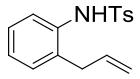
Supporting Information

Complete Reference 75:

[75] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, J. J.; Dannenberg, V. G.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzolez, C.; Pople, J. A.; Gaussian, Inc.: Wallingford, CT, 2004.

A. Experimental Procedures for Synthesis of Substrates

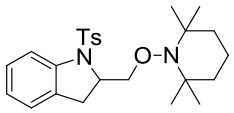
General Experimental Information: All reagents were used out of the bottle as purchased from the supplier without further purification unless otherwise specified. Solvents were purified using a commercial solvent filtration system. ^{1}H NMR spectra were recorded in $CDCl_3$ at 400 and 500 MHz. ^{13}C NMR spectra were recorded in $CDCl_3$ at 75 MHz. Spectra are reported in ppm relative to residual chloroform (7.26 ppm for ^{1}H NMRs and 77.0 ppm for ^{13}C NMRs). IR spectra were obtained neat using a Nicolet-Impact 420 FTIR. High resolution mass spectra were obtained at SUNY, Buffalo mass spectrometry facility on a ThermoFinnigan MAT XL spectrometer. Melting points are reported as uncorrected.



1

***N*-(2-Allyl-phenyl)-4-methyl-benzenesulfonamide (1)**

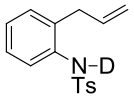
o-Allylaniline[1] (2.0 g, 15.0 mmol, 1 equiv) was dissolved in of dry CH_2Cl_2 (140 mL) and the solution was treated with *p*-toluenesulfonyl chloride (3.4 g, 18.0 mmol, 1.2 equiv) and pyridine (4.9 mL, 60.0 mmol, 4 equiv). The mixture was stirred at room temperature overnight, washed with 1 N HCl (80 mL) and extracted with CH_2Cl_2 (3 x 50 mL). The combined organic layers were washed with brine, dried over Na_2SO_4 and concentrated *in vacuo*. Flash chromatography of the resulting crude oil on SiO_2 (10% EtOAc in hexanes) afforded sulfonamide **1** (4.0 g, 95% yield) which matches the reported ^{1}H NMR data:[2] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, J = 8.0 Hz, 2H), 7.40 (d, J = 8.0 Hz, 1H), 7.23 (d, J = 8.0 Hz, 2H), 7.19 (m, 1H), 7.13-7.05 (m, 2H), 6.5 (b.s., 1H), 5.80 (m, 1H), 5.12 (dd, J = 9.0 Hz, 1.5 Hz, 1H), 4.95 (dd, J = 16.0 Hz, 1.5 Hz, 1H), 3.04 (d, J = 6.0 Hz, 2H), 2.40 (s, 3H).



2

2-(2,2,6,6-Tetramethyl-piperidin-1-yloxymethyl)-1-(toluene-4-sulfonyl)-2,3-dihyro-1*H*-indole (2)

The sulfonamide **1** (50.0 mg, 0.174 mmol, 1 equiv), $Cu(EH)_2$ (91.3 mg, 0.261 mmol, 1.5 equiv), NBu_4OAc (52.5 mg, 0.174 mmol, 1 equiv), TEMPO (81.5 mg, 0.522 mmol, 3 equiv) and toluene (1.74 mL) were combined in an oven-dried pressure tube equipped with magnetic stir bar. The reaction mixture was heated in an oil bath to 110 ^oC for 24 h. It was then cooled to room temperature, diluted with ether and filtered through a SiO_2 plug. Removal of the solvent *in vacuo* afforded the crude product. Purification by flash chromatography on SiO_2 (5-10% EtOAc in hexanes gradient) gave compound **2** (74.0 mg, 96% yield) which matches the reported characterization:[3] ^1H NMR (500 MHz, $CDCl_3$) δ 7.64 (d, J = 8.0 Hz, 1H), 7.54 (d, J = 8.0 Hz, 2H), 7.14-7.20 (m, 3H), 6.94-7.06 (m, 2H), 4.34 (m, 1H), 4.02 (m, 1H), 3.94 (m, 1H), 2.75-2.85 (m, 2H), 2.35 (s, 3H), 1.38-1.50 (m, 5H), 1.27 (m, 1 H), 1.26 (s, 3H), 1.18 (s, 3H), 0.98 (s, 3H), 0.87 (s, 3H).

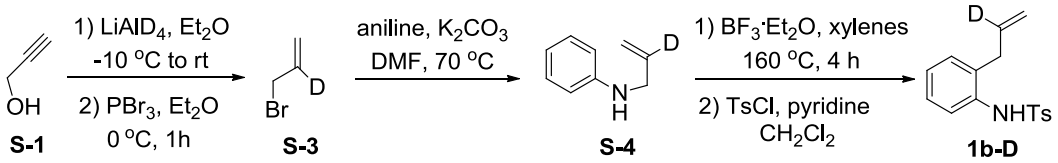


1a-D

Synthesis of deuterated substrate (1a-D)

The *N*-tosyl-*o*-allylaniline (0.30 g, 1.0 mmol, 1 equiv) was stirred in dry THF (5 mL). The solution was cooled to -78 ^oC and *n*-butyl lithium (1.6 M in hexanes, 0.45 mmol, 1.3 equiv) was added dropwise via syringe. The reaction mixture was stirred for 15 min and D_2O (3 mL) was added. The resulting solution was allowed to warm to room temperature and was stirred for another 30 minutes. The mixture was extracted with dry Et_2O (2 x 3 mL) and the combined organic layer was dried with Na_2SO_4 and concentrated *in vacuo* to give a brown solid (175 mg, 58% yield). ^1H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, J = 8.0 Hz, 2H), 7.40 (d, J = 8.0 Hz, 1H), 7.19-7.23 (m, 3H), 7.13-7.05 (m, 2H), 5.76 (m, 1H), 5.05 (d, J = 9.5 Hz, 1H), 4.90 (d, J = 17.0 Hz, 1H), 3.02 (d, J = 6.0 Hz, 2H), 2.40 (s, 3H).

Synthesis of deuterated substrate (1b-D)



A solution of $LiAlD_4$ (3.6 g, 85.6 mmol, 1.6 equiv) in dry Et_2O (285 mL) was cooled to -10 ^oC and a solution of propargyl alcohol (3.0 g, 53.5 mmol, 1 equiv) in Et_2O (33 mL) was added via addition funnel over 30 min. The resulting solution was warmed to room temperature and stirred for 14 h. The mixture was cooled to 0 ^oC and was quenched slowly with H_2O (4.0 mL). The solution was stirred for another 15 min and then 15% aqueous NaOH solution (4.0 mL) and H_2O (4.0 mL) were added. The white slurry was filtered through a short pad of Celite and was washed

with Et_2O (300 mL). The filtrate was concentrated *in vacuo* to give the crude allyl-2-d_1 alcohol[4] **S-2** as a yellow oil (3.0 g). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.22 (s, 1H), 5.09 (s, 1H), 4.08 (s, 2H), 3.0 (br.s, 1H).

The crude allyl-2-d_1 alcohol (3.0 g, 50.8 mmol, 1 equiv) was added to a stirring solution of PBr_3 (2.4 mL, 25.5 mmol, 0.5 equiv) in Et_2O (21 mL) dropwise at 0 ^{o}C. The resulting solution was stirred at 0 ^{o}C for 1 h and then carefully quenched by the addition of brine (12 mL). The layers were separated and the combined organic extracts were washed with a saturated solution of $NaHCO_3$, brine and dried over Na_2SO_4. Excess solvent was removed via careful distillation (45-50 ^{o}C). The crude allyl-2-d_1 bromide **S-3** was obtained as colorless liquid (2.1 g, 32% yield over 2 steps).[5] ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.31 (s, 1H), 5.14 (s, 1H), 3.94 (s, 2H).

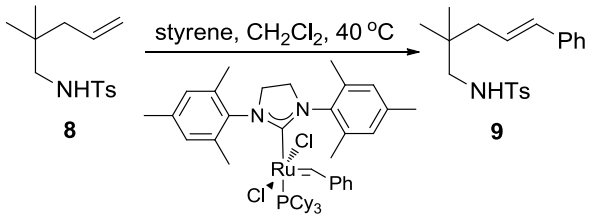
Into an oven-dried round bottom flask were added the crude allyl-2-d_1 bromide **S-3** (1.5 mL, 12.5 mmol, 1.0 equiv), aniline (4.5 mL, 37.0 mmol, 3.0 equiv), K_2CO_3 (5.0 g, 37.0 mmol, 3.0 equiv) and DMF (20 mL).[6] The flask was equipped with a stopper and the reaction mixture was heated to 70 °C overnight. The mixture was allowed to cool to room temperature and was washed with water (20 mL). The aqueous phase was extracted with Et_2O (3 x 20 mL). The combined organic layers were washed with brine, dried with Na_2SO_4 and concentrated *in vacuo*. Purification by flash chromatography on SiO_2 (10% EtOAc in hexanes) gave compound **S-4** (0.7 g, 45% yield). Data for **S-4**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18 (t, J = 7.5 Hz, 2H), 6.72 (t, J = 7.5 Hz, 1H), 6.64 (d, J = 8.0 Hz, 2H), 5.29 (s, 1H), 5.17 (s, 1H), 3.78 (s, 2H). ^{13}C NMR (75 Hz, $CDCl_3$) δ 148.0, 135.1 (t, J = 23.0 Hz), 129.2, 117.5, 116.1, 112.9, 46.4; HRMS (ESI) calcd for $[M]^+$ $C_9H_{11}DN_1$: 135.1027, found: 135.1022.

To an oven-dried pressure tube were added **S-4** (0.7 g, 5.2 mmol, 1 equiv) and xylenes (13 mL). The solution was cooled to -78 ^{o}C and $BF_3{\cdot}Et_2O$ (1.3 mL, 10.4 mmol, 2.0 equiv) was added dropwise. The resulting solution was warmed to room temperature and was heated to 160 ^{o}C for 4 h.[7] The reaction mixture was then cooled to room temperature and was placed in an ice water bath and was quenched with 6 mL of 2M NaOH. The organic layer was separated and aqueous layer was extracted with Et_2O (3 x 10 mL). The organics were combined, dried with Na_2SO_4, filtered and concentrated *in vacuo*. Purification by flash chromatography on SiO_2 (10% EtOAc in hexanes) gave *o*-allyl-2-d_1 aniline **S-5** (0.5 g, 70% yield). Data for **S-5**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.05 (t, J = 8.0 Hz, 2H), 6.75 (t, J = 7.5 Hz, 1H), 6.64 (d, J = 8.0 Hz, 1H), 5.12 (s, 1H), 5.10 s, 1H), 3.66 (br.s , 2H, 3.30 (s, 2H); HRMS (ESI) calcd for $[M+H]^+$ $C_9H_{11}DN_1$: 135.1012, found: 135.1009.

The *o*-allyl-2-d_1 aniline **S-5** (0.5 g, 3.7 mmol, 1 equiv) was dissolved in dry CH_2Cl_2 (20 mL) and the solution was treated with pyridine (1.18 mL, 14.9 mmol, 4 equiv) followed by *p*-toluenesulfonyl chloride (0.85 g, 4.5 mmol, 1.2 equiv). The mixture was stirred at room temperature for 24 h, washed with 1 N HCl (15 ml) and extracted with CH_2Cl_2 (3 x 15 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated *in vacuo*. Flash chromatography of the resulting crude compound on SiO_2 (5-10% EtOAc in hexanes) afforded compound **1b-D** as white solid (1.0 g, 96% yield). Data for **1b-D**: m.p. 62-65 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, J = 8.5 Hz, 2H), 7.41 (d, J = 8.5 Hz, 1H), 7.23 (d, J = 8.5 Hz, 2H), 7.19 (m, 1H), 7.13-7.05 (m, 2H), 6.55 (b.s., 1H), 5.11 (s, 1H), 4.93 (s, 1H), 3.00 (s, 2H), 2.39 (s, 3H); ^{13}C NMR (75 Hz, $CDCl_3$) δ 143.7, 136.7, 135.2 (t, J = 24 Hz), 134.9, 131.9, 130.4,

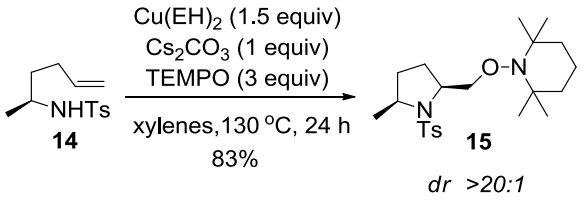
129.5, 127.6, 127.0, 126.2, 124.4, 116.9, 36.0, 21.5; IR (neat) υ 3266, 3076, 3030, 2967, 2913, 2849, 2243, 1922, 1623, 1596, 1492, 1451, 1401, 1333, 1161, 1089, 1039, 1016, 921, 817, 754, 663 cm^{-1}; HRMS (ESI) calcd for $[M]^+$ $C_{16}H_{16}DO_2N_1S_1$: 288.1037, found: 288.1036.

(*E*)-*N*-(2,2-dimethyl-5-phenylpent-4-enyl)-4-methylbenzenesulfonamide (9)



Following the procedure reported by Grubbs and co-workers,[8] a solution of *N*-(2,2-dimethylpent-4-enyl)-4-methylbenzenesulfonamide **8**[9-10] (250 mg, 0.94 mmol, 1 equiv) in CH_2Cl_2 (1.0 mL) and styrene (0.43 mL, 3.8 mmol, 4 equiv) were added simultaneously via syringe to a stirring solution of Grubb's second generation catalyst (40 mg, 0.05 mmol, 5.0 mol%) in CH_2Cl_2 (1.3 mL). The flask was fitted with a condenser and the solution was heated under reflux for 12 h. The reaction mixture was then concentrated and purified by flash chromatography on SiO_2 (5-20% EtOAc in hexanes) providing **9** as a white solid (210 mg, 65% yield). Data for **9**: mp 90-93 ^oC ^1H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, J = 8.5 Hz, 2H), 7.23-7.33 (m, 7H), 6.39 (d, J = 16.0 Hz, 1H), 6.13 (m, 1H), 4.39 (s, 1H), 2.76 (d, J = 7.0 Hz, 2H), 2.43 (s, 3H), 2.15 (d, J = 7.5 Hz, 2H), 0.94 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 143.2, 137.3, 136.9, 132.9, 129.6, 128.4, 127.0, 126.0, 125.9, 52.7, 42.8, 34.7, 25.0, 21.4; IR (neat, thin film) υ 3284, 3058, 3021, 2958, 2913, 2867, 1600, 1491, 1451, 1415, 1324, 1256, 1161, 1089, 1066, 1016, 966, 808, 735, 690, 663 cm^{-1}; HRMS (ESI) calcd for $[M+]^+$ $C_{20}H_{26}O_2N_1S_1$: 344.1679, found: 344.1670.

Procedure for the Diastereoselective Aminooxygenation Reaction (Eq. 12)

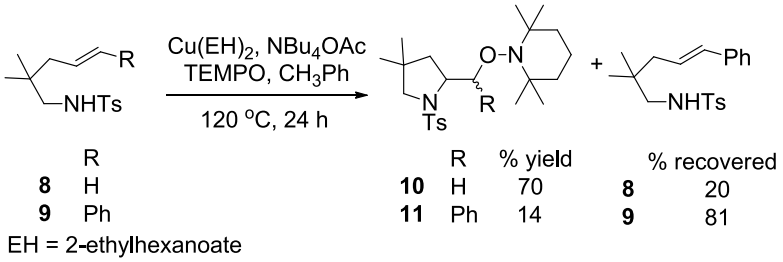


*81% yield and dr >20:1 with Bu_4NOAc (1 equiv) in place of Cs_2CO_3

Following the method we have previously reported,[11] the sulfonamide **14** (40.0 mg, 0.158 mmol, 1 equiv), $Cu(EH)_2$ (83.0 mg, 0.237 mmol, 1.5 equiv), Cs_2CO_3 (51.0 mg, 0.158 mmol, 1 equiv), TEMPO (74.0 mg, 0.474 mmol, 3 equiv) and xylenes (1.58 mL) were combined in an oven-dried pressure tube equipped with magnetic stir bar. The reaction mixture was heated in an oil bath to 130 ^oC for 24 h. It was then cooled to room temperature, diluted with ether and filtered through a SiO_2 plug. Removal of the solvent *in vacuo* afforded the crude product. Purification by flash chromatography on SiO_2 (5% ethyl acetate in hexanes) gave the disubstituted pyrrolidine **15** as white solid in 83% yield (53.5 mg). The reaction of **14** using 1 equiv of NBu_4OAc instead of Cs_2CO_3 gave **15** in 81% yield. The *cis* stereochemistry of **15** was determined by *nOe*

experiment.[12] Data for **15** matches the reported characterization:[12] $[\alpha]^{20}_{D}$ = -63.9 ^{o} (c = 1.0, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 8.0 Hz, 2H), 3.90 (dd, J = 9.0 Hz, 3.5 Hz, 1H), 3.84 (t, J = 8.0 Hz, 1H), 3.72 (m, 1H), 3.62 (m, 1H), 2.41 (s, 3H), 1.91 (m, 1H), 1.67-1.55 (m, 3H), 1.50-1.43 (m, 6H), 1.36 (d, J = 6.0 Hz, 3H), 1.18 (s, 3H), 1.16 (s, 3H), 1.09 (s, 3H), 1.08 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 143.1, 135.0, 129.5, 127.6, 78.6, 60.0, 57.4, 39.6, 32.9, 32.5, 27.3, 22.8, 21.4, 20.2, 17.0.

B. Competition Experiment



	R
8	H
9	Ph

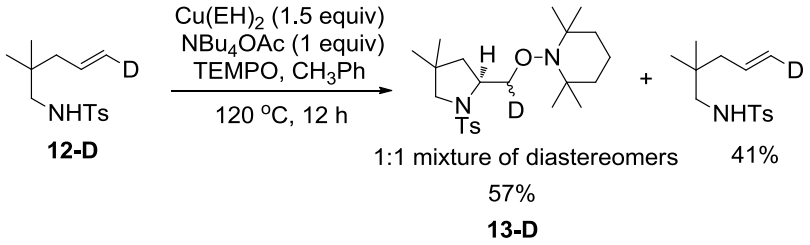
	R	% yield
10	H	70
11	Ph	14

	% recovered
8	20
9	81

An equimolar amount of **8**[9-10] (20 mg, 0.075 mmol, 1 equiv) and **9** (25.7 mg) was treated with $Cu(EH)_2$ (26.2 mg, 0.075 mmol, 1.0 equiv), NBu_4OAc (22.6 mg, 0.075 mmol, 1 equiv), TEMPO (35.2 mg, 0.225 mmol, 3 equiv) and toluene (0.8 mL). The reaction mixture was heated in an oil bath to 120 °C for 24 h, was cooled to room temperature, diluted with Et_2O and filtered through a SiO_2 plug. Solvent was removed *in vacuo* to afford the crude product. Purification by flash chromatography on SiO_2 (5-20% EtOAc in hexanes gradient) gave the TEMPO adducts **10** (22.3 mg, 70% yield) and **11** (5.1 mg, 14% yield, 4:1 d.r.). The starting olefins **8** (4 mg, 20%) and **9** (21 mg, 81%) were recovered. Spectroscopic data for compound **10** matches the previously reported characterization.[13] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (d, J = 8.5 Hz, 2H), 7.29 (d, J = 8.0 Hz, 2H), 4.20 (dd, J = 9.0 Hz, 4.0 Hz, 1H), 3.87 (t, J = 8.0 Hz, 1H), 3.69 (m, 1H), 3.11 (ABq, J_{AB} = 10.5 Hz, $\Delta\nu_{AB}$ = 21.0 Hz, 2H), 2.42 (s, 3H), 1.77-1.74 (m, 2H), 1.43-1.37 (m, 4H), 1.20 (s, 3H), 1.16 (s, 3H), 1.08 (s, 3H), 1.06 (s, 3H).

The diastereomeric ratio of compound **11** (4:1) was determined by comparing the integration of the proton peaks at 5.56 and 5.47 ppm of the crude ^{1}H NMR spectrum. Data for **11** (major diastereomer): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 (d, J = 8.5 Hz, 2H), 7.50 (d, J = 8.0 Hz, 2H), 7.27-7.32 (m, 5H), 5.56 (d, J = 4.5 Hz, 1H), 4.42 (m, 1H), 2.93 (d, J = 11.5 Hz, 1H), 2.43 (s, 3H), 2.24 (d, J = 11.0 Hz, 1H), 1.65-1.72 (m, 2H), 1.58-1.60 (m, 2H), 1.47-1.56 (m, 6H), 0.88-1.27 (m, 18H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 143.2, 139.1, 135.3, 129.5, 128.8, 127.7, 127.6, 127.1, 126.6, 86.6, 61.6, 60.7, 40.9, 40.6, 39.5, 36.7, 29.6, 26.4, 25.7, 21.5, 17.1; HRMS (ESI) calcd for $[M+H]^+$ $C_{29}H_{43}O_3N_2S_1$: 499.2989, found: 499.2989.

C. Mechanistic Analysis of C-O Bond Formation



Deuterated substrate **12-D**[3] (20 mg, 0.07 mmol, 1 equiv) was treated with $Cu(EH)_2$ (39.1 mg, 0.11 mmol, 1.5 equiv), NBu_4OAc (22.4 mg, 0.07 mmol, 1 equiv), TEMPO (34.9 mg, 0.22 mmol, 3 equiv) and toluene (1.06 mL). The reaction mixture was heated in an oil bath to 120 °C for 12 h, was cooled to room temperature, diluted with Et_2O and filtered through a SiO_2 plug. Removal of the solvent *in vacuo* afforded the crude product. Purification by flash chromatography on SiO_2

(5-10% EtOAc in hexanes gradient) gave compound **13-D** (18.1 mg, 57% yield) and the unscrambled starting material (9 mg, 41% yield). Analysis of the crude ^{1}H NMR spectrum showed two –C*H*D-OTEMP protons at 4.20 and 3.87 ppm, respectively, each integrating as 0.5 H. This indicates the presence of a 1:1 mixture of diastereomers. Data for compound **13-D**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 4.17 (m, 0.5H), 3.85 (m, 0.5H), 3.68 (m, 1H), 3.13 (ABq, J_{AB} = 10.4 Hz, $\Delta\nu_{AB}$ = 18.5 Hz, 2H), 2.43 (s, 3H), 1.78-1.75 (m, 2H), 1.45-1.42 (m, 4H), 1.20 (s, 3H), 1.16 (s, 3H), 1.08 (s, 3H), 1.06 (s, 6H), 0.55 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 143.1, 135.2, 129.4, 127.5, 79.1 (t, J = 23.0 Hz), 79.0 (t, J = 22.0 Hz), 61.4, 59.8, 58.1, 58.0, 44.1, 44.0, 39.6, 37.6, 33.1, 32.8, 26.5, 26.0, 21.5, 20.1, 17.1; IR (neat, thin film) υ 2965, 2929, 2871, 1598, 1467, 1372, 1349, 1304, 1132, 1094, 1044, 814, 663 cm^{-1}; HRMS (ESI) calcd for $[M+H]^+$ $C_{23}H_{38}{}^{2}HO_3N_2S$: 424.2739, found: 424.2743.

D. Kinetics Experiments

General Information: All reagents were used out of the bottle as purchased from the supplier without further purification unless otherwise specified. Toluene was purified using a commercial solvent filtration system. $Cu(EH)_2$ was purchased from Acros and was purified before use. $Cu(EH)_2$ was dissolved in Et_2O and the small amount of undissolved solid was filtered out. The filtrate was dried *in vacuo* and was stored in a dessicator. Reactions were monitored using Varian Prostar High Performance Liquid Chromatography. Data analysis was performed using Microsoft Office Excel 2007 software and data were plotted using SigmaPlot for Window's v. 10.0 (Systat Software, Inc, San Jose, CA).

General Procedure for Kinetics Experiments

Kinetics experiments were performed in a 16 x 100 mm sealed pressure tube. The solid reactants [substrate **1**, $Cu(EH)_2$, NBu_4OAc, TEMPO] were combined in an oven-dried pressure tube equipped with magnetic stir bar. Toluene (1.04 mL) was added via micropipette. The reaction mixture was heated to 100 ^oC using a temperature regulated oil bath and was taken out of the oil bath every 2 minutes. A 20 μL aliqout was collected using gas-tight syringe. Reactions were run up to 80-90% conversion. The aliquots collected were dried under vacuum and the residue was dissolved in 200 μL acetonitrile. The samples were analyzed using HPLC in a Microsorb-MV 100 C8 column by gradient elution (65-100% CH_3CN in H_2O). Calibration plots for substrate **1** and the TEMPO adduct **2** were used to calculate the concentrations of **1** and **2** as a function of time.

Order in substrate 1: The general procedure above was followed using substrate **1** (15 mg, 52 mmol), $Cu(EH)_2$ (109.6 mg, 312 mmol), NBu_4OAc (94.4 mg, 312 mmol) and TEMPO (48.9 mg, 312 mmol) in toluene (1.04 mL). Three separate kinetics experiments were performed and in each case a plot of $2[\mathbf{1}]^{0.5}$ versus time gave a straight line (r^2 = 0.999), indicating half-order dependence in substrate **1**. A representative plot of $2[\mathbf{1}]^{0.5}$ versus time is shown in Figure 1. Figure 2 shows the simultaneous disappearance of **1** and appearance of **2** as determined by HPLC analysis.

Figure 1. A representative plot of $2[\mathbf{1}]^{0.5}$ ($mM^{0.5}$) versus time (min) showing half-order kinetics in substrate **1**

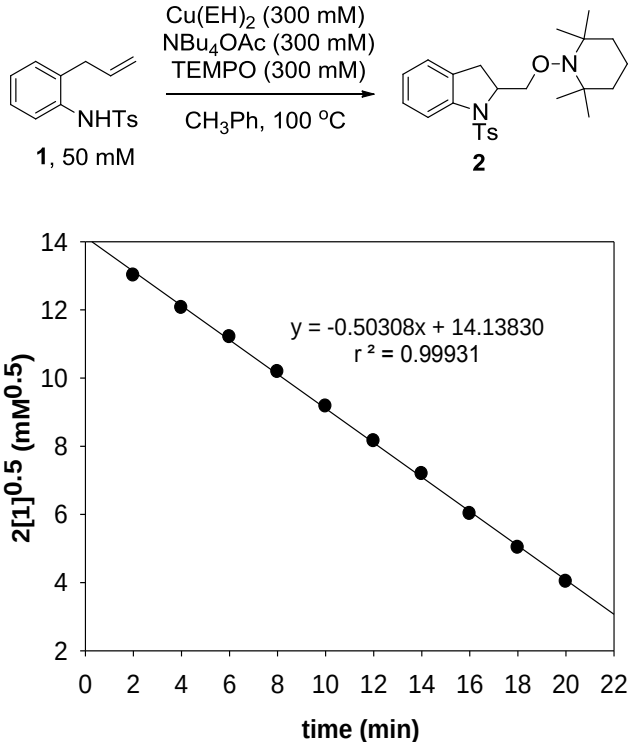
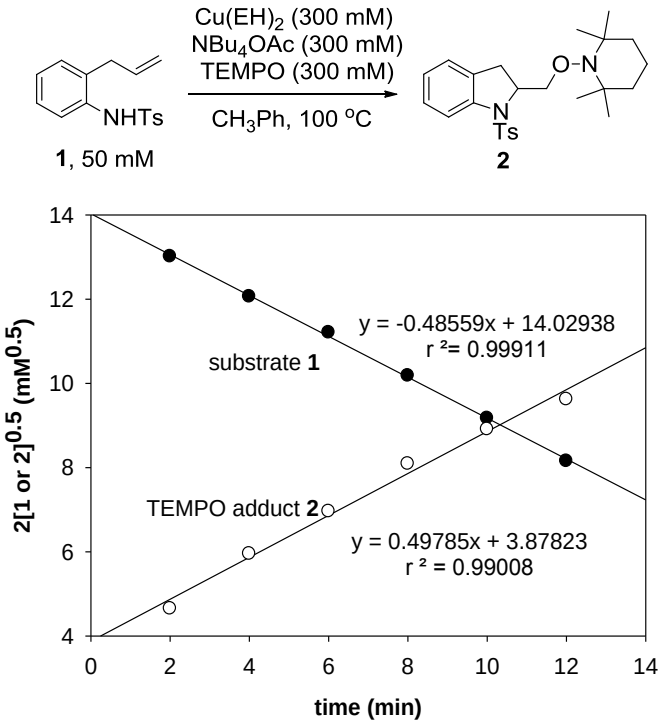


Figure 2. The loss of alkene substrate **1** and the appearance of the TEMPO adduct **2**



Effect of NBu_4OAc: The general procedure above was followed to determine the effect of the concentration of NBu_4OAc in the rate of the reaction. Substrate **1** (15 mg, 52 mmol), $Cu(EH)_2$ (109.6 mg, 312 mmol), TEMPO (48.9 mg, 312 mmol) and varying amounts of NBu_4OAc (3.8 - 156.8 mg, 12-520 mmol) were combined in toluene (1.04 mL) and the disappearance of **1** was monitored. The observed rate constant was determined from the slope of the plot of $2[\mathbf{1}]^{0.5}$ against time (a representative plot is shown in Figure 3). The reported value of k_{obs} for each [NBu_4OAc] represents an average of 2-3 kinetics experiments (Table 1). The reported error for the average k_{obs} is the square root of the sum of the squares of the standard deviation of each kinetics experiment. The data revealed that k_{obs} is optimum at a 2:1 [$Cu(EH)_2$]: [NBu_4OAc]. At concentrations higher than 200 mM, the observed rate constant decreases (Figure 4).

Figure 3. Plot of 2[**1**]$^{0.5}$ (mM$^{0.5}$) versus time (min) with [NBu_4OAc] = 200 mM and k_{obs} = 0.586 ± 0.024 mM$^{0.5}$-min^{-1}.

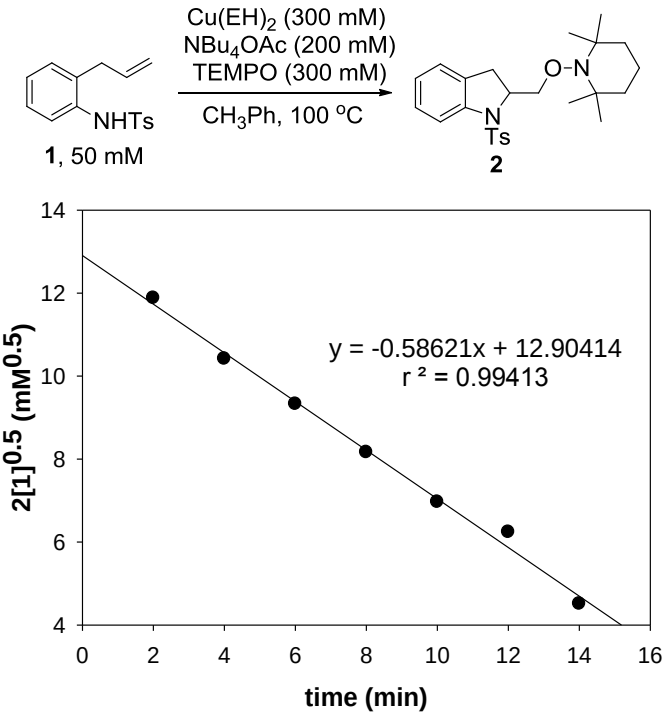
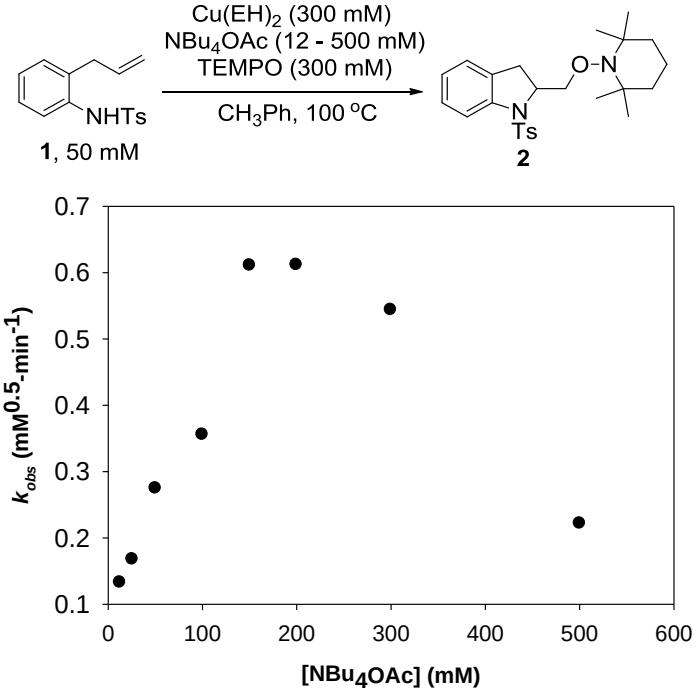


Table 1. Kinetic data for effect of the concentration of NBu_4OAc in the rate of the reaction

Entry	**[NBu_4OAc] (mM)**	**k_{obs} (mM$^{0.5}$-min^{-1})**	**Ave. k_{obs} (mM$^{0.5}$-min^{-1})**
1	11.8	0.132 ± 0.005	0.133 ± 0.010
2	12.7	0.134 ± 0.009	
3	25.1	0.177 ± 0.016	0.168 ± 0.019
4	25.5	0.168 ± 0.008	
5	25.9	0.157 ± 0.007	
6	49.6	0.254 ± 0.013	0.275 ± 0.019
7	50.8	0.266 ± 0.009	
8	50.5	0.305 ± 0.011	
9	100.4	0.377 ± 0.020	0.356 ± 0.029
10	99.1	0.335 ± 0.021	
11	151.0	0.554 ± 0.025	0.611 ± 0.033
12	150.0	0.668 ± 0.023	
13	199.5	0.586 ± 0.024	0.62 ± 0.05
14	200.0	0.657 ± 0.041	
15	305.3	0.544 ± 0.025	0.54 ± 0.05
16	305.3	0.585 ± 0.043	
17	300.0	0.503 ± 0.004	
18	500.0	0.232 ± 0.028	0.223 ± 0.033
19	500.0	0.213 ± 0.018	

Figure 4. Plot of k_{obs} ($mM^{0.5}$-min^{-1}) versus [NBu_4OAc] (mM)



Order in $Cu(EH)_2$: The order in $Cu(EH)_2$ was determined by performing a series of experiments using different concentrations of $Cu(EH)_2$ and NBu_4OAc maintained at 2:1 ratio. The general procedure above was followed using substrate **1** (15 mg, 52 mmol), TEMPO (48.9 mg, 312 mmol) and varying amounts of NBu_4OAc (47-156.8 mg, 156-520 mmol) and $Cu(EH)_2$ (109.6-364 mg, 312-1040 mmol) in toluene (1.04 mL). The disappearance of **1** was monitored and the observed rate constant was determined from the slope of the plot of $2[\mathbf{1}]^{0.5}$ against time (representative plot is given in Figure 5). The reported value of k_{obs} for each [NBu_4OAc] is an average of 2 kinetics experiments (kinetic data is given in Table 2). The reported error for the average k_{obs} is the square root of the sum of the squares of the standard deviation of each kinetics experiment. The half-order dependence in copper was determined from the plot of ln(k_{obs}) versus ln[$Cu(EH)_2$] ($m = 0.52 \pm 0.03$) (Figure 6).

Figure 5. Plot of $2[\mathbf{1}]^{0.5}$ versus time with $[Cu(EH)_2]$ = 500 mM and $[NBu_4OAc]$ = 250 mM and k_{obs} = 0.842 ± 0.019 $mM^{0.5}$-min^{-1}.

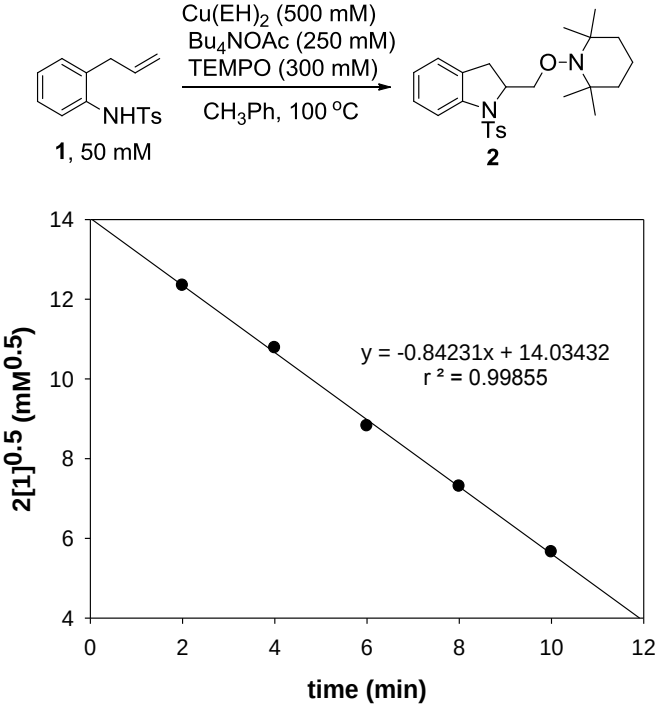
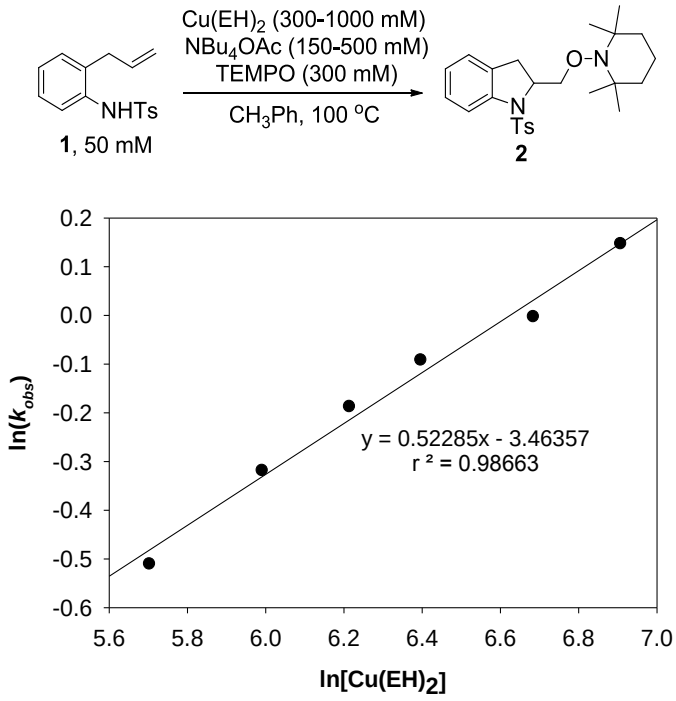


Table 2. Kinetic data for determining the order in $Cu(EH)_2$.

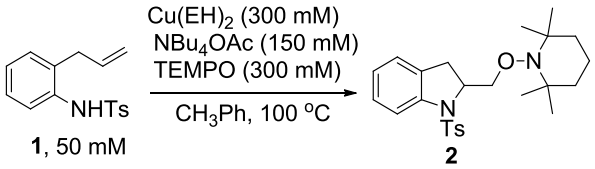
Entry	$[Cu(EH)_2]$ (mM)	NBu_4OAc (mM)	k_{obs} ($mM^{0.5}$-min^{-1})	Ave. k_{obs} ($mM^{0.5}$-min^{-1})
1	303.3	151.0	0.531 ± 0.027	0.599 ± 0.043
2	299.9	150.0	0.667 ± 0.034	
3	399.9	197.9	0.728 ± 0.027	0.727 ± 0.046
4	399.1	209.0	0.726 ± 0.037	
5	500.3	236.0	0.815 ± 0.037	0.829 ± 0.042
6	505.2	249.6	0.842 ± 0.019	
7	601.3	304.9	0.91 ± 0.09	0.912 ± 0.103
8	602.4	302.7	0.92 ± 0.05	
9	800.0	401.6	0.990 ± 0.017	1.00 ± 0.04
10	797.2	400.3	1.005 ± 0.037	
11	996.0	502.9	1.18 ± 0.09	1.16 ± 0.09
12	994.9	495.7	1.139 ± 0.012	

Figure 6. Plot of ln(k_{obs}) against ln[$Cu(EH)_2$] showing half order dependence in copper.



Order in TEMPO: The general procedure above was followed to determine the order in TEMPO using **1** (15 mg, 52 mmol), $Cu(EH)_2$ (109.6 mg, 312 mmol), NBu_4OAc (47 mg, 156 mmol) and varying amounts of TEMPO (32.5-65.0 mg, 208-416 mmol) in toluene (1.04 mL). The disappearance of **1** was monitored and the rate constant for each [TEMPO] was determined from the slope of the plot of 2[**1**]$^{0.5}$ against time (a representative plot is shown in Figure 7). The data from the experiments showed no significant change in the rate constant upon changing the concentration of TEMPO (Table 3), which suggests zero-order dependence in TEMPO.

Figure 7. A representative plot of $2[\mathbf{1}]^{0.5}$ against time with [TEMPO] = 300 mM with k_{obs} = 0.668 ± 0.023 $mM^{0.5}$-min^{-1}.



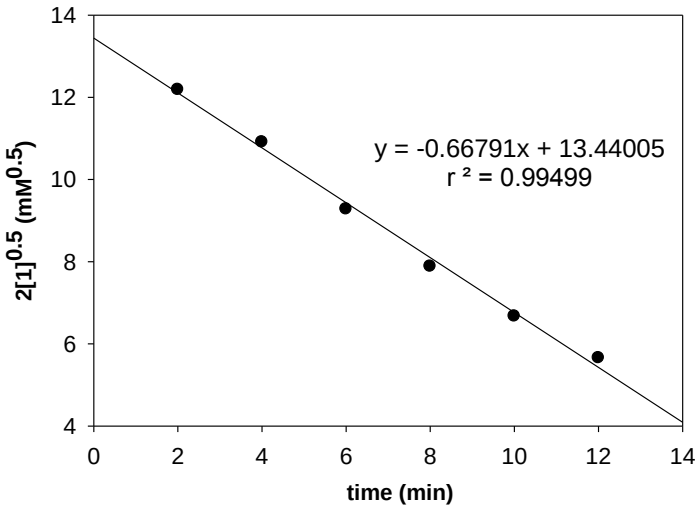


Table 3. Kinetic data for determining the order in TEMPO

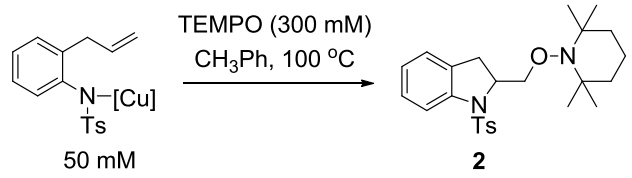
Entry	[TEMPO] (mM)	k_{obs} ($mM^{0.5}$-min^{-1})	Ave. k_{obs} ($mM^{0.5}$-min^{-1})
1	202.3	0.594 ± 0.03	0.62 ± 0.04
2	200.0	0.640 ± 0.03	
3	300.0	0.554 ± 0.025	0.611 ± 0.033
4	305.3	0.668 ± 0.023	
5	400.0	0.657 ± 0.028	0.623 ± 0.032
6	400.0	0.589 ± 0.015	

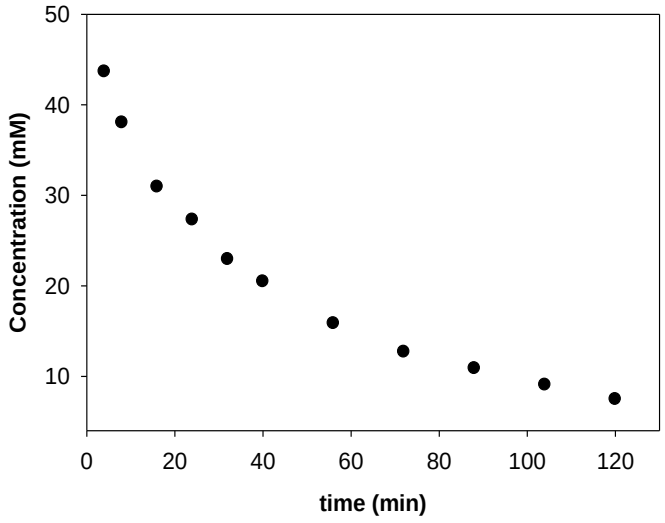
Representative Procedure for Measuring the Kinetics of [N-Cu] Intermediate

To a solution of sulfonamide **1** (15 mg, 0.052 mmol, 1 equiv) in toluene (0.502 mL) was added *n*BuLi (34 μL, 1.6 M in hexanes, 0.055 mmol, 1.05 equiv) under argon atmosphere at -78 °C. The reaction mixture was stirred for 15 min and was then warmed to room temperature. The resulting mixture was added to a solution of $Cu(EH)_2$ (18.3 mg, 0.052 mmol, 1 equiv) in toluene (0.502 mL) and was stirred for 15 min. TEMPO (48.8 mg, 0.312 mmol, 3 equiv) was then added to the mixture and was subsequently heated to 100 °C using a temperature regulated oil bath. A 20 μL aliquot was taken every 8 min using gas-tight syringe. The reaction was run up to 80-90% conversion. The aliquots collected were dried under vacuum and the residue was dissolved in

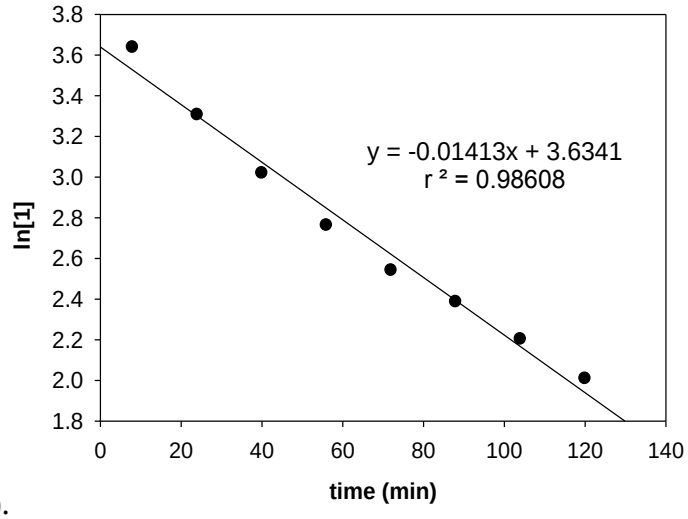
200 μL acetonitrile. The residue which was presumed to contain the amine-copper intermediate was converted to **1** when redissolved in CH_3CN and run in HPLC using CH_3CN:H_2O as solvent. The disappearance of **1** was monitored using HPLC in a Microsorb-MV 100 C8 column by gradient elution (65-100% CH_3CN in H_2O). Kinetic plots are shown in Figure 8 and Table 4 shows the effect of varying the concentration of TEMPO and $Cu(EH)_2$ in the k_{obs} value.

Figure 8. A). Kinetic plot of conversion of [N-Cu] intermediate to **2** with [TEMPO] = 300 mM. B). Plot of ln[**1**] versus time (min) with k_{obs} = 1.41(±0.07) x 10^{-2} min^{-1}.





A).



B).

Table 4. The effect of varying concentrations of TEMPO and $Cu(EH)_2$ on the observed rate constant (ave. k_{obs} = 1.6 (±0.1) x 10^{-2} min^{-1}).

Entry	R_2NLi (mM)	$Cu(EH)_2$ (mM)	TEMPO (mM)	k_{obs} (min^{-1})
1	50	50	100	1.28(±0.04) x 10^{-2}
2	50	50	200	1.78(±0.09) x 10^{-2}
3	50	50	300	1.41(±0.07) x 10^{-2}
4	50	100	200	1.76(±0.06) x 10^{-2}
			ave. k_{obs}	1.6 (±0.1) x 10^{-2}

E. Procedure for UV-Vis Spectroscopy

Stock solutions of 40 mM $Cu(EH)_2$ (35 mg dissolved in 2.5 mL toluene) and 30 mM NBu_4OAc (27 mg in 3 mL toluene) were prepared. The solutions were sonicated until all solids were dissolved. One mL of 12 mM $Cu(EH)_2$ solution was prepared by taking 0.3 mL of 40 mM $Cu(EH)_2$ solution and diluting it with 0.7 mL of toluene. Solutions of 12 mM $Cu(EH)_2$ were titrated with different concentrations of NBu_4OAc (6-20 mM). To prepare the solutions using carbonates, 1 mL of 12 mM $Cu(EH)_2$ was added to 1.95 mg of Cs_2CO_3 and 0.83 mg of K_2CO_3 weighed in separate vials. The mixtures were sonicated and the undissolved solids were carefully removed by pipetting out the liquid prior to spectroscopy. Absorption spectra were obtained using UVIKON XL spectrophotometer (Figure 9).

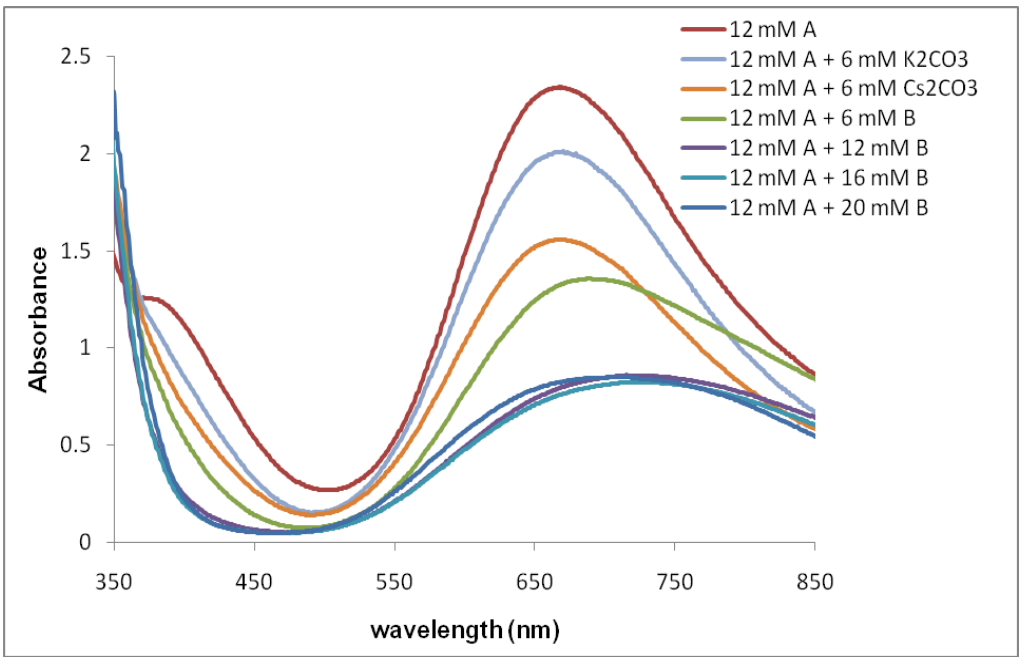


Figure 9. UV-Vis spectra of a series of $Cu(EH)_2$ (A) solution titrated with increasing amount of NBu_4OAc (B) and 6 mM of K_2CO_3 and Cs_2CO_3.

F. Electron Paramagnetic Resonance (EPR) Measurements

Stock solutions of 5 mM each of $Cu(EH)_2$, Bu_4NOAc and sulfonamide **1** in toluene were prepared. One mL of solution A was prepared by taking 100 μL of 5 mM $Cu(EH)_2$, 50 μL of 5 mM Bu_4NOAc and 850 μL of toluene. One mL of solution B was prepared by taking 100 μL each of 5 mM $Cu(EH)_2$ and 5 mM of sulfonamide **1**, 50 μL of 5 mM Bu_4NOAc and 750 μL of toluene. Solution B was heated to 50 ^oC for 15 min prior to EPR analysis. Solution C was prepared by taking 100 μL each of 5 mM $Cu(EH)_2$ and 5 mM of sulfonamide **1** (deprotonated by *n*BuLi) and 800 μL of toluene. EPR spectra were obtained using a Bruker EMX spectrometer operating at 9.85 GHz (X-band). Spectra were recorded in frozen glass of toluene at 100 K (Figure 10). Spectra are reported from 12 scans with time constant of 1.28 s, modulation amplitude of 1.0 G, and microwave power of 20 dB. EPR parameters were obtained using the software Bruker Xenon 1.1b.42 (Bruker Biospin Corporation, Billerica, MA USA).

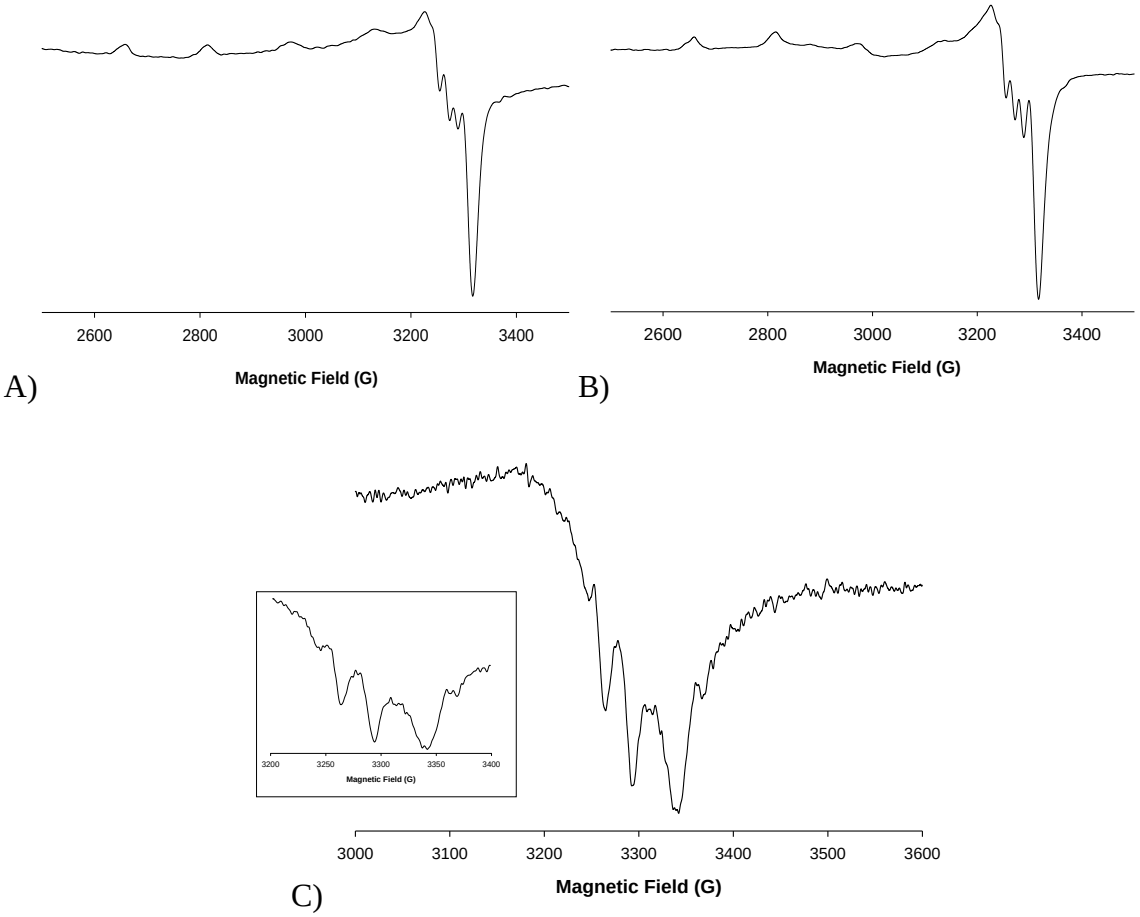
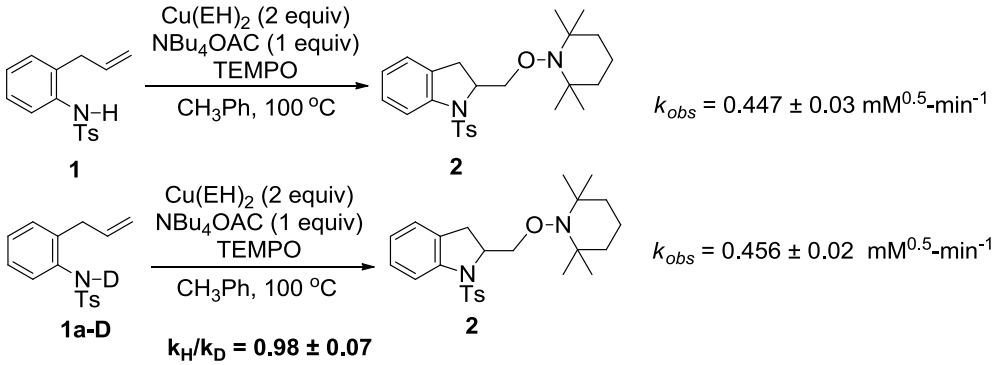


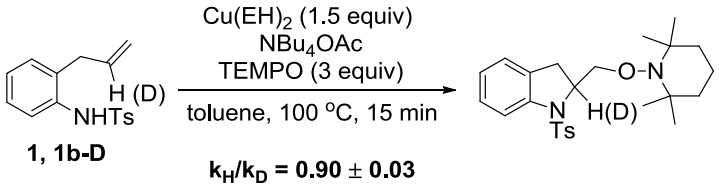
Figure 10. EPR spectra of solutions of A) 2:1 mixture of $Cu(EH)_2$ and Bu_4NOAc, B) 2:2:1 of sulfonamide **1**:$Cu(EH)_2$:Bu_4NOAc (heated at 50 ^oC for 15 min) and C) 1:1 mixture of $Cu(EH)_2$ and sulfonamide **1** (deprotonated with *n*BuLi) in frozen glass of toluene at 100 K.

G. Kinetic Isotope Effect (KIE)

Primary Kinetic Isotope Effect: The primary kinetic isotope effect was determined by studying the rate of reactions of substrate **1** and **1a-D**. The general aminooxygenation procedure (above) was followed using substrate **1** or **1a-D** (0.05 mmol, 1 equiv), $Cu(EH)_2$ (36.4 mg, 0.10 mmol, 2 equiv), NBu_4OAc (15.7 mg, 0.05 mmol, 1 equiv), TEMPO (24.2 mg, 0.15 mmol, 3 equiv) and toluene (1.04 mL). Reactions were conducted at 100 ºC and the reported value of k_{obs} represents an average of two unique kinetics experiments.



Secondary Kinetic Isotope Effect



A mixture of substrates **1** (25.0 mg) and **1b-D** (25.0 mg) was dissolved in toluene (3.46 mL). One mL aliquot was taken from this solution and was subjected to mass spectrometry to determine the isotopic ratio prior to reaction (Ro) (representative data is given in Table 5). The remaining solution was treated with $Cu(EH)_2$ (64 mg, 0.18 mmol, 1.5 equiv), NBu_4OAc (36.6 mg, 0.12 mmol, 1 equiv) and TEMPO (57.2 mg, 0.37 mmol, 3 equiv) and was heated to 100 °C for 15 min. The remaining mixture of starting olefins (**1** and **1b-D)** was isolated by flash chromatography (5% EtOAc in hexanes) and the isotopic ratio was determined by mass spectroscopy (R). Fractional conversion (F) which was corrected (Fc) using the equation given in Table 6 was determined by HPLC analysis. Six separate reactions were performed and kinetic isotope effect was determined for each case. The reported KIE is the average of these 6 experiments (0.90 ± 0.03).[14-15]

Table 5. Representative data of isotopic ratio as determined by mass spectrometry

Trial	Ro	R	R/Ro
1	1.0	0.84	
2	1.0	0.82	
3	1.0	0.84	
4	0.96	0.80	
Ave	0.99 ± 0.02	0.82 ± 0.01	0.83 ± 0.02

Table 6. Calculated KIE data and errors[14-15]

$$F_c = 1 - \frac{(1-F)(1+R_o)}{1+R}$$

$$KIE = \frac{k_H}{k_D} = \frac{\ln(1-F)}{\ln[(1-F)(R/R_o)]}$$

$$\Delta KIE = \frac{-(\Delta R/R_o)\ln(1-F)}{(R/R_o)\ln^2[(1-F)(R/R_o)]}$$

Entry	1-F	1-Fc	R/Ro	ΔR/Ro	KIE	ΔKIE
1	0.2117	0.2310	0.8323	0.02	0.8887	0.0129
2	0.2547	0.2722	0.8677	0.03	0.9017	0.0216
3	0.2541	0.2727	0.8622	0.02	0.8976	0.0144
4	0.2086	0.2267	0.8361	0.03	0.8924	0.0192
5	0.2119	0.2285	0.8569	0.04	0.9053	0.0259
6*	0.1964	0.2128	0.8466	0.04	0.9028	0.0248
				Ave. KIE	0.8971	0.03

*Reaction was run using a 2:1 ratio between $Cu(EH)_2$ and NBu_4OAc.

H. References

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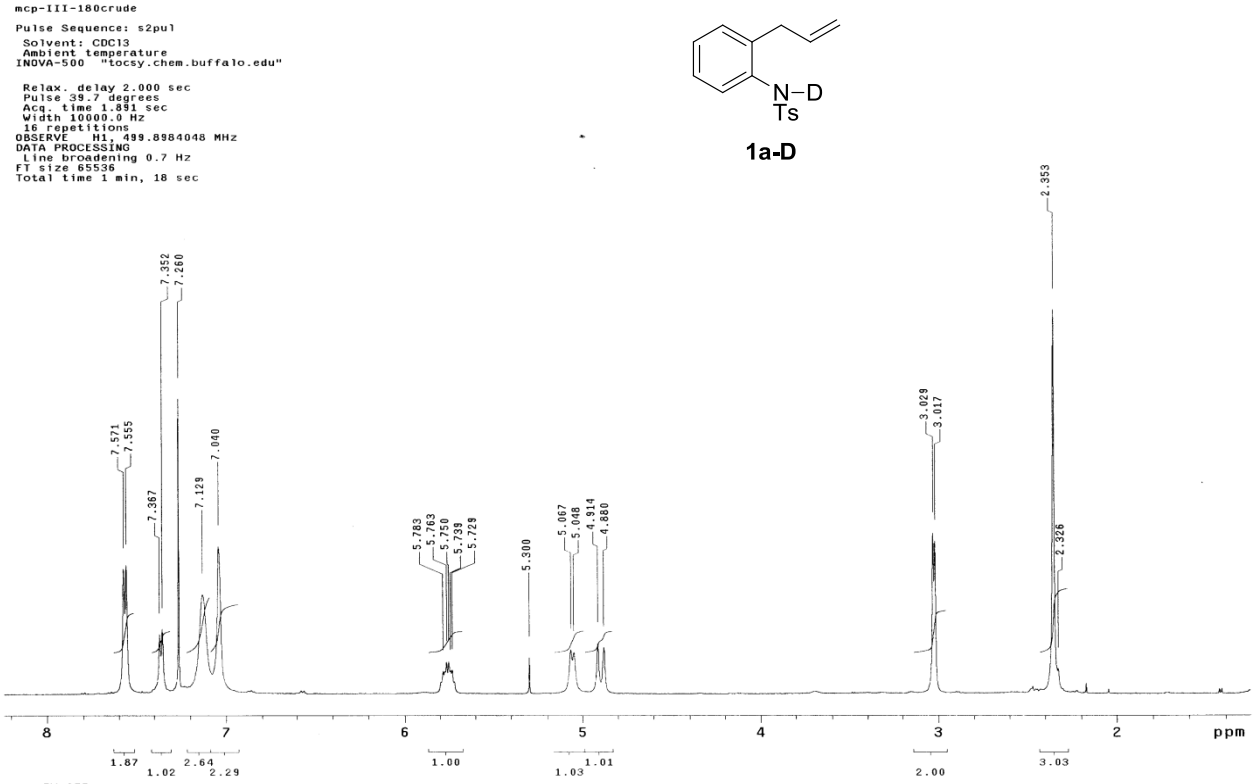
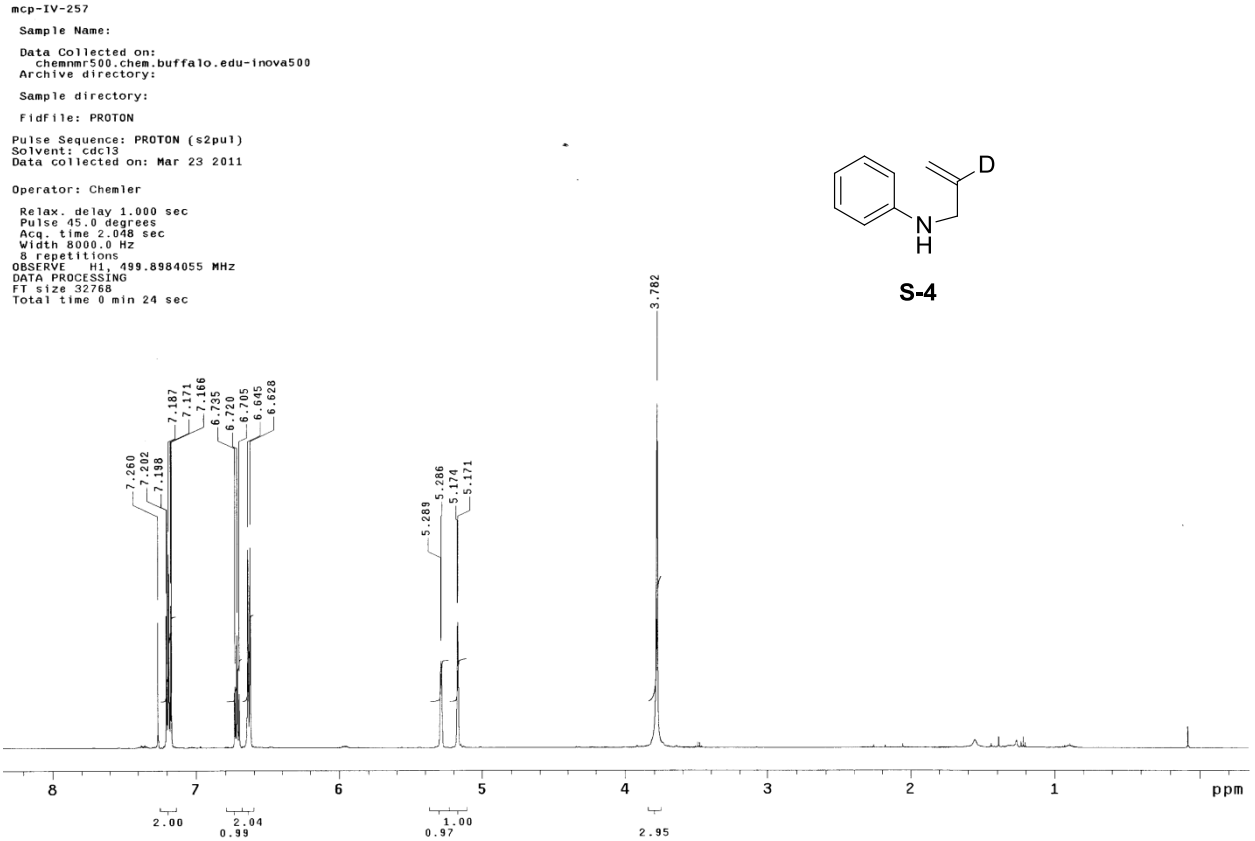
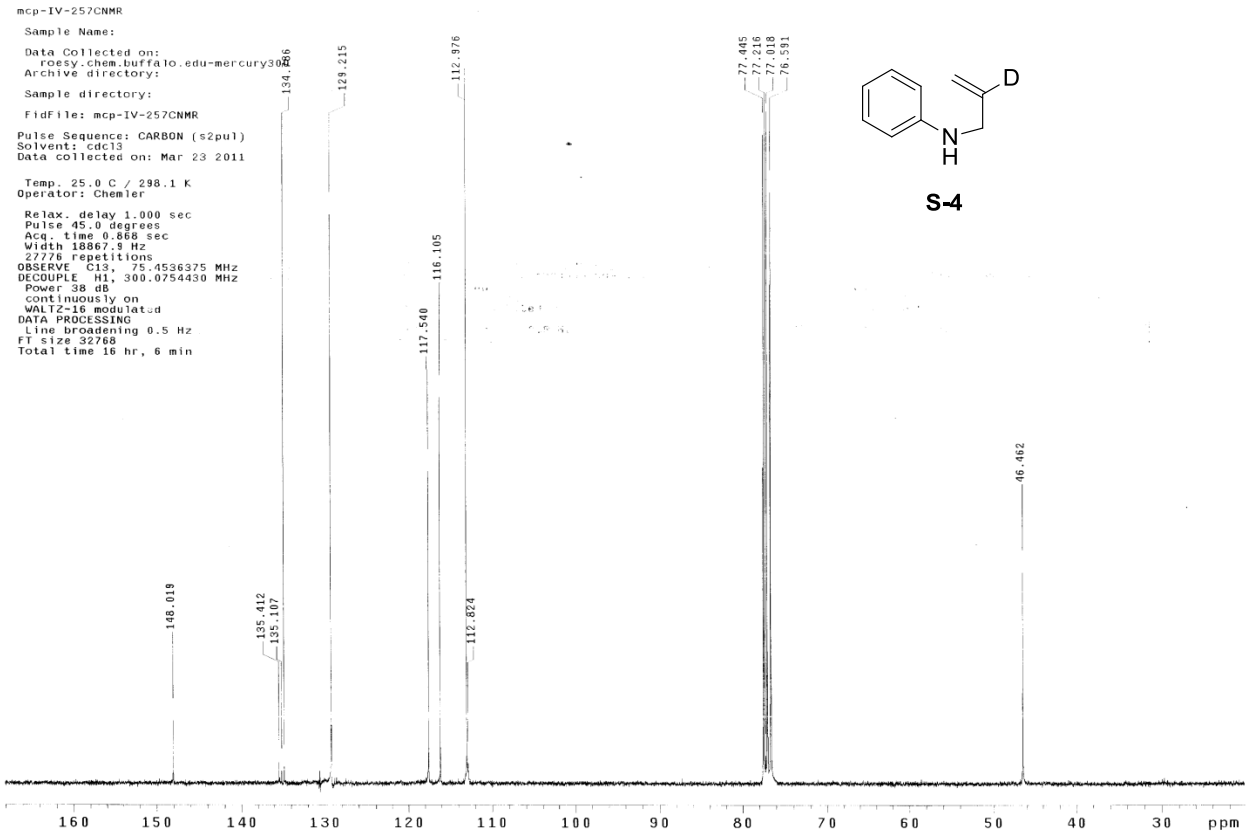
I. ^{1}H and ^{13}C NMR spectra for all new compounds



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Operator: Chemler
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112.376
77.445
77.216
77.018
76.591
117.540
116.105
148.019
135.412
135.107
112.824
46.462
D
N
H
S-4
160
150
140
130
120
110
100
90
80
70
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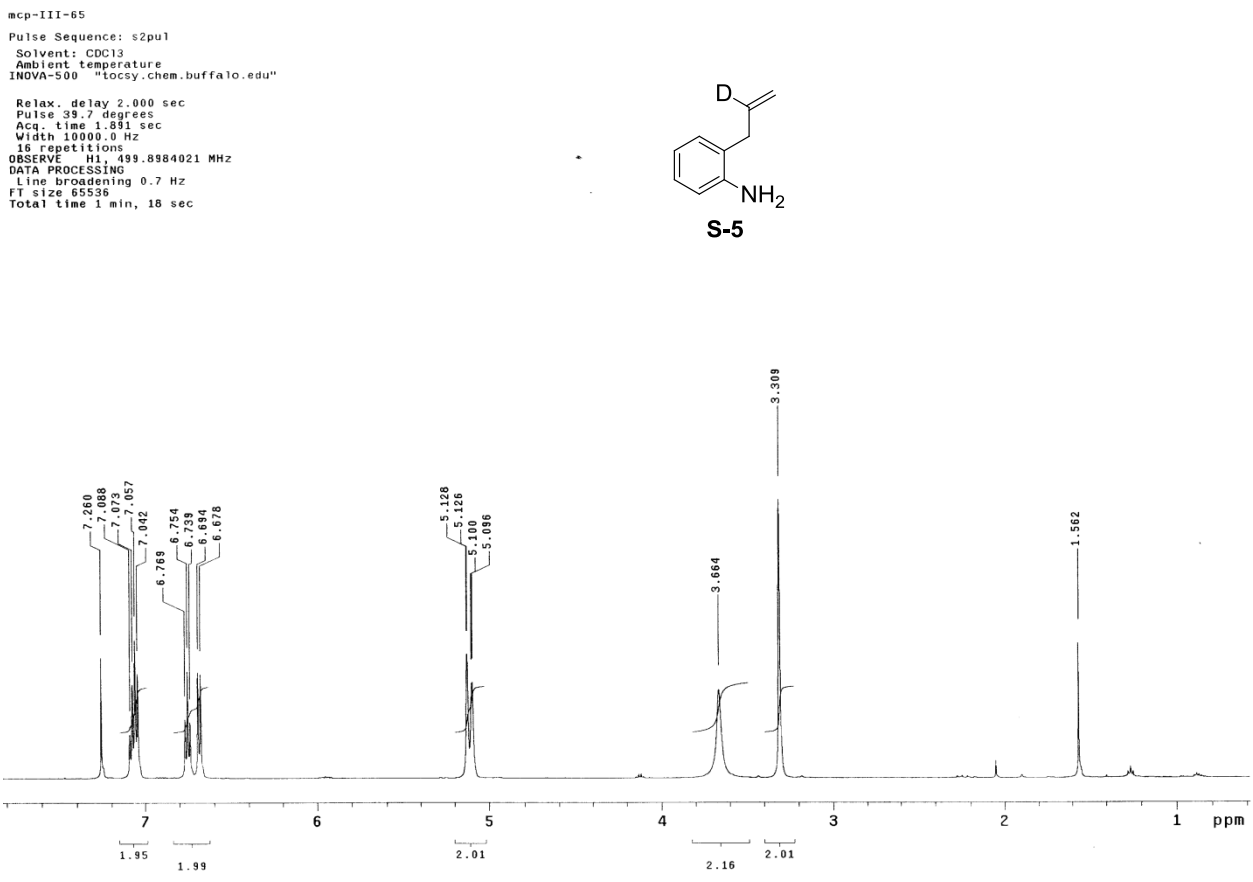
50
40
30
ppm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D
NH2
S-5
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7.088
7.073
7.057
7.042
6.769
6.754
6.738
6.694
6.678
5.128
5.126
5.100
5.096
3.664
3.309
1.562
7
6
5
4
3
2
1
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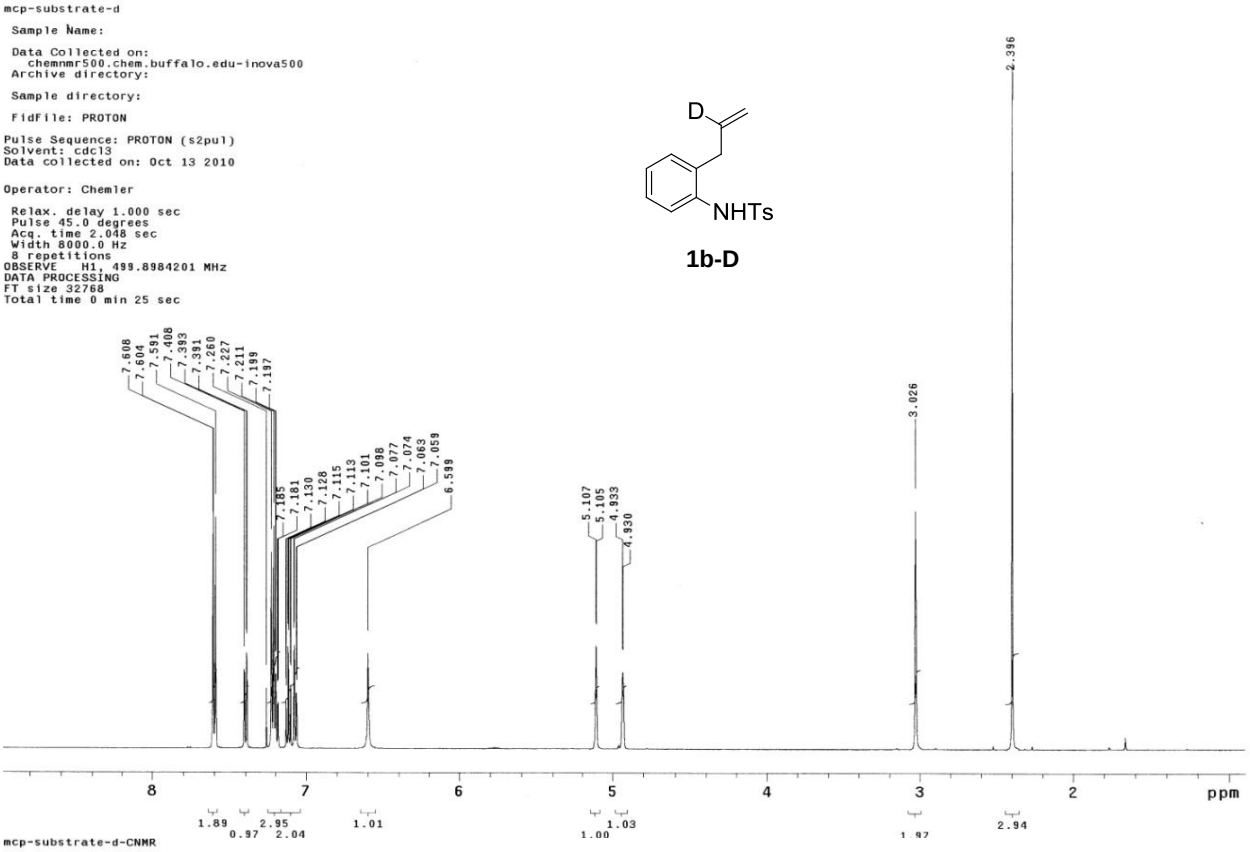
2.01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Width 8000.0 Hz
8 repetitions
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Total time 0 min 25 sec
D
NHTs
1b-D
7.608
7.604
7.591
7.408
7.393
7.391
7.260
7.227
7.211
7.199
7.197
7.185
7.181
7.130
7.128
7.115
7.113
7.101
7.098
7.077
7.074
7.063
7.059
6.599
5.107
5.105
4.933
4.930
3.026
2.396
8
7
6
5
4
3
2
ppm
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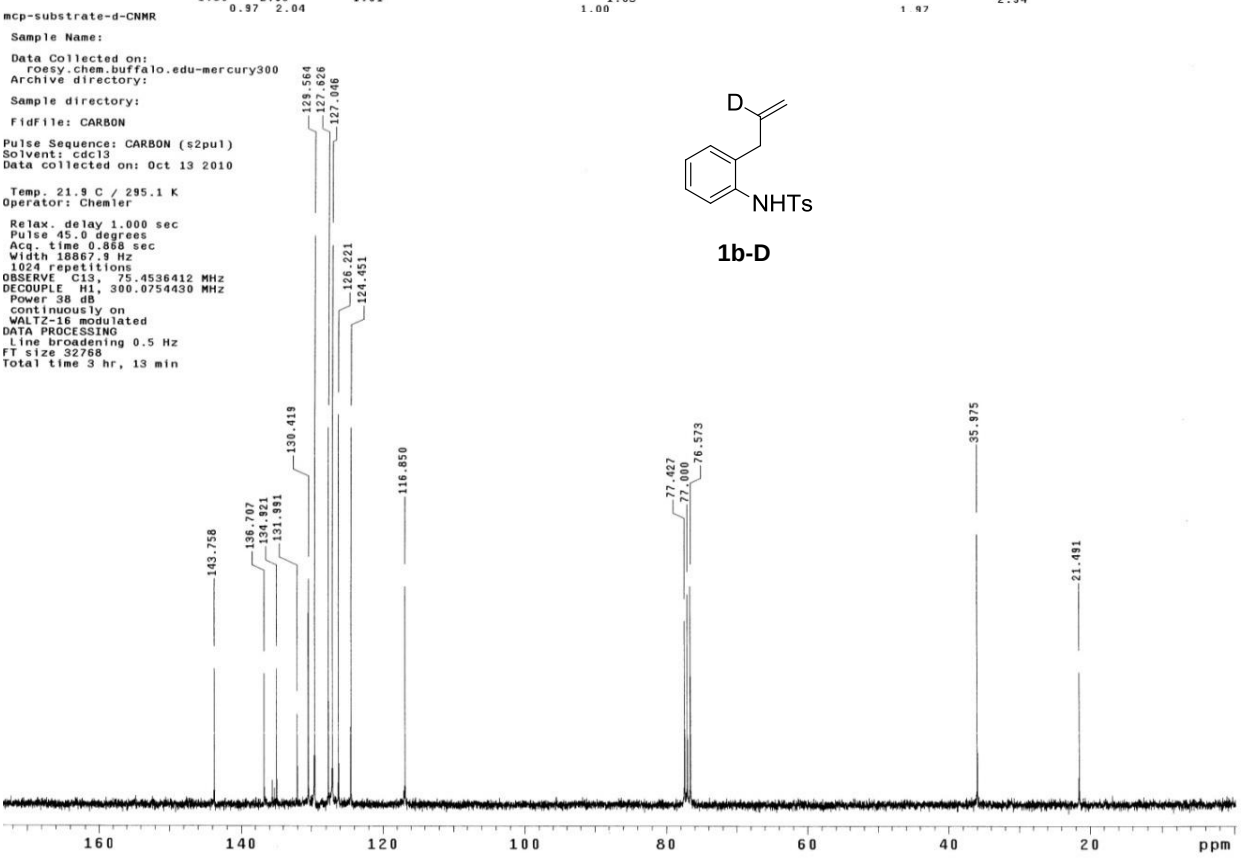
0.97
2.95
2.04
1.01
1.00
1.03
1.97
2.94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1024 repetitions
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Power 38 dB
continuously on
WALTZ-16 modulated
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NHTs
1b-D
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136.707
134.921
131.991
130.419
129.564
127.626
127.046
126.221
124.451
116.850
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77.000
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35.975
21.491
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120
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80
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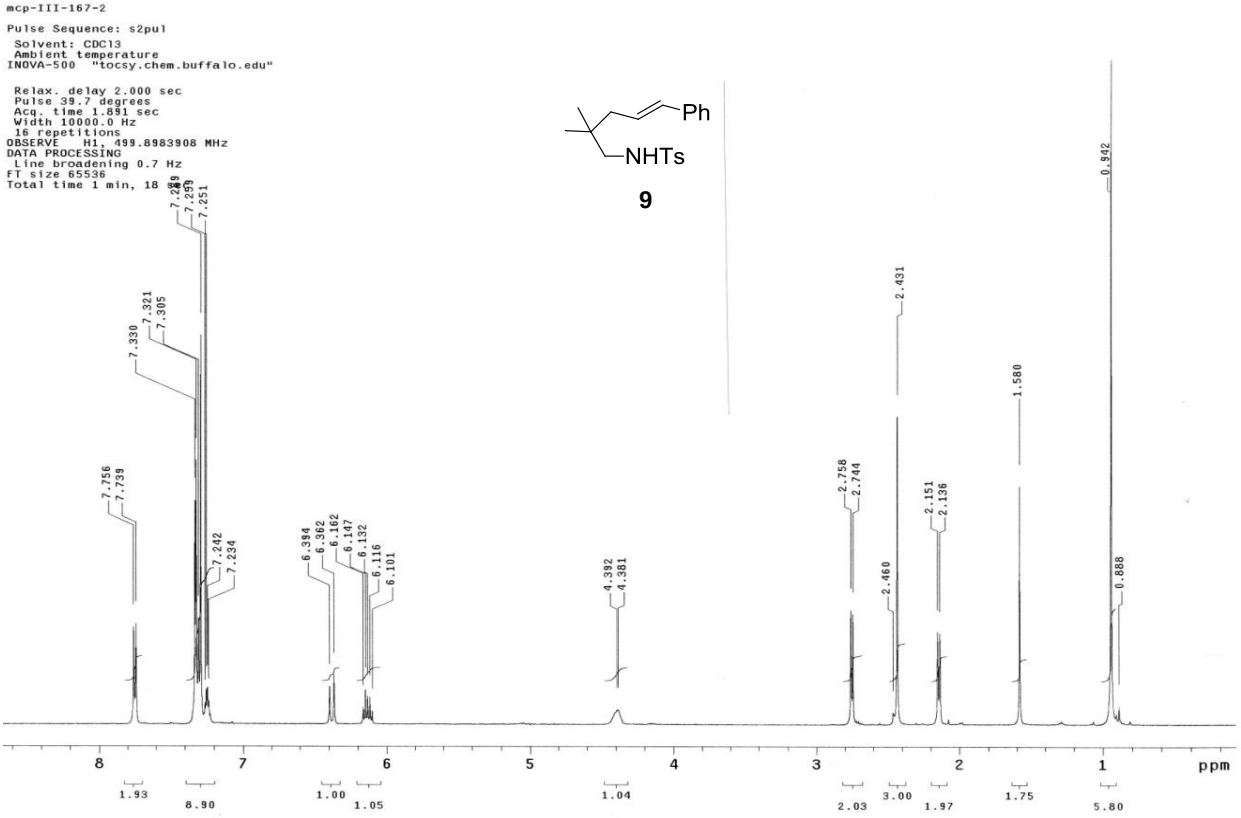
40
20
ppm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DATA PROCESSING
Line broadening 0.7 Hz
FT size 65536
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Ph
NHTs
9
7.756
7.739
7.330
7.321
7.305
7.251
7.242
7.234
6.394
6.362
6.162
6.147
6.132
6.116
6.101
4.382
4.381
2.758
2.744
2.460
2.431
2.151
2.136
1.580
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0.888
8
7
6
5
4
3
2
1
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2.03
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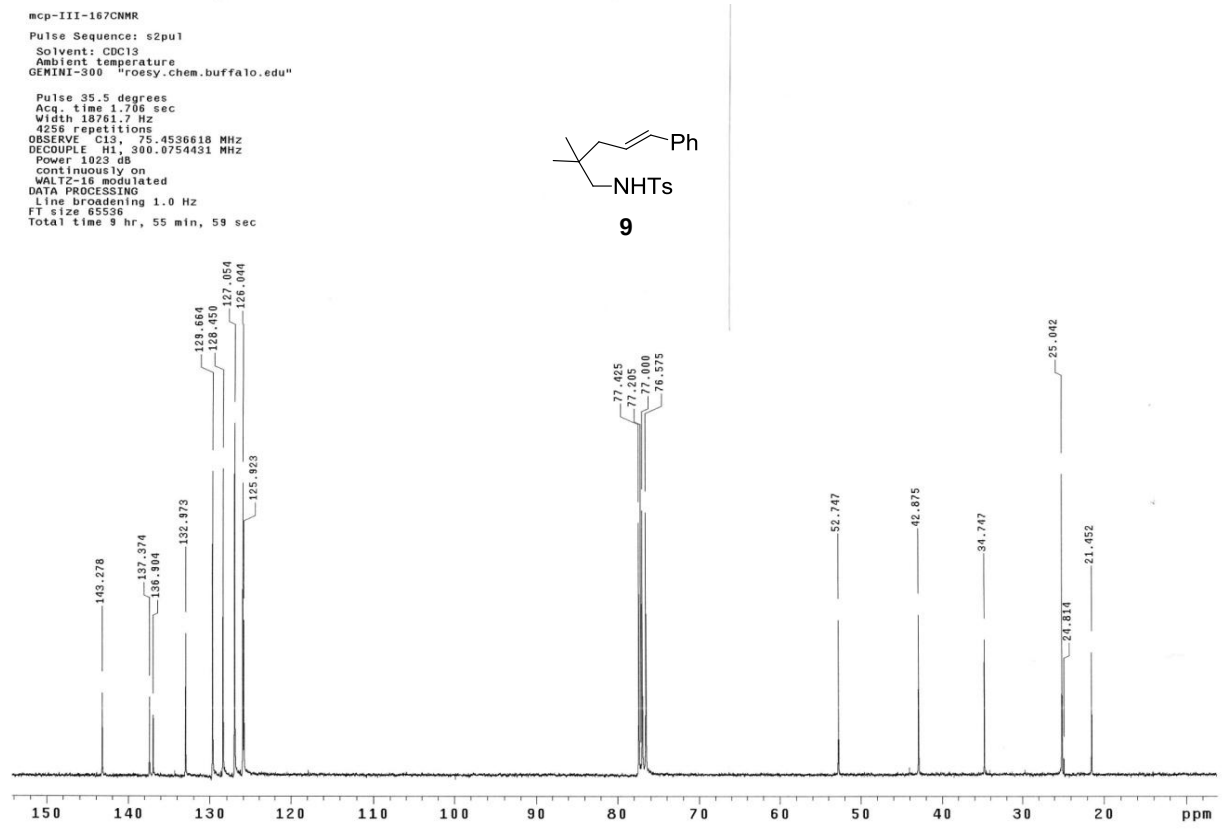
1.75
5.80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Width 18761.7 Hz
4256 repetitions
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Power 1023 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 hr, 55 min, 59 sec
Ph
NHTs
9
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137.374
136.904
132.973
129.664
128.450
127.054
126.044
125.923
77.425
77.205
77.000
76.575
52.747
42.875
34.747
25.042
24.814
21.452
150
140
130
120
110
100
90
80
70
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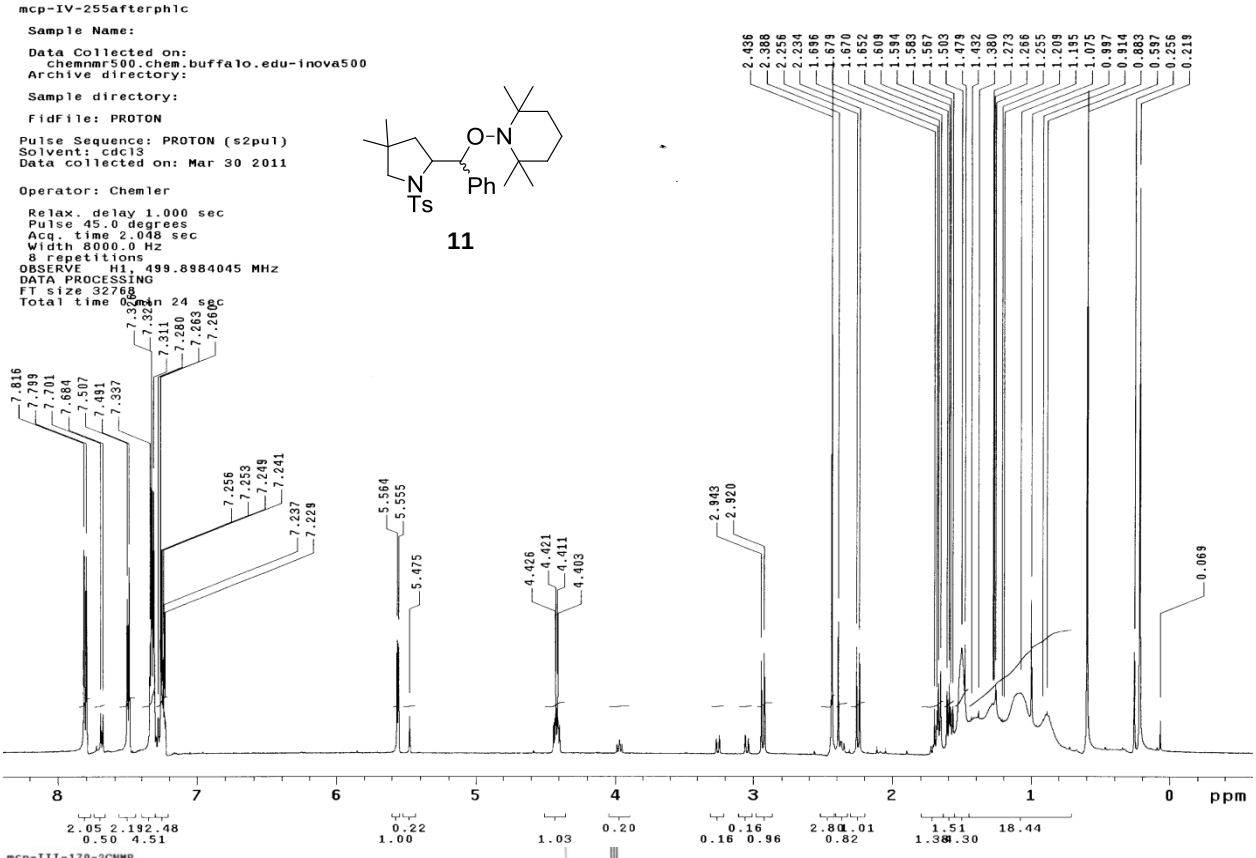
50
40
30
20
ppm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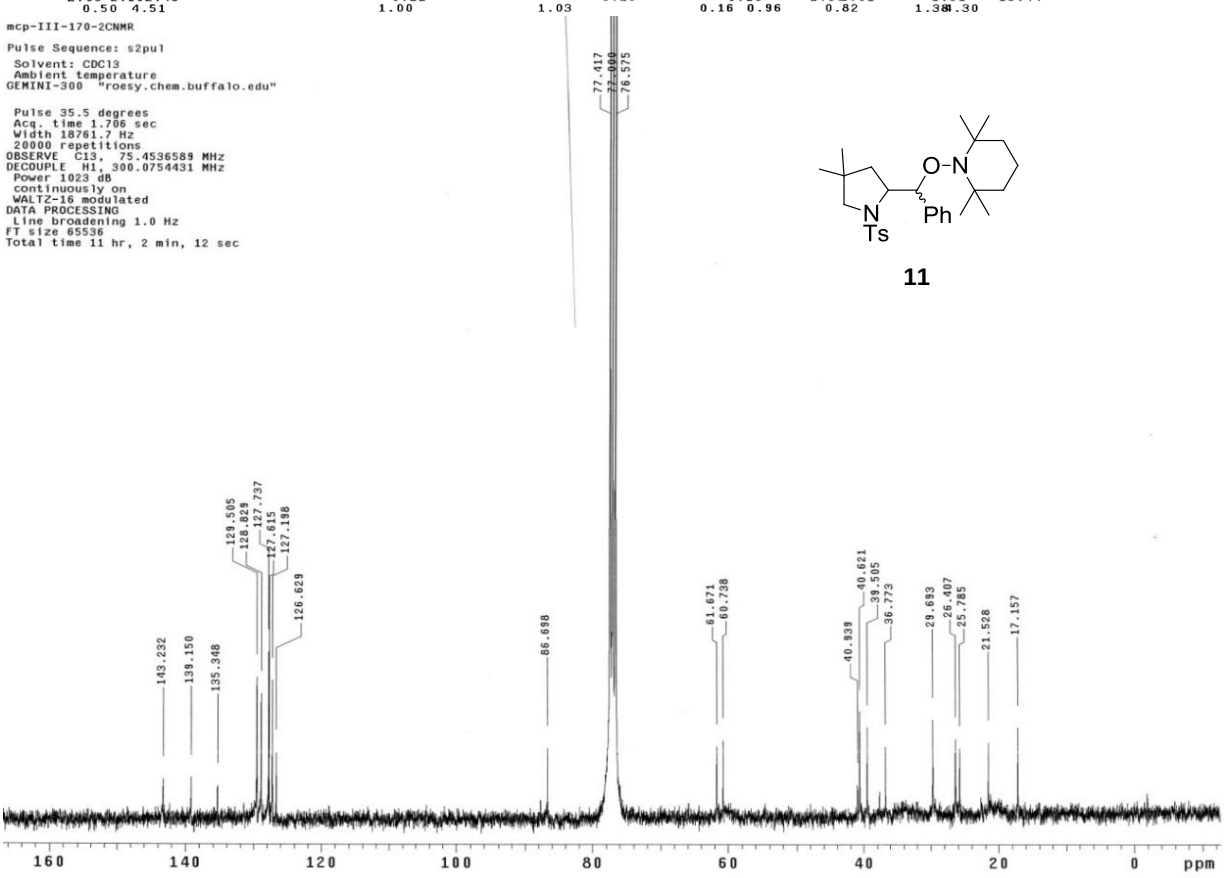
O-N
N
Ts
Ph
11
ppm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Power 1023 dB
continuously on
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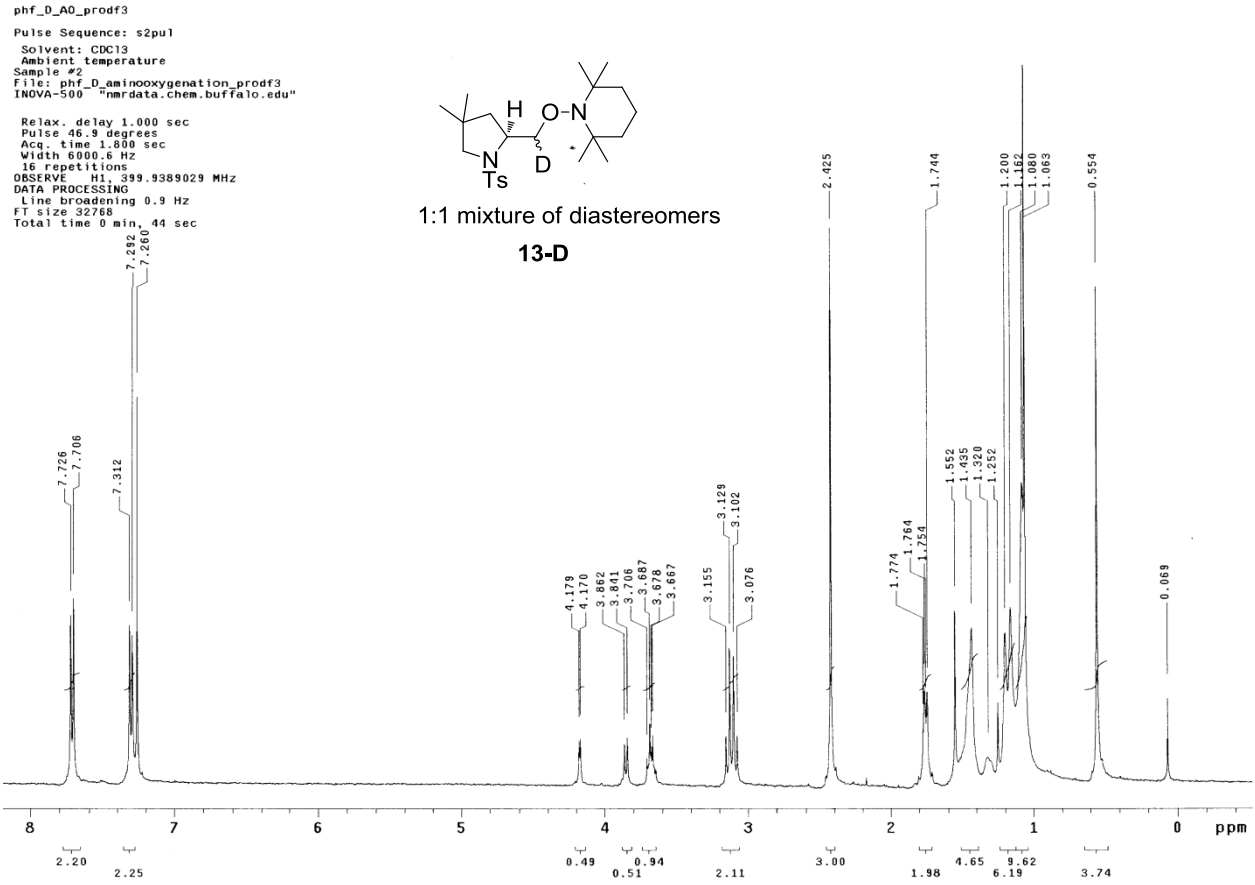
O-N
N
Ts
Ph
11
ppm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Solvent: CDCl3
Ambient temperature
Sample #2
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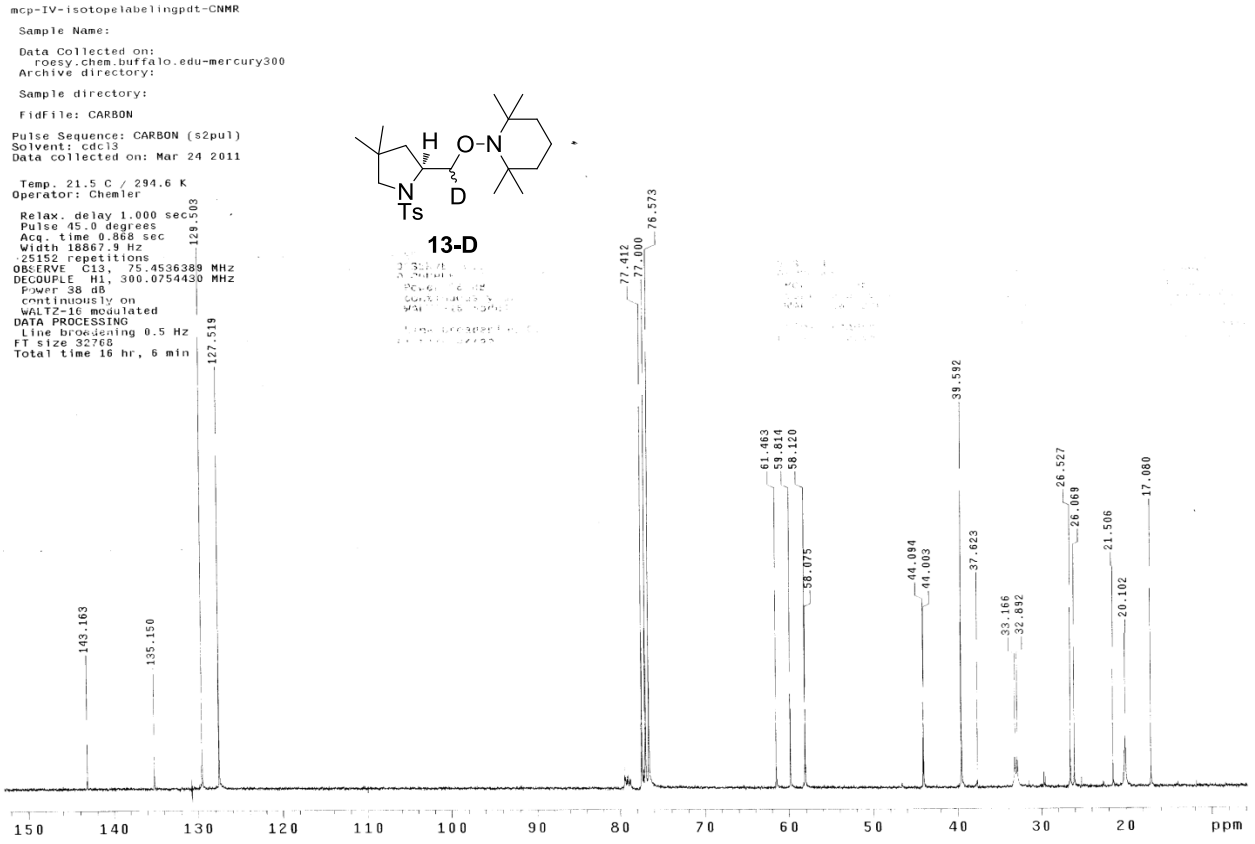
13-D
ppm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Solvent: cdcl3
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Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 16 hr, 6 min
13-D
ppm

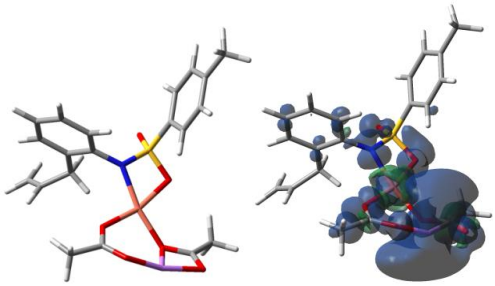
J. Theoretical Section Supporting Information

1. Calculation of [R_2N-Cu] Ground State Complexes

The ground state structures of three [R_2N-Cu] complexes derived from complexation of *N*-tosyl-2-allylaniline (**1**) with $Cu(OAc)_2$ were calculated at 25 °C and a spin density analysis was performed (Figures S-1a-c). These complexes differ in the number of acetate ligands on the copper(II) center, and the cation counterion. The first two complexes are those potentially formed from combination of the lithium amide of **1** with $Cu(OAc)_2$ (as in the EPR experiment, *vide supra*), [Ts(2-allylphenyl)N-$Cu(OAc)_2$]Li (Figure S-1a) and [Ts(2-allylphenyl)N-Cu(OAc)] (Figure S-1b). The third complex is [Ts(2-allylphenyl)N-Cu(OAc)(HOAc)] (Figure S-1c), a structure that may most closely resemble the intermediate formed under the reaction conditions involving Bu_4NOAc. These complexes all have distorted square planar Cu coordination. In all three structures, the sulfonamide oxygen also coordinates to the Cu(II) center, indicating the sulfonamide favors bidentate coordination.[1,2]

Tetrahedral twist is a description of the degree the coordination sphere deviates from square planarity.[3] The tetrahedral twist of the calculated [Ts(2-allylphenyl)N-$Cu(OAc)_2$]Li complex is 4.5°. More dramatically, the bond angles of this complex deviate from the ideal 90° by 5.1-19.2° [e.g. the N-Cu-O(sulfonamide) bond angle is 70.8°]. The tetrahedral twist of the calculated [Ts(2-allylphenyl)N-Cu(OAc)] complex is also 4.5°. The bond angles also deviate from 90° by 19.3-24.1° in this complex [e.g. the N-Cu-O (sulfonamide) bond angle is 72.0° and the O(acetate)-Cu-O(acetate) bond angle is 65.9°]. These deviations from ideal square planarity might cause significant orbital distortion resulting in the loss of the g-parallel signal in the EPR spectra (Figure 6c).

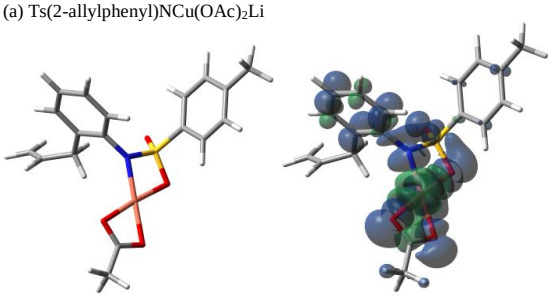
Spin density analysis revealed the majority of the spin resides on Cu. For the [Ts(2-allylphenyl)N-$Cu(OAc)_2$]Li species, 67% of the spin density resides on Cu while a total of 12% of the spin density resides on the sulfonamide ligand (delocalized through the N, Ar and SO_2) (Figure S-1a). In the [Ts(2-allylphenyl)N-Cu(OAc)] species, 53% of the spin density resides on Cu and 26% spin density is delocalized through the sulfonamide ligand (Figure S-1b). The remaining spin density is delocalized onto the acetate ligands. This indicates a significant degree of spin delocalization onto the sulfonamide ligand, but the majority still resides on Cu. This analysis is consistent with the EPR spectra observed for the [R_2N-Cu] intermediate (*vide supra*). Since the spin density on the nitrogen ligand is delocalized, with only 3.5-9.6% located on N, the N-Cu superhyperfine coupling would be expected to be small. Similar to the other two complexes, spin density calculations on the ground state structure of [Ts(2-allylphenyl)N-Cu(OAc)(HOAc)] indicate the Cu contains the majority of the spin density (57%) and the sulfonamide ligand contains 27% total spin density (Figure S-1c).



Interatomic Distances	
N-Cu	2.09 Å
Cu-O(sulfonamide)	1.98 Å
Bond Angles	
N-Cu-O(sulfonamide)	70.8°
O(acetate)-Cu-O(acetate)	96.9°

Spin densities	
Cu	67%
N	4%
O(Ac)	16%
O(S)	6%
Ar(N)	3%

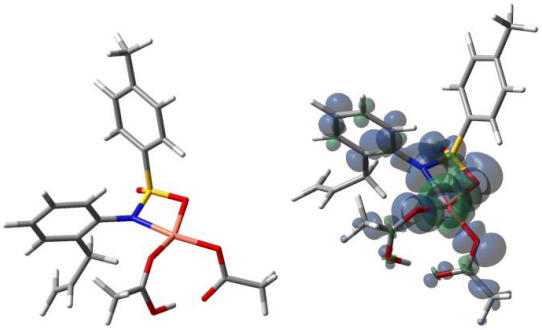
(a) Ts(2-allylphenyl)NCu(OAc)$_2$Li



Interatomic Distances	
N-Cu	1.97 Å
Cu-O(sulfonamide)	2.04 Å
Bond Angles	
N-Cu-O(sulfonamide)	72.0°
O(acetate)-Cu-O(acetate)	65.9°

Spin densities	
Cu	53%
N	10%
O(Ac)	23%
O(S)	8%
Ar(N)	6%

(b) Ts(2-allylphenyl)NCu(OAc) (**I-1B**)



Interatomic Distances	
N-Cu	1.97 Å
Cu-O(sulfonamide)	2.10 Å
Bond Angles	
N-Cu-O(sulfonamide)	70.9°
O(acetate)-Cu-O(acetate)	99.6°

Spin densities	
Cu	57%
N	11%
O(Ac)	17%
O(S)	12%
Ar(N)	3%

(c) Ts(2-allylphenyl)NCu(OAc)(HOAc) (**I-5**)

Figure S-1. Spin density analysis of potential relevant ground state [N-Cu] complexes. O(S) refers to the combined spin density of both oxygen atoms bound to sulfur and O(Ac) refers to the combined spin density on all the oxygen atoms of the acetate ligands.

2. Discussion of Computational Methods, *in Vacuo* vs. Implicit Solvation Model (Toluene)

The Density Functional Theory calculations discussed throughout this manuscript were carried out in the gas phase without the use of an implicit solvation model to account for solvent effects. The use of gase phase calculations were based upon the relatively small dielectric constant of toluene (e = 2.38), and also in part due to its greater computational cost. It is noteworthy that previous computational studies involving copper complexes and C-[Cu] bond dissociation energies have shown that the observed results of gas phase DFT calculations using the B3LYP functional were consistant with experimental findings.[4] In general, the solvent stabilizes charged species, or systems where the charge is separated/polarized.[5,6,7] We use our calculations to compare various pathways *via* relative energies. All of the complexes we have discussed in the manuscript (except for one path discussed here in the SI) have an overall charge of zero and similar degrees of charge separation throughout. Thus, we would expect solvation to lower all energies by similar amounts, thus no great change in relative energies between steps is expected. Nevertheless, in order to gage the effect that toluene would have on our computed B3LYP/GenECP gas phase findings, we carried out as a case example the geometry optimizations of the three key stationary points **I-5** (A), **TS-A** and **I-6** (from Scheme 5, Figure 8) in toluene using the IEFPCM solvation model with the keyword added [scrf=smd]. These three points correspond to the ground state, aminocupration transition state, and subsequent intermediate of pathway A. It was found that the activation barrier to aminocupration in this series was unchanged to the first decimal place (17.2 kcal/mol) while the subsequent intermediate **I-6** was lowered in energy by 2.2 kcal/mol. This latter energy change could result in a slightly endothermic rather than exothermic subsequent C-Cu bond homolysis (this is noted in the manuscript text), but the overall message of the calculations remains unchanged.

3. Comparison of the aminocupration transition states (Bu_4NOAc vs *n*BuLi as base at 100 °C) in temperatures relevant to the kinetics experiments in Figure 4 and Equation 11 (Scheme 6).

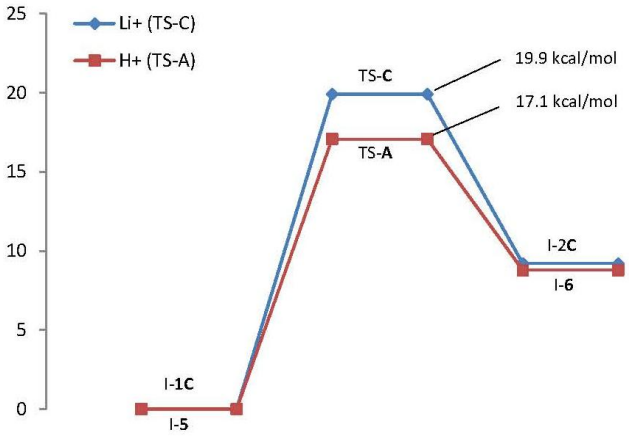
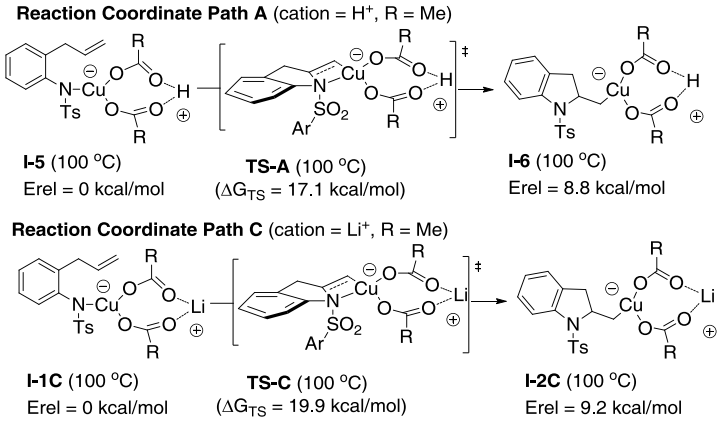


Figure S-2. In agreement with experimental results, the aminocupration of $R_2NCu(OAc)_2Li$ is calculated to be less facile than the aminocupration of $R_2NCu(OAc)(HOAc)$.

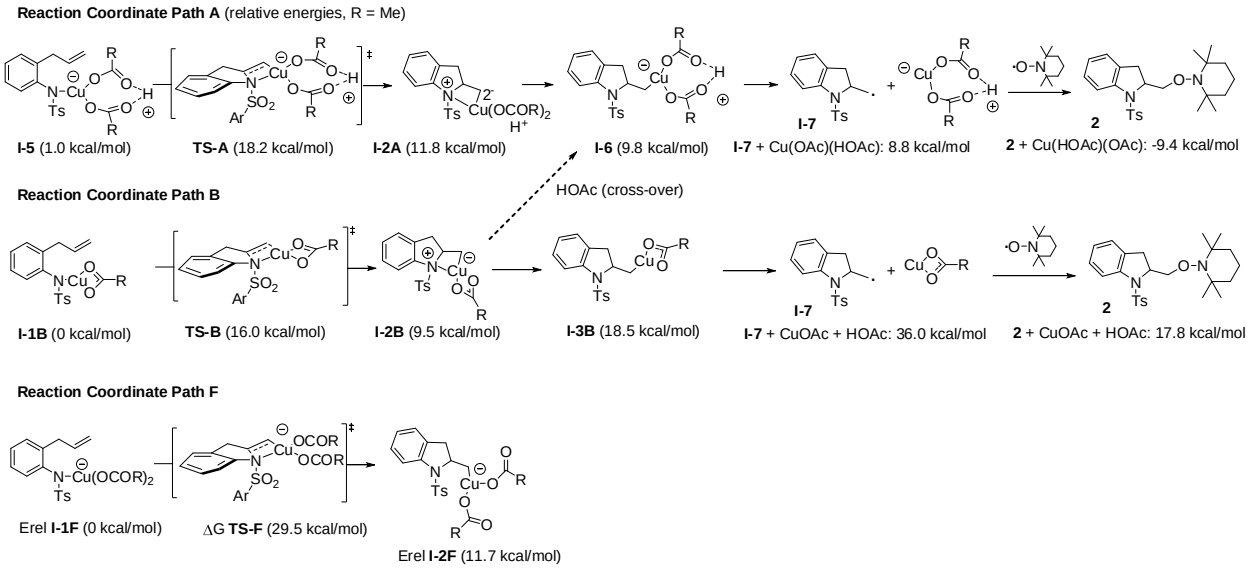


Scheme 6. Cation effects on aminocupration activation energies.

Note: Relative energies only are being compared since different atoms are involved in each path.

4. Initial Steps of an Alternative Two Acetate, Anionic Path F

An aminocupration path starting from $[R_2N\text{-}Cu(OAc)_2]^-$ (**I-1F**) was calculated and the aminocupration activation energy was found to be significantly higher than either Paths A or B, so this path was not considered further (see scheme below and Figure S-3).



Note: relative energies only are being compared with path F.

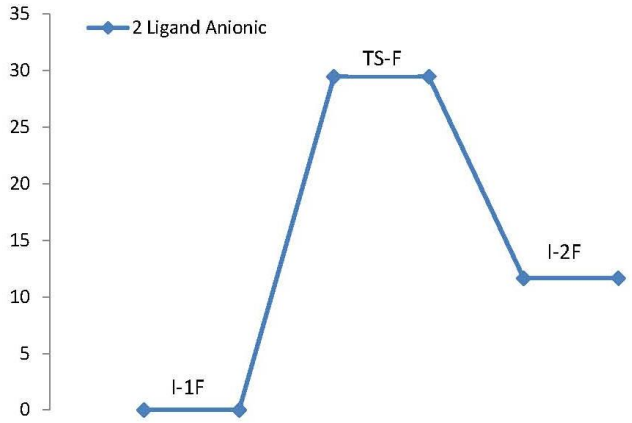
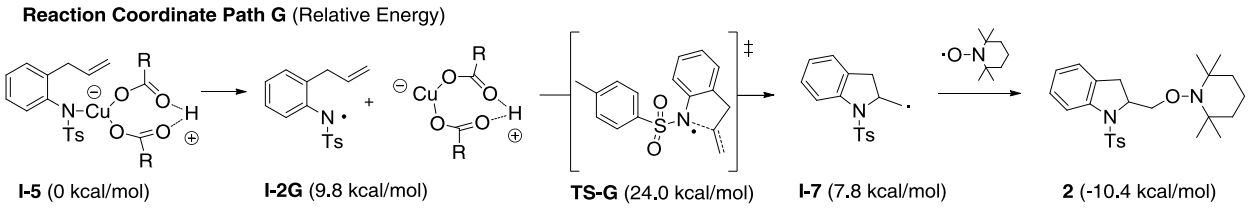


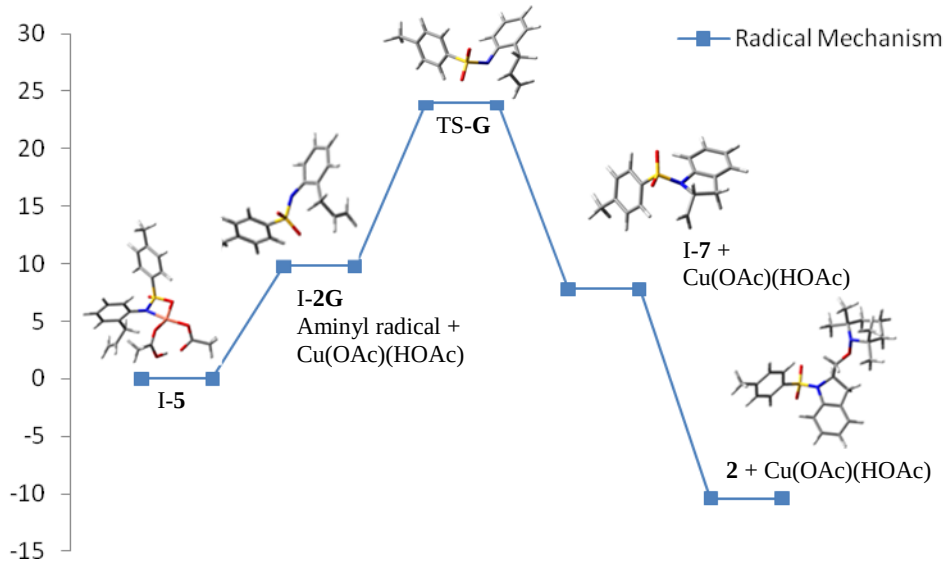
Figure S-3. Aminocupration starting from two-acetate anionic $[R_2NCu(OAc)_2]^-$; $\Delta G_{\mathbf{TSF}}$ = 29.5 kcal/mol.

5. Calculation of an Alternative, Nitrogen Radical Aminooxygenation Mechanism

Because there is evidence for a carbon radical intermediate in the aminooxygenation reaction, we also considered the possibility of a nitrogen radical pathway (Path G, Scheme below).[8] A nitrogen radical could result from the homolysis of the N-Cu bond of intermediate **I-5**; exo addition of the nitrogen radical to the alkene generates the carbon radical intermediate **I-7**. The N-Cu BDE was calculated as 9.8 kcal/mol (Figure S-4). The alkene amination transition state occurs at 24.0 kcal/mol relative to the [N-Cu] intermediate **I-5** ground state. Since the nitrogen radical pathway (Figure S-4) is overall higher in energy than the aminocupration pathway (Figure 8), we conclude it is less likely to occur. The competition experiment illustrated in Eq. 9 (vide supra) also supports the aminocupration as the dominant reaction path. It is noteworthy that the [N-Cu] BDE of intermediate **I-5**, 9.82 kcal/mol, is lower in energy than either of the aminocupration transition states (16.0 kcal/mol, **TS-A** or 17.2 kcal/mol, **TS-B**, Figure 8). Thus it is possible this bond can be broken and re-formed reversibly during the reaction and prior to N-C bond formation.



Scheme S-1. Calculated aminyl radical aminooxygenation pathway G.



.

Figure S-4. Aminyl radical potential energy landscape (Energy scale is in kcal/mol). $\Delta G_{TS\text{-}G}$ = 24.0 kcal/mol.

6. Potential energy landscape for the possible transition states in pathways D and E.

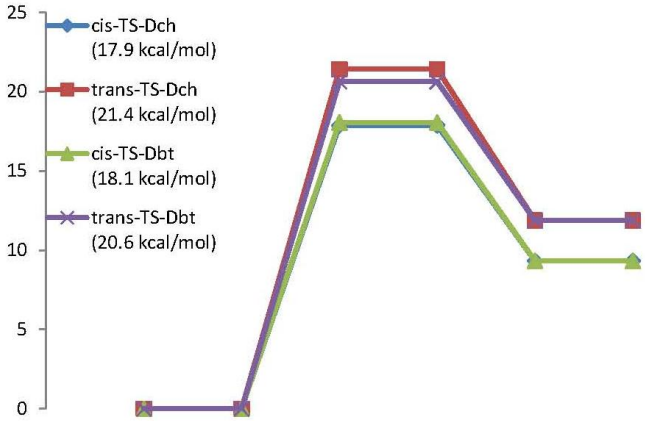


Figure S-5. Potential energy landscape for the four possible transition states in pathway D. (Energy scale in kcal/mol)

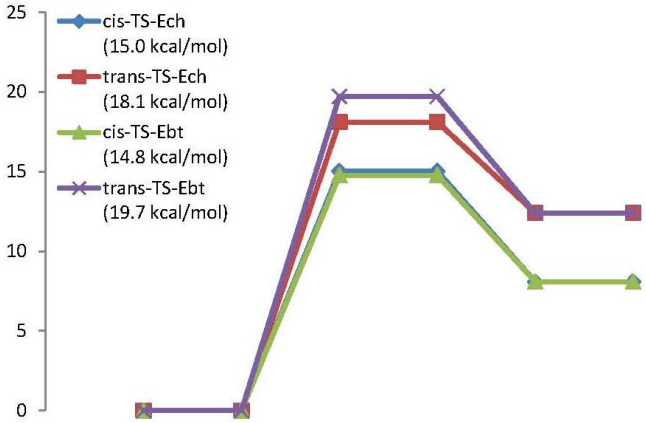
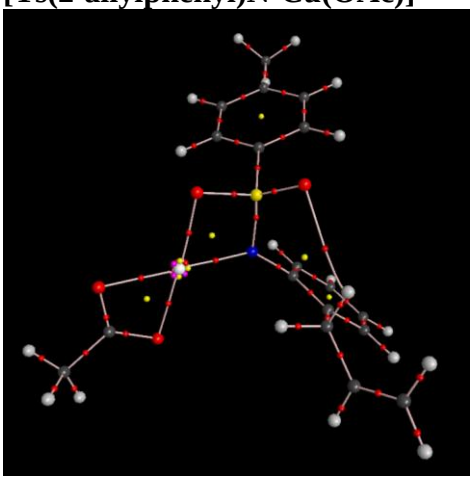


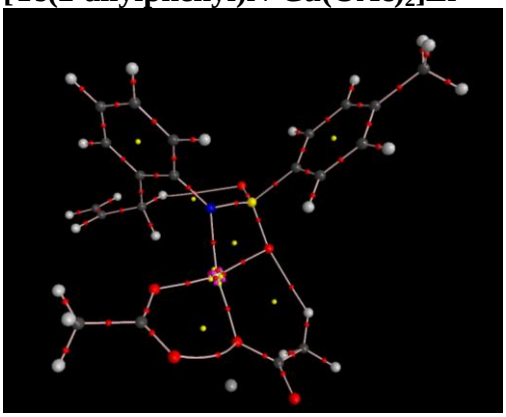
Figure S-6. Potential energy landscape for the four possible transition states in pathway E. (Energy scale in kcal/mol)

7. AIM molecular graphs; electron density (ρ) topology.

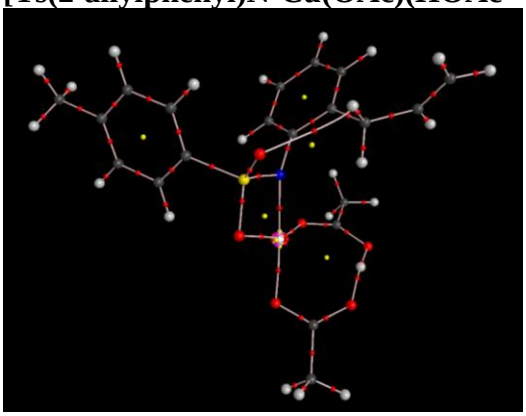
[Ts(2-allylphenyl)N-Cu(OAc)]



[Ts(2-allylphenyl)N-Cu(OAc)$_2$]Li



[Ts(2-allylphenyl)N-Cu(OAc)(HOAc



8. Thermochemical and coordinate data for all structures.

[Ts(2-allylphenyl)N-Cu(OAc)$_2$]Li

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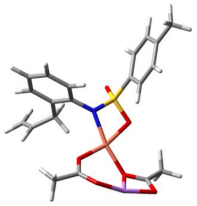
opt=calcfc freq=noraman ub3lyp/genecp gfinput

- Thermochemistry -

Zero-point correction= 0.392311 (Hartree/Particle)
Thermal correction to Energy= 0.425168
Thermal correction to Enthalpy= 0.426112
Thermal correction to Gibbs Free Energy= 0.319918
Sum of electronic and zero-point Energies= -1883.048387
Sum of electronic and thermal Energies= -1883.015530
Sum of electronic and thermal Enthalpies= -1883.014586
Sum of electronic and thermal Free Energies= -1883.120780



Cu	-1.09120100	-1.08137600	-0.20997600	H	3.61930700	1.36401200	-1.81965700
O	-1.42622600	-4.96034000	-0.03817200	C	5.25367600	-0.27510900	0.70183600
C	-1.27138700	-4.02175700	-0.84636700	H	4.29182200	-1.62425600	2.08681000
C	-0.52653100	-4.18886300	-2.14526800	H	5.88513800	1.11341500	-0.81880800
H	0.27652400	-3.44844300	-2.20760700	C	6.62709100	-0.44877000	1.30493700
H	-1.21018400	-3.98899300	-2.97812600	H	7.33961100	0.27293000	0.89444600
H	-0.12679700	-5.20045000	-2.22937300	H	6.60382000	-0.32125800	2.39346600
O	-1.81223600	-2.85973800	-0.57291500	H	7.01980600	-1.45431600	1.10681300
N	0.00028500	0.56759600	-0.01394800	C	-0.20482100	1.87662300	0.50651000
S	1.07849100	0.20279000	-1.15032200	C	-1.04468500	2.81037800	-0.14231200
C	-3.03014100	3.22111300	-1.68128900	C	0.41872500	2.21220900	1.71732800
H	-3.79838500	3.10031600	-0.91586800	C	-1.20001100	4.07216800	0.44462800
C	-3.28053300	3.99098300	-2.74167300	C	0.24809200	3.47312100	2.28370400
H	-2.53988800	4.14285000	-3.52453800	H	1.04009000	1.46480200	2.20175900
H	-4.23610300	4.49215600	-2.87238200	C	-0.56262400	4.40843600	1.63959300
C	-1.74883500	2.46636800	-1.44592500	H	-1.83417000	4.80171700	-0.05119100
H	-1.96987000	1.39050200	-1.44327300	H	0.74269900	3.72130400	3.21887900
H	-1.06089600	2.62357400	-2.28669900	H	-0.70493900	5.39741600	2.06738700
O	1.22218600	1.12486300	-2.28244900	C	-3.03770500	-1.14996500	1.96336800
O	0.57129500	-1.21013900	-1.45102000	O	-2.50387300	-0.49816300	1.00046400
C	2.70483200	0.01336900	-0.42293600	C	-4.05219200	-0.38564800	2.79735600
C	2.88257200	-0.83123200	0.67911300	H	-5.03306100	-0.86196300	2.68914400
C	3.77979600	0.71525400	-0.96587600	H	-4.11578200	0.65994400	2.49352400
C	4.15116000	-0.96865200	1.23080300	H	-3.77341200	-0.45410100	3.85365800
H	2.03907000	-1.36843900	1.10074600	O	-2.79516900	-2.34580100	2.26905000
C	5.04606400	0.56566800	-0.39762800	Li	-2.34350500	-3.67342100	1.11796600

[Ts(2-allylphenyl)N-Cu(OAc)(HOAc)]

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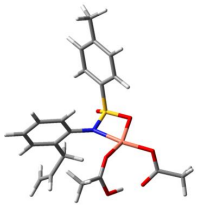
opt=calcfc freq=noraman ub3lyp/genecp gfinput

- Thermochemistry -

Zero-point correction= 0.401222 (Hartree/Particle)
Thermal correction to Energy= 0.433205
Thermal correction to Enthalpy= 0.434149
Thermal correction to Gibbs Free Energy= 0.328976
Sum of electronic and zero-point Energies= -1876.001939
Sum of electronic and thermal Energies= -1875.969956
Sum of electronic and thermal Enthalpies= -1875.969012
Sum of electronic and thermal Free Energies= -1876.074185



Cu	-1.10599300	-1.29984600	0.06774800	H	3.55123600	0.89029400	-1.62426600
O	-3.96287400	0.02109400	1.18550400	C	5.12436500	-1.29001300	0.49090000
C	-2.93888700	0.03725500	1.98586800	H	4.16626100	-2.99569000	1.40121300
C	-3.10920400	0.85151000	3.24067900	H	5.76889900	0.45547400	-0.59739700
H	-4.00826700	1.46696800	3.18957500	C	6.46794700	-1.54606400	1.13105700
H	-2.22220400	1.47304600	3.38890100	H	7.28440700	-1.13800600	0.52675700
H	-3.18534800	0.17005900	4.09552000	H	6.52707300	-1.07523300	2.12146500
O	-1.86931200	-0.57106600	1.78299800	H	6.64843400	-2.61721600	1.26977700
N	0.04784900	0.26367000	-0.24771200	C	0.30803000	1.51148000	0.38512800
S	1.00562400	-0.42592100	-1.35187800	C	-0.13042100	2.72250000	-0.19898800
C	-1.82213300	3.87038900	-1.71074900	C	0.95383900	1.52395900	1.63128500
H	-2.62759400	3.91839000	-0.97594500	C	0.12560800	3.91540500	0.49040600
C	-1.77347700	4.78319200	-2.68239800	C	1.18658800	2.72191500	2.30334500
H	-0.98718200	4.77379700	-3.43473700	H	1.26561100	0.57732300	2.06246000
H	-2.52227800	5.56597100	-2.77116100	C	0.77472200	3.92397600	1.72530300
C	-0.84630800	2.73604500	-1.54168600	H	-0.19899400	4.85164000	0.04490500
H	-1.37234000	1.77975500	-1.65686400	H	1.68925000	2.71596600	3.26686300
H	-0.10710100	2.75661900	-2.35279200	H	0.95411100	4.86708700	2.23496800
O	1.23386600	0.33742100	-2.58190300	C	-3.25417300	-2.80818500	-0.54009600
O	0.26538300	-1.75455700	-1.45018600	O	-2.07972200	-2.94463000	-0.04049800
C	2.61744500	-0.79003000	-0.65494000	C	-3.93592700	-4.08093500	-0.99843300
C	2.78183100	-1.88980900	0.19245500	H	-5.00326800	-3.91092700	-1.14933100
C	3.68841700	0.05736400	-0.94340300	H	-3.77147200	-4.88172000	-0.27220200
C	4.03249700	-2.13202600	0.75440600	H	-3.48694300	-4.39935900	-1.94644500
H	1.95118400	-2.56149800	0.38281600	O	-3.82807500	-1.69924300	-0.69017700
C	4.93222000	-0.19970800	-0.36812100	H	-3.83661200	-0.63966900	0.39724900

[Ts(2-allylphenyl)N-Cu(OAc)]

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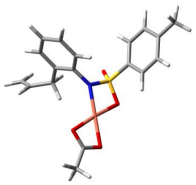
opt=calcfc freq=noraman ub3lyp/genecp gfinput

- Thermochemistry -

Zero-point correction= 0.370856 (Hartree/Particle)
Thermal correction to Energy= 0.397715
Thermal correction to Enthalpy= 0.398659
Thermal correction to Gibbs Free Energy= 0.307514
Sum of electronic and zero-point Energies= -1573.127337
Sum of electronic and thermal Energies= -1573.100478
Sum of electronic and thermal Enthalpies= -1573.099534
Sum of electronic and thermal Free Energies= -1573.190679



Cu	-1.15767200	-1.67450000	-0.12899300	H	5.16129900	1.76560100	-0.47220300
N	-0.29295500	0.07834300	0.05570300	C	6.46929400	-0.31835500	0.72705500
S	0.69083700	-0.09317100	-1.21410600	H	7.07914000	0.47544800	0.28477800
C	-3.59053900	2.75790100	-0.95208400	H	6.50176300	-0.19011300	1.81714300
H	-4.27376600	2.54759600	-0.12771900	H	6.94420000	-1.27927300	0.50076200
C	-3.95935400	3.61866500	-1.90220000	C	-0.49027200	1.30359700	0.75487100
H	-3.30569100	3.85904600	-2.73843800	C	-1.44275300	2.25424200	0.32144800
H	-4.92935700	4.10876400	-1.88605200	C	0.25948400	1.53487500	1.91751000
C	-2.28119300	2.01506600	-0.92535700	C	-1.58262800	3.42972500	1.06930900
H	-2.48190200	0.93721400	-0.99957900	C	0.10001300	2.71028900	2.64776600
H	-1.69059900	2.26278000	-1.81660400	H	0.96695100	0.77409300	2.23403600
O	0.62097900	0.94270500	-2.24930700	C	-0.82287100	3.66362300	2.21637300
O	0.28149000	-1.51965400	-1.58487000	H	-2.30301300	4.17298600	0.73995000
C	2.39825300	-0.18498200	-0.68268800	H	0.69020600	2.87828600	3.54449000
C	2.89276000	-1.36055700	-0.10899400	H	-0.95824300	4.58670500	2.77391700
C	3.20850400	0.94349300	-0.81623600	C	-3.84855100	-4.06807000	1.22448600
C	4.21221100	-1.39554700	0.33186500	H	-3.43408400	-5.07375900	1.33674700
H	2.26169500	-2.23999100	-0.03797200	H	-4.25442800	-3.71180200	2.17290900
C	4.52648000	0.88996200	-0.36337900	H	-4.65688100	-4.12314800	0.48618000
H	2.81589300	1.83888100	-1.28554300	C	-2.78880900	-3.13306000	0.71813400
C	5.04787500	-0.27249800	0.21921900	O	-2.65570900	-1.95719800	1.19550900
H	4.60426700	-2.31307300	0.76393800	O	-1.99864500	-3.47880500	-0.22342400

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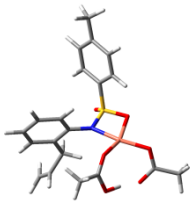
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.401222 (Hartree/Particle)
Thermal correction to Energy= 0.450085
Thermal correction to Enthalpy= 0.451299
Thermal correction to Gibbs Free Energy= 0.296804
Sum of electronic and zero-point Energies= -1876.001939
Sum of electronic and thermal Energies= -1875.953075
Sum of electronic and thermal Enthalpies= -1875.951862
Sum of electronic and thermal Free Energies= -1876.106357



Cu	-1.10584700	-1.30008400	0.06772200	C	5.12451000	-1.28952200	0.49099300
O	-3.96266400	0.02092700	1.18562200	H	4.16664000	-2.99543500	1.40110000
C	-2.93867600	0.03695800	1.98599600	H	5.76880800	0.45618600	-0.59709100
C	-3.10885800	0.85131200	3.24076000	C	6.46812500	-1.54543900	1.13113400
H	-4.00864700	1.46575800	3.19029900	H	7.28455900	-1.13758400	0.52665800
H	-2.22244100	1.47394400	3.38796100	H	6.52734200	-1.07431900	2.12139700
H	-3.18332500	0.17002500	4.09586500	H	6.64858600	-2.61655600	1.27014500
O	-1.86916200	-0.57145400	1.78312200	C	0.30777200	1.51142900	0.38514400
N	0.04779000	0.26357300	-0.24767700	C	-0.13084100	2.72237400	-0.19900700
S	1.00569200	-0.42587000	-1.35182000	C	0.95354200	1.52402600	1.63132000
C	-1.82261900	3.87003500	-1.71086800	C	0.12499700	3.91532900	0.49037100
H	-2.62813800	3.91796700	-0.97612400	C	1.18609300	2.72202700	2.30336600
C	-1.77398600	4.78282800	-2.68252600	H	1.26543900	0.57744500	2.06252400
H	-0.98764200	4.77349700	-3.43481600	C	0.77407200	3.92401700	1.72528700
H	-2.52285600	5.56553300	-2.77135000	H	-0.19972200	4.85150900	0.04484200
C	-0.84669900	2.73578600	-1.54172200	H	1.68872600	2.71617100	3.26689900
H	-1.37265000	1.77944800	-1.65685600	H	0.95331100	4.86716400	2.23493800
H	-0.10747200	2.75638700	-2.35281100	C	-3.25388300	-2.80818400	-0.54030100
O	1.23386400	0.33751300	-2.58183100	O	-2.07955100	-2.94491700	-0.04052300
O	0.26564700	-1.75461800	-1.45016700	C	-3.93598600	-4.08072600	-0.99867200
C	2.61754500	-0.78979200	-0.65486000	H	-5.00333300	-3.91048300	-1.14928400
C	2.78207400	-1.88963300	0.19242100	H	-3.77151200	-4.88167900	-0.27263400
C	3.68840000	0.05779700	-0.94319800	H	-3.48732200	-4.39903500	-1.94687500
C	4.03276400	-2.13172200	0.75438100	O	-3.82739400	-1.69905100	-0.69053400
H	1.95152500	-2.56146900	0.38268500	H	-3.83634000	-0.63964300	0.39726500
C	4.93222200	-0.19914800	-0.36791000				
H	3.55111400	0.89078000	-1.62397400				

TS-A

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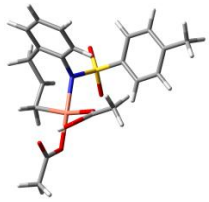
opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.400984 (Hartree/Particle)
Thermal correction to Energy= 0.448461
Thermal correction to Enthalpy= 0.449675
Thermal correction to Gibbs Free Energy= 0.301755
Sum of electronic and zero-point Energies= -1875.979746
Sum of electronic and thermal Energies= -1875.932268
Sum of electronic and thermal Enthalpies= -1875.931054
Sum of electronic and thermal Free Energies= -1876.078974



Cu	-1.65125000	-0.23486700	-0.60204000	H	3.64899400	1.59832400	-0.45992500
O	-3.84453400	-1.27553800	1.01469800	C	4.52673800	-1.69497900	-0.15394400
C	-4.03310700	-1.54050300	-0.20196600	H	3.28896700	-3.34102400	-0.79497400
C	-5.34455900	-2.18479600	-0.61768200	H	5.50459300	0.15827700	0.35704700
H	-5.50508600	-2.10452300	-1.69436800	C	5.67307800	-2.56871500	0.29706700
H	-6.17144000	-1.72302300	-0.07092500	H	5.32617000	-3.56094200	0.60350300
H	-5.32115900	-3.24563800	-0.34075900	H	6.39795000	-2.71338400	-0.51503200
O	-3.18245500	-1.31613800	-1.12997100	H	6.21301600	-2.12024500	1.13759400
N	-0.08545900	1.06687900	-0.45238700	C	0.21299900	1.68812100	0.79505900
S	1.10788400	0.97310300	-1.65799400	C	-0.36318000	2.95155900	0.98702400
C	-1.48294300	2.36024000	-1.17339000	C	0.94748100	1.07985200	1.82015900
H	-1.04353000	2.46608900	-2.16075700	C	-0.18811700	3.61560800	2.20068100
C	-2.66717500	1.59032300	-1.10091600	C	1.13268400	1.76036800	3.02451400
H	-3.33608200	1.70893300	-0.25003800	H	1.36163900	0.08939300	1.66917200
H	-3.11499000	1.22890200	-2.02222500	C	0.56817200	3.02434800	3.21549900
C	-1.15952700	3.47508900	-0.18806700	H	-0.64059900	4.59199400	2.35604900
H	-0.58484500	4.25159200	-0.70791700	H	1.70829800	1.29617500	3.82059800
H	-2.09391400	3.93389500	0.15648100	H	0.70539700	3.54439100	4.15941700
O	1.67737700	2.31196100	-1.87205500	C	-0.73613200	-2.41261200	1.43172000
O	0.42586800	0.26870600	-2.75486600	O	-0.55662100	-1.78274300	0.37966500
C	2.43000900	-0.07388000	-1.05105400	C	0.33787300	-3.30338900	2.00752700
C	2.31600200	-1.46203900	-1.15579300	H	0.03298700	-4.35021500	1.89632800
C	3.57436200	0.51774600	-0.51107200	H	0.45078000	-3.10995000	3.07834200
C	3.36645400	-2.25997300	-0.70569600	H	1.28236800	-3.14167400	1.48687400
H	1.42481100	-1.90466800	-1.58434600	O	-1.83528100	-2.39431900	2.13916600
C	4.61153200	-0.29802600	-0.06289000	H	-2.58670800	-1.86081700	1.67984700

I-2A

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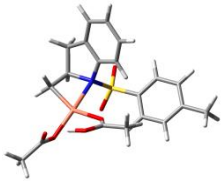
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.401934 (Hartree/Particle)
Thermal correction to Energy= 0.449465
Thermal correction to Enthalpy= 0.450678
Thermal correction to Gibbs Free Energy= 0.304531
Sum of electronic and zero-point Energies= -1875.991666
Sum of electronic and thermal Energies= -1875.944135
Sum of electronic and thermal Enthalpies= -1875.942922
Sum of electronic and thermal Free Energies= -1876.089070



Cu	-1.77850200	0.03957700	-0.35752900	H	3.88143500	0.96116300	-0.65204100
O	-4.27608900	-1.14379000	0.91798000	C	3.97328900	-2.44295300	-0.31522800
C	-4.36862800	-1.04994400	-0.33742600	H	2.34835000	-3.75750300	-0.84953100
C	-5.72601600	-1.31105300	-0.97015900	H	5.38739800	-0.86803100	0.10192200
H	-5.74278200	-1.00210700	-2.01674200	C	4.90469600	-3.55804300	0.09551500
H	-6.50089900	-0.78429000	-0.40509500	H	4.35195200	-4.43073100	0.45792600
H	-5.94975300	-2.38237600	-0.90646300	H	5.51475200	-3.88879600	-0.75544900
O	-3.40889400	-0.76262100	-1.12488900	H	5.59352800	-3.23656100	0.88348100
N	0.07857300	1.27728300	-0.44579500	C	0.66639000	1.70932600	0.80252200
S	1.23299900	0.92664800	-1.75732900	C	0.48692100	3.08055700	1.01494600
C	-0.83426600	2.46754300	-0.88833100	C	1.27898600	0.88950800	1.74800100
H	-0.75128300	2.56055600	-1.97174400	C	0.95489100	3.66015200	2.19085000
C	-2.22257300	2.01468800	-0.50721600	C	1.75410100	1.48462600	2.92059200
H	-2.54655400	2.31296800	0.49481800	H	1.36386700	-0.17770700	1.58144500
H	-2.99306000	2.17564500	-1.26002400	C	1.59769200	2.85678900	3.13927600
C	-0.25468800	3.69671900	-0.14633100	H	0.81794200	4.72270500	2.37376400
H	0.42909900	4.26396000	-0.79003300	H	2.23623700	0.86903100	3.67482500
H	-1.05716900	4.37085400	0.17036900	H	1.96329400	3.30071700	4.06104500
O	2.06757400	2.11615500	-1.96914600	C	-1.20566400	-2.33611300	1.50244600
O	0.38436300	0.40133600	-2.83032300	O	-0.83741100	-1.57195100	0.59060500
C	2.27368400	-0.38576500	-1.14158100	C	-0.22980800	-3.29270600	2.14797600
C	1.82824500	-1.70771900	-1.21034800	H	-0.62705300	-4.31162300	2.10377400
C	3.55293800	-0.07183600	-0.67585100	H	-0.11713300	-3.03612100	3.20705300
C	2.68395900	-2.72503200	-0.79256100	H	0.73912000	-3.24294600	1.64982700
H	0.83658200	-1.93407300	-1.58293800	O	-2.40407500	-2.39718800	1.99518800
C	4.39068700	-1.10457000	-0.26166000	H	-3.11204700	-1.78039100	1.50805800

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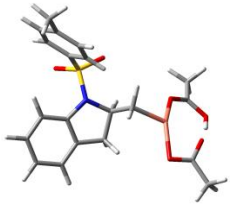
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.403376 (Hartree/Particle)
Thermal correction to Energy= 0.451379
Thermal correction to Enthalpy= 0.452592
Thermal correction to Gibbs Free Energy= 0.300389
Sum of electronic and zero-point Energies= -1875.989313
Sum of electronic and thermal Energies= -1875.941309
Sum of electronic and thermal Enthalpies= -1875.940096
Sum of electronic and thermal Free Energies= -1876.092299



Cu	-2.77557900	-0.41551800	0.72540600	H	4.93720800	-0.84859200	-1.58757000
O	-4.85344500	-0.47485500	1.20777400	C	5.33564200	-1.84255600	1.66329300
C	-4.70623300	0.65675200	1.80164000	H	3.71434000	-2.02490700	3.07669200
C	-5.90715900	1.33464600	2.41243800	H	6.69992200	-1.56260700	0.01992000
H	-5.64383800	2.32165200	2.79536900	C	6.40004000	-2.25694200	2.65144800
H	-6.29135600	0.71457000	3.23001800	H	6.57340200	-1.47155900	3.39858500
H	-6.70441200	1.41906600	1.66699500	H	6.10725500	-3.16119100	3.19746800
O	-3.55658000	1.16951500	1.88455100	H	7.35377800	-2.45616700	2.15327200
N	1.19924800	0.58583100	-0.55675500	C	1.60139400	1.94659500	-0.56347400
S	2.09145500	-0.61631800	-1.34868100	C	0.48176900	2.78645900	-0.55282700
C	-0.31806900	0.48183500	-0.53057300	C	2.89647800	2.46503800	-0.53161400
H	-0.62987600	-0.06481600	-1.42186500	C	0.64688200	4.16579900	-0.50609100
C	-0.78820100	-0.25755300	0.70491300	C	3.04850700	3.85459200	-0.49799000
H	-0.45987800	-1.30195100	0.71421100	H	3.76496600	1.81698700	-0.54163600
H	-0.53135800	0.26165000	1.63474000	C	1.93925300	4.70329500	-0.48147900
C	-0.78655900	1.96855800	-0.58799600	H	-0.22112800	4.82081700	-0.49406600
H	-1.36556100	2.16458400	-1.49998200	H	4.05047700	4.27495100	-0.48087800
H	-1.44195600	2.19239800	0.26188700	H	2.07853000	5.78015100	-0.45004900
O	2.78113100	-0.07135000	-2.52337000	C	-4.07788100	-1.93297400	-1.54157700
O	1.17196300	-1.75106000	-1.48849400	O	-3.03072700	-1.58990700	-0.97597200
C	3.35505000	-1.04025400	-0.14675600	C	-4.06234300	-2.74940700	-2.80476800
C	2.99794300	-1.37446800	1.16272200	H	-4.72345700	-2.29879700	-3.55096600
C	4.68313100	-1.10860400	-0.56568100	H	-4.44866600	-3.75179700	-2.58808200
C	3.98856300	-1.76889200	2.05596700	H	-3.04460100	-2.82474900	-3.18769200
H	1.96140200	-1.31252100	1.47761800	O	-5.28805500	-1.64149400	-1.11156100
C	5.66363700	-1.50881900	0.34402500	H	-5.24676300	-1.14225700	-0.24173600

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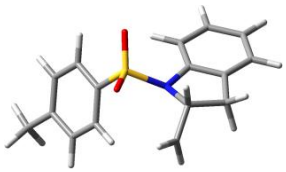
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.285077 (Hartree/Particle)
Thermal correction to Energy= 0.314376
Thermal correction to Enthalpy= 0.315590
Thermal correction to Gibbs Free Energy= 0.214831
Sum of electronic and zero-point Energies= -1222.295575
Sum of electronic and thermal Energies= -1222.266276
Sum of electronic and thermal Enthalpies= -1222.265062
Sum of electronic and thermal Free Energies= -1222.365821



N	1.03533000	-0.67747700	-0.03467100	H	-1.98051200	1.04476300	2.05905900
S	-0.15119000	-0.97715200	1.15332700	C	-4.00559600	0.71159700	-0.67989300
C	1.95130900	-1.83741600	-0.41263700	H	-3.62274500	-0.65706300	-2.30544200
H	2.27145300	-2.32773500	0.51208400	H	-4.08850600	1.94420900	1.08431200
C	1.28812400	-2.82407900	-1.30599800	C	-5.28517600	1.24586200	-1.27836200
H	1.08796000	-2.55860900	-2.34057000	H	-5.72831400	2.02307100	-0.64861700
H	0.89108100	-3.75338400	-0.91743800	H	-5.10983500	1.67664000	-2.27175200
C	3.15931300	-1.11220600	-1.07485700	H	-6.02860300	0.44843000	-1.40046900
H	4.10407100	-1.58422600	-0.78537700	C	1.78233000	0.53367300	-0.04419300
H	3.08541600	-1.18599500	-2.16848200	C	3.03721100	0.32338000	-0.62871500
O	0.12711500	-0.20881700	2.37108900	C	1.39199100	1.80170500	0.38764100
O	-0.28083100	-2.43632700	1.20686500	C	3.92722500	1.38020600	-0.77724400
C	-1.63110600	-0.28954000	0.41181300	C	2.29906000	2.85561500	0.23791600
C	-2.08778500	-0.78439200	-0.81371200	H	0.42573000	1.97126500	0.84589000
C	-2.34637200	0.68610900	1.10293600	C	3.55672500	2.65555700	-0.33533900
C	-3.26620900	-0.27849400	-1.35034700	H	4.90186900	1.21590200	-1.23061100
H	-1.52258800	-1.54923500	-1.33673300	H	2.01422100	3.84651600	0.58114500
C	-3.52873000	1.18166200	0.54883700	H	4.24688100	3.48792900	-0.43823500

2

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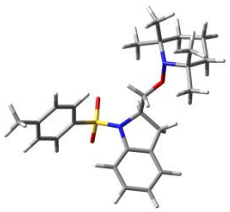
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.556596 (Hartree/Particle)
Thermal correction to Energy= 0.605086
Thermal correction to Enthalpy= 0.606299
Thermal correction to Gibbs Free Energy= 0.463938
Sum of electronic and zero-point Energies= -1705.801809
Sum of electronic and thermal Energies= -1705.753320
Sum of electronic and thermal Enthalpies= -1705.752107
Sum of electronic and thermal Free Energies= -1705.894468



N	1.22959600	0.82085600	-0.51712900	H	0.15292100	5.07142100	0.40383600
S	2.23154500	-0.07294500	-1.57900700	H	4.06891200	3.80569200	1.67294300
C	-0.22215300	0.96666800	-0.87300100	H	2.32354500	5.55978200	1.52299900
H	-0.39879800	0.55940600	-1.86817600	C	-5.23968900	0.77005100	0.22327600
C	-1.03789800	0.15617600	0.13897700	C	-5.85078500	-0.26052000	-0.73541800
H	-0.69294100	-0.88232300	0.13510900	C	-4.74851500	-1.04386100	-1.46030000
H	-0.90299000	0.55978200	1.15214800	C	-3.73742600	-1.70265300	-0.49256500
C	-0.49359800	2.49223000	-0.81544700	C	-4.23250200	0.14857100	1.22089600
H	-0.55045900	2.92261800	-1.82404200	H	-5.18638600	-1.81716900	-2.10500900
H	-1.45026800	2.69759900	-0.32581600	H	-6.51311200	-0.94579200	-0.18972100
O	3.14909100	0.81338200	-2.30183500	H	-6.48608700	0.25029800	-1.46988800
O	1.32034900	-0.96621500	-2.30324000	H	-4.71325800	1.53200000	-0.36524800
C	3.21763000	-1.06207600	-0.45465200	H	-6.02793400	1.29009000	0.78358400
C	2.59424900	-1.97758500	0.39888100	H	-4.19736700	-0.35802800	-2.11566100
C	4.60664500	-0.95817400	-0.50178700	N	-3.20412700	-0.70687900	0.51605300
C	3.37774100	-2.78131300	1.21930500	O	-2.39923400	0.22969800	-0.26678000
H	1.51243300	-2.05754100	0.41931800	C	-3.49469800	1.27301200	1.97178700
C	5.37758300	-1.77472400	0.32870900	H	-4.22208200	1.86660800	2.53662900
H	5.06904800	-0.25048900	-1.18134600	H	-2.77196100	0.85872000	2.68363100
C	4.78053800	-2.69403700	1.19862400	H	-2.97093200	1.94342300	1.28918100
H	2.89567000	-3.49206300	1.88631300	C	-4.94975600	-0.68629500	2.30563500
H	6.46119700	-1.69628400	0.29410900	H	-4.22743400	-1.29569600	2.85774200
C	5.61408100	-3.57666900	2.09693600	H	-5.43154700	-0.00506400	3.01552900
H	6.68429000	-3.41401100	1.93810500	H	-5.72956400	-1.34183200	1.91828700
H	5.39828600	-3.38282700	3.15499100	C	-4.36143200	-2.90993900	0.24383100
H	5.40429500	-4.63780900	1.91544900	H	-4.41476500	-3.75628500	-0.44961200
C	1.68722400	2.05469600	0.03678200	H	-3.73588000	-3.20645100	1.09156100
C	0.69734400	3.03948100	-0.06363300	H	-5.37478600	-2.73597500	0.60638400
C	2.90694300	2.30824900	0.66089300	C	-2.55399500	-2.26956800	-1.30071000
C	0.91821700	4.30231600	0.47457800	H	-2.93310100	-3.00648200	-2.01744200
C	3.12302700	3.58659100	1.18511100	H	-2.02498200	-1.49902500	-1.86262500
H	3.66848100	1.54095500	0.74293800	H	-1.84010100	-2.78138500	-0.64553100
C	2.14005900	4.57579100	1.10092700				

I-1B

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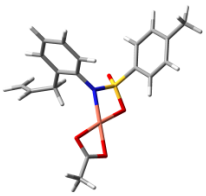
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.338049 (Hartree/Particle)
Thermal correction to Energy= 0.378466
Thermal correction to Enthalpy= 0.379679
Thermal correction to Gibbs Free Energy= 0.245903
Sum of electronic and zero-point Energies= -1646.960806
Sum of electronic and thermal Energies= -1646.920389
Sum of electronic and thermal Enthalpies= -1646.919176
Sum of electronic and thermal Free Energies= -1647.052952



Cu	-1.15767200	-1.67450000	-0.12899300	H	5.16129900	1.76560100	-0.47220300
N	-0.29295500	0.07834300	0.05570300	C	6.46929400	-0.31835500	0.72705500
S	0.69083700	-0.09317100	-1.21410600	H	7.07914000	0.47544800	0.28477800
C	-3.59053900	2.75790100	-0.95208400	H	6.50176300	-0.19011300	1.81714300
H	-4.27376600	2.54759600	-0.12771900	H	6.94420000	-1.27927300	0.50076200
C	-3.95935400	3.61866500	-1.90220000	C	-0.49027200	1.30359700	0.75487100
H	-3.30569100	3.85904600	-2.73843800	C	-1.44275300	2.25424200	0.32144800
H	-4.92935700	4.10876400	-1.88605200	C	0.25948400	1.53487500	1.91751000
C	-2.28119300	2.01506600	-0.92535700	C	-1.58262800	3.42972500	1.06930900
H	-2.48190200	0.93721400	-0.99957900	C	0.10001300	2.71028900	2.64776600
H	-1.69059900	2.26278000	-1.81660400	H	0.96695100	0.77409300	2.23403600
O	0.62097900	0.94270500	-2.24930700	C	-0.82287100	3.66362300	2.21637300
O	0.28149000	-1.51965400	-1.58487000	H	-2.30301300	4.17298600	0.73995000
C	2.39825300	-0.18498200	-0.68268800	H	0.69020600	2.87828600	3.54449000
C	2.89276000	-1.36055700	-0.10899400	H	-0.95824300	4.58670500	2.77391700
C	3.20850400	0.94349300	-0.81623600	C	-3.84855100	-4.06807000	1.22448600
C	4.21221100	-1.39554700	0.33186500	H	-3.43408400	-5.07375900	1.33674700
H	2.26169500	-2.23999100	-0.03797200	H	-4.25442800	-3.71180200	2.17290900
C	4.52648000	0.88996200	-0.36337900	H	-4.65688100	-4.12314800	0.48618000
H	2.81589300	1.83888100	-1.28554300	C	-2.78880900	-3.13306000	0.71813400
C	5.04787500	-0.27249800	0.21921900	O	-2.65570900	-1.95719800	1.19550900
H	4.60426700	-2.31307300	0.76393800	O	-1.99864500	-3.47880500	-0.22342400

TS-B

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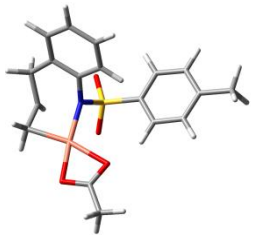
opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.337937 (Hartree/Particle)
Thermal correction to Energy= 0.376832
Thermal correction to Enthalpy= 0.378046
Thermal correction to Gibbs Free Energy= 0.252531
Sum of electronic and zero-point Energies= -1646.942067
Sum of electronic and thermal Energies= -1646.903172
Sum of electronic and thermal Enthalpies= -1646.901959
Sum of electronic and thermal Free Energies= -1647.027473



Cu	1.81459900	1.02062400	-0.00684800	C	-3.06397000	-0.89758600	-0.89894300
O	0.62302300	2.59518000	0.84943700	C	-3.37635300	1.60232300	0.30500600
C	1.70248400	3.25626400	0.85893100	H	-1.32281200	1.97153800	-0.23712400
C	1.75131300	4.68265300	1.34649800	C	-4.28241200	-0.54246000	-0.32094500
H	0.78011800	4.99051600	1.73768900	H	-2.92486600	-1.86283600	-1.37294600
H	2.03965000	5.33919900	0.51833100	C	-4.45899500	0.70787000	0.28648500
H	2.51745500	4.78142600	2.12209800	H	-3.49313300	2.57448400	0.77771500
O	2.78009400	2.70369500	0.43864000	H	-5.10813500	-1.24929400	-0.34294900
N	0.68006800	-0.60314600	-0.38509800	C	-5.78780500	1.09880900	0.88820600
S	-0.45716500	-0.43267200	-1.63850300	H	-5.65559600	1.65838300	1.82073800
C	2.43425200	-1.18873000	-1.25850400	H	-6.35406100	1.74293800	0.20253000
H	2.11059300	-1.03824300	-2.28460700	H	-6.40673800	0.22147400	1.10082800
C	3.34749900	-0.23274700	-0.75001300	C	0.53362800	-1.63906100	0.58410200
H	3.95845500	-0.48250800	0.11629100	C	1.42910200	-2.70975100	0.45126500
H	3.77416300	0.49437500	-1.43847200	C	-0.36231000	-1.59041600	1.65845300
C	2.35147200	-2.61827900	-0.74434200	C	1.41890700	-3.74255200	1.38756400
H	1.97687200	-3.26328200	-1.54854800	C	-0.37768500	-2.63878100	2.58010700
H	3.35867500	-2.96532800	-0.48445100	H	-1.03150400	-0.74354300	1.76761200
O	-0.64454100	-1.72935000	-2.30553700	C	0.50806200	-3.71129400	2.44672100
O	0.05926900	0.71997000	-2.39400000	H	2.11816200	-4.56968200	1.29252100
C	-2.01008000	0.01673400	-0.87041600	H	-1.07523200	-2.60991300	3.41249700
C	-2.15260200	1.27345700	-0.27224900	H	0.49892300	-4.51768500	3.17468200

I-2B

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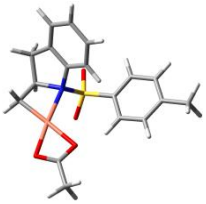
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.339740 (Hartree/Particle)
Thermal correction to Energy= 0.378694
Thermal correction to Enthalpy= 0.379907
Thermal correction to Gibbs Free Energy= 0.255549
Sum of electronic and zero-point Energies= -1646.953593
Sum of electronic and thermal Energies= -1646.914639
Sum of electronic and thermal Enthalpies= -1646.913426
Sum of electronic and thermal Free Energies= -1647.037783



Cu	2.05427700	0.79340400	0.05533300	C	-3.05483100	-0.50785400	-0.85706400
O	1.03642500	2.49498100	0.66609800	C	-2.93000500	2.07683900	0.19549200
C	2.16514700	3.08307900	0.76891600	H	-0.87349400	2.10220100	-0.44769600
C	2.22078200	4.53709300	1.17271300	C	-4.17609500	0.06118500	-0.25673600
H	1.59886600	4.69953200	2.05838100	H	-3.08567200	-1.50842500	-1.27339900
H	1.80689900	5.14983400	0.36368700	C	-4.13310900	1.35713500	0.27635300
H	3.24797600	4.84799300	1.37047100	H	-2.87683200	3.08037800	0.60985900
O	3.23216900	2.44300500	0.51655500	H	-5.09845900	-0.51116600	-0.20146900
N	0.70161500	-0.83161400	-0.45330400	C	-5.35827700	1.97828800	0.90285000
S	-0.47044700	-0.47921700	-1.75477200	H	-5.09998100	2.56331400	1.79213600
C	1.94264300	-1.57019100	-1.06313900	H	-5.85275600	2.66077900	0.19917100
H	1.91204300	-1.42313200	-2.14347100	H	-6.09057800	1.21857700	1.19331000
C	3.11429900	-0.82858300	-0.45890000	C	0.23951700	-1.70027600	0.60721000
H	3.50477500	-1.26990500	0.46349500	C	0.81983300	-2.97086700	0.52500200
H	3.91545000	-0.58195300	-1.15723700	C	-0.61009900	-1.34257700	1.65240000
C	1.73970400	-3.05207600	-0.66873000	C	0.52378600	-3.92458800	1.49460500
H	1.27337500	-3.62036200	-1.48308200	C	-0.90636600	-2.31153400	2.61556800
H	2.69984600	-3.52312700	-0.43461000	H	-1.01987900	-0.34113000	1.72185300
O	-0.88260200	-1.75117300	-2.36113300	C	-0.34895700	-3.59137500	2.53631200
O	0.21566900	0.54253900	-2.55049400	H	0.97056900	-4.91424000	1.44800500
C	-1.87601700	0.23779200	-0.92436300	H	-1.56609100	-2.05881400	3.44063000
C	-1.79784200	1.53580200	-0.40892900	H	-0.58221400	-4.32885500	3.29922600

I-3B

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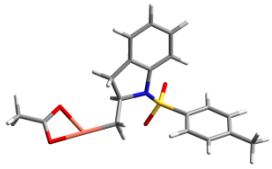
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.339828 (Hartree/Particle)
Thermal correction to Energy= 0.364989
Thermal correction to Enthalpy= 0.365933
Thermal correction to Gibbs Free Energy= 0.278639
Sum of electronic and zero-point Energies= -1646.937915
Sum of electronic and thermal Energies= -1646.912754
Sum of electronic and thermal Enthalpies= -1646.911810
Sum of electronic and thermal Free Energies= -1646.999104



Cu	3.23599800	-1.37101800	-0.54345300	C	-4.11611700	-0.54386400	1.03193600
O	5.19664900	-1.80125100	-0.53723100	C	-3.82004100	-2.08397900	-1.27732200
C	5.42387000	-0.71479800	0.08982000	H	-1.69887700	-1.78856700	-1.02596000
C	6.82252600	-0.34869600	0.51052200	C	-5.23796500	-1.05332100	0.37554200
H	7.53127600	-0.63171600	-0.27191600	H	-4.21539200	0.05237000	1.93263500
H	7.07837600	-0.91301600	1.41493600	C	-5.11047900	-1.82539700	-0.78514700
H	6.89512000	0.71806100	0.72991600	H	-3.70122600	-2.68497400	-2.17574900
O	4.44337900	0.04935000	0.37915000	H	-6.22742700	-0.84739200	0.77584800
N	-0.50987300	0.56342600	0.20558100	C	-6.32618700	-2.35664500	-1.50661300
S	-1.40990200	-0.23140700	1.41707100	H	-6.51654900	-1.79085800	-2.42799000
C	0.99075600	0.31284200	0.17242100	H	-6.19290500	-3.40562100	-1.79454800
H	1.34796900	0.26471900	1.20539500	H	-7.22390500	-2.28682000	-0.88482700
C	1.33192100	-0.97486500	-0.54856900	C	-0.76742900	1.93150400	-0.09879100
H	0.90930400	-1.85436000	-0.05015300	C	0.40767100	2.56730900	-0.51546400
H	1.04028900	-0.94336200	-1.60737600	C	-1.98517800	2.61176400	-0.06663800
C	1.55045900	1.58455500	-0.52425700	C	0.38075200	3.90386200	-0.89648200
H	2.44848900	1.94649700	-0.01467200	C	-1.99716500	3.95791300	-0.44485400
H	1.84437400	1.34476200	-1.55597100	H	-2.89765000	2.12621000	0.25725600
O	-1.88248400	0.71421600	2.43345500	C	-0.82964600	4.60525200	-0.85553100
O	-0.59574500	-1.38786700	1.80832200	H	1.29323500	4.39913200	-1.21982200
C	-2.84846200	-0.81017800	0.51618500	H	-2.93542000	4.50514600	-0.41310100
C	-2.69085600	-1.58659800	-0.63550200	H	-0.86044200	5.65228800	-1.14308500

I-1F

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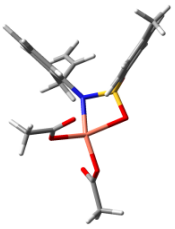
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.388669 (Hartree/Particle)
Thermal correction to Energy= 0.437589
Thermal correction to Enthalpy= 0.438802
Thermal correction to Gibbs Free Energy= 0.285745
Sum of electronic and zero-point Energies= -1875.493255
Sum of electronic and thermal Energies= -1875.444335
Sum of electronic and thermal Enthalpies= -1875.443122
Sum of electronic and thermal Free Energies= -1875.596179



Cu	-1.76120500	-0.71854600	-0.13946500	H	3.23893700	0.35357900	-2.37402000
O	-3.87795700	0.22625700	-1.20376900	C	4.29652000	-2.36487200	-0.58520800
C	-4.05540500	-1.00318100	-1.22617100	H	3.01503900	-3.51910500	0.71428400
C	-5.33021300	-1.60887500	-1.80434000	H	5.28198600	-1.01240300	-1.94316200
H	-5.86418800	-2.16137000	-1.02268900	C	5.53113000	-3.18964900	-0.30021200
H	-5.07681000	-2.32511500	-2.59373300	H	5.89478300	-3.02491800	0.72308200
H	-5.97654000	-0.82574600	-2.20770600	H	5.32770700	-4.26313800	-0.39787000
O	-3.19812900	-1.85712400	-0.76879000	H	6.34812100	-2.93793400	-0.98508400
N	-0.20188600	0.55376200	-0.05689500	C	0.38208800	1.40418600	0.91793500
S	0.52541900	0.14762900	-1.43007300	C	0.26868400	2.81049900	0.83660300
C	0.39949400	4.31091700	-1.19154100	C	1.02692000	0.82602100	2.02602300
H	1.13780800	3.73049300	-1.74204100	C	0.85241900	3.58793400	1.84678800
C	0.33052600	5.63478800	-1.35113400	C	1.58728700	1.61828500	3.02455400
H	-0.40619600	6.23819500	-0.82211500	H	1.05680800	-0.25685900	2.09093300
H	0.99792700	6.16658100	-2.02588200	C	1.50970500	3.00999300	2.93086700
C	-0.49314800	3.50267400	-0.28465300	H	0.78134800	4.67140500	1.77194100
H	-1.25373100	4.16166300	0.15608100	H	2.08125100	1.15001800	3.87310900
H	-1.01837500	2.74318200	-0.87196200	H	1.94792100	3.64028600	3.70182900
O	0.98396500	1.26231500	-2.28241700	C	-1.45801200	-1.75442400	2.35036200
O	-0.48853800	-0.80599500	-1.99911300	O	-2.19312000	-0.86718500	1.77398500
C	2.00582900	-0.82620200	-1.07635200	C	-1.78673900	-1.96709000	3.83069700
C	1.92788000	-1.91741600	-0.20300300	H	-1.60810100	-1.03747700	4.38319500
C	3.20723500	-0.49676900	-1.70163200	H	-1.16999900	-2.76639300	4.24890200
C	3.07423800	-2.67304800	0.03258100	H	-2.84739500	-2.21470300	3.94639500
H	0.99716600	-2.16187400	0.30526300	O	-0.54231100	-2.40333300	1.81549100
C	4.34434500	-1.26850500	-1.45348800				

TS-F

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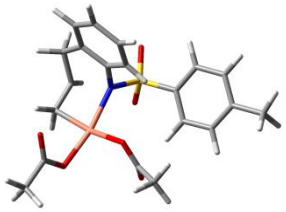
opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.388059 (Hartree/Particle)
Thermal correction to Energy= 0.435410
Thermal correction to Enthalpy= 0.436623
Thermal correction to Gibbs Free Energy= 0.289817
Sum of electronic and zero-point Energies= -1875.451013
Sum of electronic and thermal Energies= -1875.403662
Sum of electronic and thermal Enthalpies= -1875.402449
Sum of electronic and thermal Free Energies= -1875.549255



Cu	1.54830500	0.62739000	-0.47510100	H	-3.56956600	-2.04706700	-0.01672100
O	3.89772700	0.62939900	1.14429700	C	-4.59544300	1.17925600	0.48743300
C	3.92478300	1.61463200	0.39284500	H	-3.51741000	2.90946800	-0.23364100
C	5.06152700	2.64019300	0.50346300	H	-5.40004500	-0.73697000	1.06136000
H	4.65345600	3.60465700	0.82796200	C	-5.70226400	1.98447100	1.12916100
H	5.52668300	2.79962700	-0.47580900	H	-5.29900400	2.74730500	1.80647900
H	5.81251200	2.30282300	1.22263200	H	-6.30191200	2.51163700	0.37522300
O	3.05836200	1.89900400	-0.52199400	H	-6.38039500	1.34648900	1.70609500
N	0.15666100	-1.05986100	-0.59701200	C	0.22166800	-1.77922400	0.63274600
S	-1.25037400	-1.24394500	-1.51678800	C	1.08356800	-2.88444100	0.60657700
C	1.64201300	-1.83876200	-1.58513300	C	-0.40887400	-1.39184600	1.81917600
H	1.11545500	-1.94929800	-2.52866800	C	1.28300200	-3.63440100	1.76414700
C	2.64844100	-0.83783000	-1.54600500	C	-0.21714400	-2.16118700	2.96828600
H	3.47257000	-0.94108800	-0.84477000	H	-1.00361700	-0.48594700	1.83754800
H	2.85397000	-0.28270700	-2.45850100	C	0.61902800	-3.28113000	2.94237700
C	1.73774700	-3.11014200	-0.73778700	H	1.95884500	-4.48707100	1.75113400
H	1.23535400	-3.93356700	-1.26287400	H	-0.70517900	-1.86986200	3.89519400
H	2.79115300	-3.38852600	-0.61518700	H	0.77412100	-3.86537800	3.84640000
O	-1.67893600	-2.65732500	-1.48998300	C	0.03856600	2.84241700	0.30076300
O	-0.96331100	-0.60976400	-2.81097500	O	0.47414000	1.72679600	0.77531900
C	-2.54567100	-0.29309300	-0.71496300	C	-0.29806900	3.88764900	1.37301300
C	-2.52024400	1.10170800	-0.79234100	H	-0.97891400	3.45854000	2.11739500
C	-3.57377300	-0.96310700	-0.05205500	H	-0.75049800	4.77553400	0.92262100
C	-3.54543300	1.82321200	-0.18568700	H	0.61853000	4.17401300	1.90193700
H	-1.70508700	1.62449300	-1.28512200	O	-0.13150100	3.11085600	-0.89984900
C	-4.59415300	-0.22020700	0.54405300				

I-2F

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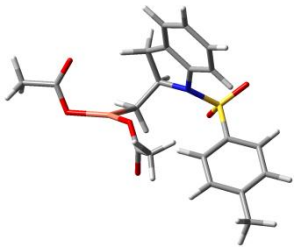
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.390007 (Hartree/Particle)
Thermal correction to Energy= 0.437713
Thermal correction to Enthalpy= 0.438926
Thermal correction to Gibbs Free Energy= 0.289660
Sum of electronic and zero-point Energies= -1875.477276
Sum of electronic and thermal Energies= -1875.429570
Sum of electronic and thermal Enthalpies= -1875.428357
Sum of electronic and thermal Free Energies= -1875.577623



Cu	-2.13006100	-1.16929100	-0.16783600	H	4.63599500	1.44045900	-0.88605300
O	-4.67201300	0.25951300	0.02565900	C	4.47764800	-1.87781300	-0.06344000
C	-4.81577100	-0.80372000	-0.59456300	H	2.61979600	-3.00842600	-0.00506400
C	-6.20411600	-1.22164000	-1.09301300	H	6.09287400	-0.45413600	-0.18807800
H	-6.45972600	-2.21308500	-0.70219300	C	5.35159400	-3.03119200	0.37334800
H	-6.19596000	-1.30003100	-2.18660300	H	4.99441600	-3.46625900	1.31481000
H	-6.96018400	-0.49580000	-0.78329600	H	5.34700800	-3.83734000	-0.37153900
O	-3.87896200	-1.64564100	-0.89100000	H	6.39067900	-2.71667200	0.51924100
N	0.40191800	1.43966700	-0.61751900	C	0.22903400	1.97119000	0.68532300
S	1.84172700	1.61208700	-1.46746400	C	-1.09868300	2.37977500	0.86562200
C	-0.92145500	1.40858400	-1.35332200	C	1.16865900	2.07519300	1.71043200
H	-0.77644700	1.96216100	-2.28814900	C	-1.50451400	2.88647700	2.09419500
C	-1.37935200	-0.00282400	-1.67336400	C	0.74883800	2.60170100	2.93660700
H	-2.25863900	0.03255200	-2.32599700	H	2.19664900	1.76278700	1.56681300
H	-0.59165600	-0.59109100	-2.15534200	C	-0.57463200	3.00001500	3.13568600
C	-1.88393900	2.19224900	-0.41022900	H	-2.53778900	3.19185400	2.24114100
H	-2.15304300	3.16706200	-0.84189100	H	1.46868600	2.69087400	3.74695500
H	-2.81093800	1.62842100	-0.25447900	H	-0.88497000	3.39492600	4.09992100
O	2.54252600	2.84793800	-1.08363100	C	-0.20595200	-2.45842100	1.38318000
O	1.51587200	1.37922200	-2.88053600	O	-1.06010500	-1.48848300	1.40723400
C	2.84521200	0.24848400	-0.86856600	C	0.45420800	-2.73226500	2.73850400
C	2.27677400	-1.00392600	-0.62776100	H	1.14859700	-1.91529600	2.96945400
C	4.21711100	0.45499700	-0.71212700	H	1.00558600	-3.67610600	2.71728100
C	3.09469600	-2.05483500	-0.21921000	H	-0.29773900	-2.75215900	3.53385500
H	1.20967400	-1.17043700	-0.71889400	O	0.11693600	-3.12211600	0.38585200
C	5.02360700	-0.61191900	-0.31417300				

(OAc)(HOAc) Cu(I) (110 °C)

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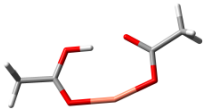
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.114591 (Hartree/Particle)
Thermal correction to Energy= 0.131354
Thermal correction to Enthalpy= 0.132567
Thermal correction to Gibbs Free Energy= 0.056632
Sum of electronic and zero-point Energies= -653.670140
Sum of electronic and thermal Energies= -653.653377
Sum of electronic and thermal Enthalpies= -653.652164
Sum of electronic and thermal Free Energies= -653.728099



Cu	0.08972900	-1.12074700	-0.00002600	H	-3.90896700	1.30774700	0.88834200
O	1.18365400	1.35017800	-0.00018100	H	-3.90724600	1.32685400	-0.87436200
C	2.10615200	0.49736400	-0.00003200	C	3.54900300	0.96471700	0.00032800
O	1.93623900	-0.77988300	0.00011000	H	4.06149800	0.56821300	0.88320500
C	-2.18763600	0.41038900	-0.00045400	H	4.06407900	0.56245100	-0.87838800
O	-1.78870500	-0.77527000	-0.00028300	H	3.60396200	2.05419800	-0.00294700
C	-3.65998600	0.71706300	0.00063900	O	-1.42112900	1.46328400	-0.00069200
H	-4.23816300	-0.20683800	-0.00919600	H	-0.40296400	1.28535100	-0.00040600

OAc Cu(I) (110 °C)

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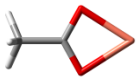
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.050872 (Hartree/Particle)
Thermal correction to Energy= 0.059544
Thermal correction to Enthalpy= 0.060758
Thermal correction to Gibbs Free Energy= 0.007854
Sum of electronic and zero-point Energies= -424.589041
Sum of electronic and thermal Energies= -424.580369
Sum of electronic and thermal Enthalpies= -424.579155
Sum of electronic and thermal Free Energies= -424.632059



Cu	1.30468500	-0.00022200	0.00386000	C	-2.57908800	0.00007000	0.00562900
O	-0.44595500	-1.11332600	-0.00924300	H	-2.91731400	-0.03064800	1.04813600
C	-1.06303400	0.00065500	-0.01502800	H	-2.96825700	0.91092700	-0.45354500
O	-0.44542600	1.11423000	-0.00919800	H	-2.96650700	-0.88542900	-0.50260400

HOAc (110 °C)

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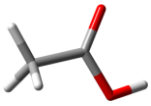
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.062023 (Hartree/Particle)
Thermal correction to Energy= 0.068731
Thermal correction to Enthalpy= 0.069945
Thermal correction to Gibbs Free Energy= 0.025016
Sum of electronic and zero-point Energies= -229.015587
Sum of electronic and thermal Energies= -229.008878
Sum of electronic and thermal Enthalpies= -229.007665
Sum of electronic and thermal Free Energies= -229.052594



O	0.64568600	1.20201900	0.00001800	H	-1.68533200	-0.69151400	0.88206300
C	0.09249300	0.12562300	0.00000000	H	-1.91752600	0.84835200	-0.00005300
C	-1.39757600	-0.10985600	-0.00000700	O	0.77867400	-1.04660600	-0.00001100
H	-1.68531600	-0.69159700	-0.88202700	H	1.72379200	-0.80314500	0.00000100

Tempo (110 °C)

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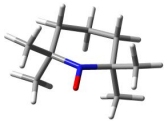
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.263368 (Hartree/Particle)
Thermal correction to Energy= 0.282776
Thermal correction to Enthalpy= 0.283990
Thermal correction to Gibbs Free Energy= 0.211474
Sum of electronic and zero-point Energies= -483.447721
Sum of electronic and thermal Energies= -483.428313
Sum of electronic and thermal Enthalpies= -483.427099
Sum of electronic and thermal Free Energies= -483.499615



C	-1.36073200	0.59053900	1.24717300	H	1.90768000	0.45011200	2.42312300
C	-2.12489100	0.14140800	0.00000000	H	0.95425100	1.89090400	2.02861000
C	-1.36073200	0.59053900	-1.24717300	C	0.07136400	-1.45949300	1.76108300
C	0.07136400	0.02351800	-1.33128700	H	1.08577200	-1.86108200	1.68435000
C	0.07136400	0.02351800	1.33128700	H	-0.26294000	-1.54944700	2.80100900
H	-1.89525300	0.30475800	-2.16158500	H	-0.59053900	-2.07239600	1.14150200
H	-2.26645900	-0.94678100	0.00000000	C	0.89265000	0.84283900	-2.34092500
H	-3.12932500	0.58209900	0.00000000	H	1.90768000	0.45011200	-2.42312300
H	-1.30610900	1.68793600	1.24566600	H	0.41189800	0.80269100	-3.32483900
H	-1.89525300	0.30475800	2.16158500	H	0.95425100	1.89090400	-2.02861000
H	-1.30610900	1.68793600	-1.24566600	C	0.07136400	-1.45949300	-1.76108300
N	0.75681200	0.14853100	0.00000000	H	-0.26294000	-1.54944700	-2.80100900
O	2.01777100	-0.09991000	0.00000000	H	1.08577200	-1.86108200	-1.68435000
C	0.89265000	0.84283900	2.34092500	H	-0.59053900	-2.07239600	-1.14150200
H	0.41189800	0.80269100	3.32483900				

I-1D

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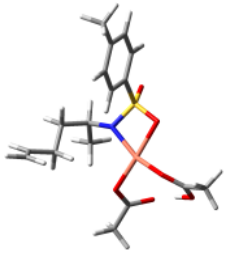
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.406350 (Hartree/Particle)
Thermal correction to Energy= 0.458204
Thermal correction to Enthalpy= 0.459481
Thermal correction to Gibbs Free Energy= 0.294872
Sum of electronic and zero-point Energies= -1762.885616
Sum of electronic and thermal Energies= -1762.833762
Sum of electronic and thermal Enthalpies= -1762.832485
Sum of electronic and thermal Free Energies= -1762.997094



O	-2.61155500	0.94646500	0.46925400	H	1.11949200	3.89327300	-1.11239600
C	-3.72241700	0.69243000	-0.12167500	O	0.07840000	-1.74017800	-0.70166300
C	-4.80358600	1.75089400	-0.02545800	O	1.20233500	-0.78651900	-2.79872000
H	-5.76660300	1.27696900	0.18454200	H	1.08522700	1.80092600	-2.30050100
H	-4.56765000	2.49319700	0.73893000	C	-0.97226800	2.35148100	-2.20804700
H	-4.89061600	2.25207300	-0.99665400	H	-0.84368200	3.31829900	-2.70980600
O	-3.93464100	-0.35153000	-0.78934300	H	-1.25419600	1.60745000	-2.95977500
Cu	-1.29421700	-0.42110900	0.05286200	H	-1.78945300	2.43998100	-1.48760200
O	-1.96758900	-1.84690000	1.30639100	H	1.82833500	2.61682100	-0.12866600
C	-2.82382700	-2.73663100	1.15750400	C	2.55657000	-0.77121200	-0.55118800
C	-2.78356800	-3.99159900	1.98591400	C	3.64581900	-1.27034400	-1.26677500
H	-2.30730700	-4.78198000	1.39340900	C	2.69499200	-0.38411200	0.78529200
H	-2.19215100	-3.82577300	2.88716400	C	4.88216700	-1.38428200	-0.63158900
H	-3.79474600	-4.32089900	2.23594900	H	3.51906500	-1.55992800	-2.30411900
N	0.16472100	0.62691100	-0.83195600	C	3.93696500	-0.50379400	1.40220500
S	0.95624000	-0.66949600	-1.35606700	H	1.84507300	0.01686700	1.32764200
C	0.59096400	4.34486200	1.57668800	C	5.04921600	-1.00375900	0.70650300
H	0.90274300	5.29410500	1.13523500	H	5.73121100	-1.77507500	-1.18693900
C	0.81033100	4.13651000	2.87596000	H	4.04677900	-0.20184300	2.44091600
H	0.51612300	3.20788200	3.36212600	C	6.39856900	-1.09888900	1.37800600
H	1.28340000	4.88540700	3.50602600	H	7.03032100	-1.85598600	0.90267500
C	0.32918900	1.93133800	-1.51420800	H	6.93433500	-0.14200400	1.32057100
C	-0.05187900	3.36355000	0.63396200	H	6.30140100	-1.35240400	2.43904400
H	-0.97650800	3.80241100	0.23329700	O	-3.79518400	-2.68630400	0.28848900
H	-0.35036600	2.46147400	1.17903500	H	-3.80441500	-1.78599900	-0.19838900
C	0.87934000	2.98859000	-0.53462800				

***cis*-TS-D_{ch}**

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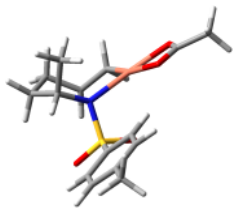
opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.406492 (Hartree/Particle)
Thermal correction to Energy= 0.456322
Thermal correction to Enthalpy= 0.457598
Thermal correction to Gibbs Free Energy= 0.304075
Sum of electronic and zero-point Energies= -1762.866187
Sum of electronic and thermal Energies= -1762.816358
Sum of electronic and thermal Enthalpies= -1762.815081
Sum of electronic and thermal Free Energies= -1762.968604



O	-0.54327200	1.73132900	0.10161600	H	0.13091400	-3.33245000	2.99211300
C	-0.82978000	2.68506100	0.83788600	O	1.76413900	-2.84689300	-0.92203800
C	0.15566000	3.79849800	1.09860500	O	0.45651100	-1.04543400	-2.17006900
H	0.11564700	4.10426100	2.14748900	H	1.58445400	-1.52868500	1.70554800
H	1.16288600	3.47868000	0.82812000	C	-0.11692900	-0.63618000	2.64743100
H	-0.12094400	4.66801800	0.49077900	H	0.19448800	-0.88601700	3.66840600
O	-1.97675100	2.84433000	1.44628300	H	0.21486900	0.38068600	2.42289700
Cu	-1.52232600	-0.10060500	-0.41381400	H	-1.21219500	-0.64878300	2.61479800
O	-3.01807500	0.75901500	-1.36013100	H	0.80364600	-3.75211700	1.40608100
C	-3.93104500	1.17419800	-0.57260100	C	2.51609400	-0.34477500	-0.63323700
C	-5.23486800	1.63552300	-1.20089000	C	2.38351200	0.99918400	-0.99382300
H	-5.33695600	2.71770700	-1.05965800	C	3.70061100	-0.82331900	-0.06955500
H	-5.26988400	1.40397300	-2.26677500	C	3.44979600	1.86604200	-0.76774000
H	-6.07535200	1.16271300	-0.68316500	H	1.46527700	1.35422300	-1.44504300
N	0.04197200	-1.30897800	0.27088200	C	4.75426400	0.06292600	0.15534700
S	1.17666000	-1.49543000	-0.96521300	H	3.80066900	-1.87900600	0.15851200
C	-1.34916700	-2.71162200	-0.06240900	C	4.64613600	1.41755800	-0.18458400
H	-0.76906100	-3.26676200	-0.79582800	H	3.35816500	2.90887800	-1.06301900
C	-2.47955200	-1.99334400	-0.53648400	H	5.67958500	-0.30871000	0.58840100
H	-3.31143900	-1.82168500	0.14461800	C	5.78303400	2.37771600	0.07311800
H	-2.71755200	-2.01701000	-1.59594700	H	6.72668300	1.84801300	0.23615800
C	0.49312100	-1.62664700	1.65162200	H	5.92106600	3.06832600	-0.76617600
C	-1.30391500	-3.28345900	1.33552100	H	5.58923700	2.98797800	0.96519000
H	-1.56202900	-4.34904600	1.27715700	O	-3.81100800	1.22846200	0.68431400
H	-2.06553600	-2.80151000	1.95958500	H	-2.66237400	2.12592500	1.17128800
C	0.09810500	-3.09349600	1.92288100				

***cis*-I-2D**

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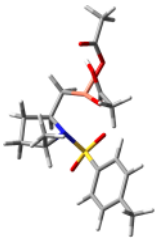
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.407122 (Hartree/Particle)
Thermal correction to Energy= 0.457394
Thermal correction to Enthalpy= 0.458671
Thermal correction to Gibbs Free Energy= 0.301450
Sum of electronic and zero-point Energies= -1762.876555
Sum of electronic and thermal Energies= -1762.826283
Sum of electronic and thermal Enthalpies= -1762.825006
Sum of electronic and thermal Free Energies= -1762.982227



O	-0.75440500	1.67530600	0.21840200	H	0.48613100	-3.08369800	3.27380200
C	-1.18868000	2.62712600	0.89588600	O	2.06219500	-2.79514200	-1.05344100
C	-0.29467200	3.79661500	1.23522500	O	0.50214300	-1.11829400	-2.17464300
H	-0.43374300	4.08634300	2.28040500	H	1.99601000	-1.61158500	1.53385700
H	0.74957600	3.54694000	1.04218900	C	0.50778800	-0.48631500	2.58669800
H	-0.58142100	4.65508300	0.61674600	H	1.03367000	-0.56825100	3.54532100
O	-2.39514400	2.72956800	1.35826400	H	0.76160800	0.47296000	2.12834800
Cu	-1.59322700	-0.12518200	-0.34734300	H	-0.56937200	-0.49168100	2.78721800
O	-3.18373500	0.52816500	-1.37123400	H	1.14287800	-3.79704200	1.78834900
C	-4.18339800	0.87030900	-0.66433700	C	2.52271200	-0.22525700	-0.68455900
C	-5.53086400	0.97266600	-1.35941400	C	2.18640200	1.11270300	-0.90708600
H	-5.87346000	2.01309700	-1.33221300	C	3.81413800	-0.59008300	-0.29653900
H	-5.47169700	0.63201000	-2.39438200	C	3.15842700	2.09070900	-0.70885600
H	-6.26704300	0.37707000	-0.80965400	H	1.18696500	1.38460400	-1.22204700
N	0.23637400	-1.50148300	0.32248000	C	4.77047900	0.40524700	-0.10190100
S	1.33091500	-1.51895500	-1.03057600	H	4.06377600	-1.63846600	-0.17381500
C	-0.80303900	-2.65361300	0.15617100	C	4.45923600	1.75750500	-0.29969200
H	-0.34360300	-3.42080000	-0.47796800	H	2.90587400	3.13275900	-0.89014600
C	-2.05832200	-2.06931400	-0.44373000	H	5.77763200	0.12491500	0.19567700
H	-2.96693000	-2.23843300	0.13895200	C	5.49288100	2.83395700	-0.07006400
H	-2.20820200	-2.27082100	-1.50460600	H	6.50909000	2.42985300	-0.10984100
C	0.91184100	-1.64234400	1.67090200	H	5.41269900	3.63087100	-0.81715700
C	-0.92882700	-3.19853600	1.58340700	H	5.36226300	3.29955700	0.91582700
H	-1.27042700	-4.23811300	1.57242700	O	-4.13797600	1.13203900	0.57430600
H	-1.66911000	-2.61286300	2.14261700	H	-3.05750000	1.96730800	1.02655300
C	0.46957100	-3.02651100	2.18041000				

I-3D

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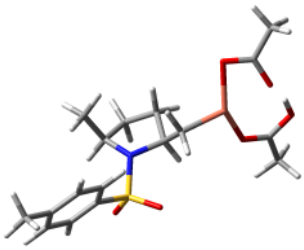
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.408400 (Hartree/Particle)
Thermal correction to Energy= 0.459096
Thermal correction to Enthalpy= 0.460372
Thermal correction to Gibbs Free Energy= 0.297983
Sum of electronic and zero-point Energies= -1762.875589
Sum of electronic and thermal Energies= -1762.824893
Sum of electronic and thermal Enthalpies= -1762.823617
Sum of electronic and thermal Free Energies= -1762.986006



O	-3.08914000	-1.35071700	-0.68122500	H	0.34082200	-1.07298400	3.93888900
C	-4.18400700	-1.90667800	-0.84405400	O	2.69255700	-2.61792900	0.17294800
C	-4.29263000	-3.39308800	-1.05256700	O	1.46427400	-1.26718200	-1.59387400
H	-4.58577600	-3.58699300	-2.09063800	H	2.50478200	-1.40319900	2.29750100
H	-3.33346500	-3.87054700	-0.85185400	C	2.13748200	0.64372100	2.86919400
H	-5.07370600	-3.80805400	-0.40892300	H	2.44636400	0.48159700	3.90916700
O	-5.34239500	-1.28282100	-0.86525000	H	2.98523800	1.06448300	2.31979300
Cu	-2.66882400	0.67992400	-0.36920500	H	1.33165100	1.38611900	2.86376400
O	-3.40463600	2.42312400	0.58861600	H	0.38038700	-2.34255000	2.70043400
C	-4.53494900	2.22919300	0.06640800	C	3.68177300	-0.27489600	-0.50328200
C	-5.70088300	3.13695100	0.37320000	C	3.53690400	1.06341300	-0.88382800
H	-6.54438400	2.54280700	0.74033300	C	4.94487000	-0.83069000	-0.31269300
H	-5.42417500	3.88933900	1.11308600	C	4.67326600	1.84493100	-1.06164300
H	-6.02786900	3.62813600	-0.54971300	H	2.54648000	1.48212200	-1.02971800
N	1.31301600	-0.48620900	0.80355900	C	6.07554000	-0.03150800	-0.49718900
S	2.22960500	-1.31710200	-0.34166000	H	5.03262300	-1.87270400	-0.02495500
C	-0.19216200	-0.52859800	0.61354800	C	5.96004700	1.31180300	-0.87159600
H	-0.45848100	-1.45335300	0.09326600	H	4.56391700	2.88640800	-1.35526000
C	-0.68566100	0.65713400	-0.18662700	H	7.06243200	-0.46253800	-0.34810600
H	-0.35464300	0.62570400	-1.23000600	C	7.18233700	2.17814400	-1.06425800
H	-0.44733300	1.61740000	0.28230800	H	8.10490600	1.60054800	-0.95196200
C	1.68788200	-0.67864200	2.23815400	H	7.19143400	2.63750900	-2.06008700
C	-0.71541500	-0.57990500	2.06353600	H	7.20875100	2.99612800	-0.33319100
H	-1.66690000	-1.11919500	2.11544600	O	-4.69764000	1.25374000	-0.75758500
H	-0.89291500	0.43787100	2.43149300	H	-5.21531100	-0.28831400	-0.77771100
C	0.40429300	-1.25831100	2.86140000				

I-4D/E

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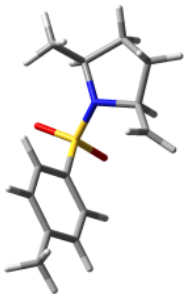
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.290285 (Hartree/Particle)
Thermal correction to Energy= 0.320721
Thermal correction to Enthalpy= 0.321997
Thermal correction to Gibbs Free Energy= 0.217461
Sum of electronic and zero-point Energies= -1109.182967
Sum of electronic and thermal Energies= -1109.152531
Sum of electronic and thermal Enthalpies= -1109.151254
Sum of electronic and thermal Free Energies= -1109.255791



N	1.50935800	0.05735200	-0.08350500	H	1.82040300	-1.84470400	-2.03304200
S	0.48863700	-0.85289800	0.91526500	H	2.41849100	-0.29248400	-2.66184000
C	1.74693000	1.47622000	0.32559000	H	4.31431800	0.41728900	0.61851000
H	1.96518800	1.51868000	1.40187400	C	-1.15461900	-0.40190700	0.35369300
C	0.59565300	2.36350600	0.01170400	C	-1.55477200	-0.72821800	-0.94580600
H	0.08445200	2.26945100	-0.94063000	C	-2.03722000	0.20806500	1.24219700
H	0.33418500	3.18633600	0.66767700	C	-2.84765600	-0.41997500	-1.35443200
C	2.77970300	-0.61000200	-0.53501600	H	-0.86135500	-1.21521900	-1.62349900
C	3.04470800	1.80572600	-0.45351500	C	-3.33315000	0.50677900	0.81631700
H	3.56079700	2.66658600	-0.01859500	H	-1.70800500	0.43992700	2.24911700
H	2.79743400	2.04883900	-1.49330100	C	-3.75719500	0.20297600	-0.48230000
C	3.84054600	0.49892700	-0.36672800	H	-3.16200200	-0.67033400	-2.36506700
H	4.62854900	0.42563000	-1.12321100	H	-4.02441100	0.98267800	1.50735400
O	0.72654100	-2.25776700	0.55854400	C	-5.15646800	0.53261800	-0.94593800
O	0.60569800	-0.41543900	2.31524900	H	-5.75604900	0.96217000	-0.13771100
H	3.00308300	-1.46136500	0.11267700	H	-5.14135200	1.25500500	-1.77180600
C	2.63388100	-1.11588900	-1.97091300	H	-5.67543400	-0.36177800	-1.31141700
H	3.55804900	-1.60910800	-2.29625100				

15

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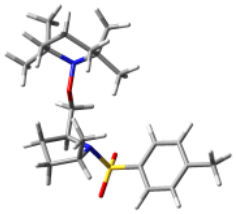
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.562220 (Hartree/Particle)
Thermal correction to Energy= 0.613717
Thermal correction to Enthalpy= 0.614994
Thermal correction to Gibbs Free Energy= 0.466306
Sum of electronic and zero-point Energies= -1592.687734
Sum of electronic and thermal Energies= -1592.636237
Sum of electronic and thermal Enthalpies= -1592.634960
Sum of electronic and thermal Free Energies= -1592.783648



N	0.95585000	-1.34833900	0.06422300	H	5.68789100	4.16188600	-0.14475500
S	2.31756200	-1.42518200	-0.95183900	H	5.14396300	3.97485400	1.52311700
C	-0.23209100	-2.10003200	-0.48089300	H	6.62286000	3.16675900	0.98529500
H	0.10130300	-2.75877000	-1.29047900	C	-2.53767800	1.83735100	-0.30185100
C	-1.27963200	-1.17765800	-1.10523200	C	-2.73274600	2.09118400	1.21293800
H	-0.79325000	-0.50149200	-1.81370500	C	-4.12830900	1.69827400	1.71440800
H	-1.99772300	-1.79234800	-1.66340800	C	-4.44791100	0.24537500	1.34076600
C	1.20413300	-1.75218900	1.48654100	C	-4.28743900	-0.03890800	-0.17196700
C	-0.73052800	-2.95650700	0.70507200	H	-4.17838900	1.82040200	2.80383800
H	-1.13438900	-3.91295300	0.35855400	H	-1.98065500	1.50858700	1.75980700
H	-1.52759700	-2.42895000	1.23514200	H	-2.53109400	3.14878100	1.42901200
C	0.50269500	-3.11750600	1.60234100	H	-3.77026800	-0.42056100	1.89022500
H	0.25133300	-3.37596000	2.63642700	H	-5.46839500	-0.01597200	1.65081000
O	3.13750600	-2.61712100	-0.67186900	H	-4.88791600	2.37458600	1.30094900
O	1.81140400	-1.19869900	-2.31171100	N	-2.94925800	0.43523100	-0.69314400
H	2.28059800	-1.85757600	1.64576700	O	-1.95576200	-0.44538200	-0.08423700
C	0.65850600	-0.68353800	2.43704400	C	-3.31758800	2.86827500	-1.14952100
H	0.82061900	-0.98259400	3.47975700	H	-2.78423500	3.82479500	-1.11958800
H	1.16805100	0.27054800	2.26800400	H	-3.37044700	2.54271700	-2.19295100
H	-0.41264500	-0.52378800	2.27969000	H	-4.33078200	3.06107300	-0.79561400
H	1.16551400	-3.89449900	1.20509200	C	-1.05245300	2.02624400	-0.66308400
C	3.26507000	0.00529000	-0.43285200	H	-0.89592900	1.89183800	-1.73974200
C	4.48883900	-0.17887400	0.20845400	H	-0.75020500	3.04768100	-0.40393400
C	2.79920000	1.28794700	-0.73773100	H	-0.41167400	1.32876800	-0.12295800
C	5.24463700	0.93960000	0.56510600	C	-4.40697400	-1.55487200	-0.41875000
H	4.84400800	-1.18406700	0.40844800	H	-4.32316500	-1.78626600	-1.48641600
C	3.56581000	2.39051300	-0.37511900	H	-3.64998200	-2.12050000	0.12596000
H	1.85754300	1.41445100	-1.26056700	C	-5.42527700	0.61170600	-0.99130400
C	4.79728300	2.23600900	0.28387800	H	-5.18288000	0.59788500	-2.05841200
H	6.20097200	0.79936000	1.06267600	H	-6.34306700	0.03186000	-0.84385800
H	3.20844300	3.38953900	-0.61334800	H	-5.65055800	1.63821400	-0.70221100
C	5.60939200	3.44582400	0.68130500	H	-5.39181300	-1.89505000	-0.07950600

***cis*-TS-D_{bt}**

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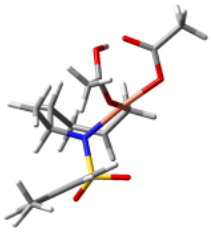
opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.406722 (Hartree/Particle)
Thermal correction to Energy= 0.456519
Thermal correction to Enthalpy= 0.457795
Thermal correction to Gibbs Free Energy= 0.304462
Sum of electronic and zero-point Energies= -1762.866054
Sum of electronic and thermal Energies= -1762.816257
Sum of electronic and thermal Enthalpies= -1762.814980
Sum of electronic and thermal Free Energies= -1762.968314



O	-3.08518800	0.86321400	-1.29953200	H	-1.86053100	-1.60480300	2.35675600
C	-3.86396600	1.34860900	-0.41419100	H	-0.82353800	-2.76025200	3.20021700
C	-5.18563400	1.92672600	-0.88861200	O	1.65767600	-2.99757400	-0.67778400
H	-5.99341700	1.57393500	-0.24041700	O	0.52351100	-1.26735900	-2.17773600
H	-5.15040900	3.01872600	-0.79708500	H	1.04757100	-2.28444800	1.72932900
H	-5.38842100	1.66037300	-1.92741200	C	0.52524600	-0.31371200	2.45061500
Cu	-1.56538900	-0.07427500	-0.46874900	H	0.74444200	-0.56449500	3.49555300
O	-0.42371300	1.71735900	-0.17538200	H	1.39571200	0.19988900	2.03347700
C	-0.54449000	2.67400700	0.59994200	H	-0.32404700	0.37729200	2.43973900
C	0.51906100	3.73854100	0.70943600	C	2.49237000	-0.51082100	-0.56820900
H	0.54468800	4.15621000	1.71847200	C	2.48212800	0.76620300	-1.13426600
H	1.49039900	3.32401400	0.43502800	C	3.57920700	-0.95116400	0.19125500
H	0.27613400	4.55100300	0.01394100	C	3.57129700	1.60867200	-0.91864100
O	-1.57911400	2.87856800	1.37862600	H	1.64080800	1.08533400	-1.73716900
N	-0.09470700	-1.34068200	0.23546400	C	4.65470500	-0.08985800	0.40321800
S	1.13068300	-1.63761800	-0.88824800	H	3.59083100	-1.96325100	0.58112200
C	-1.51590200	-2.71883300	-0.17958800	C	4.66787700	1.20130200	-0.14300000
H	-0.99332200	-3.21861000	-0.99006400	H	3.57763000	2.59590800	-1.37493700
C	-2.62754600	-1.91626500	-0.54671200	H	5.50482600	-0.43280500	0.98781300
H	-3.41229000	-1.72689000	0.18390100	C	5.82930000	2.13467600	0.10381800
H	-2.92553600	-1.88033100	-1.59095900	H	6.75662300	1.58176300	0.28506300
C	0.19936500	-1.58913300	1.66795100	H	5.99267400	2.80473300	-0.74674100
C	-1.41581300	-3.37813900	1.18044700	H	5.64798300	2.76502700	0.98475000
H	-0.64650700	-4.15718200	1.15052900	O	-3.59249600	1.38185000	0.82043700
H	-2.37188800	-3.85488500	1.42764000	H	-2.33726700	2.21241200	1.18649600
C	-1.03724400	-2.31856200	2.22043400				

***trans*-TS-D_{ch}**

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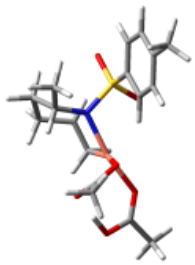
opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.406896 (Hartree/Particle)
Thermal correction to Energy= 0.456620
Thermal correction to Enthalpy= 0.457897
Thermal correction to Gibbs Free Energy= 0.305228
Sum of electronic and zero-point Energies= -1762.861287
Sum of electronic and thermal Energies= -1762.811563
Sum of electronic and thermal Enthalpies= -1762.810286
Sum of electronic and thermal Free Energies= -1762.962955



O	-2.96700900	-0.87223900	-1.38261000	H	1.84512200	1.53480500	3.29705800
C	-4.05685600	-1.32225700	-1.00057400	H	1.96356400	0.15721200	2.18678500
C	-5.09612000	-1.79450100	-1.98397900	H	2.63057600	1.73782300	1.72392000
H	-4.77138700	-1.58704400	-3.00368600	C	0.17513300	3.15227100	1.75603600
H	-6.05072300	-1.29921800	-1.78014100	H	0.14360100	3.49562500	2.79683500
H	-5.25353000	-2.87094300	-1.85611700	H	-0.32374400	1.12523300	2.26323500
Cu	-1.46877300	0.04600100	-0.30403500	O	2.00398200	2.58710100	-0.95145900
O	-0.80648300	-1.71186900	0.54054000	O	0.55002400	0.87413100	-2.14583500
C	-1.47937600	-1.80733700	1.61219900	H	0.97576400	3.69453600	1.24105100
C	-1.11895800	-2.89818000	2.60395600	C	2.56455800	0.03060400	-0.63557400
H	-1.13649800	-2.49662400	3.62127200	C	3.90372700	0.41740700	-0.71137500
H	-0.14141600	-3.33044600	2.38179000	C	2.21043600	-1.30545800	-0.42763100
H	-1.87761600	-3.68846100	2.55461400	C	4.89969600	-0.54800600	-0.56791700
O	-2.45416300	-1.03546300	1.88334200	H	4.15263200	1.45827500	-0.88575400
N	0.15427800	1.22372800	0.27239400	C	3.22276600	-2.25127900	-0.27891600
S	1.31125900	1.28394100	-0.94971700	H	1.17065200	-1.60387800	-0.35015900
C	-1.17303500	2.65274900	-0.27781200	C	4.57808200	-1.89340200	-0.34670400
H	-0.53319500	3.09142100	-1.03861700	H	5.94327900	-0.24952300	-0.63237500
C	-2.30753600	1.92429300	-0.72643800	H	2.95213300	-3.29123500	-0.11148100
H	-3.18779000	1.90111300	-0.08404700	C	5.65980200	-2.93134300	-0.16276200
H	-2.48786100	1.84836000	-1.79545100	H	6.60734100	-2.60591500	-0.60386500
C	0.44462900	1.64129200	1.67332100	H	5.84334200	-3.12553400	0.90250600
C	-1.16471800	3.37441200	1.04867800	H	5.38039400	-3.88600500	-0.62154900
H	-1.34250900	4.44078000	0.85570200	O	-4.41927300	-1.43842900	0.25295400
H	-1.99091200	3.01175000	1.67277100	H	-3.65363500	-1.20498600	0.89356200
C	1.80779000	1.23770800	2.24256100				

***trans*-TS-D_{bt}**

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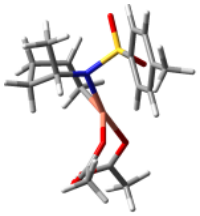
opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.406102 (Hartree/Particle)
Thermal correction to Energy= 0.456085
Thermal correction to Enthalpy= 0.457361
Thermal correction to Gibbs Free Energy= 0.302698
Sum of electronic and zero-point Energies= -1762.860815
Sum of electronic and thermal Energies= -1762.810833
Sum of electronic and thermal Enthalpies= -1762.809556
Sum of electronic and thermal Free Energies= -1762.964220



O	2.86671400	0.62740900	-1.58339400	H	-1.80200800	-2.02309400	3.25751000
C	3.95472500	0.97333600	-1.01276900	H	-2.62265000	-1.66507300	1.73540000
C	5.11954000	1.33538500	-1.91882000	H	-1.59589200	-3.09432500	1.85248300
H	5.29249900	2.41647400	-1.86252100	C	0.80629500	-1.69309200	2.45519700
H	4.92103100	1.05628900	-2.95499300	H	1.58249300	-0.92049500	2.38768100
H	6.02865000	0.84355300	-1.55971500	H	0.63534700	-1.89280600	3.51863800
Cu	1.47469500	-0.14944600	-0.46835100	H	-0.67139100	-0.16034100	2.05634600
O	0.78281300	1.70055300	0.43625700	O	-1.83935600	-2.74945800	-0.88910000
C	1.29225300	2.47748800	1.25803300	O	-0.46439900	-0.99195500	-2.10370400
C	0.47639800	3.56100100	1.92251900	C	-2.55976300	-0.22300300	-0.64222100
H	0.69933800	4.51947900	1.43927000	C	-3.87276100	-0.69441100	-0.59195900
H	0.75159400	3.65325900	2.97650500	C	-2.28236300	1.14542300	-0.56534400
H	-0.58907500	3.34984000	1.81997200	C	-4.91821700	0.21885500	-0.45488200
O	2.54558600	2.46380200	1.62171300	H	-4.06246100	-1.75979300	-0.66432100
N	-0.11445100	-1.21536000	0.33210000	C	-3.34118000	2.03909700	-0.42313700
S	-1.23261000	-1.40774400	-0.91249300	H	-1.26009200	1.50573000	-0.59200300
C	1.24687200	-2.69285100	0.20660800	C	-4.67212900	1.59531600	-0.37063600
H	0.62166400	-3.35211000	-0.38909100	H	-5.94174800	-0.14566700	-0.41677400
C	2.35736000	-2.08320600	-0.43525000	H	-3.13086200	3.10433600	-0.35890700
H	3.24090800	-1.84292600	0.15367500	C	-5.80832900	2.58289300	-0.25033000
H	2.51310900	-2.25084800	-1.49687100	H	-6.00691800	3.07167000	-1.21315700
C	-0.48104700	-1.20206200	1.76683400	H	-6.73417000	2.09307600	0.06697400
C	1.26874900	-2.95507300	1.70233300	H	-5.57712200	3.37461000	0.47109400
H	0.61107500	-3.79694700	1.94039100	O	4.12302700	1.03936600	0.23553800
H	2.28279700	-3.23286100	2.01050700	H	3.11851700	1.80102800	1.06305900
C	-1.69689500	-2.05249800	2.16678000				

***trans*-I-2D**

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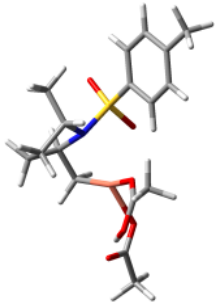
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.406868 (Hartree/Particle)
Thermal correction to Energy= 0.457216
Thermal correction to Enthalpy= 0.458493
Thermal correction to Gibbs Free Energy= 0.301069
Sum of electronic and zero-point Energies= -1762.872368
Sum of electronic and thermal Energies= -1762.822019
Sum of electronic and thermal Enthalpies= -1762.820742
Sum of electronic and thermal Free Energies= -1762.978166



O	3.16514400	0.42532100	-1.48873400	H	-2.24918600	-1.96603700	3.17497900
C	4.22585000	0.74161600	-0.86419200	H	-2.88425900	-1.91398600	1.52756000
C	5.51767800	0.79425300	-1.66257700	H	-1.74395100	-3.18146500	1.98446200
H	5.87538200	1.82932900	-1.70180900	C	0.43114900	-1.51606000	2.59457100
H	5.37325100	0.41830200	-2.67671200	H	1.12134000	-0.66559100	2.56090500
H	6.28586300	0.20733000	-1.14882900	H	0.18004000	-1.70351900	3.64318500
Cu	1.60878900	-0.16889500	-0.40365700	H	-1.11952100	-0.15903600	1.85622000
O	0.87695500	1.62985900	0.35331700	O	-1.99575800	-2.72923900	-1.06469900
C	1.39971100	2.51025200	1.06648200	O	-0.47613700	-0.98347100	-2.11636400
C	0.57198500	3.66544500	1.58082600	C	-2.55323400	-0.17060100	-0.67003600
H	0.74053500	4.53489200	0.93426600	C	-3.89221200	-0.56368800	-0.61253300
H	0.88532900	3.93987000	2.59112900	C	-2.19175400	1.17788200	-0.60265400
H	-0.48955400	3.41263800	1.56204100	C	-4.87864100	0.40982500	-0.46289200
O	2.64491400	2.54779200	1.41593600	H	-4.14834400	-1.61450400	-0.69352800
N	-0.25179900	-1.37886000	0.37757400	C	-3.19448900	2.13243800	-0.44484900
S	-1.31548900	-1.42806900	-0.99404900	H	-1.15052400	1.47682900	-0.64728100
C	0.74222000	-2.57124600	0.38565300	C	-4.54842300	1.76940300	-0.37739100
H	0.22097600	-3.45344300	-0.00393800	H	-5.92171000	0.10697000	-0.41722200
C	1.92825900	-2.15246300	-0.45680700	H	-2.92004400	3.18289900	-0.38379100
H	2.90352600	-2.40933500	-0.03986700	C	-5.62416600	2.82108300	-0.24907200
H	1.85715400	-2.40193500	-1.51616100	H	-5.94141500	3.17726800	-1.23809700
C	-0.81779700	-1.20529600	1.75582400	H	-6.51226700	2.42802500	0.25607200
C	1.04918300	-2.74069600	1.89559300	H	-5.26894300	3.69228600	0.31103200
H	0.59822900	-3.66500800	2.27021100	O	4.28960900	1.01817800	0.37025000
H	2.12644600	-2.80906400	2.06881800	H	3.26520300	1.80524500	0.95453700
C	-1.99295900	-2.12504500	2.12105000				

I-1E

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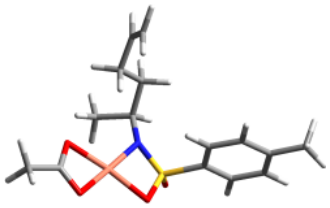
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.343164 (Hartree/Particle)
Thermal correction to Energy= 0.385667
Thermal correction to Enthalpy= 0.386944
Thermal correction to Gibbs Free Energy= 0.247144
Sum of electronic and zero-point Energies= -1533.845378
Sum of electronic and thermal Energies= -1533.802875
Sum of electronic and thermal Enthalpies= -1533.801599
Sum of electronic and thermal Free Energies= -1533.941399



Cu	1.61563000	-1.04282300	-0.24374000	C	-2.27201800	-0.70587100	0.16129800
N	0.33963700	-0.04082000	0.87579800	C	-3.48152400	-1.20402400	0.64811100
S	-0.74370800	-1.23009000	0.93589800	C	-2.24309300	0.16261100	-0.93389500
C	1.01934300	4.24662400	-0.05300800	C	-4.67057600	-0.82846500	0.02415700
H	0.95463400	5.03108300	0.70412900	H	-3.48316300	-1.87101300	1.50317200
C	0.81484900	4.56732800	-1.33158200	C	-3.44048800	0.52770000	-1.54229800
H	0.86998200	3.82142100	-2.12270200	H	-1.29758300	0.55564400	-1.29253300
H	0.59234300	5.58559300	-1.63991500	C	-4.67154000	0.04022700	-1.07534300
C	0.47097900	0.93200100	1.98465700	H	-5.61364300	-1.21745600	0.39987300
C	1.32706300	2.86535600	0.45950700	H	-3.42049700	1.20417100	-2.39318800
H	2.31268400	2.87313800	0.94604400	C	-5.96533600	0.46681800	-1.72674500
H	1.40138100	2.16531000	-0.38072300	H	-6.76474400	-0.25758600	-1.54187600
C	0.26841700	2.36943200	1.46305700	H	-6.30258500	1.43533300	-1.33406100
H	0.24417000	3.04548200	2.33016100	H	-5.85028200	0.57922700	-2.81012700
O	-0.06016700	-2.18691200	-0.04879600	C	3.72382400	-1.00445500	-1.28317800
O	-1.09770700	-1.76064200	2.25817100	C	5.08296200	-1.01376000	-1.92129000
H	-0.33424000	0.73280900	2.70447300	H	5.75874400	-1.61968100	-1.30598500
C	1.80256900	0.72292400	2.71823200	H	5.03016400	-1.46860300	-2.91329500
H	1.92879600	1.46817800	3.51291800	H	5.48407000	0.00014200	-1.98066300
H	1.82519500	-0.27188400	3.17532800	O	3.37415500	-0.07148000	-0.48374000
H	2.65179500	0.80414800	2.03200900	O	2.88504500	-1.94098700	-1.49736900
H	-0.72183600	2.42708400	0.99424400				

***cis*-TS-E_{bt}**

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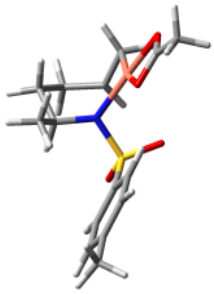
opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.343147 (Hartree/Particle)
Thermal correction to Energy= 0.383889
Thermal correction to Enthalpy= 0.385166
Thermal correction to Gibbs Free Energy= 0.254952
Sum of electronic and zero-point Energies= -1533.829654
Sum of electronic and thermal Energies= -1533.788911
Sum of electronic and thermal Enthalpies= -1533.787635
Sum of electronic and thermal Free Energies= -1533.917848



O	-2.87334000	2.29237400	-0.23125900		O	-0.14892600	-0.30258600	-2.16910000
C	-1.85382900	2.99209400	0.10326700		H	0.35436400	-2.55563800	1.19819200
C	-1.96179100	4.49726000	0.10181000		C	0.23193500	-0.81948700	2.48723500
H	-2.92673600	4.80759500	0.51182500		H	0.37611600	-1.37350000	3.42273200
H	-1.14329700	4.94177900	0.67147400		H	1.19721400	-0.40928800	2.18003200
H	-1.91028700	4.85683600	-0.93265700		H	-0.44462000	0.01994400	2.68378700
Cu	-1.84635600	0.58975200	-0.06203900		C	1.98617400	-0.41164900	-0.57462400
N	-0.65028400	-1.03802700	0.14606300		C	2.05302100	0.96675700	-0.34139500
S	0.45073000	-1.15559500	-1.12675800		C	3.10628600	-1.22796800	-0.41183900
C	-2.36620900	-1.93475500	-0.49424000		C	3.26464400	1.51719800	0.06683000
H	-2.00200100	-2.23320700	-1.47335900		H	1.17500100	1.59445800	-0.45223800
C	-3.30407900	-0.86866100	-0.46556400		C	4.31099900	-0.65283600	-0.00631600
H	-3.98764200	-0.78470100	0.37862600		H	3.03025500	-2.29080200	-0.61327200
H	-3.67009200	-0.47229000	-1.41039700		C	4.41059000	0.72280600	0.23752300
C	-0.35323100	-1.74322400	1.41412000		H	3.32130400	2.58642300	0.25634200
C	-2.31073100	-2.99138900	0.58841400		H	5.18733300	-1.28412700	0.11802200
H	-1.70247200	-3.83396100	0.24252000		C	5.72002900	1.34714500	0.65737600
H	-3.32328700	-3.36276000	0.78781900		H	6.15258300	1.94001500	-0.15893100
C	-1.68235200	-2.38578600	1.84872500		H	5.58515500	2.02363700	1.50917800
H	-2.34496300	-1.62026800	2.27475200		H	6.45520400	0.58744200	0.94017500
H	-1.51471000	-3.13835300	2.62716500		O	-0.77083300	2.41000500	0.40565500
O	0.73203400	-2.57371500	-1.40840800					

***cis*-I-2E**

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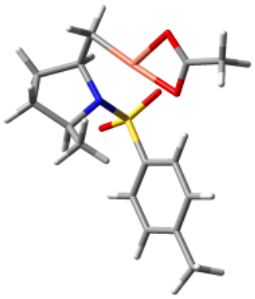
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.344891 (Hartree/Particle)
Thermal correction to Energy= 0.385865
Thermal correction to Enthalpy= 0.387142
Thermal correction to Gibbs Free Energy= 0.256549
Sum of electronic and zero-point Energies= -1533.840158
Sum of electronic and thermal Energies= -1533.799183
Sum of electronic and thermal Enthalpies= -1533.797907
Sum of electronic and thermal Free Energies= -1533.928500



O	-3.05096200	2.35970100	-0.12154300
C	-1.96810700	3.00399900	0.03336500
C	-1.96342400	4.51388900	-0.00683000
H	-2.98044400	4.90789800	0.03154800
H	-1.37227300	4.90661500	0.82596300
H	-1.48451100	4.84500600	-0.93559100
Cu	-1.94847400	0.59797800	-0.00145100
N	-0.67967000	-1.18593700	0.07231100
S	0.49517400	-1.22720400	-1.23134400
C	-1.95315000	-1.99715800	-0.35603000
H	-1.84463200	-2.25694600	-1.41050800
C	-3.10021600	-1.03052400	-0.15671900
H	-3.65248000	-1.15636300	0.77975600
H	-3.77690800	-0.93311800	-1.00737400
C	-0.18597600	-1.73599900	1.39675900
C	-1.89809900	-3.23242700	0.55059800
H	-1.23487900	-3.98657100	0.11125600
H	-2.88943500	-3.67661400	0.68120400
C	-1.30100000	-2.69510500	1.85338000
H	-2.05569400	-2.14179700	2.42571500
H	-0.90269800	-3.47921400	2.50521300
O	0.87456200	-2.62657700	-1.47600900
O	-0.12707600	-0.43002300	-2.29359800
H	0.71735300	-2.32580900	1.19933200
C	0.12903800	-0.63086200	2.40141500
H	0.45470000	-1.07763400	3.34838800
H	0.92009500	0.03418000	2.04662000
H	-0.76162300	-0.02383900	2.60098400
C	1.92763600	-0.37293300	-0.59038500
C	1.90395000	1.01635800	-0.42887300
C	3.07977900	-1.11810000	-0.32818200
C	3.05716800	1.65124900	0.02583200
H	1.00333700	1.58950100	-0.62222700
C	4.22274800	-0.45762600	0.11968400
H	3.07680400	-2.19098600	-0.48615700
C	4.23066800	0.93189000	0.30332200
H	3.04363500	2.72915900	0.16598400
H	5.12294000	-1.03115100	0.32530500
C	5.47809200	1.64676300	0.76425400
H	5.99232600	2.12034200	-0.08232300
H	5.24181600	2.43934600	1.48253600
H	6.18593100	0.95781200	1.23540300
O	-0.87369300	2.37004300	0.20700600

I-3E

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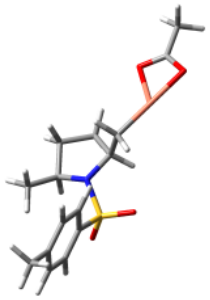
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.344974 (Hartree/Particle)
Thermal correction to Energy= 0.386131
Thermal correction to Enthalpy= 0.387407
Thermal correction to Gibbs Free Energy= 0.251472
Sum of electronic and zero-point Energies= -1533.823756
Sum of electronic and thermal Energies= -1533.782600
Sum of electronic and thermal Enthalpies= -1533.781323
Sum of electronic and thermal Free Energies= -1533.917258



O	-4.61042600	0.11348400	-0.75562700		O	0.96060800	-0.18830400	2.18024700
C	-5.45209000	-0.64197400	-0.16537300		H	0.95799500	3.12699300	-0.12953100
C	-6.93156800	-0.42469800	-0.35056400		C	1.92975400	2.17175100	-1.79829800
H	-7.12869400	0.53918700	-0.82259000		H	1.95349600	3.06673800	-2.43128200
H	-7.33173800	-1.22487200	-0.98361800		H	2.89687400	2.09655600	-1.29336700
H	-7.43576100	-0.48733600	0.61791700		H	1.80641900	1.29330300	-2.44105200
Cu	-3.13548300	-1.05969600	0.14698200		C	2.99752000	-0.14625100	0.48834600
N	0.57123400	1.04425200	0.00686300		C	2.74083400	-1.29454800	-0.26666100
S	1.64691300	0.74106100	1.27176000		C	4.30422100	0.28300500	0.71256500
C	-0.89564300	0.79836400	0.28879700		C	3.80755300	-2.00438500	-0.80749500
H	-1.05744800	0.80799200	1.36848100		H	1.71901000	-1.61725200	-0.43708000
C	-1.30049500	-0.55922700	-0.26724700		C	5.36353100	-0.44299600	0.16381000
H	-0.74092000	-1.37358800	0.21512500		H	4.48103600	1.17452300	1.30443600
H	-1.19612600	-0.61890500	-1.35657600		C	5.13528000	-1.59204000	-0.60173600
C	0.77365300	2.28131600	-0.80640200		H	3.61003800	-2.89466500	-1.40019400
C	-1.58516200	2.00458400	-0.38628700		H	6.38342200	-0.10801400	0.33528400
H	-1.71711600	2.80784700	0.34858700		C	6.28045300	-2.37595200	-1.19797900
H	-2.57205700	1.74331700	-0.77697300		H	6.28482500	-3.41090300	-0.83438200
C	-0.59894400	2.45130700	-1.47014300		H	6.20555300	-2.42010900	-2.29159600
H	-0.66734300	1.80070900	-2.35144100		H	7.24663600	-1.92846600	-0.94621300
H	-0.75929600	3.48163900	-1.80342800		O	-5.02670100	-1.59385100	0.56805800
O	2.20496600	2.00119700	1.78717600					

***cis*-TS-E_{ch}**

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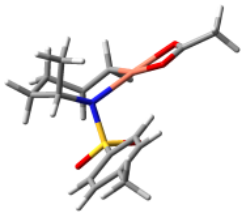
opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.343301 (Hartree/Particle)
Thermal correction to Energy= 0.383902
Thermal correction to Enthalpy= 0.385179
Thermal correction to Gibbs Free Energy= 0.255946
Sum of electronic and zero-point Energies= -1533.830087
Sum of electronic and thermal Energies= -1533.789486
Sum of electronic and thermal Enthalpies= -1533.788210
Sum of electronic and thermal Free Energies= -1533.917442



Cu	-1.83685600	0.59616400	-0.09757800	H	0.84805900	-1.91373200	1.41830900
O	-2.87402500	2.29363100	-0.30036400	C	-0.60983600	-0.92328200	2.63667400
C	-1.89104300	2.99208100	0.12940500	H	-0.31548100	-1.44801900	3.55306500
C	-2.00983600	4.49624100	0.15526900	H	-0.10345000	0.04634900	2.61076100
H	-1.80623900	4.88535000	-0.84953600	H	-1.68902300	-0.73702600	2.68796200
H	-3.02581900	4.79316900	0.42788500	H	-0.41509000	-3.76016700	0.62406500
H	-1.28480500	4.92605700	0.84960800	C	1.99839500	-0.35059900	-0.54901000
N	-0.60088200	-1.01459800	0.17021200	C	2.03370300	1.00432600	-0.20053000
S	0.46953200	-1.08946500	-1.12995600	C	3.14528200	-1.14368000	-0.48730300
C	-2.30150200	-1.93777400	-0.40996000	C	3.24179700	1.55416400	0.21955400
H	-1.86499200	-2.38810200	-1.29853200	H	1.13779900	1.61587600	-0.23800400
C	-3.23739500	-0.88512100	-0.60101300	C	4.34512300	-0.56916800	-0.06703400
H	-4.00924400	-0.73036200	0.15207100	H	3.09169100	-2.18801300	-0.77478700
H	-3.49386500	-0.58379400	-1.61415400	C	4.41385400	0.78361200	0.28943100
C	-0.23725800	-1.75306500	1.40399600	H	3.27472500	2.60484600	0.49775400
C	-2.36666900	-2.84655300	0.79559700	H	5.24151500	-1.18252200	-0.01942200
H	-2.85279700	-3.78219000	0.48889700	C	5.71935800	1.40992700	0.71852900
H	-3.00096400	-2.39396800	1.56672000	H	6.46235700	0.65061100	0.98160400
C	-0.95459000	-3.11761100	1.32772400	H	6.14415700	2.02256000	-0.08745200
H	-0.97532400	-3.62257900	2.30037000	H	5.58236300	2.06738500	1.58437800
O	0.76802900	-2.48910400	-1.48150400	O	-0.82778900	2.41111000	0.49988800
O	-0.15613900	-0.20536900	-2.13201400				

***trans*-TS-E_{ch}**

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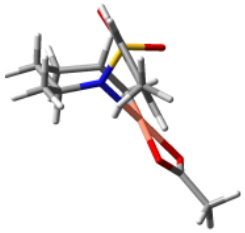
opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.343602 (Hartree/Particle)
Thermal correction to Energy= 0.384108
Thermal correction to Enthalpy= 0.385385
Thermal correction to Gibbs Free Energy= 0.255648
Sum of electronic and zero-point Energies= -1533.824574
Sum of electronic and thermal Energies= -1533.784067
Sum of electronic and thermal Enthalpies= -1533.782790
Sum of electronic and thermal Free Energies= -1533.912527



Cu	1.86526000	0.69658400	-0.05576200	C	-1.92667100	-0.36230100	-0.50368100
N	0.73317300	-0.99750400	0.24505400	C	-3.10843500	-1.09987900	-0.59420100
S	-0.39614800	-1.15671600	-1.01056500	C	-1.94027500	0.98113000	-0.11661600
C	2.39832700	-1.80846300	-0.47333300	C	-4.31872900	-0.48427800	-0.27756100
H	1.94415400	-2.24435900	-1.35956400	H	-3.07295600	-2.13559500	-0.91353800
C	3.27666100	-0.70082200	-0.67885500	C	-3.16046800	1.57140900	0.20530300
H	4.09809600	-0.55652700	0.02214000	H	-1.02456100	1.55952700	-0.04826700
H	3.45918300	-0.36290400	-1.69674900	C	-4.36500300	0.85462600	0.13248100
C	0.58645100	-1.74055400	1.53290800	H	-5.24138000	-1.05447800	-0.35291000
C	2.61440200	-2.78073200	0.66546800	H	-3.17515500	2.61367800	0.51471600
H	3.08766400	-3.68377800	0.25899700	C	-5.67403000	1.50834700	0.50641400
H	3.31086800	-2.34671600	1.39403500	H	-6.52673000	0.97577900	0.07355000
C	-0.82571600	-1.84840500	2.11283800	H	-5.81155400	1.51924000	1.59588000
H	-0.75922900	-2.32701800	3.09670400	H	-5.71294800	2.54878500	0.16601700
H	-1.28566700	-0.86533800	2.24244500	C	1.83050700	3.08432700	0.26127700
H	-1.47717400	-2.46255000	1.48513900	O	2.80611300	2.45714000	-0.27669600
C	1.27507000	-3.09915500	1.33552200	O	0.82753400	2.43409800	0.68539700
H	1.41145600	-3.62152100	2.28975000	C	1.87994700	4.58992300	0.35446400
H	1.18562500	-1.15480200	2.24283900	H	1.61267200	5.01550700	-0.62011600
O	-0.70130600	-2.57744600	-1.25730000	H	1.17101000	4.95171000	1.10198400
O	0.20720700	-0.34673100	-2.08599800	H	2.89343300	4.92200600	0.59443900
H	0.65821200	-3.72910700	0.68548100				

***trans*-TS-E_{bt}**

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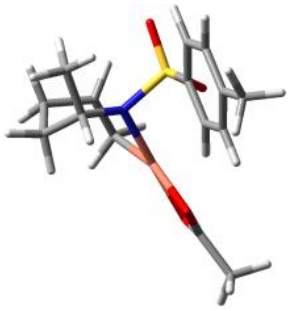
opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.343591 (Hartree/Particle)
Thermal correction to Energy= 0.384078
Thermal correction to Enthalpy= 0.385354
Thermal correction to Gibbs Free Energy= 0.256644
Sum of electronic and zero-point Energies= -1533.823024
Sum of electronic and thermal Energies= -1533.782537
Sum of electronic and thermal Enthalpies= -1533.781260
Sum of electronic and thermal Free Energies= -1533.909971



Cu	1.86197700	0.57666800	-0.11438700	H	-0.35431500	-3.62318600	0.77670600
O	0.93657600	2.35412400	0.67998000	C	1.68507400	-2.05934000	2.00883100
C	1.96573000	2.95360500	0.24440400	H	2.25805000	-1.16629600	2.28950700
C	2.09160400	4.45450100	0.33805300	H	1.59350400	-2.68379700	2.90399800
H	1.80057800	4.89499800	-0.62305600	H	-0.11688200	-0.86227100	2.12380800
H	3.12897200	4.73792000	0.53366500	O	-0.78274900	-2.33419900	-1.62306800
H	1.43312600	4.84691700	1.11582200	O	0.20523900	-0.03212100	-2.04739700
O	2.90103600	2.27898700	-0.30861500	C	-1.97984800	-0.24786400	-0.52564900
N	0.61705600	-1.03751500	0.16308800	C	-3.16910500	-0.96887200	-0.65406500
S	-0.45849500	-0.98543500	-1.13123500	C	-1.96996300	1.04322400	0.01238300
C	2.32353900	-1.97468300	-0.40503200	C	-4.36332300	-0.38925600	-0.22779000
H	1.88255000	-2.46253800	-1.26983200	H	-3.14977700	-1.96372000	-1.08581700
C	3.23487900	-0.91033400	-0.64164900	C	-3.17493700	1.59809700	0.43840000
H	4.03113800	-0.73341300	0.08047700	H	-1.04575200	1.60532600	0.10743600
H	3.45524100	-0.62720000	-1.66831600	C	-4.38652500	0.89914100	0.32336900
C	0.30006600	-1.64497900	1.47632900	H	-5.29120700	-0.94725300	-0.32692700
C	2.40718700	-2.79851300	0.86642500	H	-3.17253800	2.59798400	0.86566500
H	1.94747700	-3.77848000	0.70529700	C	-5.68637500	1.53338000	0.75781800
H	3.45912600	-2.96634800	1.12373600	H	-6.44510400	0.77838800	0.98739700
C	-0.67808700	-2.82993600	1.45500300	H	-5.54941600	2.16113300	1.64480500
H	-0.75331100	-3.24065300	2.46847500	H	-6.09269100	2.17597600	-0.03454700
H	-1.67989400	-2.52067200	1.14889500				

***trans*-I-2E**

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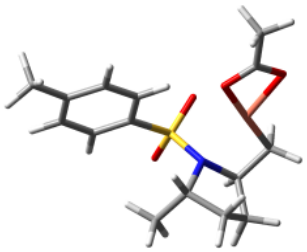
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.345310 (Hartree/Particle)
Thermal correction to Energy= 0.386144
Thermal correction to Enthalpy= 0.387420
Thermal correction to Gibbs Free Energy= 0.257223
Sum of electronic and zero-point Energies= -1533.833538
Sum of electronic and thermal Energies= -1533.792703
Sum of electronic and thermal Enthalpies= -1533.791427
Sum of electronic and thermal Free Energies= -1533.921624



Cu	1.97253900	0.51148900	-0.15121300	H	-0.51899300	-3.65739300	1.07100400
O	1.12535500	2.25916800	0.58272600	C	1.42434400	-1.93466600	2.18328500
C	2.17340600	2.88426100	0.20031700	H	1.97343300	-1.01426700	2.41537600
C	2.25478400	4.38245300	0.37567200	H	1.26780300	-2.47712700	3.12064900
H	1.52990300	4.86181400	-0.29216300	H	-0.36405600	-0.69577200	1.92907700
H	3.25612300	4.74850000	0.14284600	O	-0.98617000	-2.44435500	-1.60087800
H	1.98265900	4.65072900	1.40120500	O	0.17682200	-0.26124500	-2.17987000
O	3.12879100	2.24488000	-0.33422600	C	-1.92880400	-0.20452900	-0.54179100
N	0.59000200	-1.22192900	0.12532200	C	-3.17995700	-0.82598800	-0.57564800
S	-0.52985600	-1.10514500	-1.20572800	C	-1.78378700	1.11465200	-0.10034700
C	1.83012500	-2.10844000	-0.23303400	C	-4.29892400	-0.11847600	-0.14089400
H	1.50877400	-2.86196600	-0.95935700	H	-3.26681900	-1.84262300	-0.94327200
C	2.87911800	-1.15202800	-0.76537400	C	-2.91688400	1.79615700	0.33974300
H	3.87476700	-1.27340700	-0.33417700	H	-0.81529100	1.60538600	-0.07947800
H	2.91583800	-1.07488000	-1.85369800	C	-4.18679000	1.19949200	0.32358400
C	0.09286800	-1.59049300	1.49712900	H	-5.27406700	-0.59829100	-0.16548900
C	2.17618800	-2.75978100	1.12570800	H	-2.80902200	2.81668600	0.69838400
H	1.83977100	-3.80126700	1.14553200	C	-5.40645900	1.97053000	0.76801500
H	3.25665400	-2.76209800	1.29235800	H	-6.20271400	1.30166300	1.10985900
C	-0.90221000	-2.75910200	1.56281400	H	-5.16755900	2.66340700	1.58158000
H	-1.08984800	-2.99512400	2.61665700	H	-5.81282200	2.56795700	-0.05883600
H	-1.86096900	-2.51113600	1.10444100				

HOAc (130 °C)

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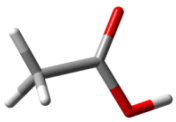
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.062023 (Hartree/Particle)
Thermal correction to Energy= 0.069290
Thermal correction to Enthalpy= 0.070567
Thermal correction to Gibbs Free Energy= 0.022655
Sum of electronic and zero-point Energies= -229.015587
Sum of electronic and thermal Energies= -229.008320
Sum of electronic and thermal Enthalpies= -229.007043
Sum of electronic and thermal Free Energies= -229.054955



O	0.64568600	1.20201900	0.00001800	H	-1.68533200	-0.69151400	0.88206300
C	0.09249300	0.12562300	0.00000000	H	-1.91752600	0.84835200	-0.00005300
C	-1.39757600	-0.10985600	-0.00000700	O	0.77867400	-1.04660600	-0.00001100
H	-1.68531600	-0.69159700	-0.88202700	H	1.72379200	-0.80314500	0.00000100

TEMPO (130 °C)

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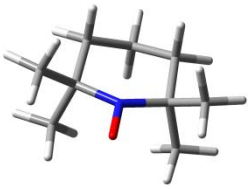
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.263368 (Hartree/Particle)
Thermal correction to Energy= 0.284757
Thermal correction to Enthalpy= 0.286034
Thermal correction to Gibbs Free Energy= 0.207637
Sum of electronic and zero-point Energies= -483.447721
Sum of electronic and thermal Energies= -483.426332
Sum of electronic and thermal Enthalpies= -483.425055
Sum of electronic and thermal Free Energies= -483.503452



C	-1.36073200	0.59053900	1.24717300	H	1.90768000	0.45011200	2.42312300
C	-2.12489100	0.14140800	0.00000000	H	0.95425100	1.89090400	2.02861000
C	-1.36073200	0.59053900	-1.24717300	C	0.07136400	-1.45949300	1.76108300
C	0.07136400	0.02351800	-1.33128700	H	1.08577200	-1.86108200	1.68435000
C	0.07136400	0.02351800	1.33128700	H	-0.26294000	-1.54944700	2.80100900
H	-1.89525300	0.30475800	-2.16158500	H	-0.59053900	-2.07239600	1.14150200
H	-2.26645900	-0.94678100	0.00000000	C	0.89265000	0.84283900	-2.34092500
H	-3.12932500	0.58209900	0.00000000	H	1.90768000	0.45011200	-2.42312300
H	-1.30610900	1.68793600	1.24566600	H	0.41189800	0.80269100	-3.32483900
H	-1.89525300	0.30475800	2.16158500	H	0.95425100	1.89090400	-2.02861000
H	-1.30610900	1.68793600	-1.24566600	C	0.07136400	-1.45949300	-1.76108300
N	0.75681200	0.14853100	0.00000000	H	-0.26294000	-1.54944700	-2.80100900
O	2.01777100	-0.09991000	0.00000000	H	1.08577200	-1.86108200	-1.68435000
C	0.89265000	0.84283900	2.34092500	H	-0.59053900	-2.07239600	-1.14150200
H	0.41189800	0.80269100	3.32483900				

OAc Cu(I) (130 °C)

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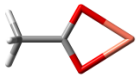
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.050872 (Hartree/Particle)
Thermal correction to Energy= 0.060216
Thermal correction to Enthalpy= 0.061493
Thermal correction to Gibbs Free Energy= 0.005074
Sum of electronic and zero-point Energies= -424.589041
Sum of electronic and thermal Energies= -424.579697
Sum of electronic and thermal Enthalpies= -424.578420
Sum of electronic and thermal Free Energies= -424.634839



Cu	1.30468500	-0.00022200	0.00386000	C	-2.57908800	0.00007000	0.00562900
O	-0.44595500	-1.11332600	-0.00924300	H	-2.91731400	-0.03064800	1.04813600
C	-1.06303400	0.00065500	-0.01502800	H	-2.96825700	0.91092700	-0.45354500
O	-0.44542600	1.11423000	-0.00919800	H	-2.96650700	-0.88542900	-0.50260400

(OAc)(HOAc) Cu(I) (130 °C)

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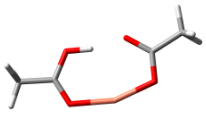
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=403.15

- Thermochemistry -

Zero-point correction= 0.114591 (Hartree/Particle)
Thermal correction to Energy= 0.132718
Thermal correction to Enthalpy= 0.133995
Thermal correction to Gibbs Free Energy= 0.052646
Sum of electronic and zero-point Energies= -653.670140
Sum of electronic and thermal Energies= -653.652013
Sum of electronic and thermal Enthalpies= -653.650736
Sum of electronic and thermal Free Energies= -653.732085



Cu	0.08972900	-1.12074700	-0.00002600	H	-3.90896700	1.30774700	0.88834200
O	1.18365400	1.35017800	-0.00018100	H	-3.90724600	1.32685400	-0.87436200
C	2.10615200	0.49736400	-0.00003200	C	3.54900300	0.96471700	0.00032800
O	1.93623900	-0.77988300	0.00011000	H	4.06149800	0.56821300	0.88320500
C	-2.18763600	0.41038900	-0.00045400	H	4.06407900	0.56245100	-0.87838800
O	-1.78870500	-0.77527000	-0.00028300	H	3.60396200	2.05419800	-0.00294700
C	-3.65998600	0.71706300	0.00063900	O	-1.42112900	1.46328400	-0.00069200
H	-4.23816300	-0.20683800	-0.00919600	H	-0.40296400	1.28535100	-0.00040600

I-1C

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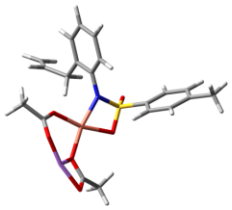
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=373.15

- Thermochemistry -

Zero-point correction= 0.392311 (Hartree/Particle)
Thermal correction to Energy= 0.440361
Thermal correction to Enthalpy= 0.441543
Thermal correction to Gibbs Free Energy= 0.291463
Sum of electronic and zero-point Energies= -1883.048387
Sum of electronic and thermal Energies= -1883.000337
Sum of electronic and thermal Enthalpies= -1882.999155
Sum of electronic and thermal Free Energies= -1883.149235



Cu	-1.09120100	-1.08137600	-0.20997600	H	3.61930700	1.36401300	-1.81965700
O	-1.42622500	-4.96034000	-0.03817200	C	5.25367600	-0.27510800	0.70183600
C	-1.27138600	-4.02175700	-0.84636700	H	4.29182200	-1.62425500	2.08681000
C	-0.52653000	-4.18886300	-2.14526800	H	5.88513800	1.11341600	-0.81880800
H	0.27652500	-3.44844300	-2.20760700	C	6.62709100	-0.44876900	1.30493700
H	-1.21018300	-3.98899300	-2.97812600	H	7.33961100	0.27293100	0.89444600
H	-0.12679600	-5.20045000	-2.22937300	H	6.60382000	-0.32125700	2.39346600
O	-1.81223500	-2.85973800	-0.57291500	H	7.01980600	-1.45431500	1.10681300
N	0.00028500	0.56759600	-0.01394800	C	-0.20482100	1.87662300	0.50651000
S	1.07849100	0.20279000	-1.15032200	C	-1.04468500	2.81037800	-0.14231200
C	-3.03014100	3.22111300	-1.68128900	C	0.41872500	2.21220900	1.71732800
H	-3.79838500	3.10031500	-0.91586800	C	-1.20001200	4.07216800	0.44462800
C	-3.28053400	3.99098300	-2.74167300	C	0.24809200	3.47312100	2.28370400
H	-2.53988900	4.14285000	-3.52453800	H	1.04009000	1.46480200	2.20175900
H	-4.23610400	4.49215500	-2.87238200	C	-0.56262500	4.40843600	1.63959300
C	-1.74883500	2.46636800	-1.44592500	H	-1.83417100	4.80171700	-0.05119100
H	-1.96987000	1.39050200	-1.44327300	H	0.74269900	3.72130400	3.21887900
H	-1.06089600	2.62357400	-2.28669900	H	-0.70494000	5.39741600	2.06738700
O	1.22218600	1.12486300	-2.28244900	C	-3.03770500	-1.14996500	1.96336800
O	0.57129500	-1.21013900	-1.45102000	O	-2.50387300	-0.49816300	1.00046400
C	2.70483200	0.01336900	-0.42293600	C	-4.05219200	-0.38564900	2.79735600
C	2.88257200	-0.83123100	0.67911300	H	-5.03306100	-0.86196400	2.68914400
C	3.77979600	0.71525500	-0.96587600	H	-4.11578200	0.65994300	2.49352400
C	4.15116000	-0.96865100	1.23080300	H	-3.77341200	-0.45410200	3.85365800
H	2.03907000	-1.36843900	1.10074600	O	-2.79516900	-2.34580100	2.26905000
C	5.04606400	0.56566900	-0.39762800	Li	-2.34350400	-3.67342100	1.11796600

TS-C

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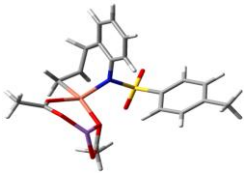
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=373.15

- Thermochemistry -

Zero-point correction= 0.392076 (Hartree/Particle)
Thermal correction to Energy= 0.438708
Thermal correction to Enthalpy= 0.439890
Thermal correction to Gibbs Free Energy= 0.296443
Sum of electronic and zero-point Energies= -1883.021863
Sum of electronic and thermal Energies= -1882.975231
Sum of electronic and thermal Enthalpies= -1882.974049
Sum of electronic and thermal Free Energies= -1883.117496



Cu	-1.67655300	-0.04013200	-0.35385800	H	4.08341400	0.97864600	-0.76340300
O	-3.22280800	-1.58948300	2.19050900	C	4.33220600	-1.84498600	1.15592200
C	-3.84367900	-0.68253200	1.57769800	H	2.74340000	-3.28458000	1.39844100
C	-5.19645400	-0.25371900	2.12683900	H	5.68724400	-0.22917500	0.70955000
H	-5.12088800	-0.09658800	3.20697500	C	5.31157000	-2.59830300	2.02412200
H	-5.91574700	-1.06539200	1.96659400	H	5.82086800	-3.38342100	1.44962100
H	-5.56069200	0.65042300	1.63630700	H	6.08362800	-1.93536300	2.42752200
O	-3.45503700	-0.08929100	0.51394500	H	4.80832300	-3.08818600	2.86463000
N	0.11641900	0.92771500	-0.61630700	C	0.39645500	1.92907800	0.36507500
S	1.40536400	0.38395500	-1.58861500	C	0.05311900	3.24268300	0.01365200
C	-1.06172800	2.06627300	-1.87183000	C	0.90090000	1.64397600	1.63907900
H	-0.64547500	1.67427300	-2.79542400	C	0.22808700	4.27465900	0.93360800
C	-2.35667200	1.62554800	-1.52595000	C	1.08871200	2.68658800	2.54870200
H	-2.95453300	2.18091000	-0.80879600	H	1.14488900	0.62111900	1.90695800
H	-2.90586600	0.99828100	-2.22687100	C	0.75391700	3.99691300	2.19882000
C	-0.49884900	3.39202800	-1.38659100	H	-0.04594000	5.29267900	0.66787300
H	0.30031600	3.71149900	-2.06521700	H	1.48468200	2.47133200	3.53716500
H	-1.28863900	4.15208900	-1.41504000	H	0.88912100	4.80227000	2.91531700
O	2.12656600	1.55265200	-2.11742100	C	-1.49487500	-3.11548500	-0.72031900
O	0.78890300	-0.56896000	-2.52142200	O	-1.11416700	-2.01745600	-0.13014900
C	2.53133200	-0.48517800	-0.49664100	C	-1.38049000	-3.20943000	-2.22458900
C	2.13832100	-1.68561500	0.10278000	H	-0.48532200	-2.69098000	-2.57561300
C	3.80368000	0.04724800	-0.28403700	H	-2.24864500	-2.70947900	-2.67385200
C	3.04236800	-2.35117400	0.92697800	H	-1.38711400	-4.25419800	-2.54149400
H	1.13830800	-2.07432900	-0.05950300	O	-1.96022700	-4.05670800	-0.03839500
C	4.69438800	-0.63900500	0.54121100	Li	-2.08858500	-2.75957700	1.39614100

I-2C

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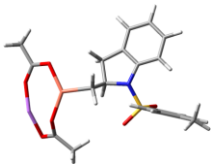
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=373.15

- Thermochemistry -

Zero-point correction= 0.393569 (Hartree/Particle)
Thermal correction to Energy= 0.440805
Thermal correction to Enthalpy= 0.441987
Thermal correction to Gibbs Free Energy= 0.293329
Sum of electronic and zero-point Energies= -1883.034327
Sum of electronic and thermal Energies= -1882.987091
Sum of electronic and thermal Enthalpies= -1882.985909
Sum of electronic and thermal Free Energies= -1883.134567



Cu	-2.80316500	-0.51391600	0.86355600	H	4.74663100	-0.68050300	-1.77709300
O	-5.49017400	0.08998600	0.22603400	C	5.46020800	-1.68359300	1.41667400
C	-5.01261700	1.06002100	0.87911200	H	3.97922700	-1.91247200	2.96972900
C	-5.91412100	2.24079300	1.18022700	H	6.66178900	-1.36743900	-0.34383600
H	-5.36326100	3.04945700	1.66236200	C	6.62146600	-2.07218900	2.30040600
H	-6.72728700	1.91046300	1.83628900	H	6.94284100	-1.22594600	2.92193400
H	-6.37243000	2.59645200	0.25198700	H	6.35155700	-2.88788300	2.97995800
O	-3.81284600	1.11070500	1.31562500	H	7.48535200	-2.39252500	1.70980100
N	1.11100800	0.70263200	-0.39976500	C	1.51866900	2.06446700	-0.43108900
S	1.93256500	-0.49992600	-1.27245900	C	0.40423700	2.90991700	-0.38767800
C	-0.40462300	0.61642100	-0.33190100	C	2.81714000	2.57370800	-0.44512400
H	-0.74267600	0.07142100	-1.21537600	C	0.57974200	4.28860100	-0.35343000
C	-0.82229300	-0.12017600	0.92357500	C	2.97900800	3.96244100	-0.42487100
H	-0.41762900	-1.13423000	0.97994100	H	3.68086800	1.91983300	-0.47743300
H	-0.65529700	0.45041900	1.84241500	C	1.87558300	4.81745700	-0.37535300
C	-0.87079100	2.10145000	-0.38322700	H	-0.28295900	4.94953000	-0.31701600
H	-1.47040700	2.29531100	-1.28163500	H	3.98326900	4.37692100	-0.44388000
H	-1.50995300	2.32781900	0.47719300	H	2.02228900	5.89351900	-0.35450300
O	2.49551400	0.03307200	-2.51711800	C	-3.35344400	-2.86775100	-0.95115800
O	1.00379800	-1.63860100	-1.30957200	O	-3.35665600	-2.27907600	0.21606700
C	3.30691800	-0.91078500	-0.19724500	C	-2.10953500	-3.61348600	-1.36521700
C	3.07738000	-1.26185100	1.13592900	H	-2.25590600	-4.09469100	-2.33328700
C	4.59216800	-0.94985100	-0.73783600	H	-1.86954300	-4.36644500	-0.60663700
C	4.15377500	-1.64210600	1.93114900	H	-1.25508600	-2.92859800	-1.41625100
H	2.07324500	-1.22601700	1.54557200	O	-4.37213800	-2.81471600	-1.67386400
C	5.65908100	-1.33550800	0.07484700	Li	-5.16621400	-1.57310600	-0.43325200

I-5 (100 °C)

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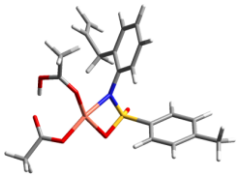
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=373.15

- Thermochemistry -

Zero-point correction= 0.401222 (Hartree/Particle)
Thermal correction to Energy= 0.447933
Thermal correction to Enthalpy= 0.449115
Thermal correction to Gibbs Free Energy= 0.300807
Sum of electronic and zero-point Energies= -1876.001939
Sum of electronic and thermal Energies= -1875.955228
Sum of electronic and thermal Enthalpies= -1875.954046
Sum of electronic and thermal Free Energies= -1876.102354



Cu	-1.10584700	-1.30008400	0.06772200	H	3.55111400	0.89078000	-1.62397400
O	-3.96266400	0.02092700	1.18562200	C	5.12451000	-1.28952100	0.49099300
C	-2.93867600	0.03695800	1.98599600	H	4.16664000	-2.99543500	1.40110000
C	-3.10885800	0.85131200	3.24076000	H	5.76880800	0.45618700	-0.59709100
H	-4.00864700	1.46575800	3.19029900	C	6.46812500	-1.54543800	1.13113400
H	-2.22244100	1.47394400	3.38796100	H	7.28455900	-1.13758300	0.52665800
H	-3.18332500	0.17002500	4.09586500	H	6.52734200	-1.07431800	2.12139700
O	-1.86916200	-0.57145400	1.78312200	H	6.64858600	-2.61655500	1.27014500
N	0.04779000	0.26357300	-0.24767700	C	0.30777200	1.51142900	0.38514400
S	1.00569200	-0.42587000	-1.35182000	C	-0.13084100	2.72237400	-0.19900700
C	-1.82261900	3.87003500	-1.71086800	C	0.95354200	1.52402600	1.63132000
H	-2.62813800	3.91796700	-0.97612400	C	0.12499700	3.91532900	0.49037100
C	-1.77398700	4.78282800	-2.68252600	C	1.18609300	2.72202700	2.30336600
H	-0.98764300	4.77349700	-3.43481600	H	1.26543900	0.57744500	2.06252400
H	-2.52285700	5.56553300	-2.77135000	C	0.77407200	3.92401700	1.72528700
C	-0.84669900	2.73578600	-1.54172200	H	-0.19972300	4.85150900	0.04484200
H	-1.37265000	1.77944800	-1.65685600	H	1.68872600	2.71617100	3.26689900
H	-0.10747200	2.75638700	-2.35281100	H	0.95331000	4.86716400	2.23493800
O	1.23386400	0.33751300	-2.58183100	C	-3.25388300	-2.80818400	-0.54030100
O	0.26564700	-1.75461800	-1.45016700	O	-2.07955100	-2.94491700	-0.04052300
C	2.61754500	-0.78979200	-0.65486000	C	-3.93598600	-4.08072600	-0.99867200
C	2.78207400	-1.88963300	0.19242100	H	-5.00333300	-3.91048300	-1.14928400
C	3.68840000	0.05779700	-0.94319800	H	-3.77151200	-4.88167900	-0.27263400
C	4.03276400	-2.13172200	0.75438100	H	-3.48732200	-4.39903500	-1.94687500
H	1.95152500	-2.56146900	0.38268500	O	-3.82739400	-1.69905100	-0.69053400
C	4.93222200	-0.19914700	-0.36791000	H	-3.83634000	-0.63964300	0.39726500

TS-A (100 °C)

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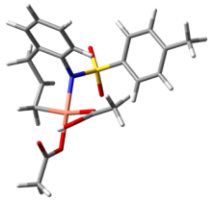
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=373.15

- Thermochemistry -

Zero-point correction= 0.400984 (Hartree/Particle)
Thermal correction to Energy= 0.446337
Thermal correction to Enthalpy= 0.447519
Thermal correction to Gibbs Free Energy= 0.305588
Sum of electronic and zero-point Energies= -1875.979746
Sum of electronic and thermal Energies= -1875.934392
Sum of electronic and thermal Enthalpies= -1875.933211
Sum of electronic and thermal Free Energies= -1876.075142



Cu	-1.65125000	-0.23486700	-0.60204000	H	3.64899400	1.59832400	-0.45992500
O	-3.84453400	-1.27553800	1.01469800	C	4.52673800	-1.69497900	-0.15394400
C	-4.03310700	-1.54050300	-0.20196600	H	3.28896700	-3.34102400	-0.79497400
C	-5.34455900	-2.18479600	-0.61768200	H	5.50459300	0.15827700	0.35704700
H	-5.50508600	-2.10452300	-1.69436800	C	5.67307800	-2.56871500	0.29706700
H	-6.17144000	-1.72302300	-0.07092500	H	5.32617000	-3.56094200	0.60350300
H	-5.32115900	-3.24563800	-0.34075900	H	6.39795000	-2.71338400	-0.51503200
O	-3.18245500	-1.31613800	-1.12997100	H	6.21301600	-2.12024500	1.13759400
N	-0.08545900	1.06687900	-0.45238700	C	0.21299900	1.68812100	0.79505900
S	1.10788400	0.97310300	-1.65799400	C	-0.36318000	2.95155900	0.98702400
C	-1.48294300	2.36024000	-1.17339000	C	0.94748100	1.07985200	1.82015900
H	-1.04353000	2.46608900	-2.16075700	C	-0.18811700	3.61560800	2.20068100
C	-2.66717500	1.59032300	-1.10091600	C	1.13268400	1.76036800	3.02451400
H	-3.33608200	1.70893300	-0.25003800	H	1.36163900	0.08939300	1.66917200
H	-3.11499000	1.22890200	-2.02222500	C	0.56817200	3.02434800	3.21549900
C	-1.15952700	3.47508900	-0.18806700	H	-0.64059900	4.59199400	2.35604900
H	-0.58484500	4.25159200	-0.70791700	H	1.70829800	1.29617500	3.82059800
H	-2.09391400	3.93389500	0.15648100	H	0.70539700	3.54439100	4.15941700
O	1.67737700	2.31196100	-1.87205500	C	-0.73613200	-2.41261200	1.43172000
O	0.42586800	0.26870600	-2.75486600	O	-0.55662100	-1.78274300	0.37966500
C	2.43000900	-0.07388000	-1.05105400	C	0.33787300	-3.30338900	2.00752700
C	2.31600200	-1.46203900	-1.15579300	H	0.03298700	-4.35021500	1.89632800
C	3.57436200	0.51774600	-0.51107200	H	0.45078000	-3.10995000	3.07834200
C	3.36645400	-2.25997300	-0.70569600	H	1.28236800	-3.14167400	1.48687400
H	1.42481100	-1.90466800	-1.58434600	O	-1.83528100	-2.39431900	2.13916600
C	4.61153200	-0.29802600	-0.06289000	H	-2.58670800	-1.86081700	1.67984700

I-6 (100 °C)

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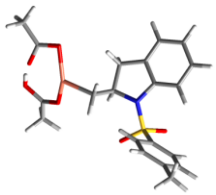
opt=calcfc freq=noraman ub3lyp/genecp gfinput temperature=373.15

- Thermochemistry -

Zero-point correction= 0.403376 (Hartree/Particle)
Thermal correction to Energy= 0.449242
Thermal correction to Enthalpy= 0.450424
Thermal correction to Gibbs Free Energy= 0.304333
Sum of electronic and zero-point Energies= -1875.989313
Sum of electronic and thermal Energies= -1875.943446
Sum of electronic and thermal Enthalpies= -1875.942264
Sum of electronic and thermal Free Energies= -1876.088356



Cu	-2.77557900	-0.41551800	0.72540600	H	4.93720800	-0.84859200	-1.58757000
O	-4.85344500	-0.47485500	1.20777400	C	5.33564200	-1.84255600	1.66329300
C	-4.70623300	0.65675200	1.80164000	H	3.71434000	-2.02490700	3.07669200
C	-5.90715900	1.33464600	2.41243800	H	6.69992200	-1.56260700	0.01992000
H	-5.64383800	2.32165200	2.79536900	C	6.40004000	-2.25694200	2.65144800
H	-6.29135600	0.71457000	3.23001800	H	6.57340200	-1.47155900	3.39858500
H	-6.70441200	1.41906600	1.66699500	H	6.10725500	-3.16119100	3.19746800
O	-3.55658000	1.16951500	1.88455100	H	7.35377800	-2.45616700	2.15327200
N	1.19924800	0.58583100	-0.55675500	C	1.60139400	1.94659500	-0.56347400
S	2.09145500	-0.61631800	-1.34868100	C	0.48176900	2.78645900	-0.55282700
C	-0.31806900	0.48183500	-0.53057300	C	2.89647800	2.46503800	-0.53161400
H	-0.62987600	-0.06481600	-1.42186500	C	0.64688200	4.16579900	-0.50609100
C	-0.78820100	-0.25755300	0.70491300	C	3.04850700	3.85459200	-0.49799000
H	-0.45987800	-1.30195100	0.71421100	H	3.76496600	1.81698700	-0.54163600
H	-0.53135800	0.26165000	1.63474000	C	1.93925300	4.70329500	-0.48147900
C	-0.78655900	1.96855800	-0.58799600	H	-0.22112800	4.82081700	-0.49406600
H	-1.36556100	2.16458400	-1.49998200	H	4.05047700	4.27495100	-0.48087800
H	-1.44195600	2.19239800	0.26188700	H	2.07853000	5.78015100	-0.45004900
O	2.78113100	-0.07135000	-2.52337000	C	-4.07788100	-1.93297400	-1.54157700
O	1.17196300	-1.75106000	-1.48849400	O	-3.03072700	-1.58990700	-0.97597200
C	3.35505000	-1.04025400	-0.14675600	C	-4.06234300	-2.74940700	-2.80476800
C	2.99794300	-1.37446800	1.16272200	H	-4.72345700	-2.29879700	-3.55096600
C	4.68313100	-1.10860400	-0.56568100	H	-4.44866600	-3.75179700	-2.58808200
C	3.98856300	-1.76889200	2.05596700	H	-3.04460100	-2.82474900	-3.18769200
H	1.96140200	-1.31252100	1.47761800	O	-5.28805500	-1.64149400	-1.11156100
C	5.66363700	-1.50881900	0.34402500	H	-5.24676300	-1.14225700	-0.24173600

I-2G

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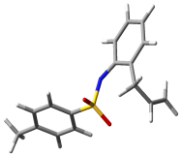
opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.284514 (Hartree/Particle)
Thermal correction to Energy= 0.314461
Thermal correction to Enthalpy= 0.315674
Thermal correction to Gibbs Free Energy= 0.211669
Sum of electronic and zero-point Energies= -1222.289768
Sum of electronic and thermal Energies= -1222.259821
Sum of electronic and thermal Enthalpies= -1222.258608
Sum of electronic and thermal Free Energies= -1222.362613



N	0.42186300	0.60210700	-0.11454000	C	-4.71314100	0.43688600	-0.29588900
S	-0.35378800	-0.76022800	0.48125300	H	-4.45030800	-0.53189900	-2.20416100
C	3.03534900	-2.29379200	-0.32826600	H	-4.63910200	1.30785200	1.67535400
H	2.77219700	-3.31615800	-0.06090400	C	-6.15995700	0.79794500	-0.53701500
C	3.48565300	-2.03858900	-1.55627800	H	-6.43575500	1.72008900	-0.01472100
H	3.75159300	-1.03767200	-1.88565100	H	-6.36683300	0.93527000	-1.60346700
H	3.59140000	-2.83415400	-2.28837300	H	-6.82882400	0.00593500	-0.17449900
C	2.85681200	-1.29769700	0.80381200	C	1.73408400	0.91482600	-0.06843200
H	1.94612800	-1.53557400	1.35544300	C	2.88561500	0.15116700	0.37645100
H	3.67337400	-1.45218500	1.52494300	C	1.95881200	2.25723600	-0.54354100
O	-0.17190500	-0.83916000	1.94209700	C	4.12639500	0.78661600	0.35059400
O	-0.06097300	-1.93145500	-0.35812700	C	3.20702200	2.84014800	-0.55486500
C	-2.05058800	-0.28092700	0.17416900	H	1.07884200	2.79622700	-0.87747900
C	-2.65175700	-0.62896700	-1.03561300	C	4.30758600	2.10071100	-0.09627800
C	-2.75831200	0.41148400	1.15707400	H	4.99345600	0.22341700	0.68608700
C	-3.97754400	-0.26401800	-1.26234300	H	3.33417100	3.85866900	-0.90954000
H	-2.08974800	-1.18427900	-1.77893700	H	5.30146700	2.53919200	-0.09103600
C	-4.08324100	0.76752400	0.91280200				
H	-2.27819400	0.65576300	2.09861000				

TS-G

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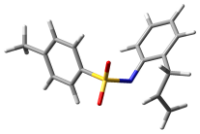
opt=(calcfc,ts,noeigen) freq=noraman ub3lyp/genecp gfinput temperature=383.15

- Thermochemistry -

Zero-point correction= 0.283624 (Hartree/Particle)
Thermal correction to Energy= 0.312508
Thermal correction to Enthalpy= 0.313721
Thermal correction to Gibbs Free Energy= 0.213683
Sum of electronic and zero-point Energies= -1222.270042
Sum of electronic and thermal Energies= -1222.241159
Sum of electronic and thermal Enthalpies= -1222.239945
Sum of electronic and thermal Free Energies= -1222.339984



N	0.95199400	-0.64207400	-0.66760500
S	0.01566000	-1.37529300	0.56928700
C	2.86317000	-1.64730600	-0.34954300
H	2.40679200	-2.48492200	0.16930300
C	3.23345800	-1.84955900	-1.66045500
H	3.81436100	-1.11118000	-2.20780900
H	2.87774200	-2.71387800	-2.21161200
C	3.43465900	-0.51944700	0.48937300
H	3.30006000	-0.75622500	1.55113300
H	4.51255900	-0.42425800	0.30881500
O	0.45717300	-0.97262500	1.91593900
O	-0.05154100	-2.79981900	0.21955700
C	-1.59118800	-0.64195900	0.26957200
C	-2.35601400	-1.08684700	-0.81331900
C	-2.06021600	0.35815700	1.12172300
C	-3.60477900	-0.51543200	-1.03739400
H	-1.97626900	-1.87312600	-1.45702500
C	-3.31618200	0.91598700	0.88243200
H	-1.45065700	0.67940000	1.95932400
C	-4.10548900	0.49115500	-0.19496700
H	-4.20550400	-0.85807100	-1.87654700
H	-3.68940600	1.69240500	1.54569900
C	-5.47611900	1.07896200	-0.43310600
H	-5.59043200	2.04641800	0.06568200
H	-5.67133800	1.22058000	-1.50182100
H	-6.26053900	0.41479300	-0.04668800
C	1.44666100	0.65949600	-0.38924500
C	2.73204700	0.78361700	0.16455800
C	0.72155200	1.80557800	-0.74573500
C	3.27646700	2.05051100	0.36940400
C	1.26992300	3.06813300	-0.51615000
H	-0.25710300	1.69701800	-1.20107200
C	2.54430600	3.19423100	0.04060500
H	4.27725200	2.14499300	0.78460100
H	0.70459900	3.95471200	-0.79064100
H	2.97476300	4.17844000	0.20280400

9. Theoretical Section Supporting Information References

(1) AIM analyses were performed on the three ground state structures in Fig. 8. In each, a bond critical point (3,-1) was located between the sulfonamide oxygen and Cu, which is indicative of the existence of a bond. Furthermore, a ring critical point (3,+1) was present in each ground state structure at the center of the Cu-O-S-N ring.

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