3, 145.6, 137.5, 137.4, 135.6, 134.8, 132.6, 130.5, 129.5, 129.4, 129.0, 128.96, 128.8, 128.7, 128.4, 126.4, 122.4, 122.2, 78.8, 74.8, 51.6, 46.1, 34.0, 29.1, 28.4, 27.2, 25.9, 24.1, 23.8, 23.2, 22.2, 21.7, 20.2, 20.2. IR (neat) 2961, 2961, 2622, 1452, 1370, 1337, 1233, 1088, 1031, 881 cm^{-1}. HRMS (FD) calcd. for $C_{39}H_{45}N_3OCuBr$: 713.2042, found: 713.2040.



L3

((4S,5S)-1-(2-(diisopropylcarbamoyl)-4-isopropylphenyl)-4,5-diphenyl-3-(2,4,6-triisopropylphenyl)imidazolidin-2-ylidene)copper(III) bromide (**L3**CuBr)

Colorless solid. 0.366 g (0.448 mmol, 32% yield in 4 steps). Mp : 245.2 °C. R_f = 0.26 [hexane/EtOAc = 5:1 (v/v)]. $[\alpha]^{26.7}_D$ = -116.0 (*c* = 0.125, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, J = 6.9 Hz, 2H), 7.29 (t, *J* = 7.3 Hz, 3H), 7.24 (s, 5H), 7.06 (d, *J* = 1.8 Hz, 1H), 7.03 (s, 3H), 6.75 (d, *J* = 1.8 Hz, 1H), 6.46 (d, *J* = 9.6 Hz, 1H), 5.10 (d, *J* = 10.1 Hz, 1H), 3.82 (sept, *J* = 6.9 Hz , 1H), 3.64 (sept, *J* = 6.9 Hz, 1H), 3.41 (sept, *J* = 6.9 Hz, 1H), 2.85 (sept, *J* = 6.9 Hz, 2H), 2.68 (sept, *J* = 6.9 Hz, 1H), 1.85 (d, *J* = 6.9 Hz, 3H), 1.67 (d, *J* = 6.9 Hz, 3H), 1.50 (t, *J* = 6.9 Hz, 6H), 1.29 (d, *J* = 6.4 Hz, 3H), 1.23 (d, *J* = 6.9 Hz, 6H), 1.20-1.11 (m, 12H), 0.13 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 169.3, 149.5, 149.0, 147.2, 145.5, 137.6, 136.9, 134.8, 133.1, 132.1, 130.4, 129.2, 128.8, 128.6, 128.6, 128.1, 127.6, 124.3, 124.2, 122.2, 122.0, 78.7, 74.7, 51.4, 45.9, 33.8, 33.3, 28.9, 28.2, 27.0, 25.7, 23.9, 23.7, 23.6, 23.1, 22.8, 22.1, 21.5, 20.0, 20.0. IR (neat) 3032, 2964, 1864, 1594, 1571, 1543, 1472, 1424, 1382, 1338, 1204, 1177, 1121, 1089, 1035, 994, 952. HRMS (FD) calcd. for $C_{46}H_{59}BrCuN_3O$: 811.3137, found: 811.3138.

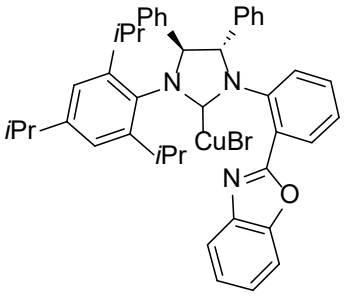


L4

((4S,5S)-1-(2-(dimethylcarbamoyl)naphthalen-1-yl)-4,5-diphenyl-3-(2,4,6-

triisopropylphenyl)imidazolidin-2-ylidene)copper(III) bromide (**L4**CuBr)

Colorless solid. 0.107 g (0.140 mmol, 20% yield in 4 steps). Mp : 241.9 °C. R_f = 0.44 [hexane/EtOAc = 1:1 (v/v)]. $[\alpha]^{24.3}_D$ = -93.1 (*c* = 0.25, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.2 Hz, 1H), 7.82 (d, *J* = 7.3 Hz, 1H), 7.74 (d, *J* = 7.3 Hz, 1H), 7.44-7.27 (m, 10H), 7.13 (d, *J* = 1.8 Hz, 1H), 7.08-7.03 (m, 3H), 6.79 (d, *J* = 1.8 Hz, 1H), 6.57 (d, *J* = 11.0 Hz, 1H), 5.48 (d, *J* = 11.4 Hz, 1H), 3.60 (sept, *J* = 6.9 Hz, 1H), 3.36 (s, 3H), 3.07 (s, 3H), 2.89 (sept, *J* = 6.9 Hz, 1H), 2.73 (sept, *J* = 6.9 Hz , 1H), 1.72 (d, *J* = 6.9 Hz, 3H), 1.59 (d, *J* = 6.9 Hz, 3H), 1.25 (d, *J* = 7.3 Hz, 6H), 1.20 (d, *J* = 6.9 Hz, 3H), 0.31 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.1, 169.5, 149.9, 147.0, 145.6, 134.8, 133.9, 133.8, 133.7, 133.7, 131.5, 130.4, 129.8, 129.3, 129.1, 128.9, 128.7, 128.6, 128.4, 127.9, 127.2, 127.0, 123.2, 123.0, 122.3, 122.0, 76.0, 74.0, 40.6, 34.9, 33.9, 29.4, 28.5, 26.9, 25.9, 24.2, 23.8, 23.7, 22.2. IR (neat) 3033, 2962, 2922, 2861, 2309, 1595, 1569, 1542, 1471, 1446, 1424, 1385, 1317, 1220, 1178, 1120, 1094, 1034, 993, 953. HRMS (FD) calcd. for $C_{46}H_{59}BrCuN_3O$: 763.2198, found: 763.2198.



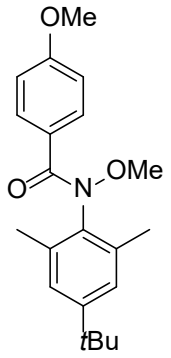
L5

((4S,5S)-1-(2-(benzo[d]oxazol-2-yl)phenyl)-4,5-diphenyl-3-(2,4,6-triisopropylphenyl)imidazolidin-2-ylidene)copper(III) bromide (**L5**CuBr)

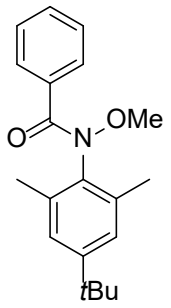
Colorless solid. 0.162 g (0.212 mmol, 15% yield in 4 steps). Mp : 168.7 °C. R_f = 0.34 [hexane/EtOAc = 2:1 (v/v)]. $[\alpha]^{24.5}_D$ = +11.8 (*c* = 0.20, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 7.8 Hz, 1H), 7.90 (t, *J* = 4.1 Hz, 1H), 7.71 (t, *J* = 4.4 Hz, 1H), 7.61-7.60 (m, 2H), 7.50-7.47 (m, 3H), 7.39-7.32 (m, 8H), 7.26 (s, 1H), 7.21 (d, *J* = 7.8 Hz, 1H), 7.04 (s, 1H), 6.71 (s, 1H), 6.42 (d, *J* = 11.4 Hz, 1H), 5.26 (d, *J* = 11.4 Hz, 1H), 3.39 (sept, *J* = 6.9 Hz, 1H), 2.94 (sept, *J* = 6.9 Hz, 1H), 2.82 (sept, *J* = 6.9 Hz, 1H), 1.53 (d, *J* = 6.9 Hz, 3H), 1.49 (d, *J* = 6.4 Hz, 3H), 1.21 (d, *J* = 6.4 Hz, 6H), 0.64 (d, *J* = 6.9 Hz, 3H), 0.34 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.5, 160.2, 150.4, 149.7, 147.5, 145.7, 142.2, 138.4, 137.7, 134.1, 132.3, 131.9, 130.9, 130.5, 129.9, 129.2, 129.1, 128.5, 128.5, 125.9, 125.8, 124.8, 122.2, 122.1, 119.8, 111.2, 79.5, 73.6, 34.0, 29.0, 28.2, 26.1, 25.9, 24.4, 23.9, 23.8, 22.0. IR (neat) 3033, 2854, 2409, 1649, 1629, 1593, 1569, 1543, 1487, 1472, 1419, 1386, 1356, 1307, 1178, 1121, 1094, 1036, 994, 952, 825. HRMS (FD) calcd. for $C_{43}H_{43}BrCuN_3O$: 759.1885,

found: 759.1884.

13. Analytical data of 1

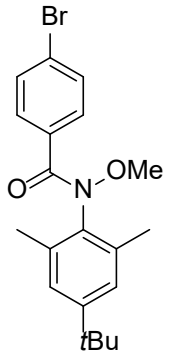


***N*-(4-(*tert*-butyl)-2,6-dimethylphenyl)-*N*,4-dimethoxybenzamide (1a).** Colorless solid. 0.266 g (0.78 mmol, 54% yield in 3 steps). Mp : 102.4 °C. R_f = 0.44 [hexane/EtOAc = 2:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ. 7.89 (d, *J* = 8.2 Hz, rotamer), 7.29 (d, *J* = 8.2 Hz, 2H), 7.13 (S, rotamer), 7.02 (s, 2H), 6.96 (d, *J* = 8.2 Hz, rotamer), 6.66 (d, *J* = 8.2 Hz, 2H), 3.86 (s, 3H) 3.86 (s, rotamer), 3.74 (s, 3H), 3.53 (s, rotamer) , 2.35 (s, rotamer), 2.25 (s, 6H), 1.32 (s, rotamer), 1.27 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.8, 166.7, 161.4, 161.2, 152.2, 151.7, 136.3, 136.1, 135.3, 133.2, 130.5, 130.1, 126.6, 136.1, 125.8, 125.5, 113.2, 112.9, 60.8, 60.4, 55.2, 55.1, 34.4, 31.2, 31.1, 18.8, 18.6. IR (neat) 2996, 2963, 2901, 2837, 2561, 2509, 2057, 1922, 1737, 1636, 1605, 1509, 1463, 1438, 1414, 1361, 1305, 1256, 1237, 1203, 1172, 1150, 1123, 1022, 1003, 979, 924, 890, 880, 846, 835, 811, cm^{-1}. HRMS (FD) calcd. for $C_{21}H_{27}NO_3$: 341.1991, found: 341.1990.

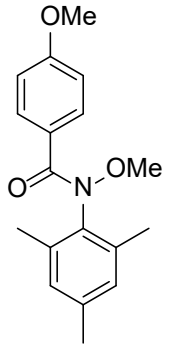


***N*-(4-(*tert*-butyl)-2,6-dimethylphenyl)-*N*-methoxybenzamide (1b).** Colorless solid. 0.178 g (0.571 mmol, 35% yield in 3 steps). Mp : 79.4 °C. R_f = 0.52 [hexane/EtOAc = 2:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ. 7.81 (d, *J* = 7.3 Hz, 2H), 7.49-7.46 (m, 3H), 7.33-7.28 (m, rotamer), 7.18-7.15 (m, 2H, rotamer), 7.00 (s, 2H), 3.87 (s, rotamer), 3.49 (s, 3H), 2.38 (s, 6H), 2.26 (s, rotamer), 1.32 (s, 9H), 1.26 (s, rotamer). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.7, 167.0, 152.4, 151.8, 136.3, 136.1, 134.8, 134.8, 134.0, 132.7, 130.5, 130.3, 128.0, 127.9, 127.6, 125.8, 125.6, 60.8, 60.4, 34.4, 31.2, 31.1, 18.8, 18.6. IR (neat) 2963, 2869,

1658, 1601, 1578, 1483, 1446, 1363, 1239, 1039, 1022, 968, 927, 871, 837, 770 cm^{-1}. HRMS (ESI) calcd. for $C_{20}H_{25}NO_2$ $(M+Na)^+$ 334.1777, found 334.1778.

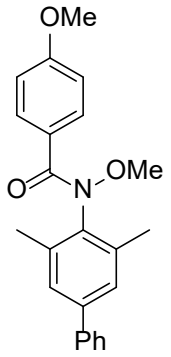


4-bromo-*N*-(4-(*tert*-butyl)-2,6-dimethylphenyl)-*N*-methoxybenzamide (1c) Colorless solid. 0.215 g (0.551 mmol, 34% yield in 3 steps). Mp : 75.8 °C. R_f = 0.24 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ. 7.71 (d, *J* = 8.7 Hz, 2H), 7.60 (d, *J* = 8.7, 2H), 7.30 (d, *J* = 8.7 Hz, rotamer), 7.19 (d, *J* = 8.7 Hz, rotamer), 7.14 (s, 2H), 7.03 (s, rotamer), 3.86 (s, rotamer), 3.49 (s, 3H), 2.36 (s, 6H), 2.25 (s, rotamer), 1.32 (s, 9H), 1.28 (s, rotamer). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 166.0, 152.7, 152.1, 136.3, 136.0, 134.5, 133.5, 132.8, 132.4, 131.1, 130.9, 129.8, 129.7, 126.0, 125.6, 125.2, 124.9, 60.9, 60.4, 34.4, 31.2, 31.1, 18.8, 18.6. IR (neat) 2965, 2409, 2360, 2349, 2342, 1658, 1591, 1483, 1396, 1363, 1220, 1012, 772 cm^{-1}. HRMS (ESI) calcd. for $C_{20}H_{24}BrNO_2$ $(M+Na)^+$: 412.0883, found: 412.0883.

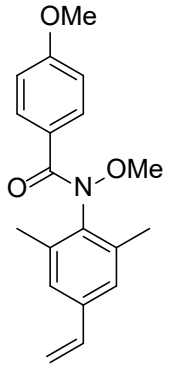


***N*-mesityl-*N*,4-dimethoxybenzamide (1d)** Colorless solid. 0.183 g (0.612 mmol, 22% yield in 2 steps). Mp : 65.8 °C. R_f = 0.44 [hexane/EtOAc = 2:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.8 Hz, rotamer), 7.29 (d, *J* = 8.2 Hz, 2H), 6.96 (s, rotamer), 6.85 (s, 2H), 6.67 (d, *J* = 8.0 Hz, 2H), 3.87 (s, rotamer), 3.85 (s, 3H), 3.74 (s, 3H), 3.53 (s, rotamer), 2.32 (s, rotamer), 2.26 (s, 3H), 2.22 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.7, 166.6, 161.3, 161.1, 139.0, 138.7, 136.7, 136.4, 135.2, 133.2, 130.3, 129.9, 129.4, 129.0, 126.4, 125.9, 113.0, 112.8, 60.5, 60.1, 55.1, 54.9, 20.8, 18.3, 18.1. IR (neat) 2962, 2931, 2409,

2359, 2349, 1567, 1459, 1416, 1368, 1304, 1175, 1134, 1028, 971, 884, 853 cm^{-1}. HRMS (ESI) calcd. for $C_{18}H_{21}NO_3$ $(M+Na)^+$: 322.1414, found: 322.1414.



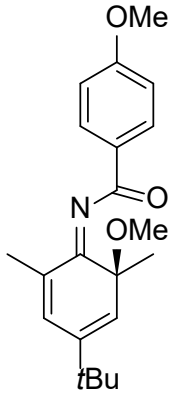
***N*-(3,5-dimethyl-[1,1'-biphenyl]-4-yl)-*N*,4-dimethoxybenzamide (1e)** Colorless solid. 0.448 g (1.24 mmol, 20% yield in 5 steps). Mp : 128.5 °C. R_f = 0.40 [hexane/EtOAc = 2:1 (v/v)]. ^1H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.8 Hz, rotamer), 7.57 (m, rotamer), 7.43 (t, *J* = 6.9 Hz, 4H), 7.37-7.33 (m, 3H, rotamer) , 7.28 (s, 2H), 6.98 (d, *J* = 8.2 Hz, rotamer), 6.68 (d, *J* = 8.2 Hz, 2H), 3.90 (s, 3H), 3.89 (s, rotamer), 3.74 (s, 3H), 3.58 (s, rotamer), 2.43 (s, rotamer), 2.33 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 166.4, 161.3, 161.1, 141.5, 140.1, 139.4, 137.2, 136.9, 136.8, 135.0, 130.3, 129.8, 128.4, 127.4, 127.2, 127.0, 126.8, 126.6, 126.0, 125.6, 112.9, 112.8, 60.6, 60.2, 54.9, 54.8, 18.5, 18.3. IR (neat) 2384, 2360, 2349, 2299, 1748, 1648, 1606, 1509, 1373, 1255, 1220, 1175, 1030, 772 cm^{-1}. HRMS (ESI) calcd. for $C_{23}H_{23}NO_3$ $(M+Na)^+$: 384.1570, found: 384.1570.



***N*-(2,6-dimethyl-4-vinylphenyl)-N,4-dimethoxybenzamide (1f)** Colorless oil. 0.198 g (0.635 mmol, 22% yield in 5 steps). R_f = 0.48 [hexane/EtOAc = 2:1 (v/v)]. ^1H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.3 Hz, rotamer), 7.30 (d, *J* = 8.7 Hz, 2H), 7.19 (s, rotamer), 7.09 (s, 2H), 6.97 (d, *J* = 7.8 Hz, rotamer), 6.71-6.58 (m, 3H, rotamer), 5.74 (d, *J* = 17.4 Hz, 1H, rotamer), 5.28 (d, *J* = 11.0 Hz, 1H, rotamer), 3.88 (s, rotamer), 3.86 (s, 3H), 3.74 (s, 3H), 3.54 (s, rotamer), 2.36 (s, rotamer), 2.26 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.8, 166.6,

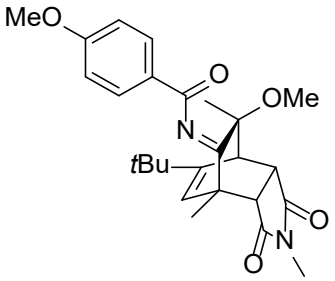
161.5, 161.4, 138.1, 137.3, 137.3, 137.0, 136.2, 135.8, 135.4, 130.5, 130.1, 126.6, 126.3, 125.9, 115.1, 114.7, 113.2, 113.1, 60.8, 60.4, 55.3, 55.1, 18.7, 18.4. IR (neat) 2932, 2839, 1650, 1605, 1575, 1509, 1459, 1440, 1416, 1349, 1304, 1252, 1175, 1141, 1111, 1026, 968, 913, 876, 840 cm^{-1}. HRMS (ESI) calcd. for $C_{19}H_{21}NO_3$ $(M+Na)^+$: 334,1414, found: 334.1414.

14. Analytical data of 2 and 4



(*S,E*)-*N*-(4-(*tert*-butyl)-6-methoxy-2,6-dimethylcyclohexa-2,4-dien-1-ylidene)-4-methoxybenzamide (2a) Colorless solid. 19.8 mg (0.058 mmol, 58% yield). Mp : 108.6 °C. R_f = 0.54 [hexane/EtOAc = 2:1 (v/v)]. $[\alpha]^{24.5}_D$ = -246.2 (*c* = 0.20, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ. 7.85 (d, *J* = 8.7 Hz, 2H), 6.90 (d, *J* = 9.2 Hz, 2H), 6.63 (d, *J* = 0.92 Hz, 1H), 5.67 (d, *J* = 0.92 Hz, 1H), 3.85 (s, 3H), 2.66 (s, 3H), 2.08 (s, 3H), 1.50 (s, 3H), 1.21 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) 178.8, 169.2, 162.6, 143.0, 133.6, 132.6, 130.8, 129.1, 127.8, 113.3, 80.4, 55.3, 54.4, 34.0, 28.7, 28.3, 18.2. IR (neat) 3160, 2962, 2869, 2566, 1789, 1633, 1599, 1508, 1454, 1416, 1383,1365, 1313, 1297, 1248, 1199, 1182, 1160, 1086, 1065, 1042, 1022, 969, 954, 924, 896, 865, 843, 803 cm^{-1}. HRMS (FD) calcd. for $C_{21}H_{27}NO_3$: 341.1991, found: 341.1991.

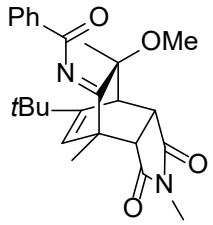
HPLC analysis DAICEL CHIRALPAK IC-3 4.6 × 250 mm (Hexane/IPA = 85/15, 1.0 ml/min, 220 nm, 30 ℃) 18.4 min (minor), 20.9 min (major), er = 83 : 17.



***N*-((3a*S*,4*S*,7*S*,9*S*,*Z*)-5-(*tert*-butyl)-9-methoxy-2,7,9-trimethyl-1,3-dioxo-2,3,3a,4,7,7a-hexahydro-1*H*-4,7-ethanoisoindol-8-ylidene)-4-methoxybenzamide (4aa)** Colorless solid. 28.5 mg (0.063 mmol, 63% yield). Mp : 181.9 °C. R_f = 0.44 [hexane/EtOAc = 2:1 (v/v)]. $[\alpha]^{26.9}_D$ = +110.4 (*c* = 0.14, $CHCl_3$). ^1H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.7 Hz, 2H), 6.89 (d, *J* = 8.7 Hz, 2H), 5.67 (d, *J* = 1.8 Hz, 1H), 3.86 (s, 3H), 3.52 (t, *J* = 2.3 Hz, 1H), 3.45 (dd, *J* = 8.0, 2.5 Hz, 1H), 3.11 (s, 3H), 2.90 (s, 3H), 2.86 (d, *J* = 8.2 Hz, 1H), 1.72 (s,

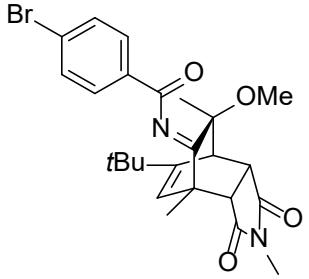
3H), 1.39 (s, 3H), 1.01 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.4, 178.1, 175.9, 174.0, 162.8, 152.6, 130.5, 126.9, 125.0, 113.4, 78.8, 55.4, 49.6, 48.8, 46.6, 43.2, 40.7, 34.1, 29.5, 24.8, 21.8, 17.9. IR (neat) 2957, 2839, 2409, 1774, 1699, 1658, 1602, 1577, 1509, 1435, 1381, 1288, 1251, 1220, 1165, 1107, 1062, 1026, 980, 915, 877, 851, 772, 675, 614 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{32}N_2O_5$ $(M+Na)^+$: 475.2203, found: 475.2203.

SFC analysis DAICEL CHIRALPAK IA-3/SFC 4.6 × 150 mm (CO_2/MeOH = 95/5, 3.0 ml/min, 254 nm, 40 ℃) 4.9 min (minor), 7.0 min (major), er = 91 : 9.



***N*-((3a*S*,4*S*,7*S*,9*S*,*Z*)-5-(*tert*-butyl)-9-methoxy-2,7,9-trimethyl-1,3-dioxo-2,3,3a,4,7,7a-hexahydro-1*H*-4,7-ethanoisoindol-8-ylidene)benzamide (4ba)** Colorless solid. 21.1 mg (0.050 mmol, 50% yield). Mp : 191.9 °C. R_f = 0.40 [hexane/EtOAc = 2:1 (v/v)]. $[\alpha]^{26.4}_D$ = +50.8 (*c* = 0.15, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.3 Hz, 2H), 7.50 (t, *J* = 6.6 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 2H), 5.68 (d, *J* = 1.8 Hz, 1H), 3.51 (t, *J* = 2.5 Hz, 1H), 3.43 (dd, *J* = 8.4, 2.6 Hz, 1H), 3.08 (s, 3H), 2.90 (s, 3H), 2.86 (d, *J* = 8.2 Hz, 1H), 1.74 (s, 3H), 1.40 (s, 3H), 1.01 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.1, 178.0, 175.8, 174.6, 152.6, 134.4, 132.2, 128.3, 128.1, 124.9, 78.8, 49.5, 48.9, 46.5, 43.1, 40.7, 34.1, 29.5, 24.8, 21.8, 17.9. IR (neat) 2956, 2870, 2835, 2409, 2369, 2349, 2321, 1775, 1605, 1545, 1508, 1434, 1383, 1289, 1106, 1053, 1020, 976, 915, 840 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{30}N_2O_4$ $(M+Na)^+$: 445.2098, found: 445.2098.

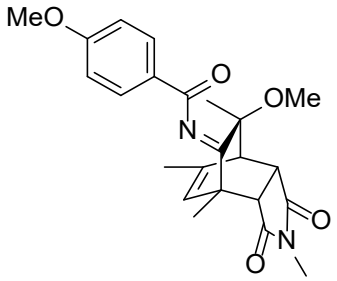
SFC analysis DAICEL CHIRALPAK IA-3/SFC 4.6 × 150 mm (CO_2/MeOH = 95/5, 3.0 ml/min, 254 nm, 40 ℃) 2.6 min (minor), 3.3 min (major), er = 87 : 13.



4-bromo-*N*-((3a*S*,4*S*,7*S*,9*S*,*Z*)-5-(*tert*-butyl)-9-methoxy-2,7,9-trimethyl-1,3-dioxo-2,3,3a,4,7,7a-hexahydro-1*H*-4,7-ethanoisoindol-8-ylidene)benzamide (4ca) Colorless solid. 14.0 mg (0.028 mmol, 28% yield). Mp : 188.5 °C. R_f = 0.50 [hexane/EtOAc = 2:1

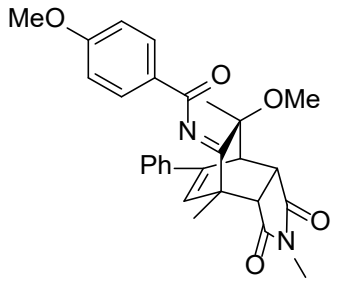
(v/v)]. $[\alpha]^{26.6}_{D}$ = +106.6 (*c* = 0.15, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.7 Hz, 2H), 7.54 (d, *J* = 8.2 Hz, 2H), 5.68 (d, *J* = 2.3 Hz, 1H), 3.51 (t, *J* = 2.3 Hz, 1H), 3.39 (dd, *J* = 7.8, 2.3 Hz, 1H), 3.08 (s, 3H), 2.90 (s, 3H), 2.82 (d, *J* = 8.2 Hz, 1H), 1.73 (s, 3H), 1.38 (s, 3H), 1.01 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.3, 177.9, 175.7, 175.6, 152.7, 133.3, 131.4, 129.9, 127.1, 124.7, 79.0, 49.5, 49.0, 46.4, 43.1, 40.7, 34.1, 29.5, 24.8, 21.8, 17.8. IR (neat) 2957, 2834, 2373, 2321, 1774, 1605, 1587, 1509, 1434, 1382, 1288, 1250, 1173, 1106, 1068, 1010, 980, 952, 877, 852 cm^{-1}. HRMS (ESI) calcd. for $C_{25}H_{29}BrN_2O_4$ $(M+Na)^+$: 523.1203, found: 523.1203.

SFC analysis DAICEL CHIRALPAK IA-3/SFC 4.6 × 150 mm (CO_2/MeOH = 95/5, 3.0 ml/min, 254 nm, 40 ℃) 3.5 min (minor), 5.2 min (major), er = 92 : 8.

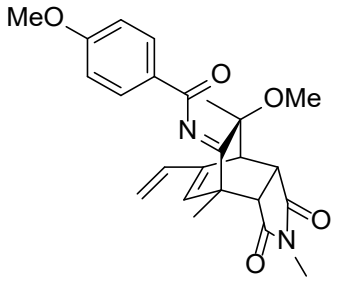


4-methoxy-*N*-((3a*S*,4*S*,7*S*,9*S*,*Z*)-9-methoxy-2,5,7,9-tetramethyl-1,3-dioxo-2,3,3a,4,7,7a-hexahydro-1*H*-4,7-ethanoisoindol-8-ylidene)benzamide (4da) Colorless solid. 21.8 mg (0.053 mmol, 53% yield). Mp : 135.4 °C. R_f = 0.28 [hexane/EtOAc = 2:1 (v/v)]. $[\alpha]^{26.6}_{D}$ = +69.6 (*c* = 0.17, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.7 Hz, 2H), 6.89 (d, *J* = 8.7 Hz, 2H), 5.52 (s, 1H), 3.86 (s, 3H), 3.37 (dd, J = 8.0, 3.0 Hz, 1H), 3.20 (t, *J* = 2.1 Hz, 1H), 3.10 (s, 3H), 2.94 (s, 3H), 2.88 (d, *J* = 8.2 Hz, 1H), 1.82 (s, 3H), 1.64 (s, 3H), 1.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.1, 178.0, 175.7, 173.4, 162.8, 141.7, 130.4, 126.7, 125.5, 113.3, 78.0, 55.3, 49.6, 48.2, 47.3, 40.5, 24.9, 21.9, 20.5, 17.4. IR (neat) 3033, 2527, 2370, 2347, 2322, 1702, 1647, 1511, 1435, 1384, 1220, 772 cm^{-1}. HRMS (ESI) calcd. for $C_{23}H_{26}N_2O_5$ $(M+Na)^+$: 433.1734, found: 433.1734.

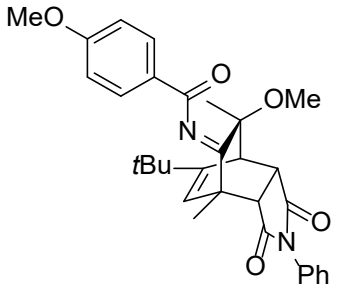
SFC analysis DAICEL CHIRALPAK IA-3/SFC 4.6 × 150 mm (CO_2/MeOH = 95/5, 3.0 ml/min, 254 nm, 40 ℃) 5.9 min (minor), 7.4 min (major), er = 87 : 13.



4-methoxy-*N*-((3a*S*,4*S*,7*S*,9*S*,*Z*)-9-methoxy-2,7,9-trimethyl-1,3-dioxo-5-phenyl-2,3,3a,4,7,7a-hexahydro-1*H*-4,7-ethanoisoindol-8-ylidene)benzamide (4ea) Colorless solid. 14.2 mg (0.030 mmol, 30% yield). Mp : 165.3 °C. R_f = 0.34 [hexane/EtOAc = 2:1 (v/v)]. $[\alpha]^{26.7}_D$ = +17.7 (*c* = 0.07, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.7 Hz, 2H), 7.38-7.30 (m, 5H), 6.91 (d, *J* = 8.7 Hz, 2H), 6.09 (d, *J* = 1.4 Hz, 1H), 3.87 (s, 4H), 3.55 (dd, *J* = 8.2, 2.7 Hz, 1H), 3.13 (s, 3H), 3.01 (d, *J* = 8.2 Hz, 1H), 2.85 (s, 3H), 1.79 (s, 3H), 1.37 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.3, 177.9, 175.6, 173.1, 162.8, 143.8, 136.9, 130.5, 128.9, 128.6, 126.7, 126.2, 125.4, 113.4, 78.5, 55.3, 49.7, 48.7, 47.8, 45.6, 40.7, 25.0, 21.0, 17.7. IR (neat) 3033, 2374, 2352, 2321, 1704, 1607, 1544, 1509, 1339, 1220, 772 cm^{-1}. HRMS (ESI) calcd. for $C_{28}H_{28}N_2O_5$ $(M+Na)^+$: 495.1890, found: 495.1891.
SFC analysis DAICEL CHIRALPAK IA-3/SFC 4.6 × 150 mm (CO_2/MeOH = 95/5, 3.0 ml/min, 254 nm, 40 ℃)10.1 min (minor), 13.8 min (major), er = 84 : 16.



4-methoxy-*N*-((3a*S*,4*S*,7*S*,9*S*,*Z*)-9-methoxy-2,7,9-trimethyl-1,3-dioxo-5-vinyl-2,3,3a,4,7,7a-hexahydro-1*H*-4,7-ethanoisoindol-8-ylidene)benzamide (4fa) Colorless solid. 6.3 mg (0.015 mmol, 15% yield). Mp : 142.0 °C. R_f = 0.32 [hexane/EtOAc = 2:1 (v/v)]. $[\alpha]^{26.7}_D$ = +98.2 (*c* = 0.09, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.7 Hz, 2H), 6.90 (d, *J* = 8.7 Hz, 2H), 6.34 (dd, *J* = 17.4, 11.0 Hz, 1H), 5.76 (s, 1H), 5.46 (d, *J* = 17.4 Hz, 1H), 5.20 (d, *J* = 10.5 Hz, 1H), 3.86 (s, 3H), 3.72 (s, 1H), 3.45 (dd, *J* = 8.0, 3.0 Hz, 1H), 3.14 (s, 3H), 2.95 (d, *J* = 7.8 Hz, 1H), 2.90 (s, 3H), 1.71 (s, 3H), 1.36 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.1, 177.4, 175.6, 172.8, 162.8, 142.0, 133.7, 130.5, 129.1, 126.7, 116.1, 113.4, 78.1, 55.4, 49.7, 48.7, 47.7, 41.2, 40.2, 25.0, 20.4, 17.4. IR (neat) 2981, 2940, 2373, 2352, 2321, 1777, 1702, 1606, 1543, 1509, 1434, 1384, 1290, 1255, 1220, 1176, 1134, 981, 772 cm^{-1}. HRMS (ESI) calcd. for $C_{24}H_{26}N_2O_5$ $(M+Na)^+$: 445.1734, found: 445.1734.
SFC analysis DAICEL CHIRALPAK IA-3/SFC 4.6 × 150 mm (CO_2/MeOH = 95/5, 3.0 ml/min, 254 nm, 40 ℃) 6.9 min (minor), 8.9 min (major), er = 81 : 19.

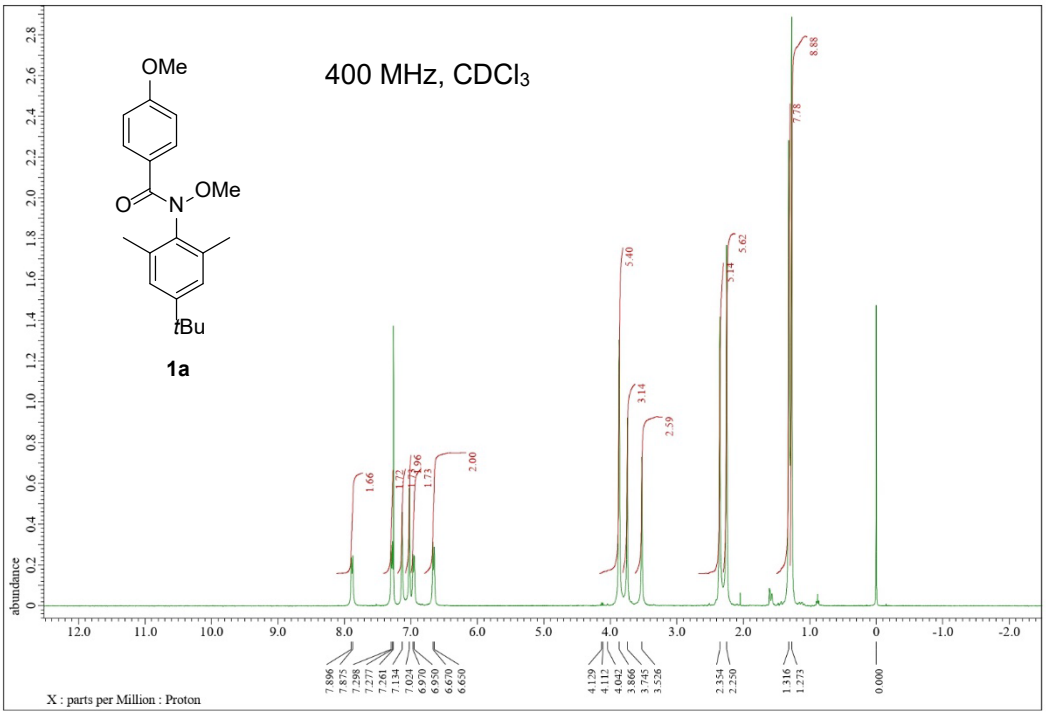


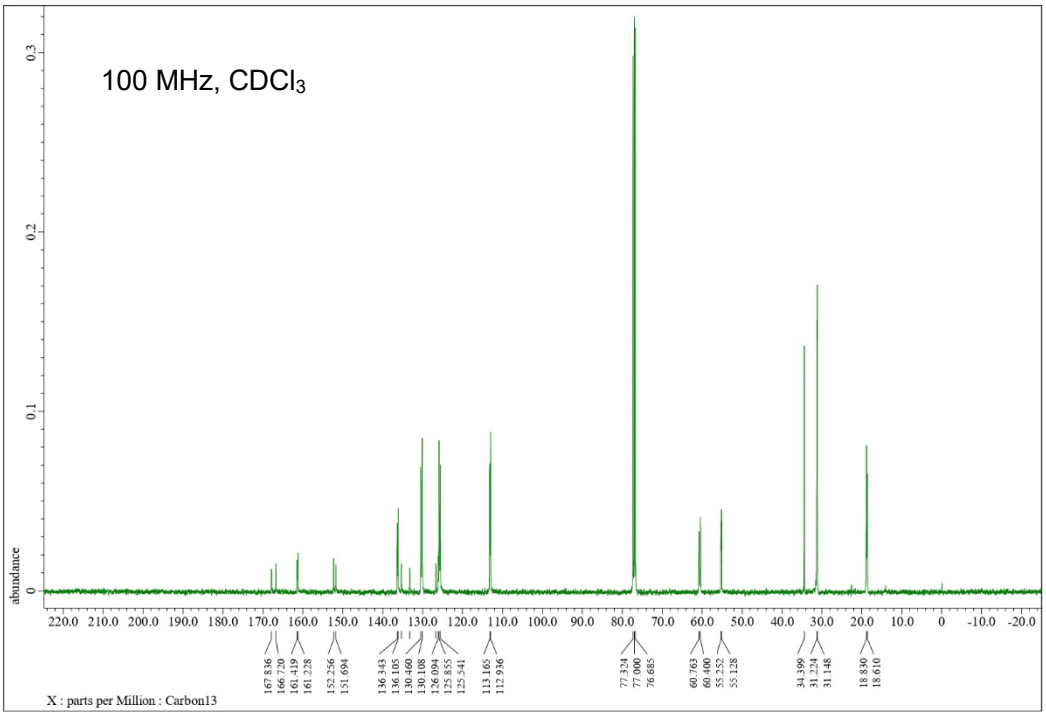
***N*-((3a*S*,4*S*,7*S*,9*S*,*Z*)-5-(*tert*-butyl)-9-methoxy-7,9-dimethyl-1,3-dioxo-2-phenyl-2,3,3a,4,7,7a-hexahydro-1H-4,7-ethanoisoindol-8-ylidene)-4-methoxybenzamide (4ab)**

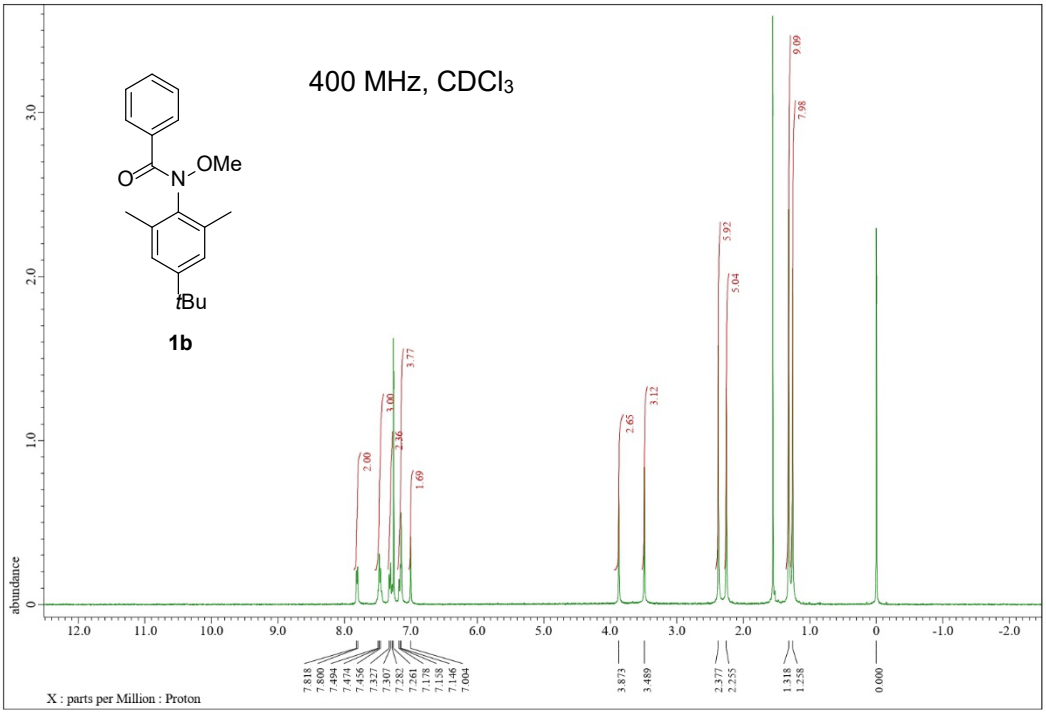
Colorless solid. 29.8 mg (0.058 mmol, 58% yield). Mp : 198.7 °C. R_f = 0.44 [hexane/EtOAc = 2:1 (v/v)]. $[\alpha]^{26.8}_D$ = +10.8 (*c* = 0.18, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.7 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.20 (d, *J* = 7.8 Hz, 2H), 6.91 (d, *J* = 8.7 Hz, 2H), 5.80 (d, *J* = 1.4 Hz, 1H), 3.87 (s, 3H), 3.65 (dd, J = 8.5, 3.0 Hz, 1H), 3.61 (s, 1H), 3.14 (s, 3H), 3.03 (d, *J* = 8.7 Hz, 1H), 1.77 (s, 3H), 1.44 (s, 3H), 1.06 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.3, 176.9, 174.8, 173.9, 162.8, 152.9, 131.7, 130.5, 129.1, 128.6, 126.8, 126.2, 124.9, 113.4, 78.8, 55.4, 49.6, 48.6, 46.9, 43.4, 40.9, 34.2, 29.7, 21.8, 17.9. IR (neat) 2953, 2373, 2352, 2373, 2321, 1713, 1659, 1602, 1543, 1509, 1374, 1315, 1253, 1220, 1167, 1112, 1031, 772 cm^{-1}. HRMS (ESI) calcd. for $C_{31}H_{34}N_2O_5$ $(M+Na)^+$: 537.2360, found: 537.2360.

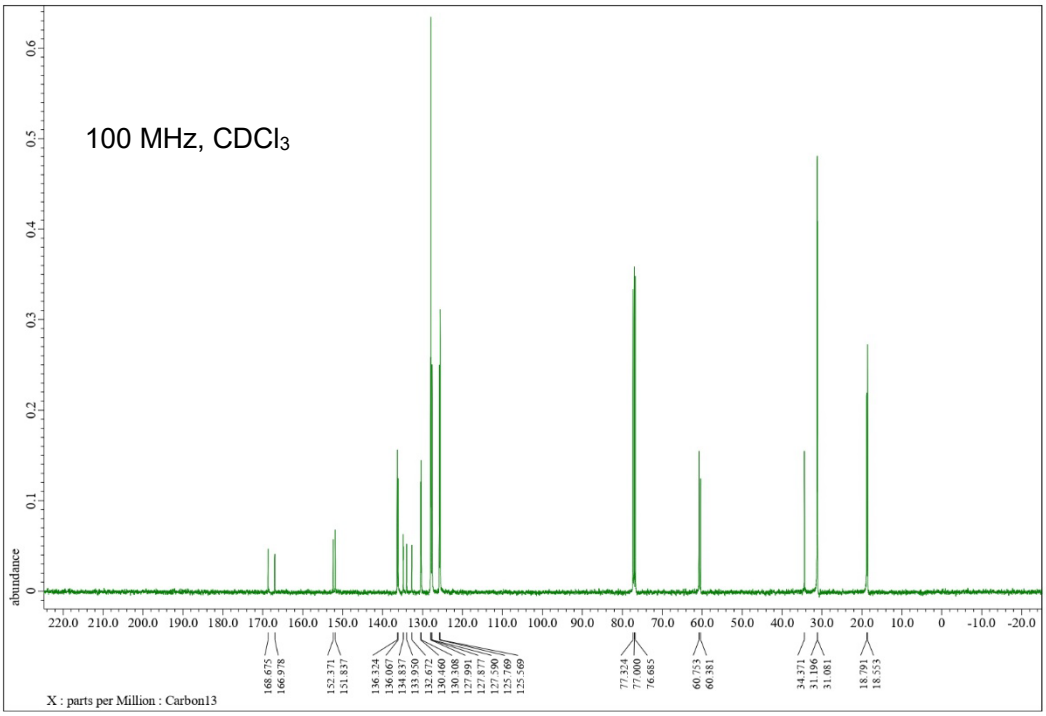
SFC analysis DAICEL CHIRALPAK IA-3/SFC 4.6 × 150 mm (CO_2/MeOH = 95/5, 3.0 ml/min, 254 nm, 40 ℃) 3.7 min (minor), 6.2 min (major), er = 84 : 16.

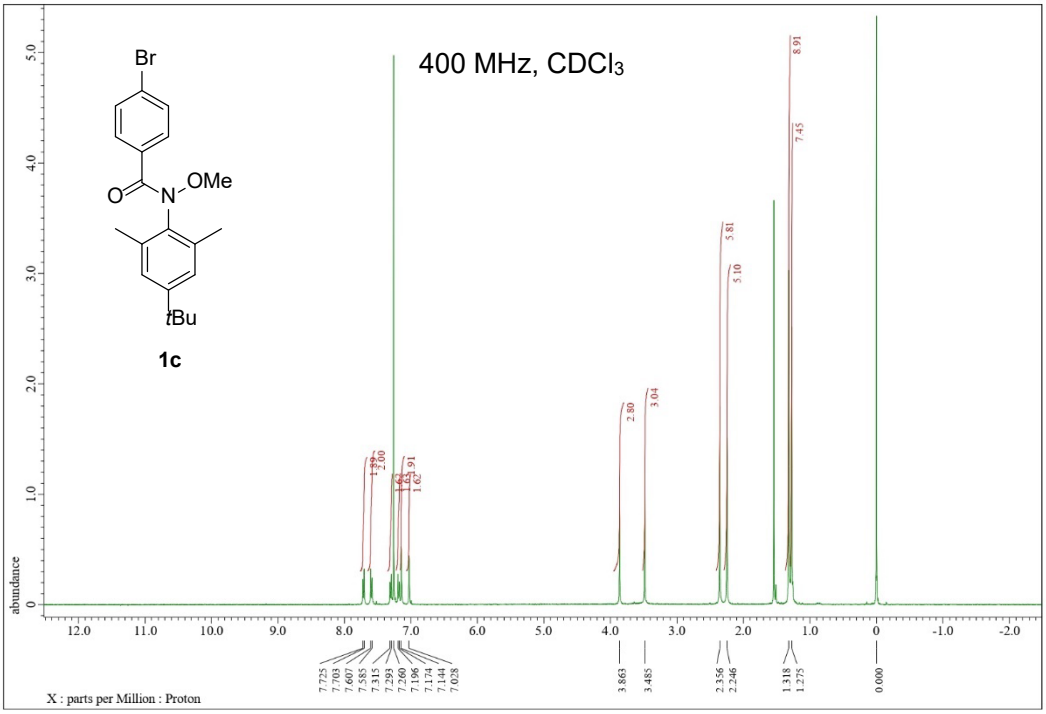
15. ^{1}H and ^{13}C NMR chart of 1

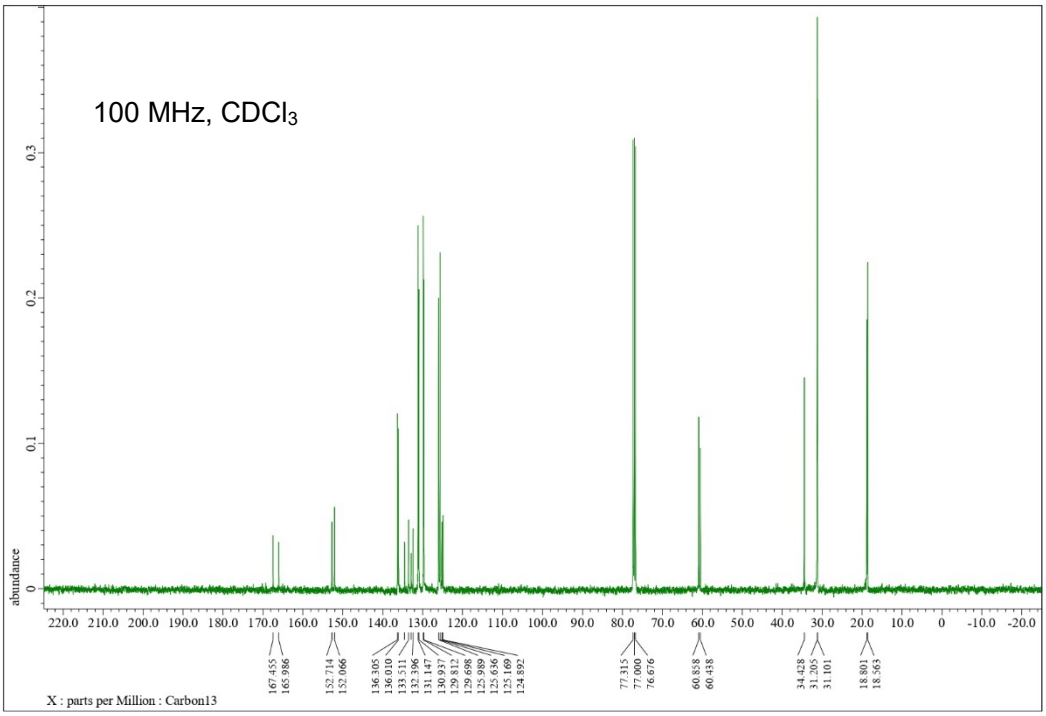


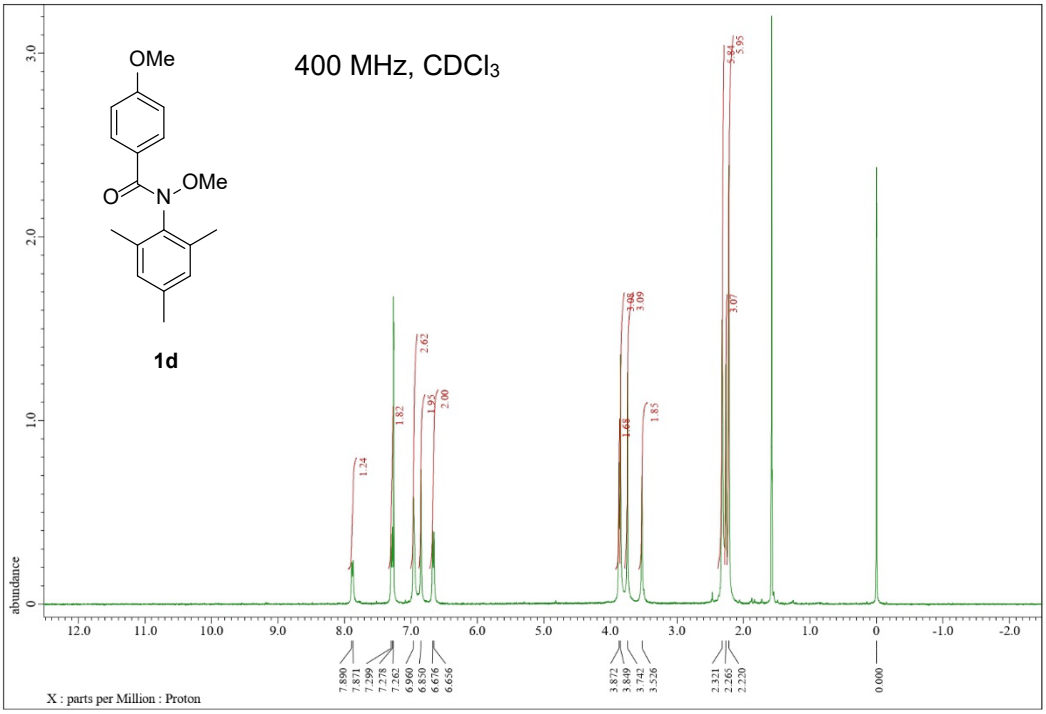


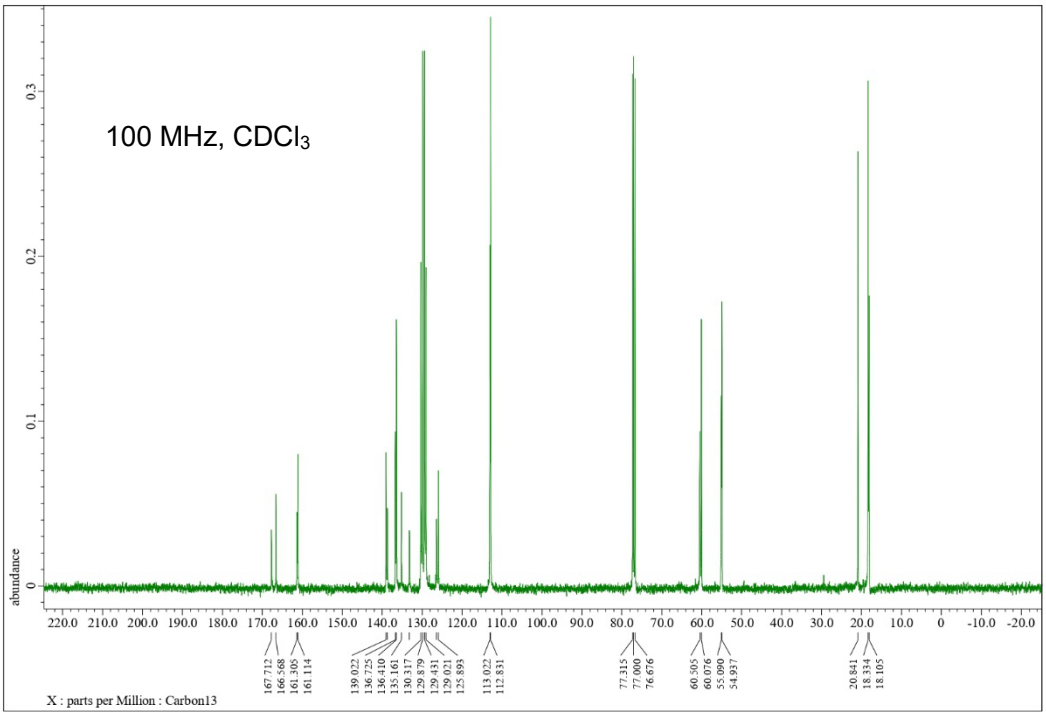

400 MHz, CDCl3
OMe
tBu
1b
abundance
X : parts per Million : Proton

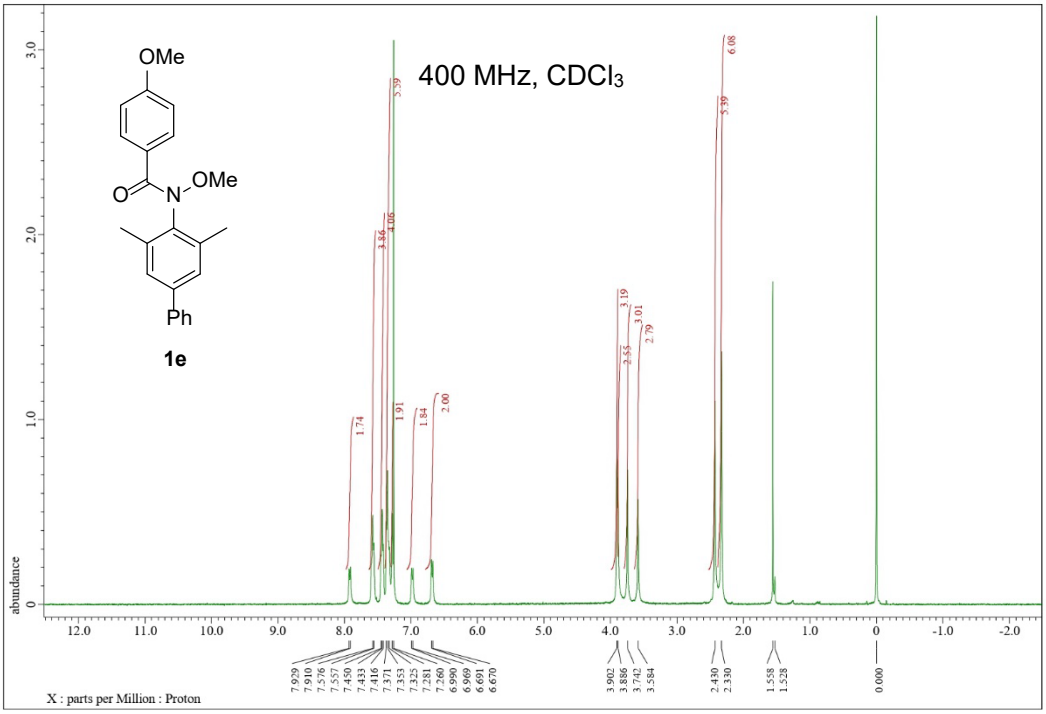

100 MHz, CDCl3
abundance
X : parts per Million : Carbon13

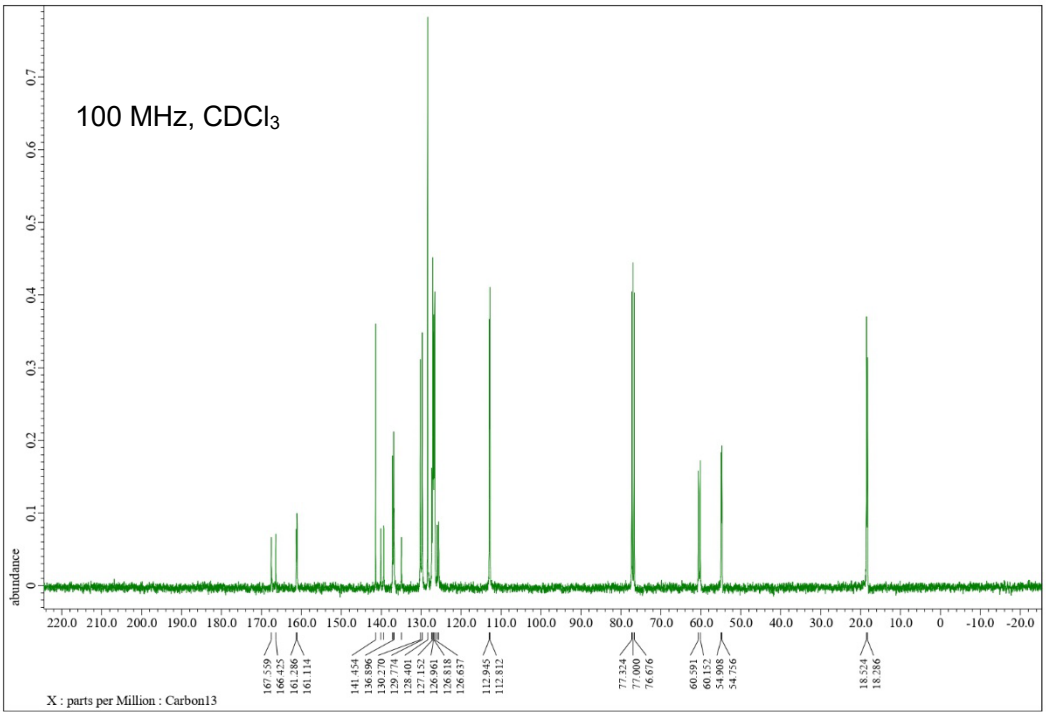

Br
O
N
OMe
tBu
1c
400 MHz, CDCl3
abundance
X : parts per Million : Proton

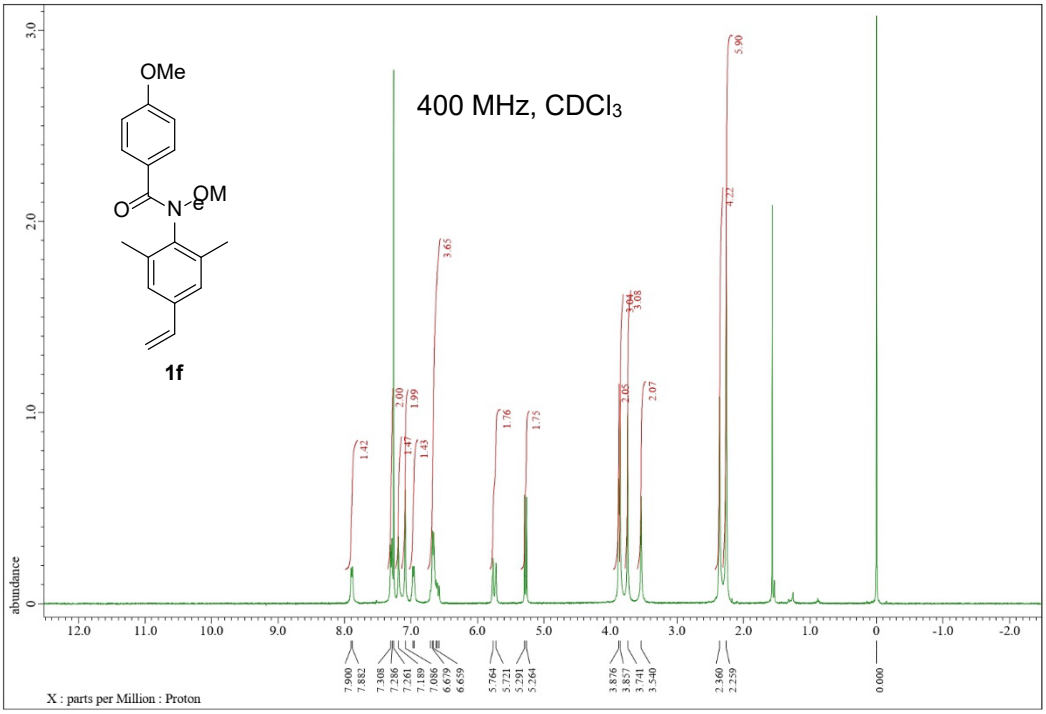

100 MHz, CDCl3
abundance
X : parts per Million : Carbon13

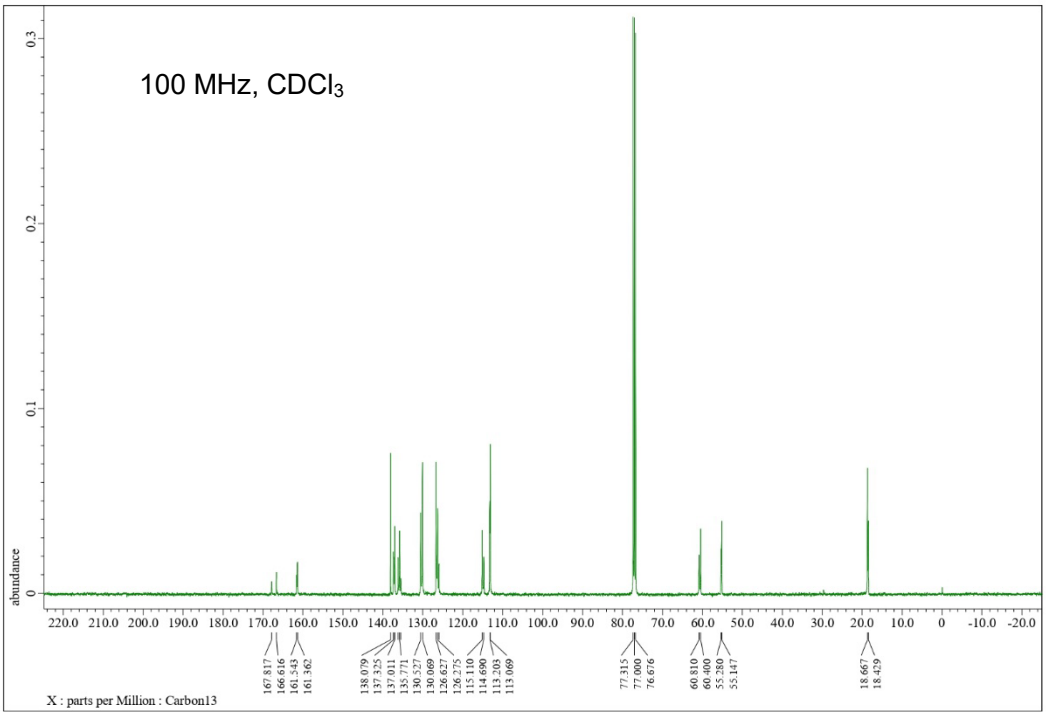

400 MHz, CDCl3
OMe
N
OMe
O
1d
abundance
X : parts per Million : Proton


100 MHz, CDCl3
abundance
X : parts per Million : Carbon13

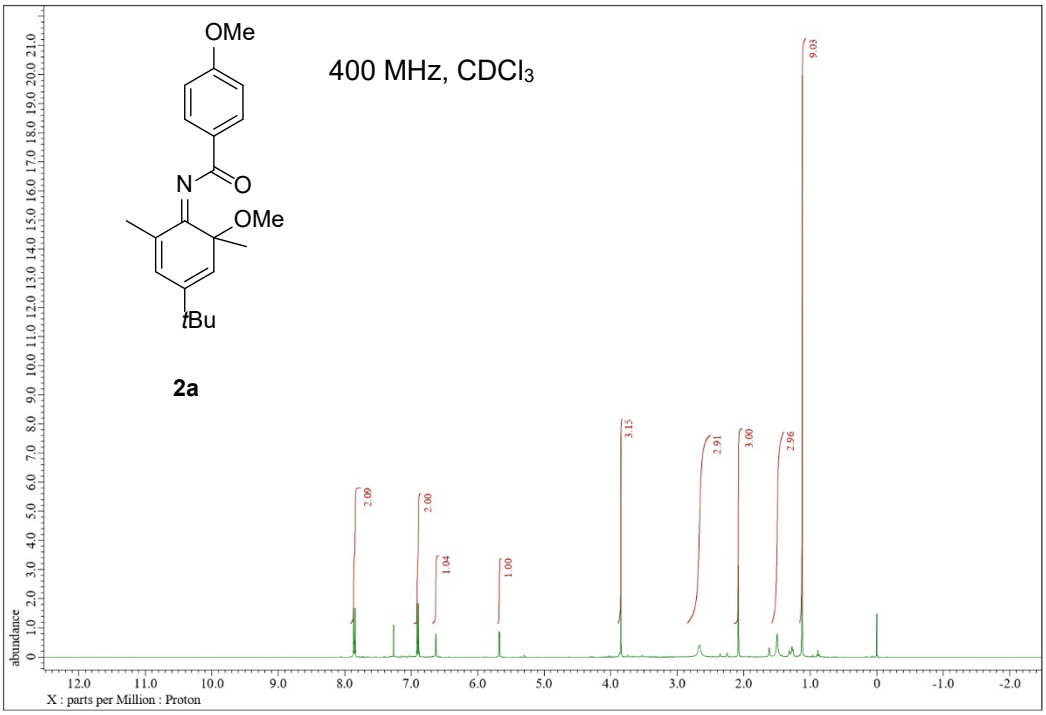

OMe
O
N
OMe
Ph
1e
400 MHz, CDCl3
abundance
X : parts per Million : Proton

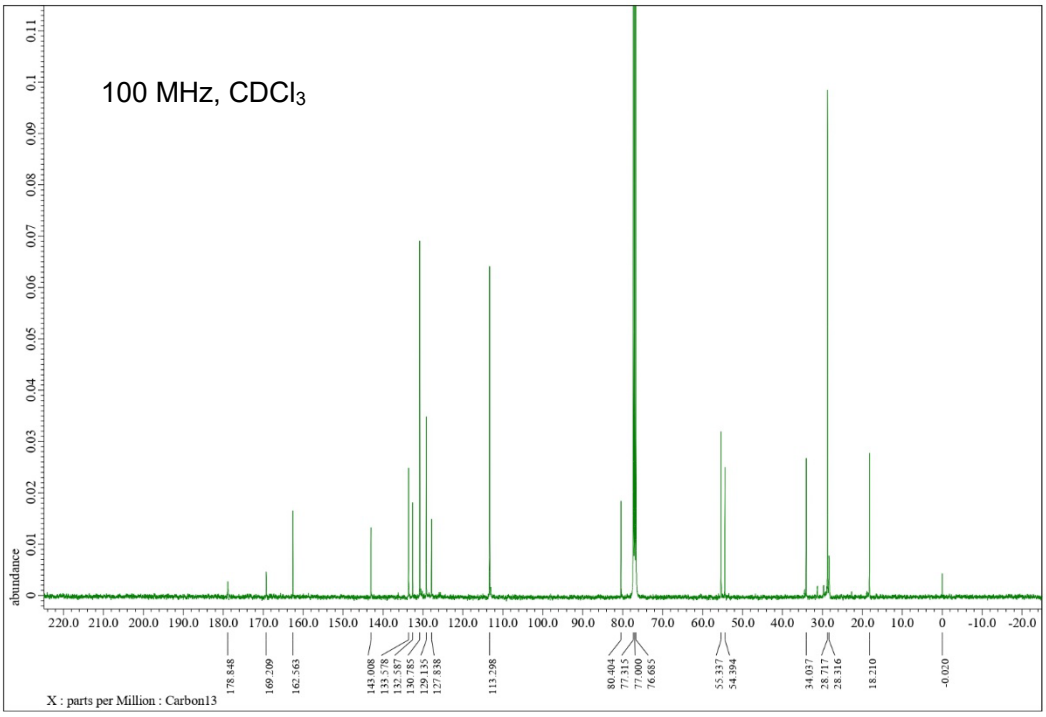

100 MHz, CDCl3
abundance
X : parts per Million : Carbon13

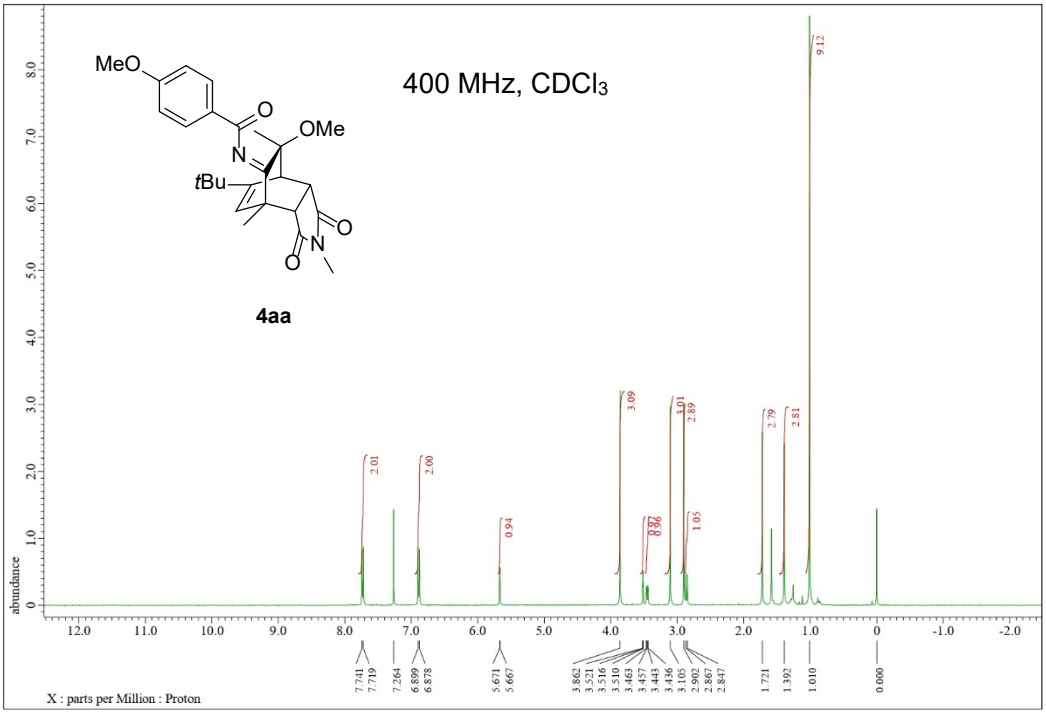

OMe
OM
1f
400 MHz, CDCl3
abundance
X : parts per Million : Proton

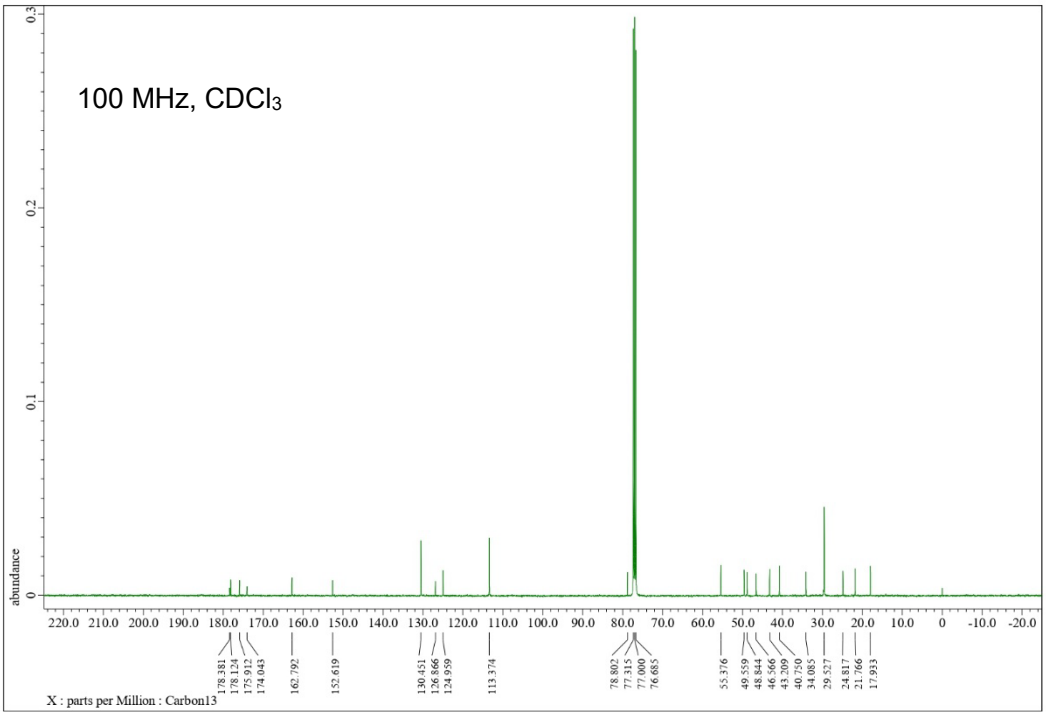

100 MHz, CDCl3
abundance
X : parts per Million : Carbon13

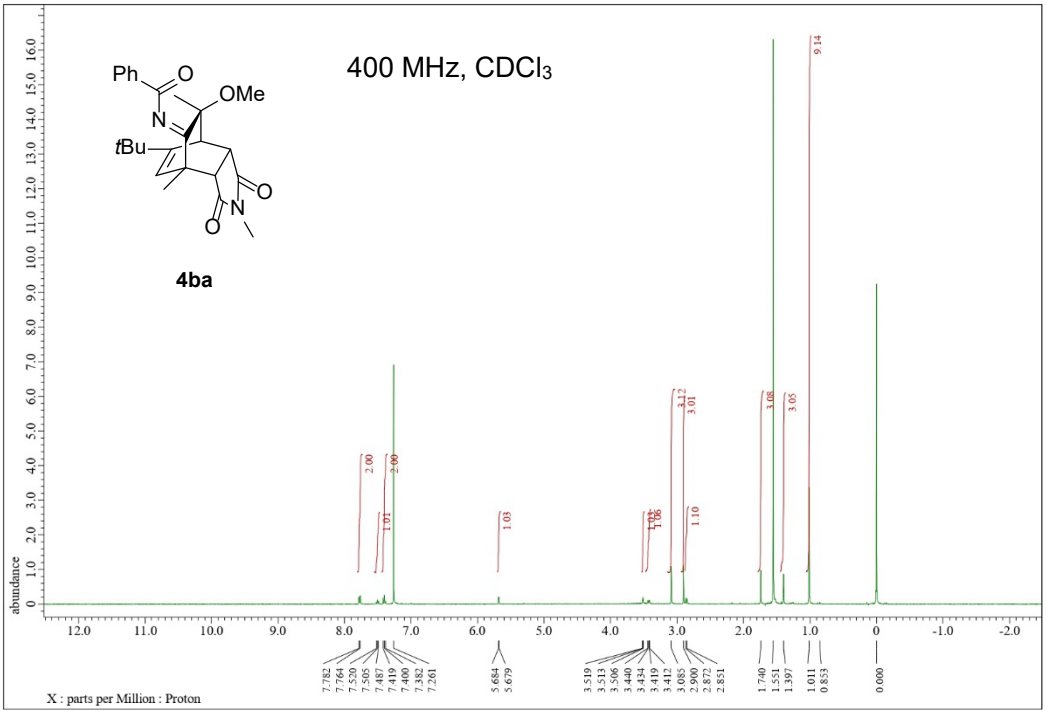
16. ^{1}H and ^{13}C NMR charts of 2 and 4

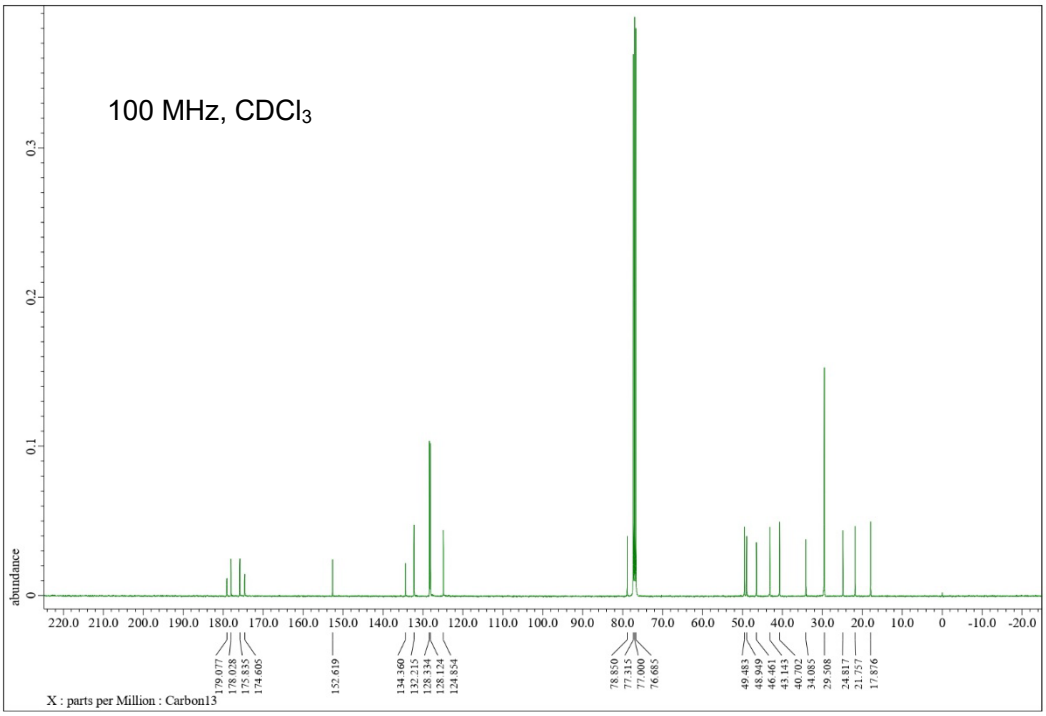


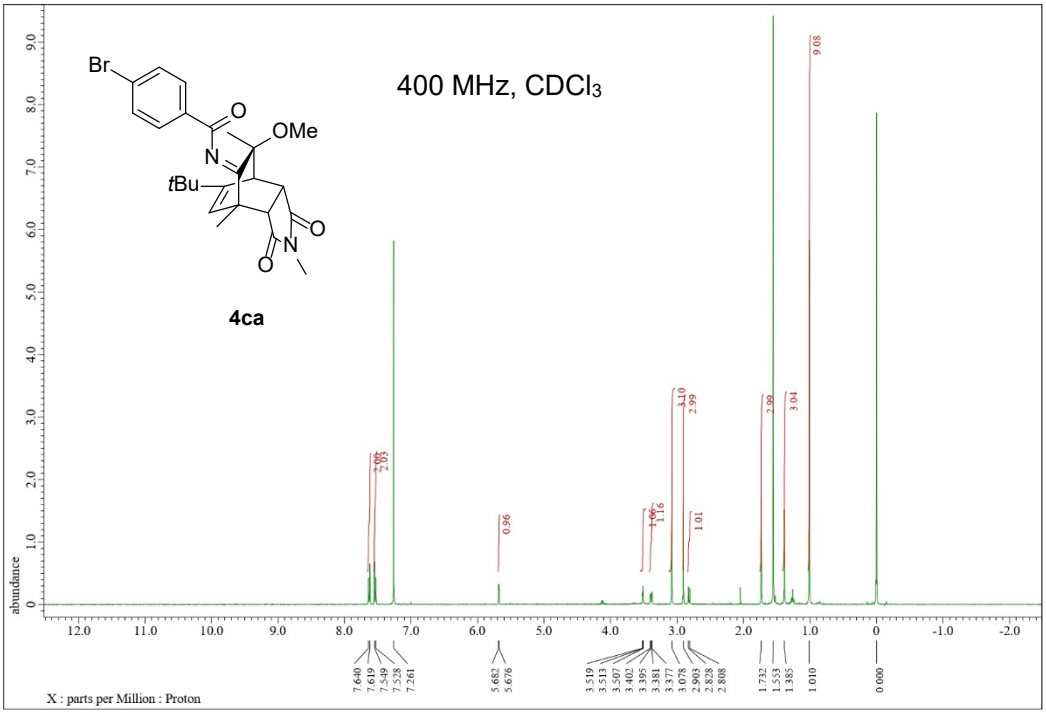


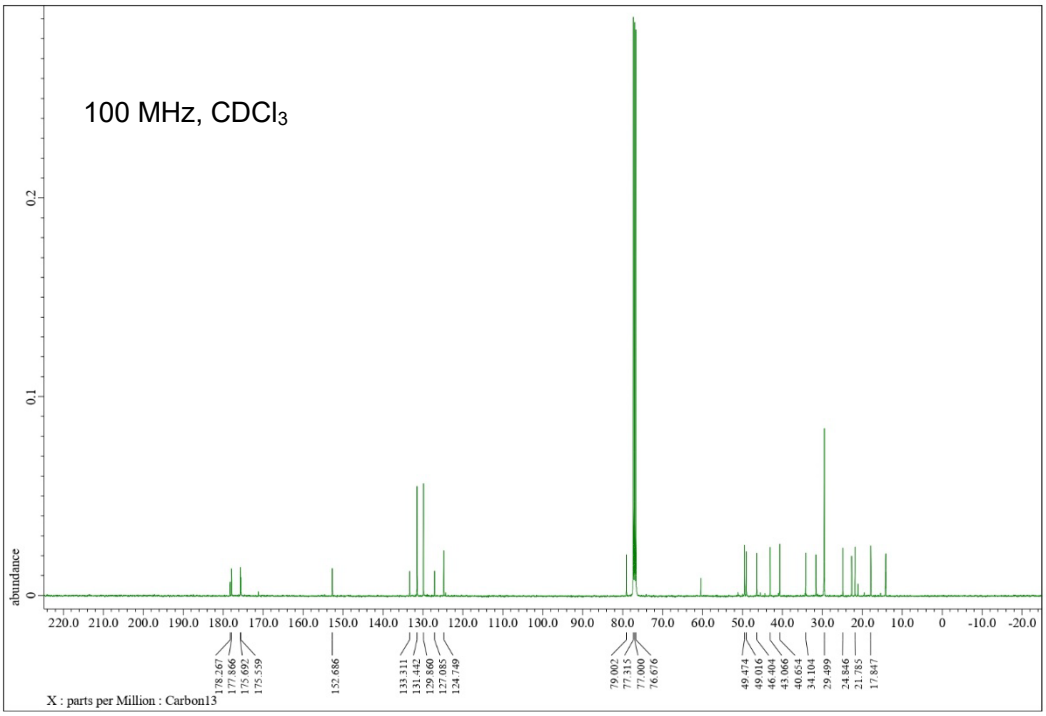

MeO
O
OMe
N
tBu
O
N
O
400 MHz, CDCl3
4aa
abundance
X : parts per Million : Proton

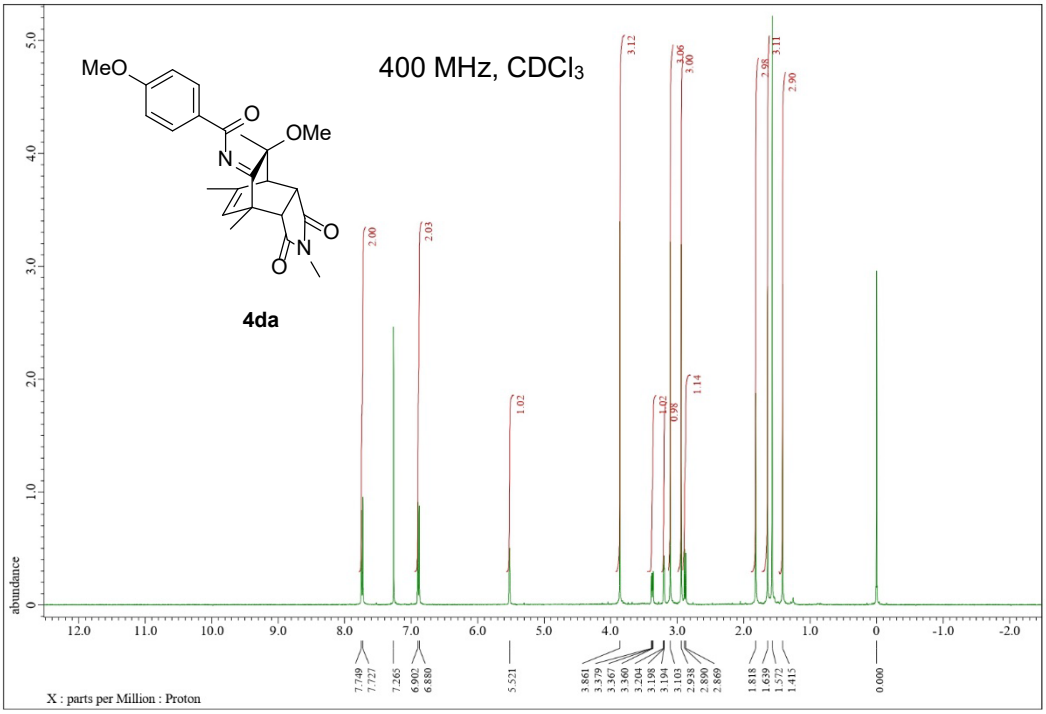

100 MHz, CDCl3
abundance
X : parts per Million : Carbon13

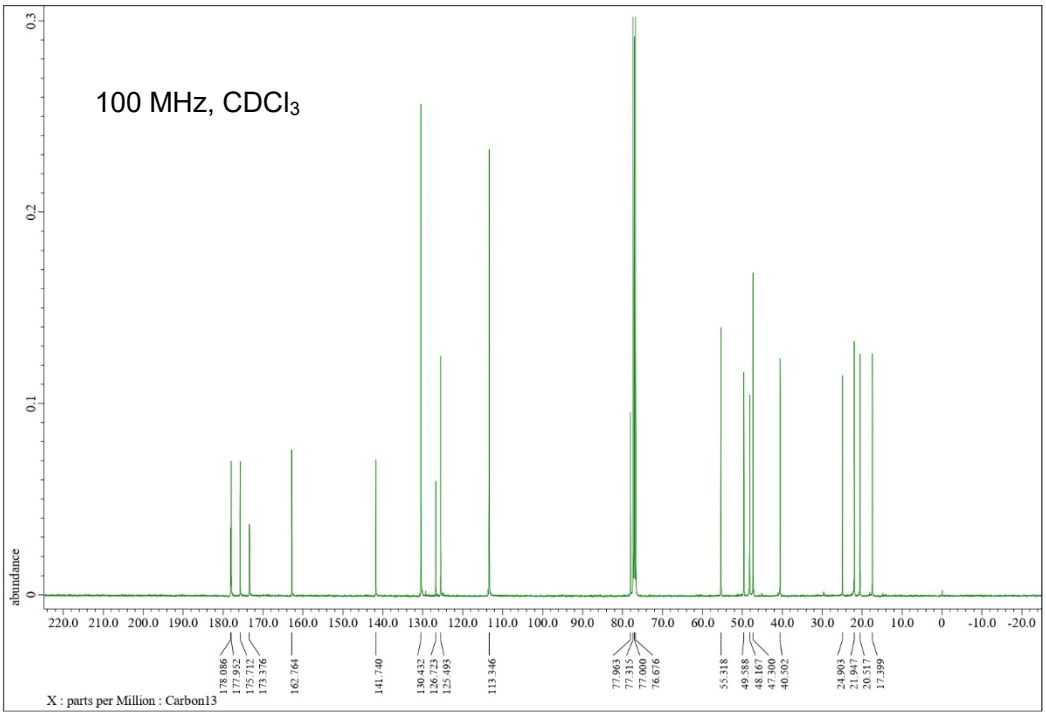

400 MHz, CDCl3
Ph
O
OMe
N
tBu
O
N
O
4ba
abundance
X : parts per Million : Proton

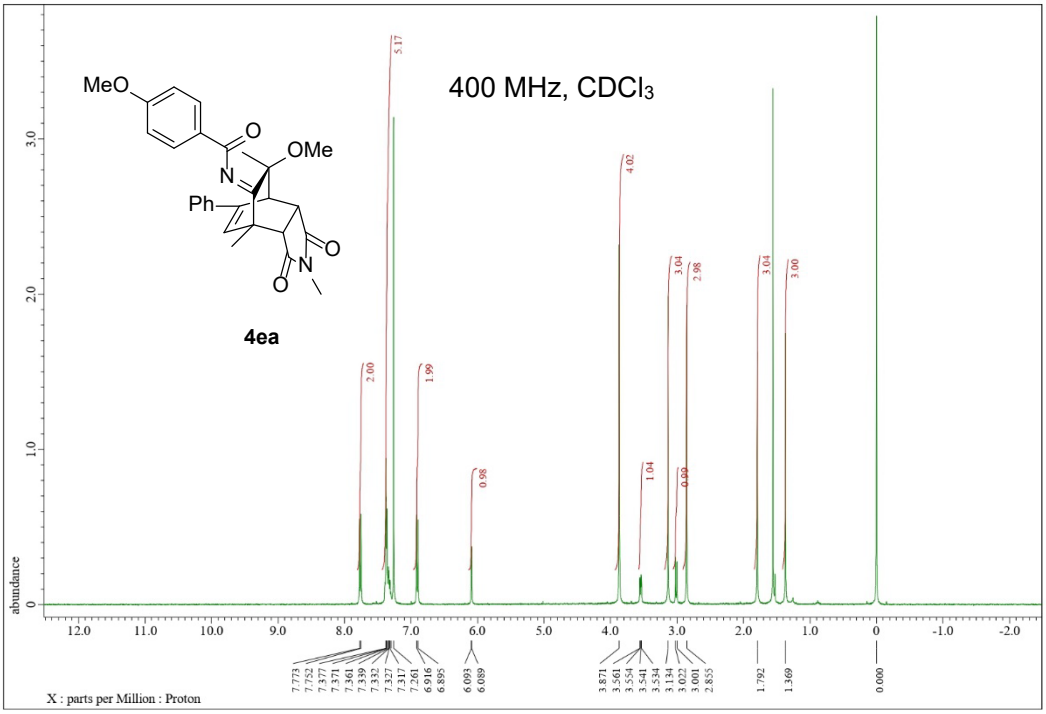

100 MHz, CDCl3
abundance
X : parts per Million : Carbon13

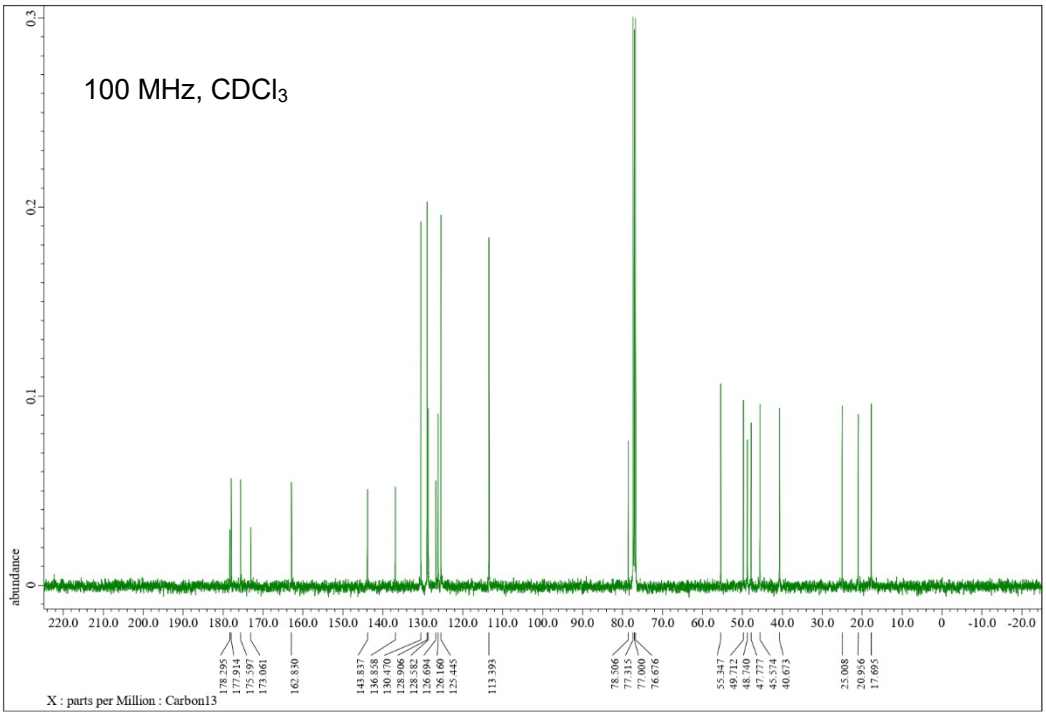

400 MHz, CDCl3
Br
O
OMe
N
tBu
O
N
O
4ca
abundance
X : parts per Million : Proton

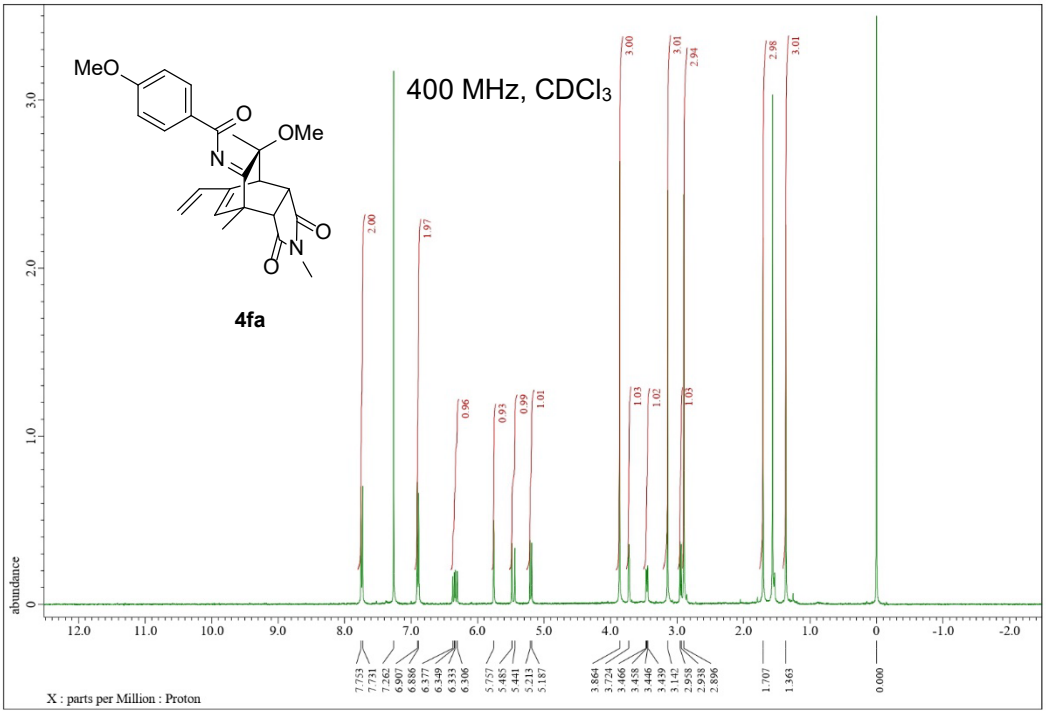

100 MHz, CDCl3
abundance
X : parts per Million : Carbon13

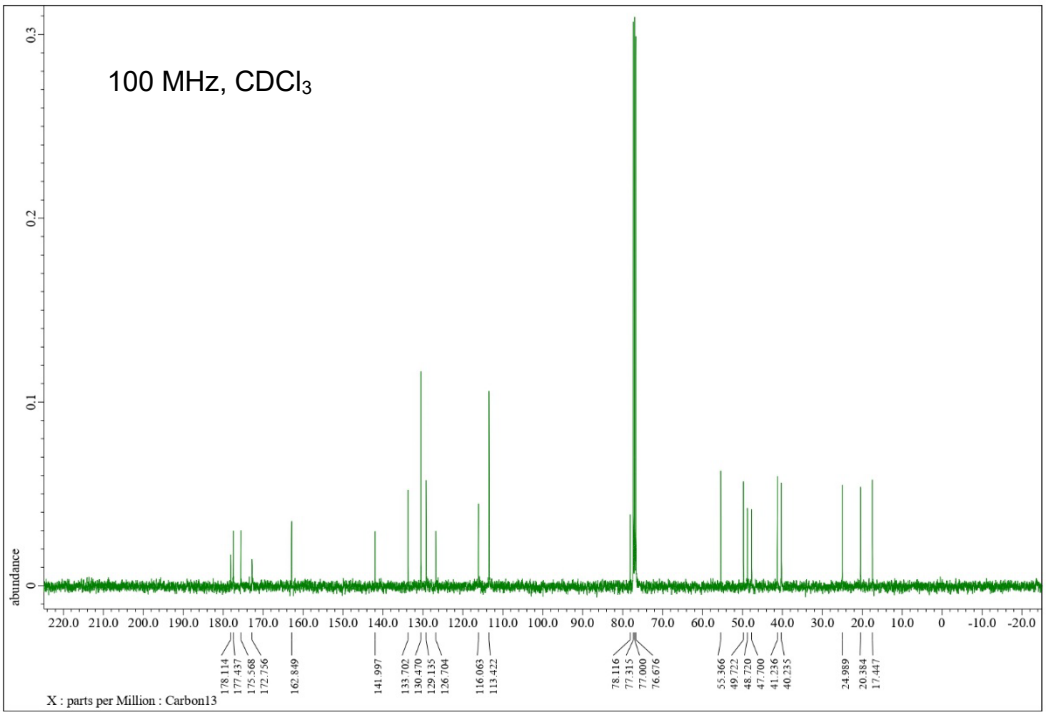

MeO
O
OMe
N
O
N
O
4da
400 MHz, CDCl3
abundance
X : parts per Million : Proton

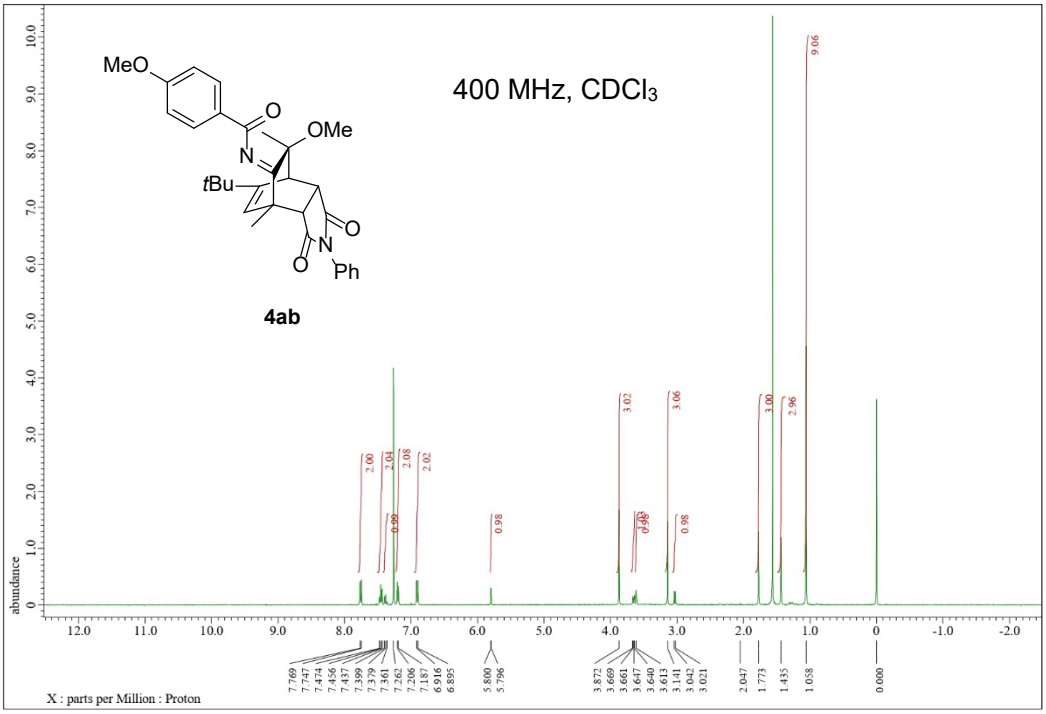

100 MHz, CDCl3
abundance
X : parts per Million : Carbon13

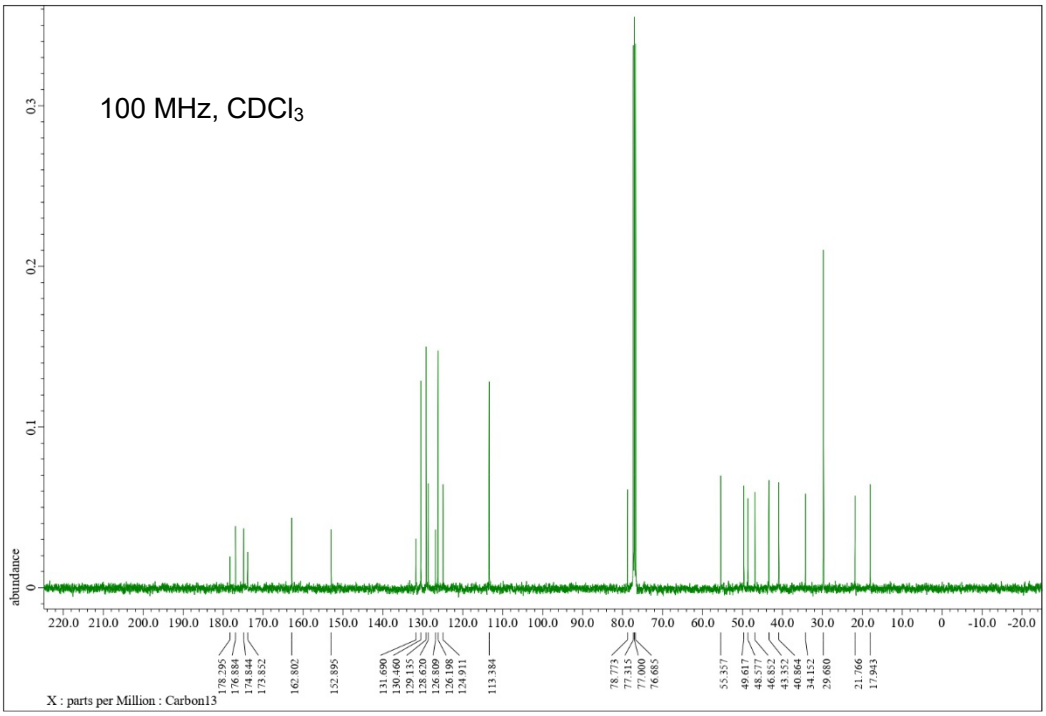

400 MHz, CDCl3
MeO
O
OMe
N
Ph
O
N
O
4ea
abundance
X : parts per Million : Proton


100 MHz, CDCl3
abundance
X : parts per Million : Carbon13

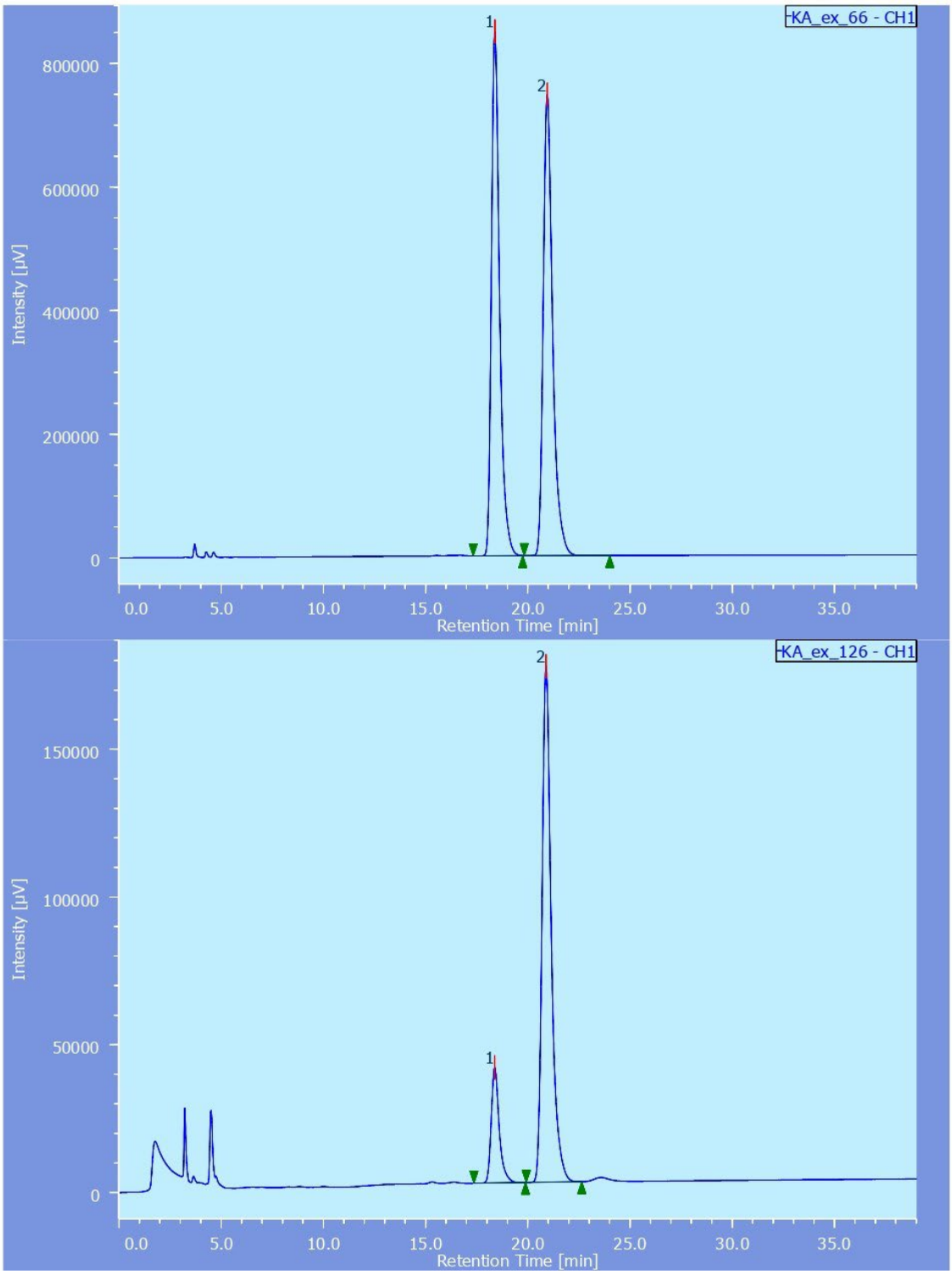

MeO
O
N
OMe
O
N
O
4fa
400 MHz, CDCl3
abundance
X : parts per Million : Proton


100 MHz, CDCl3
abundance
X : parts per Million : Carbon13

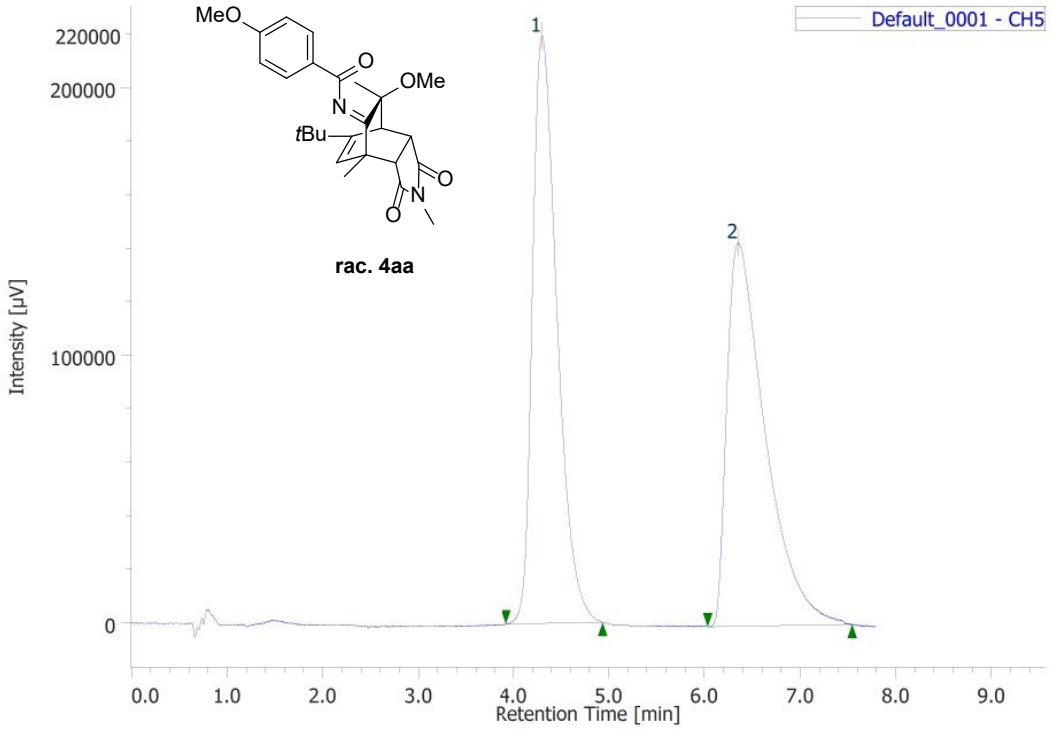

MeO
O
OMe
N
tBu
O
N
O
Ph
4ab
400 MHz, CDCl3
abundance
X : parts per Million : Proton

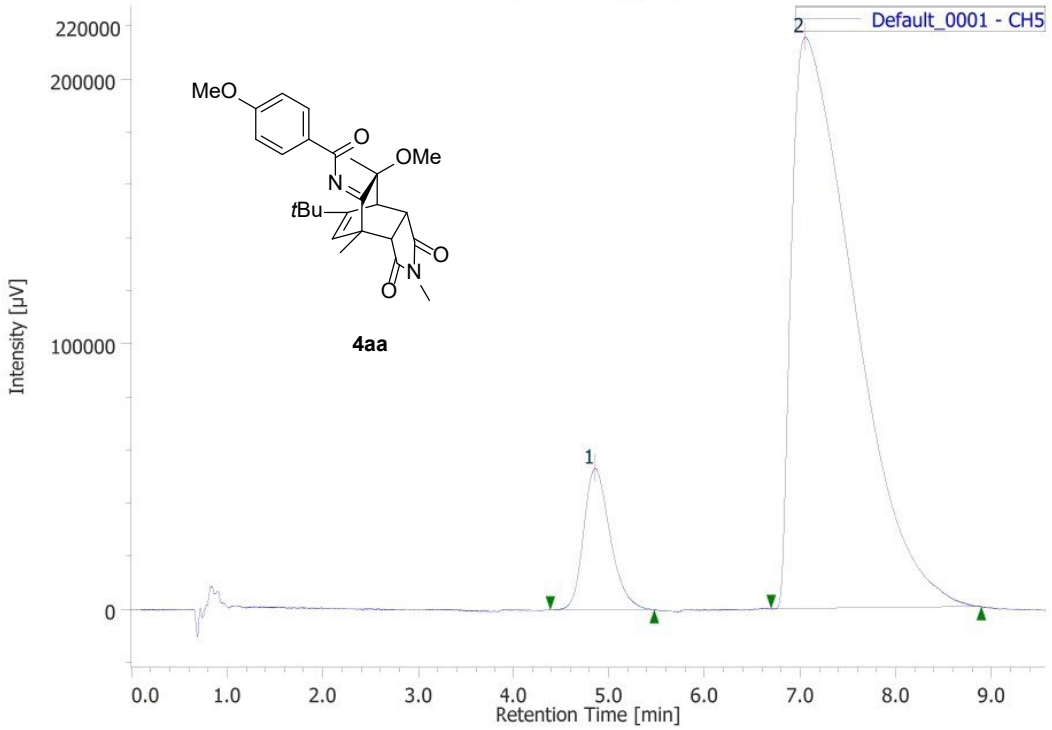

100 MHz, CDCl3
abundance
X : parts per Million : Carbon13

17. HPLC charts of 2 and 4

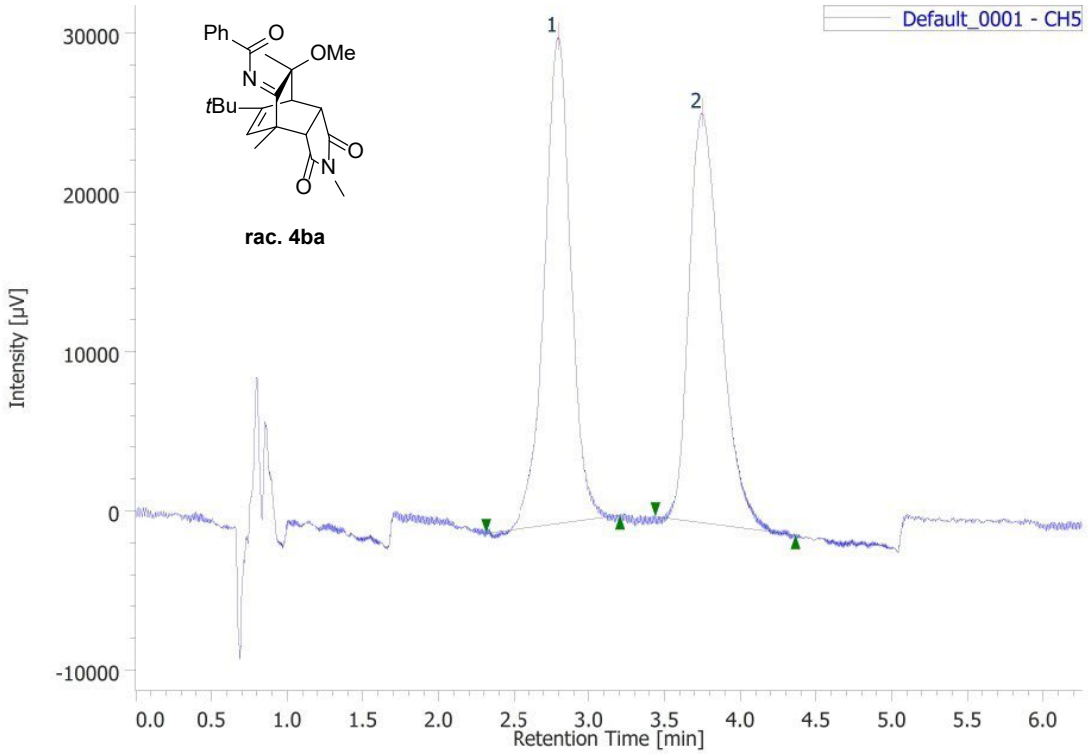


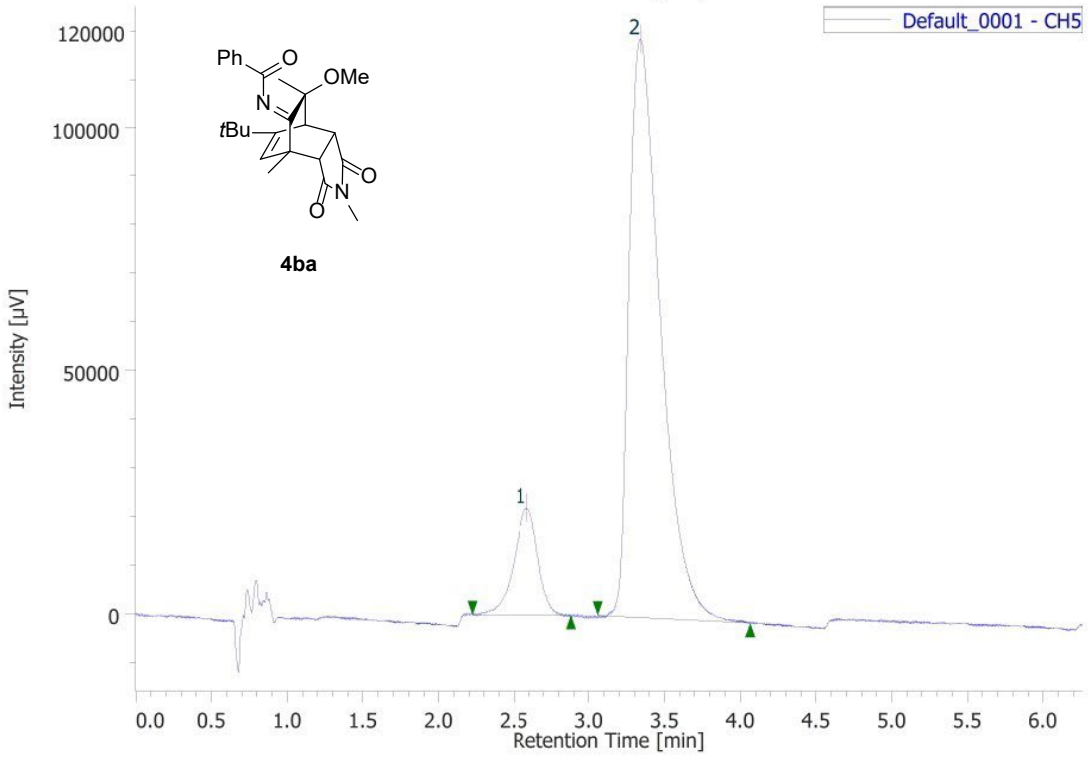
2a	Peak 1	Peak 2
Retention time (min)	18.375	20.883
Area (%)	16.401	83.599



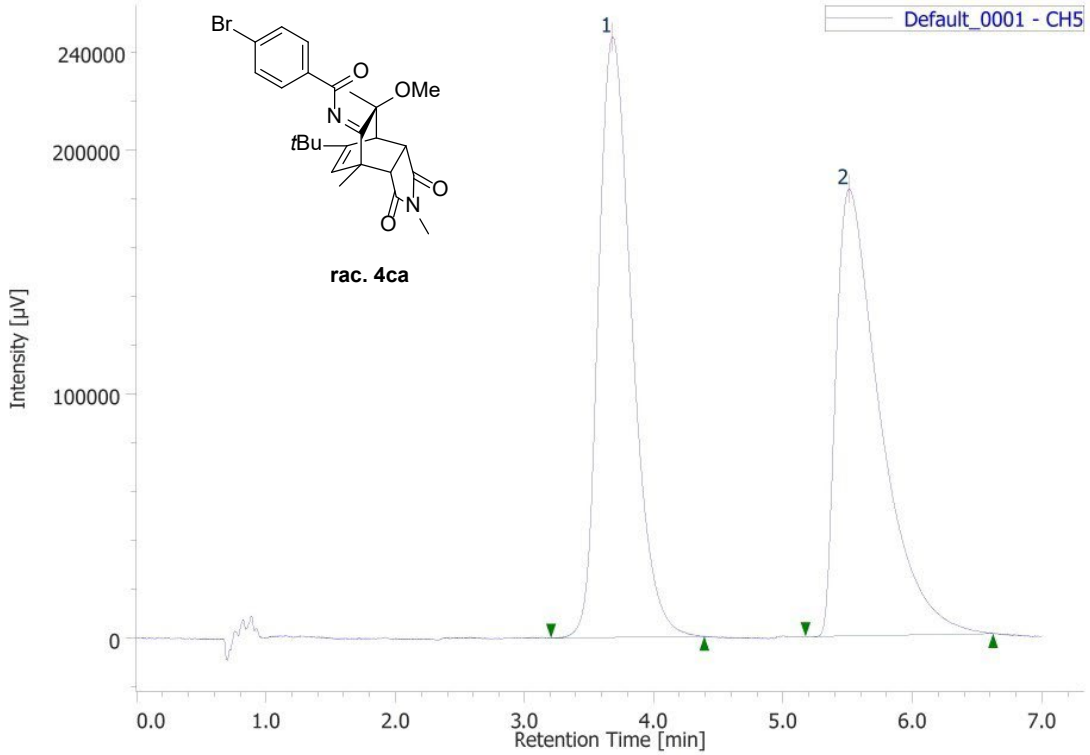


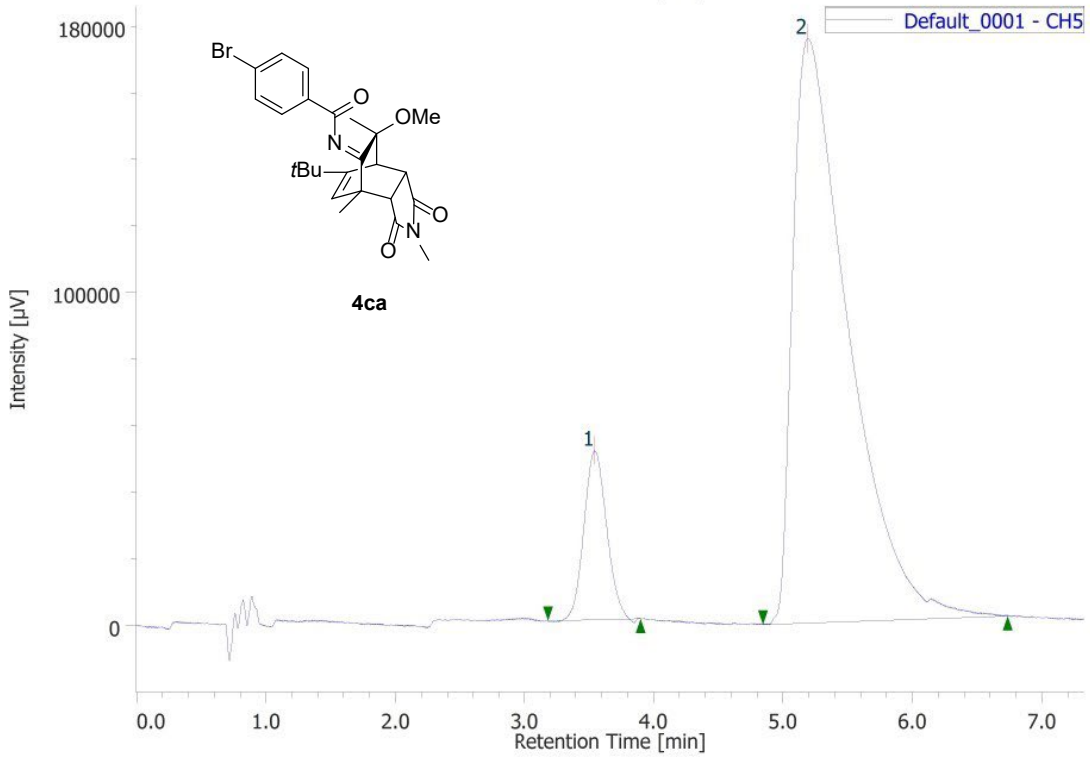
4aa	Peak 1	Peak 2
Retention time (min)	4.858	7.047
Area (%)	9.520	90.480



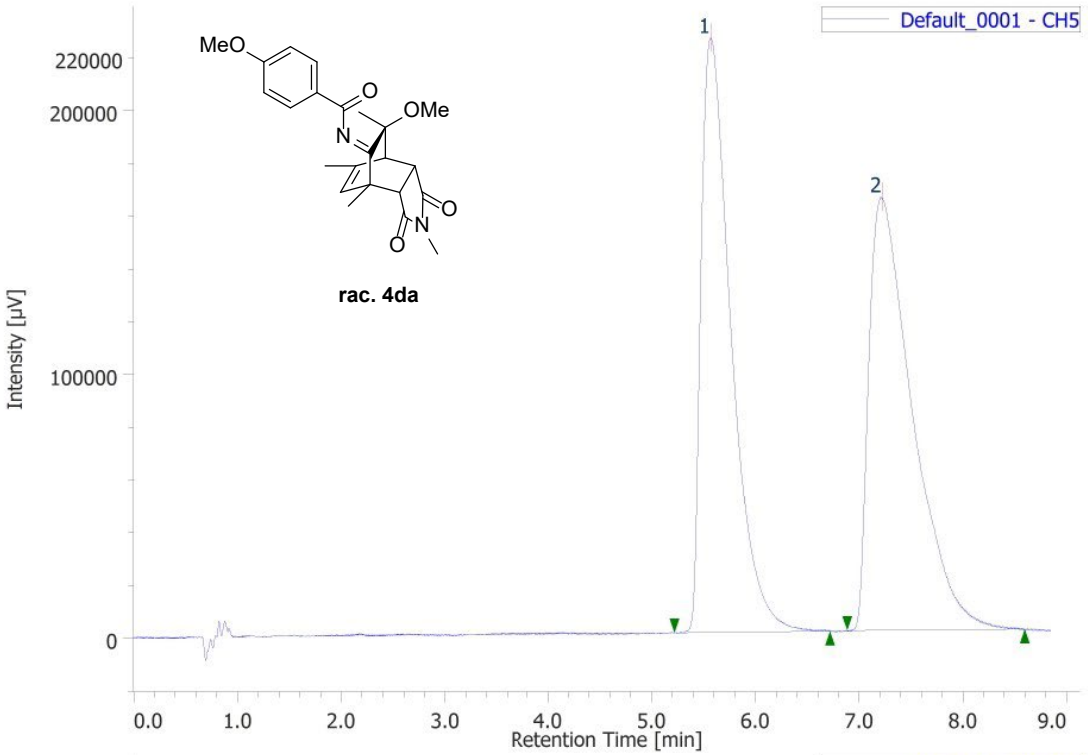


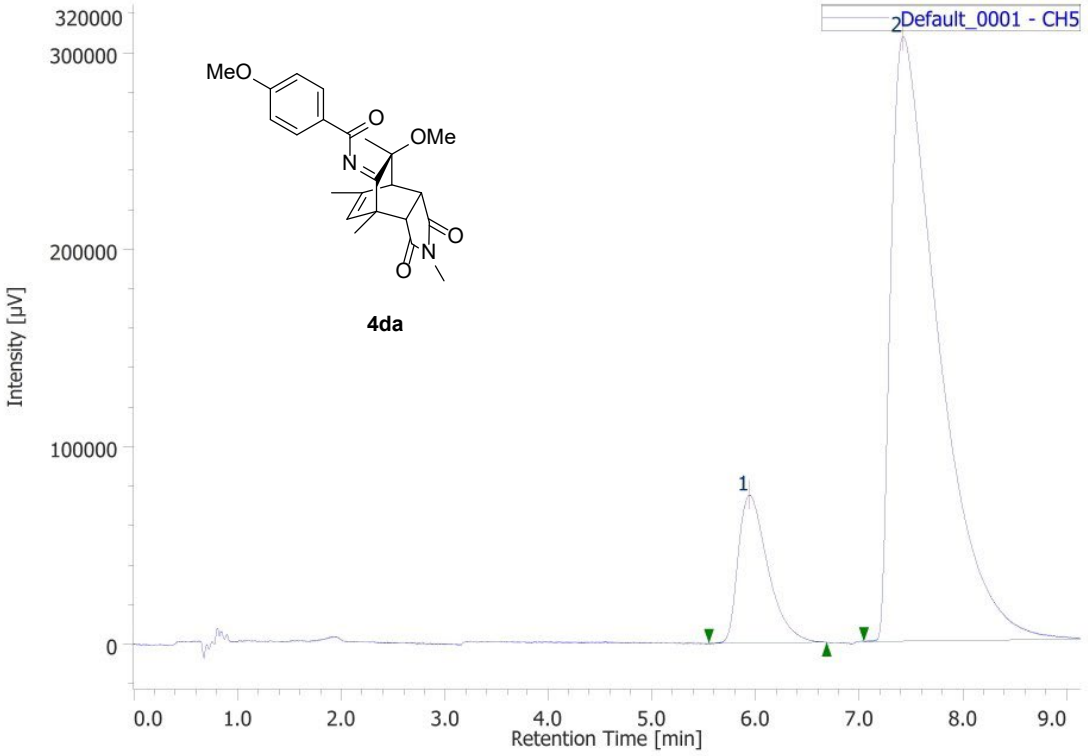
4ba	Peak 1	Peak 2
Retention time (min)	2.587	3.343
Area (%)	12.5451	87.455



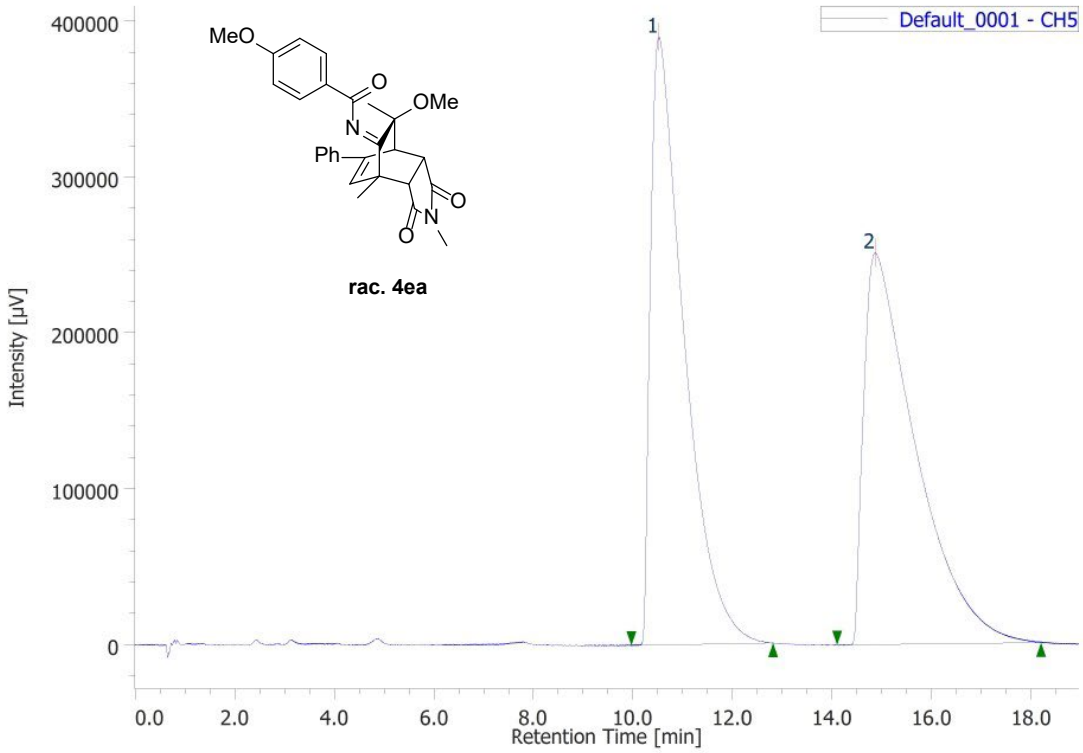


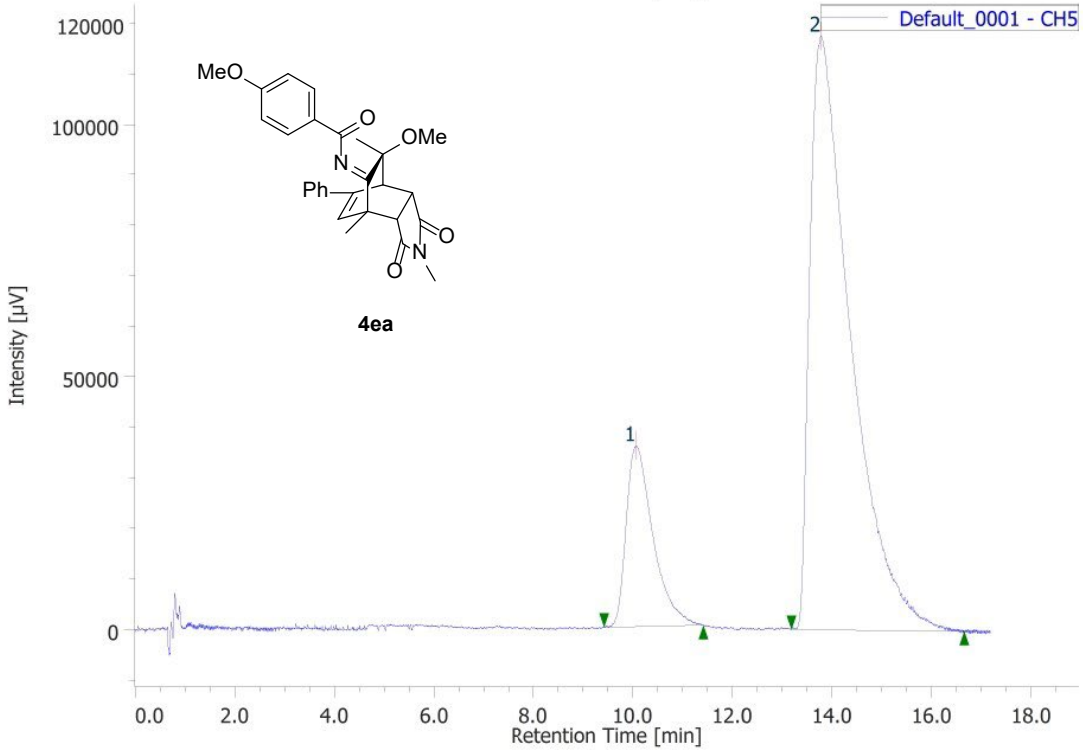
4ca	Peak 1	Peak 2
Retention time (min)	3.547	5.188
Area (%)	10.551	89.449



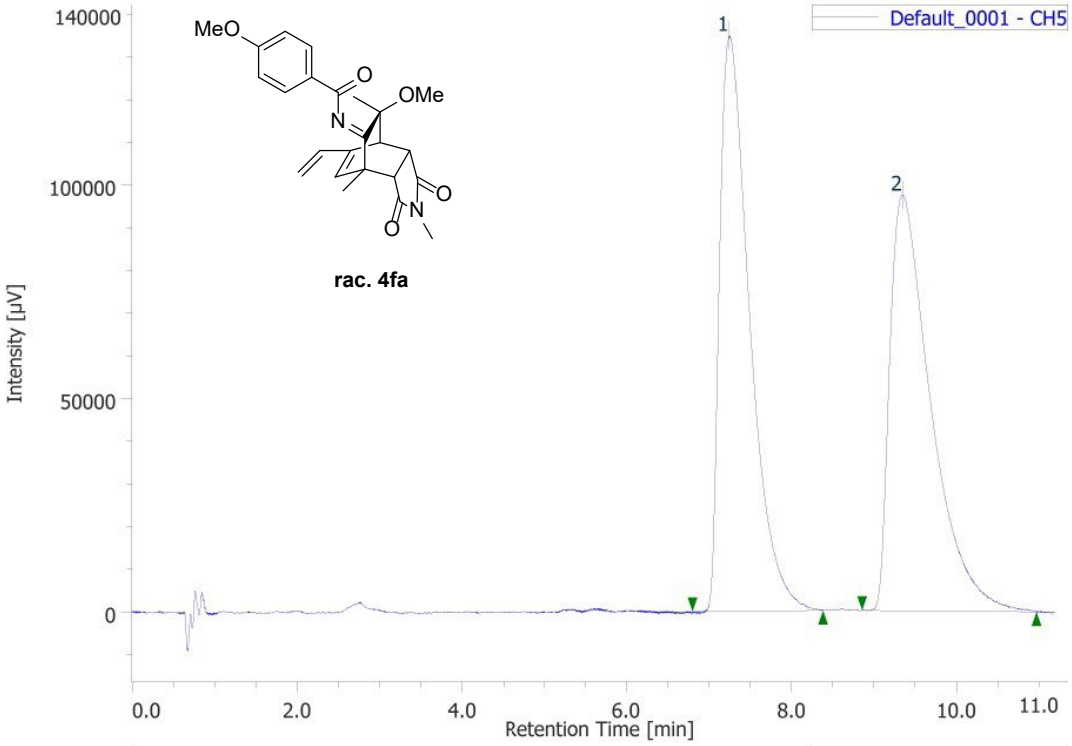


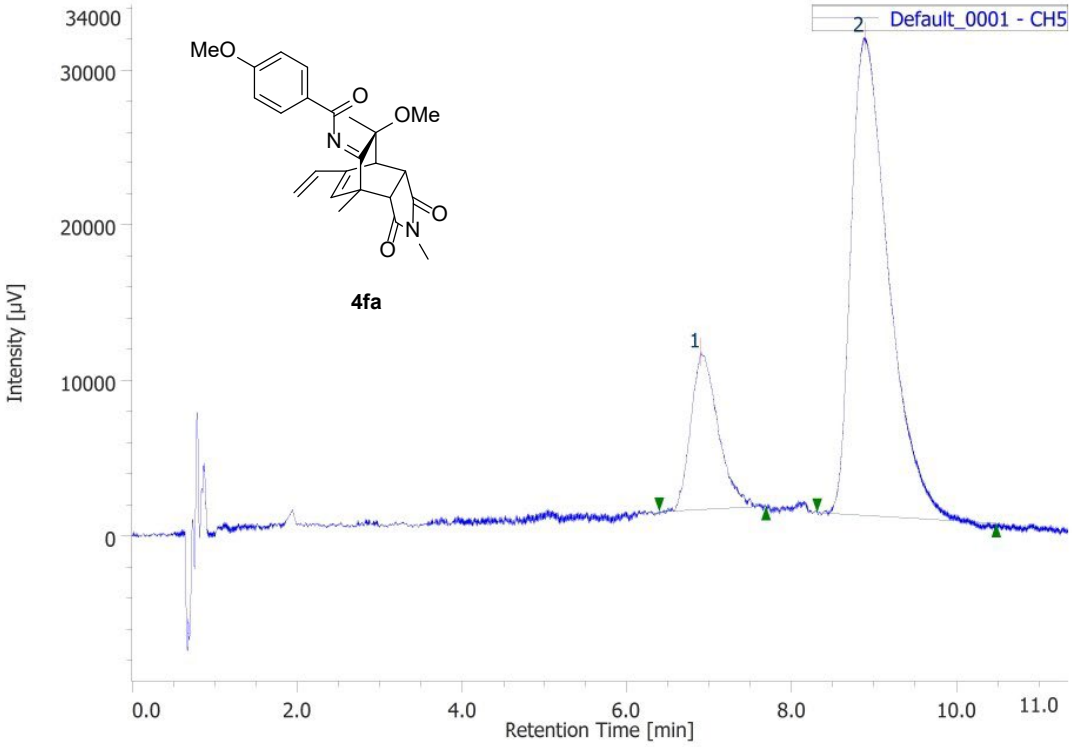
4da	Peak 1	Peak 2
Retention time (min)	5.943	7.420
Area (%)	13.150	86.850



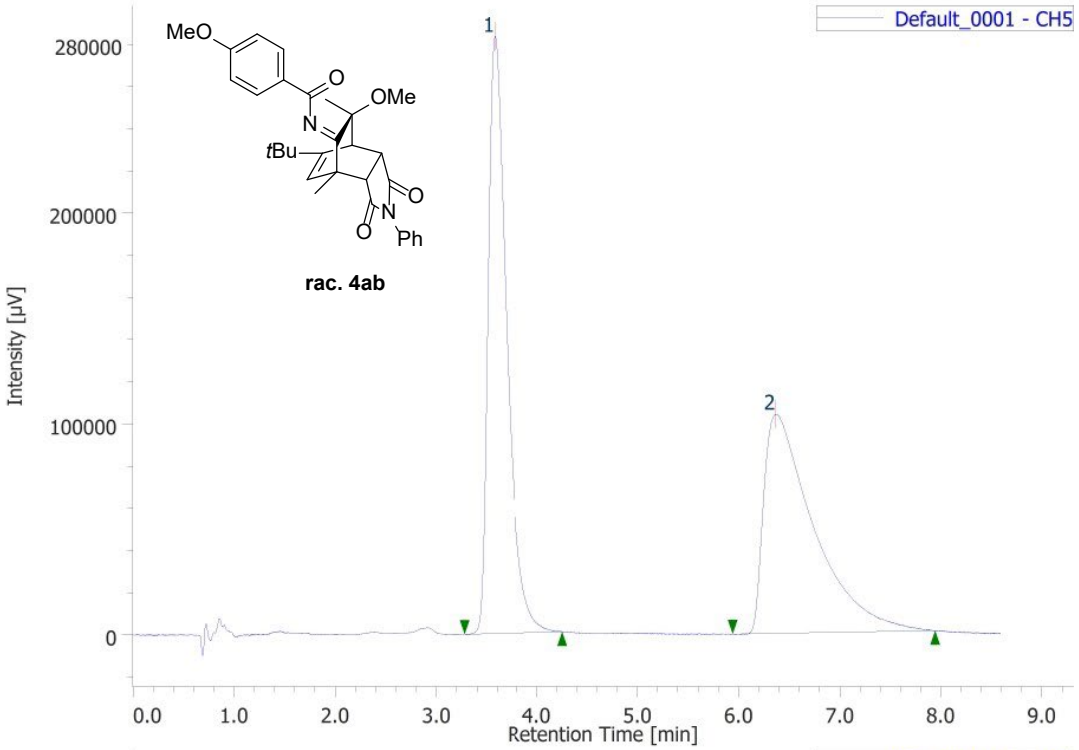


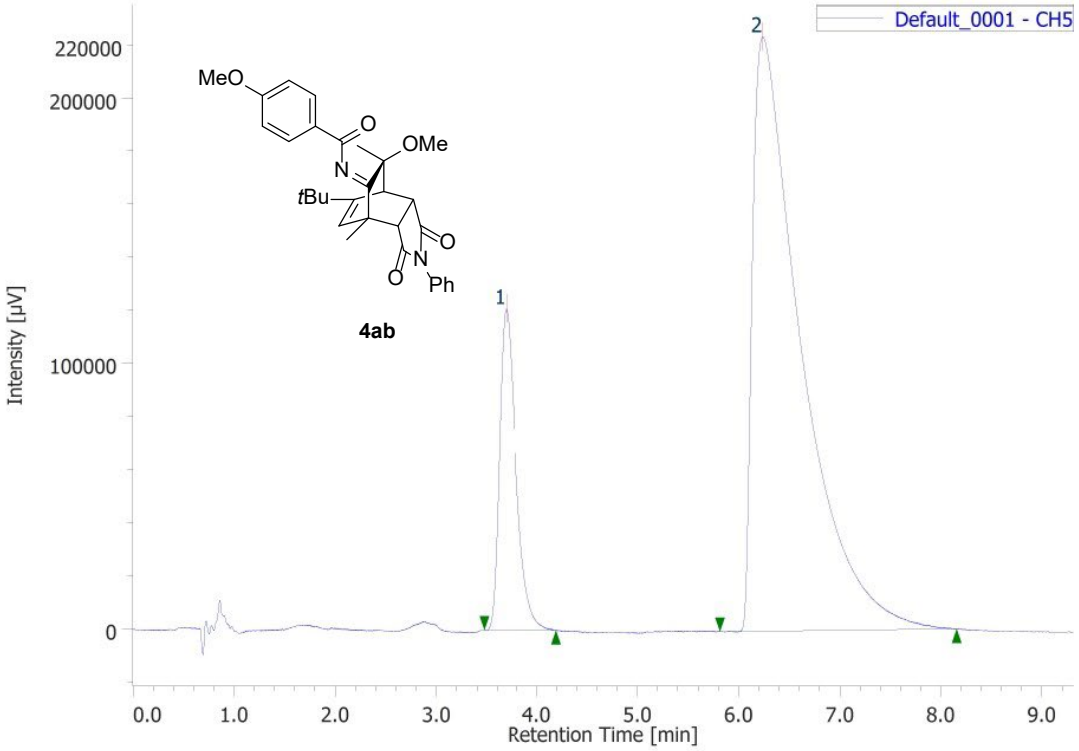
4ea	Peak 1	Peak 2
Retention time (min)	10.077	13.780
Area (%)	16.619	83.381





4fa	Peak 1	Peak 2
Retention time (min)	6.905	8.887
Area (%)	19.256	80.744





4ab	Peak 1	Peak 2
Retention time (min)	3.693	6.237
Area (%)	15.782	84.218