

Insights into the Mechanisms of Cu(I)-Catalyzed Heterocyclization of α -Acyl- α -alkynyl Ketene Dithioacetals to form 3-Cyanofurans: the Roles of NH_4OAc

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Table S1. Exploring the effects of methods B3LYP, CAM-B3LYP, M06, BLYP, B3P86, B3PW91 and BHandHLYP by comparing the activation free energy barriers from **in1** to **ts1** (the geometric structures of **in1** and **ts1** are optimized using B3LYP (CAM-B3LYP, M06, BLYP, B3P86, B3PW91 and BHandHLYP)/6-31G* in gas phase, and the single point energies are obtained at the PCM//M06-2x/6-311++G** calculated level in solution phase).

Species	Activation Free Energy Barriers (kJ/mol)						
	B3LYP	CAM-B3LYP	M06	BLYP	B3P86	B3PW91	BHandHLYP
ts1	72.4	71.1	73.9	66.5	70.2	69.7	76.9

Table S1 shows that the effects of DFT functionals B3LYP, CAM-B3LYP, M06, BLYP, B3P86, B3PW91 and BHandHLYP on the activation free energy barriers are very small.

Table S2. Exploring the effects of basis sets 6-31G*, 6-31G**, 6-31+G* and 6-311G* by comparing the activation free energy barriers from **in1** to **ts1** (the geometric structures of **in1** and **ts1** are optimized using B3LYP/6-31G* (6-31G**, 6-31+G* and 6-311G*) in gas phase, and the single point energies are obtained at the PCM//M06-2x/6-311++G** calculated level in solution phase).

Species	Activation Free Energy Barriers (kJ/mol)			
	6-31G*	6-31G**	6-31+G*	6-311G*
ts1	72.4	72.2	73.8	72.8

Table S2 shows that the effects of basis sets 6-31G*, 6-31G**, 6-31+G* and 6-311G* on the activation free energy barriers are very small.

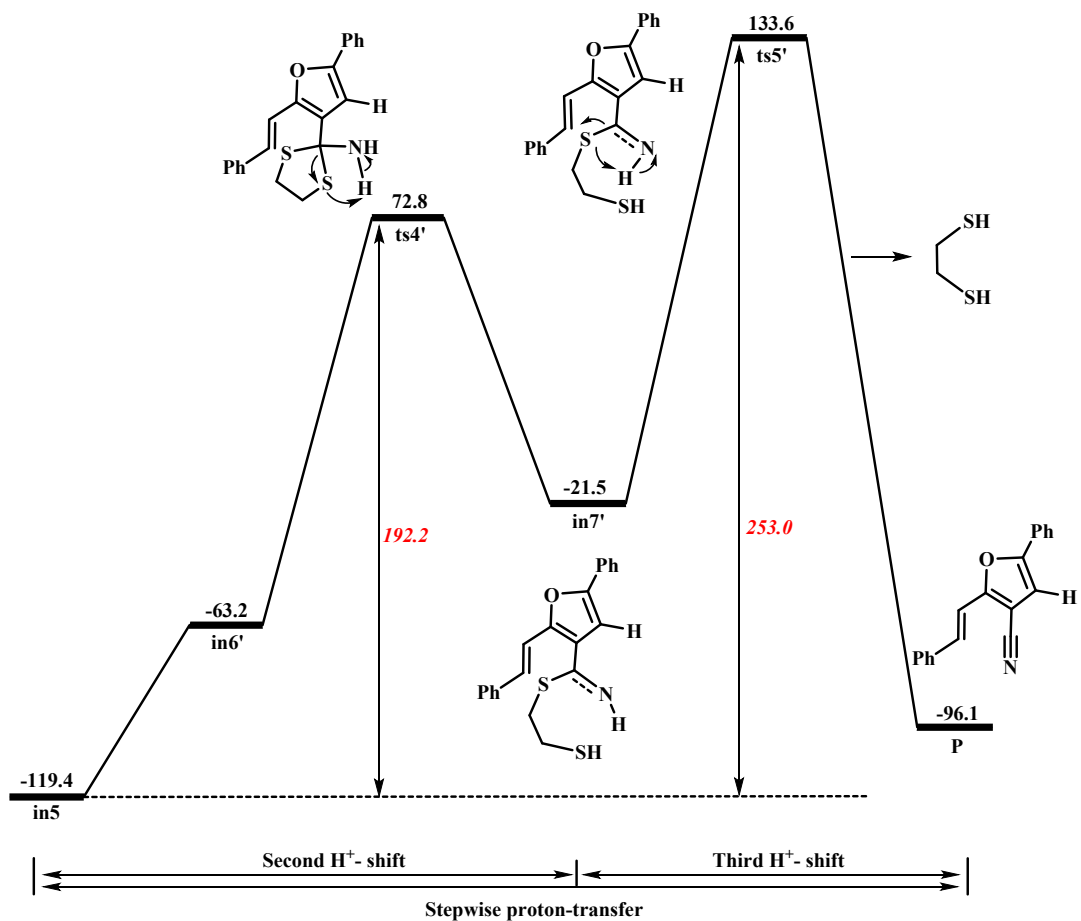


Figure S1. DFT-computed energy profile for the proton-transfer reactions in the absence of CuBr.

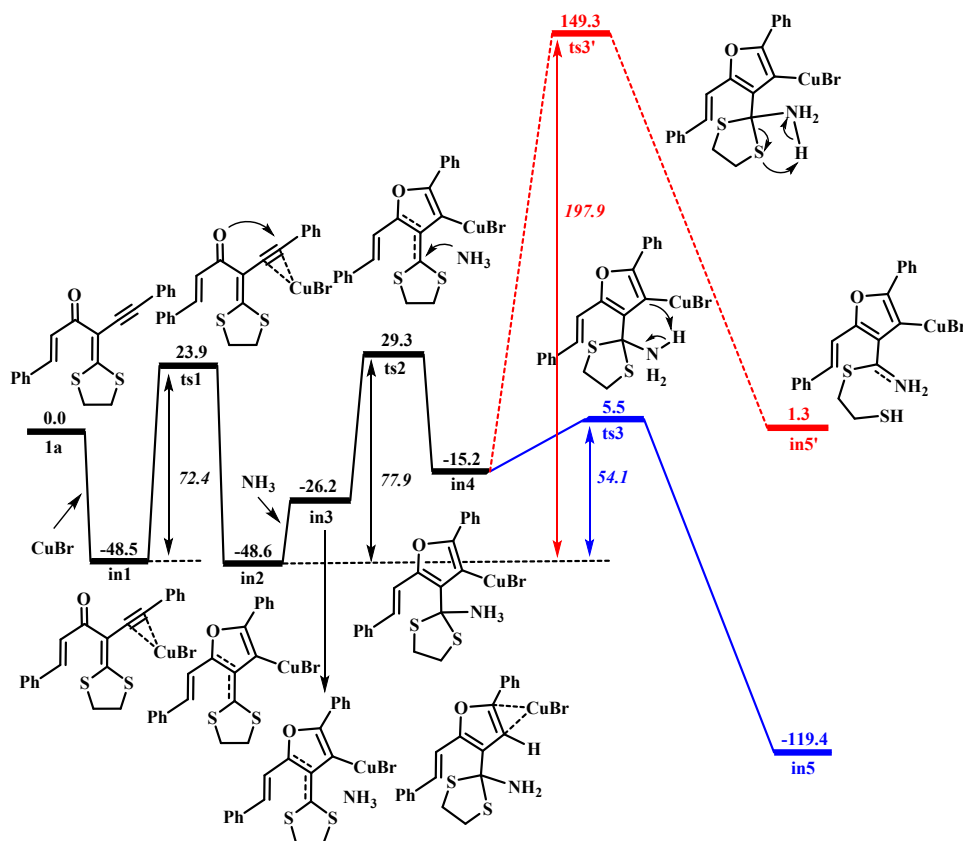


Figure S2. Comparing the free energy barriers of **ts3'** vs. **ts3**.

Based on the Arrhenius equation (K. J. Laidler, *J. Chem. Educ.*, 1984, **61**(6), 494-498; S. R. Logan, *J. Chem. Educ.*, 1982, **59**(4), 279-281),

$$\mathbf{in5/in5'} = \exp(-\Delta G_{ts3}/RT) / \exp(-\Delta G_{ts3'}/RT) \dots \dots \dots \mathbf{Eq\ S1}$$

$$\mathbf{in5/in5'} = \exp[(\Delta G_{ts3'} - \Delta G_{ts3})/RT] \dots \dots \dots \mathbf{Eq\ S2}$$

$\Delta G_{ts3} = 54.1$ kJ/mol; $\Delta G_{ts3'} = 197.9$ kJ/mol; $R = 8.314$ J/mol·K; $T = 383.15$ K.

ΔG_{ts3} and $\Delta G_{ts3'}$ are the free energy barriers of **ts3** and **ts3'**.

Theoretical calculation result (yields),

$$\mathbf{in5/in5'} = 4.03 \times 10^{19}:1$$

An **in5/in5'** = **4.03 × 10¹⁹:1** is predicted by the theoretical calculations based on the energy difference of **ts3** and **ts3'**, and the similar calculations have been widely reported in previous literatures (H. Han, T. Zhang, S.-D. Yang, Y. Lan and J.-B. Xia, *Org. Lett.*, 2019, **21**, 1749-1754; H. Jiang, Q. Li, Q. Qi, C. Yang and D. Zhang, *Chinese J. Org. Chem.*, 2018, **38**, 825-831; Z. Yu, T. Zhang, R. Bai and Y. Lan, *Catal. Sci. Technol.*, 2019, **9**, 646-651; D. Wei, Q. Liu, L. Sun, S.-J. Li, X. Li, L.-B. Qu and Y. Lan, *Chem. -Asian J.*, 2019 (<https://doi.org/10.1002/asia.201900076>)). Therefore, the formation of **in5'** is quite disadvantageous when compared with that of **in5** (**in5/in5'** = **4.03 × 10¹⁹:1**).

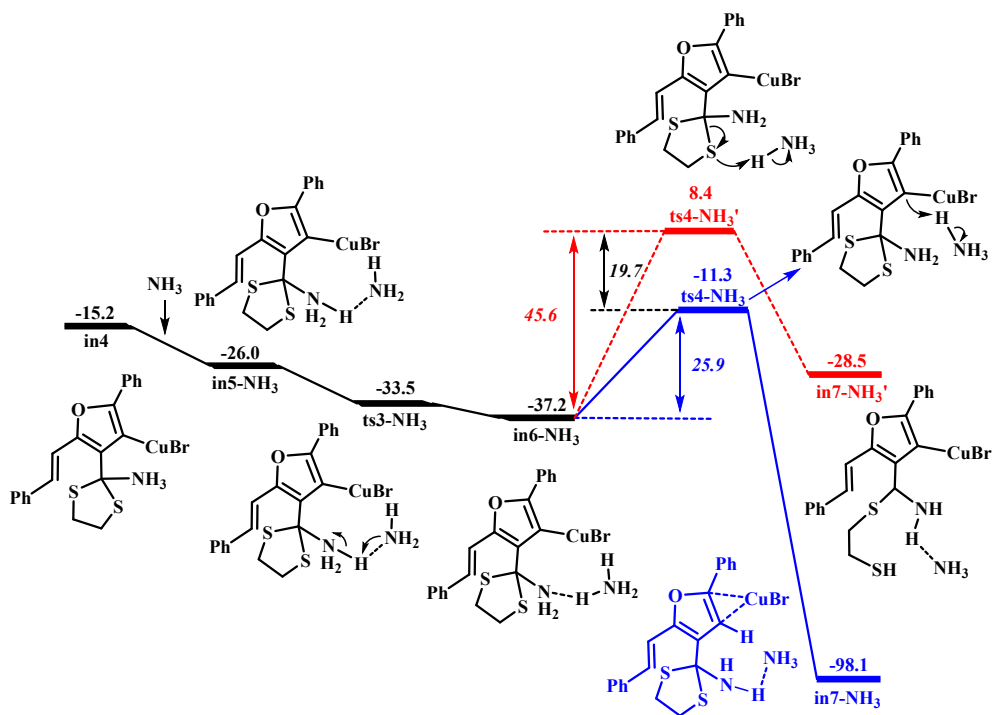


Figure S3. Comparing the free energy barriers of **ts4-NH₃'** vs. **ts4-NH₃**.

Based on the Arrhenius equation (K. J. Laidler, *J. Chem. Educ.*, 1984, **61**(6), 494-498; S. R. Logan, *J. Chem. Educ.*, 1982, **59**(4), 279-281),

$$\mathbf{in7-NH_3/in7-NH_3'} = \exp(-\Delta G_{ts4-NH_3}/RT) / \exp(-\Delta G_{ts4-NH_3'}/RT) \dots \dots \dots \mathbf{Eq\ S3}$$

$$\mathbf{in7-NH_3/in7-NH_3'} = \exp[(\Delta G_{ts4-NH_3'} - \Delta G_{ts4-NH_3})/RT] \dots \dots \dots \mathbf{Eq\ S4}$$

$\Delta G_{ts4-NH_3} = 25.9$ kJ/mol; $\Delta G_{ts4-NH_3'} = 45.6$ kJ/mol; $R = 8.314$ J/mol·K; $T = 383.15$ K.

ΔG_{ts4-NH_3} and $\Delta G_{ts4-NH_3'}$ are the free energy barriers of **ts4-NH₃** and **ts4-NH₃'**.

Theoretical calculation result (yields),

$$\mathbf{in7-NH_3/in7-NH_3'} = \mathbf{493:1}$$

An **in7-NH₃/in7-NH₃'=493:1** is predicted by the theoretical calculations based on the energy difference of **ts4-NH₃** and **ts4-NH₃'**, and the similar calculations have been widely reported in previous literatures (H. Han, T. Zhang, S.-D. Yang, Y. Lan and J.-B. Xia, *Org. Lett.*, 2019, **21**, 1749-1754; H. Jiang, Q. Li, Q. Qi, C. Yang and D. Zhang, *Chinese J. Org. Chem.*, 2018, **38**, 825-831; Z. Yu, T. Zhang, R. Bai and Y. Lan, *Catal. Sci. Technol.*, 2019, **9**, 646-651; D. Wei, Q. Liu, L. Sun, S.-J. Li, X. Li, L.-B. Qu and Y. Lan, *Chem. -Asian J.*, 2019 (<https://doi.org/10.1002/asia.201900076>)). Therefore, the formation of **in7-NH₃'** is quite disadvantageous when compared with that of **in7-NH₃** (**in7-NH₃/in7-NH₃'=493:1**).

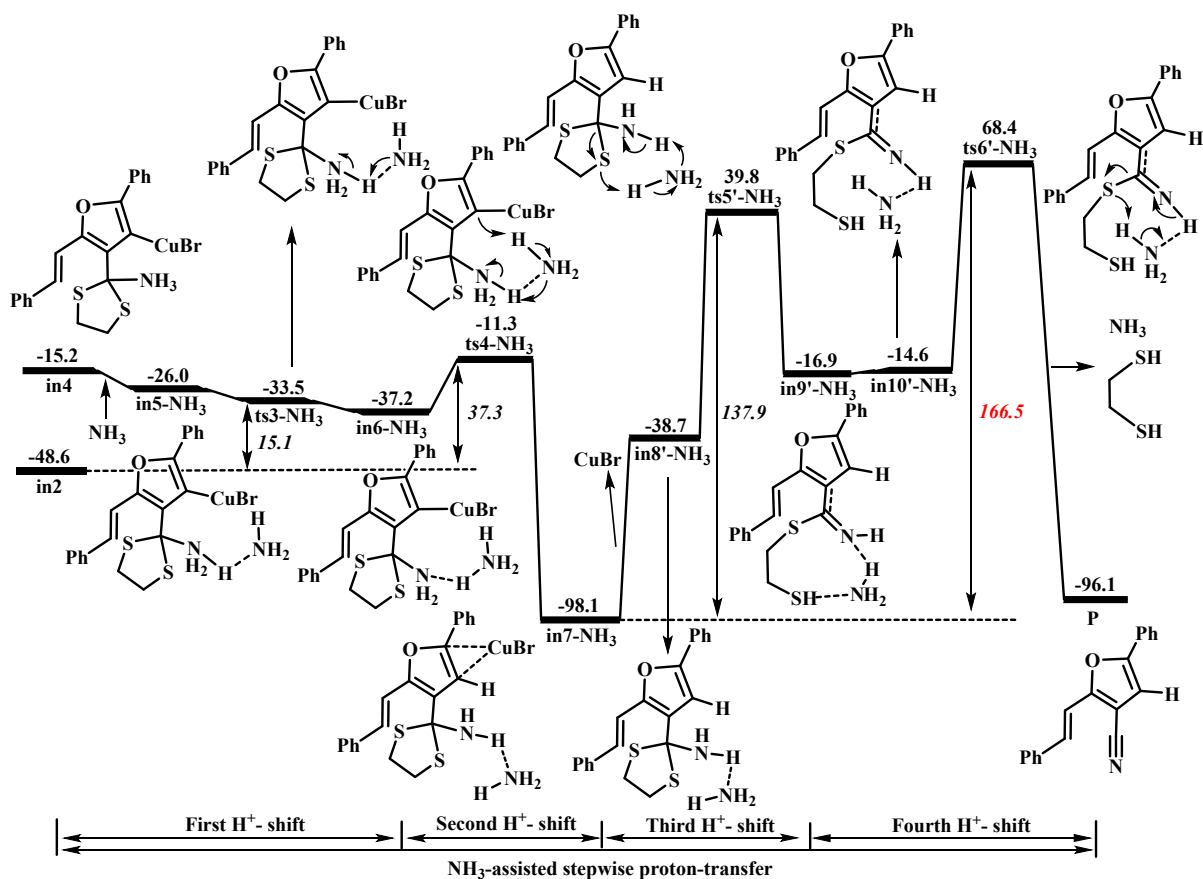


Figure S4. DFT-computed energy profile for the NH_3 -assisted proton-transfer reactions.

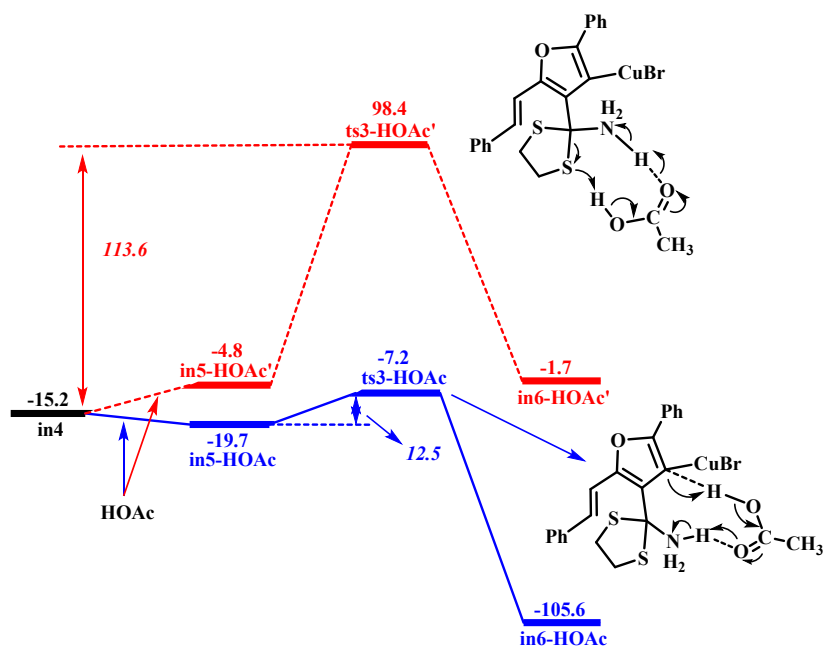


Figure S5. Comparing the free energy barriers of **ts3-HOAc'** vs. **ts3-HOAc**.

Based on the Arrhenius equation (K. J. Laidler, *J. Chem. Educ.*, 1984, **61**(6), 494-498; S. R. Logan, *J. Chem. Educ.*, 1982, **59**(4), 279-281),

$$\text{in6-HOAc}/\text{in6-HOAc}' = \exp(-\Delta G_{\text{ts3-HOAc}}/RT) / \exp(-\Delta G_{\text{ts3-HOAc}'}/RT) \dots \text{Eq S5}$$

$$\text{in6-HOAc}/\text{in6-HOAc}' = \exp[(\Delta G_{\text{ts3-HOAc}} - \Delta G_{\text{ts3-HOAc}'})/RT] \dots \text{Eq S6}$$

$\Delta G_{\text{ts3-HOAc}} = 12.5$ kJ/mol; $\Delta G_{\text{ts3-HOAc}'} = 113.6$ kJ/mol; $R = 8.314$ J/mol·K; $T = 383.15$ K.

$\Delta G_{\text{ts3-HOAc}}$ and $\Delta G_{\text{ts3-HOAc}'}$ are the free energy barriers of **ts3-HOAc** and **ts3-HOAc'**.

Theoretical calculation result (yields),

$$\text{in6-HOAc}/\text{in6-HOAc}' = 5.8 \times 10^{13}:1$$

An **in6-HOAc/in6-HOAc'** = $5.8 \times 10^{13}:1$ is predicted by the theoretical calculations based on the energy difference of **ts3-HOAc** and **ts3-HOAc'**, and the similar calculations have been widely reported in previous literatures (H. Han, T. Zhang, S.-D. Yang, Y. Lan and J.-B. Xia, *Org. Lett.*, 2019, **21**, 1749-1754; H. Jiang, Q. Li, Q. Qi, C. Yang and D. Zhang, *Chinese J. Org. Chem.*, 2018, **38**, 825-831; Z. Yu, T. Zhang, R. Bai and Y. Lan, *Catal. Sci. Technol.*, 2019, **9**, 646-651; D. Wei, Q. Liu, L. Sun, S.-J. Li, X. Li, L.-B. Qu and Y. Lan, *Chem. -Asian J.*, 2019 (<https://doi.org/10.1002/asia.201900076>)). Therefore, the formation of **in6-HOAc'** is quite disadvantageous when compared with that of **in6-HOAc** (**in6-HOAc/in6-HOAc'** = $5.8 \times 10^{13}:1$).

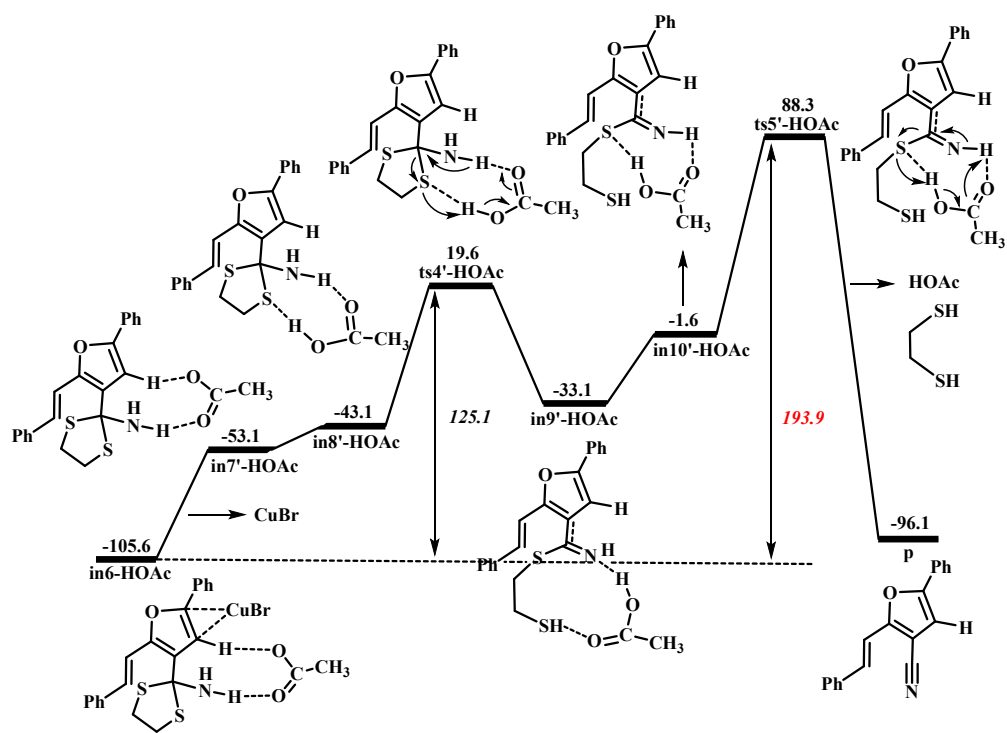


Figure S6. DFT-computed energy profile for the HOAc-assisted proton-transfer reactions in the absence of CuBr.

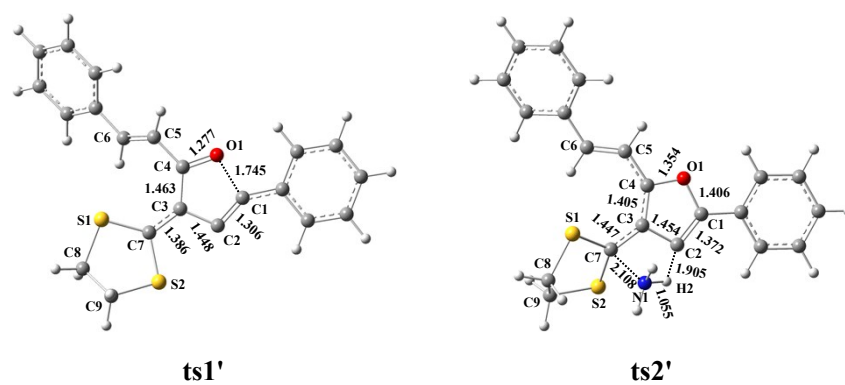
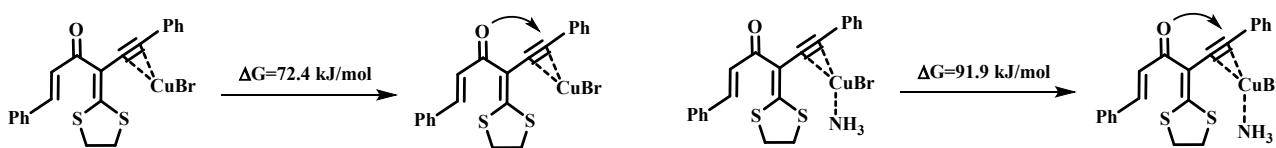


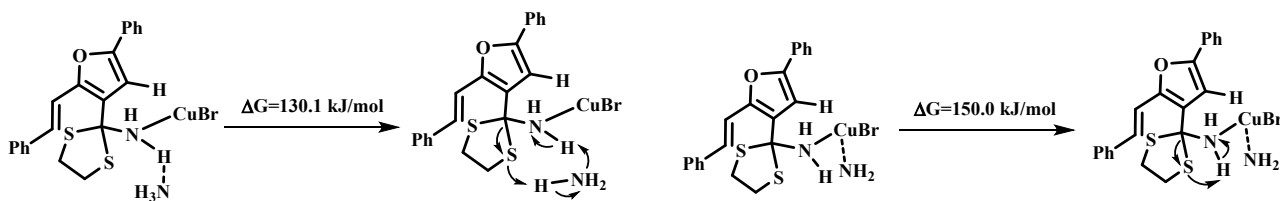
Figure S7. Optimized geometries involved in the intramolecular cycloaddition and the intermolecular addition in the absence of CuBr.

Scheme S1. The coordination effects of NH₃ with CuBr on the process of intramolecular cyclization.



The influence of NH₃ on the intramolecular cyclization is considered. The molecule of NH₃ as a ligand coordinates with the metal catalyst CuBr, but the participation of NH₃ do not alter the reaction mechanism of intramolecular cyclization process (see Scheme S1). In the present situations, the activation free energy of CuBr(NH₃)-catalyzed reaction is 91.9 kJ/mol, which is 19.5 kJ/mol higher than that of CuBr-catalyzed case without NH₃ as the ligand. This means that the effect of NH₃ on the process of intramolecular cyclization is negative.

Scheme S2. The effects of NH₃ (as the proton shuttle or the catalyst ligand) on the proton-transfer process.



The influence of NH₃ on the proton-transfer process is also considered. As shown in Figures 1 vs. 3, NH₃ as the proton shuttle can assist proton-transfer by reducing the rate-determining free energy barrier of whole Cu(I)-catalyzed reactions. In addition, the calculation shows that the molecule of NH₃ (as a ligand) coordinated with the metal catalyst CuBr can also promote proton-transfer reaction (160.8 vs. 150.0 kJ/mol, see Figure 1 vs. Scheme S2). However, the activation free energy of CuBr(NH₃)-catalyzed proton-transfer process is 150.0 kJ/mol, which is 19.9 kJ/mol higher than that of CuBr-catalyzed case with NH₃ as the proton shuttle (see Scheme S2). It should be noted that 150.0 kJ/mol is higher than the rate-determining free energy barrier of whole Cu(I)-catalyzed reactions (130.1 kJ/mol, see Figures 1 and 3). Therefore, the roles of NH₃ as the ligand is unfavorable when compared with that of NH₃ as the proton shuttle.

Intrinsic Reaction Coordinates

When the animation of transition state's vibrations cannot easily confirm the reliability of transition states, the intrinsic reaction coordinate (IRC) calculations is conducted to unambiguously identify the transition states, which are connected with the reactants and the products.

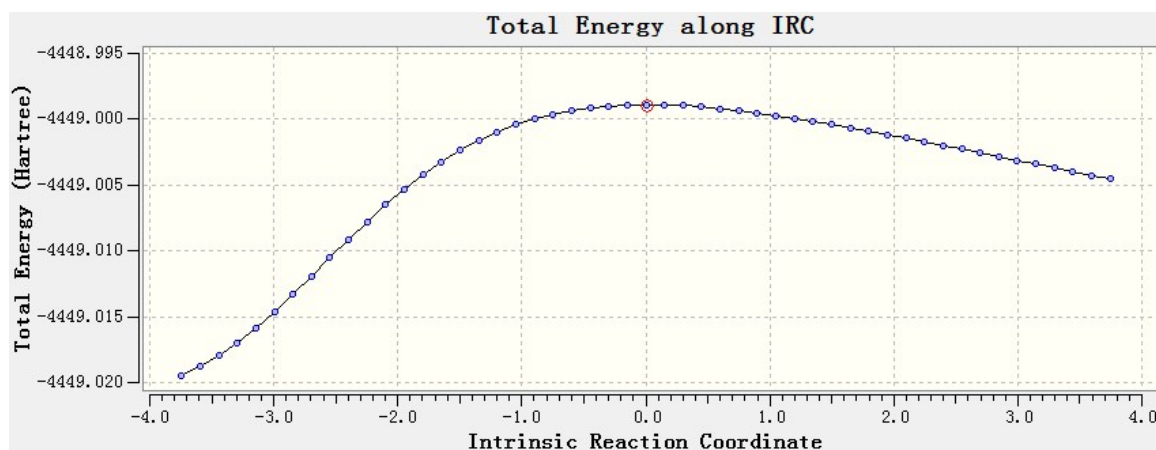


Figure S8. IRC of **ts1**.

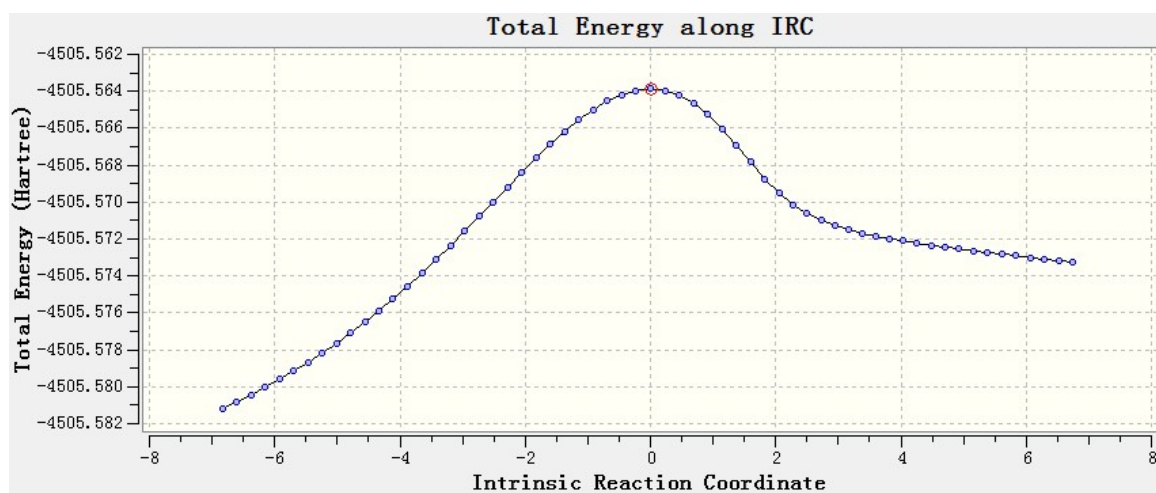


Figure S9. IRC of **ts2**.

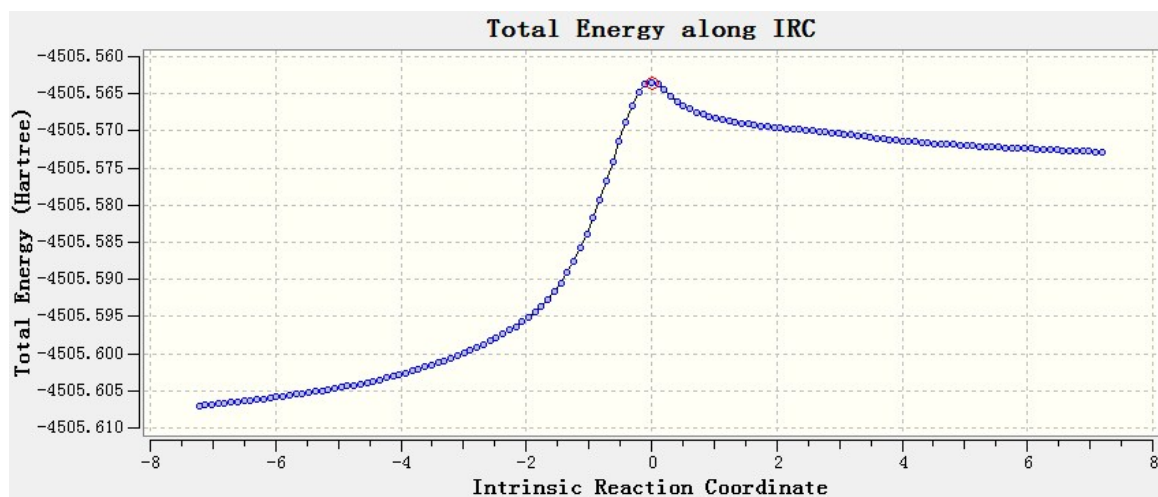


Figure S10. IRC of **ts3**.

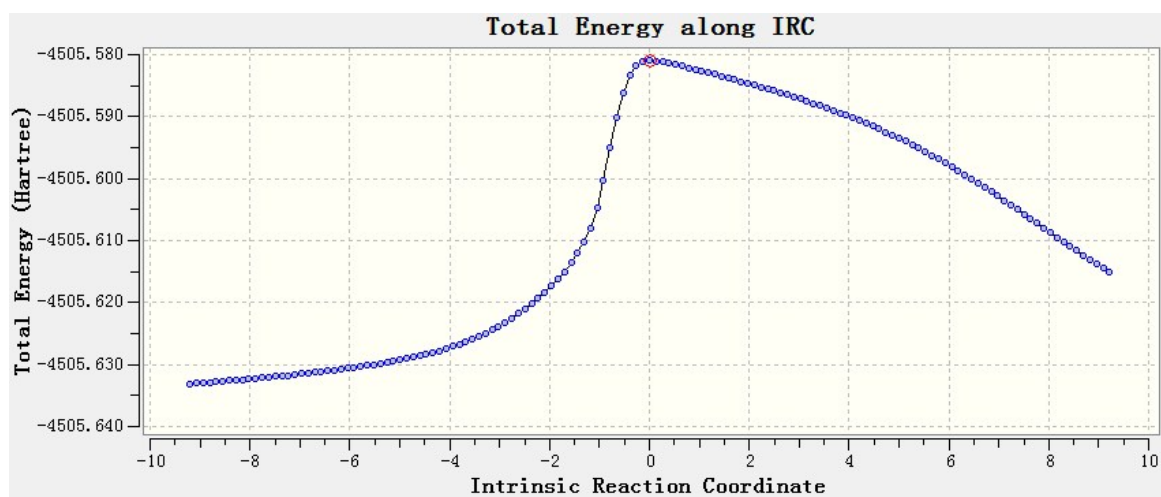


Figure S11. IRC of **ts4**.

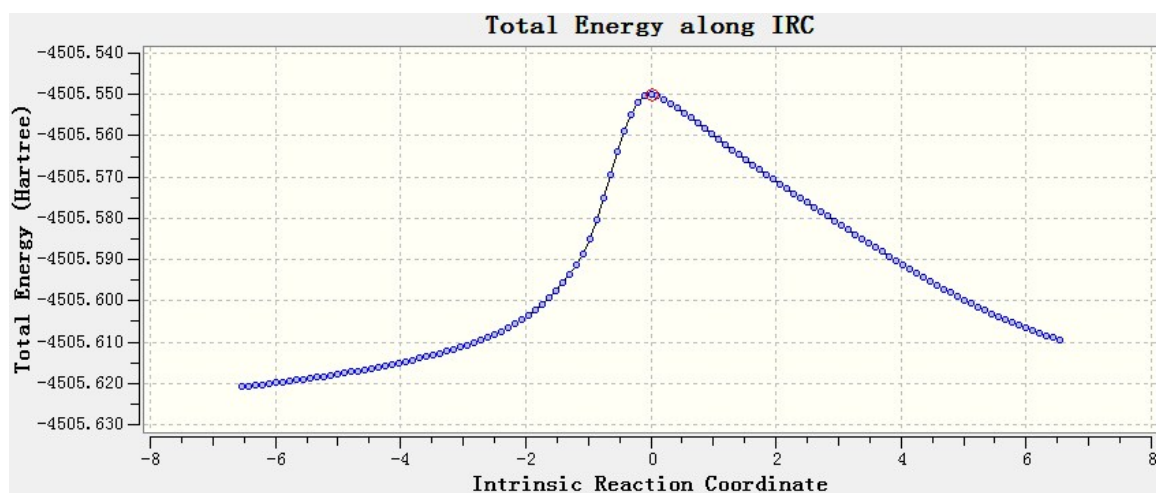


Figure S12. IRC of **ts5**.

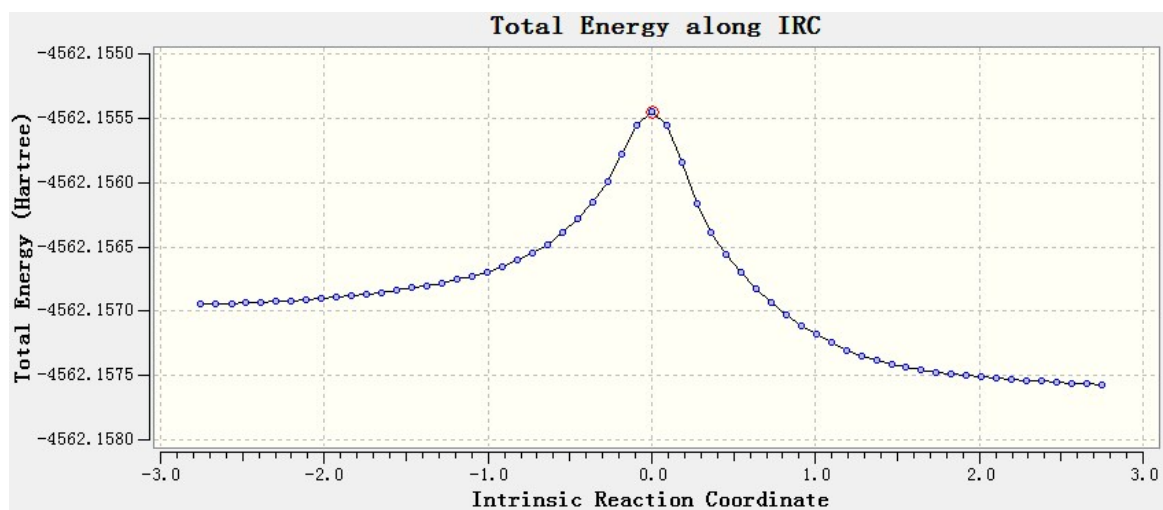


Figure S13. IRC of **ts3-NH₃**.

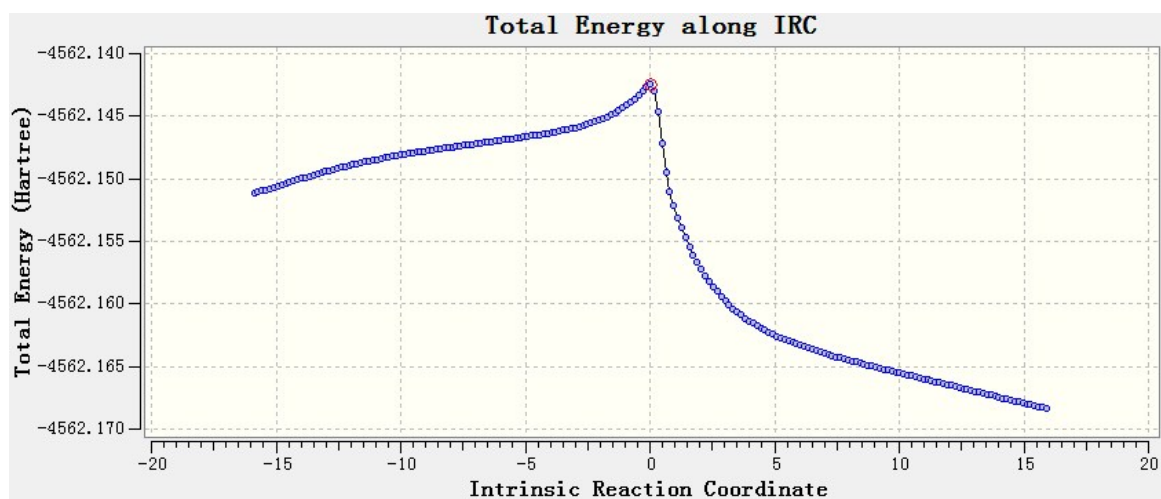


Figure S14. IRC of ts4-NH_3 .

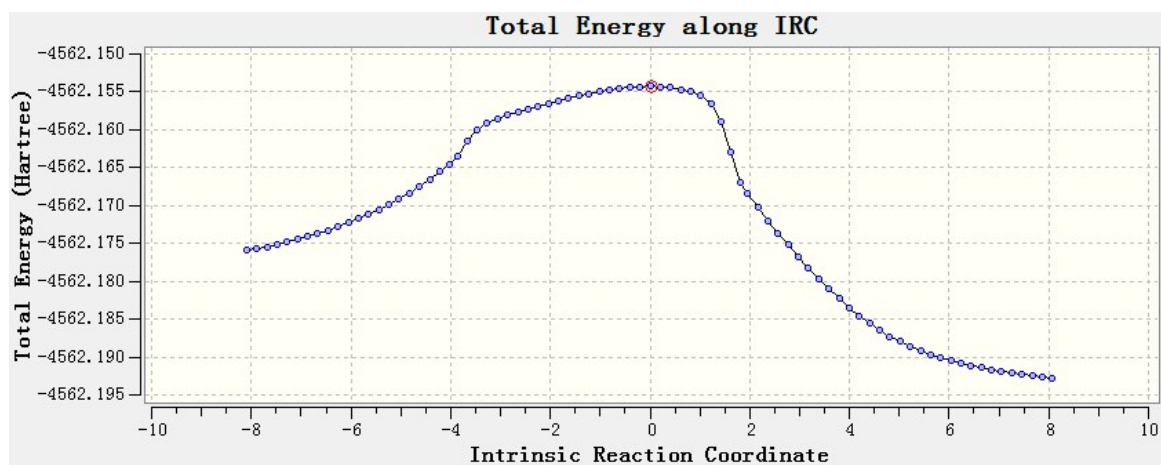


Figure S15. IRC of $ts5-NH_3$.

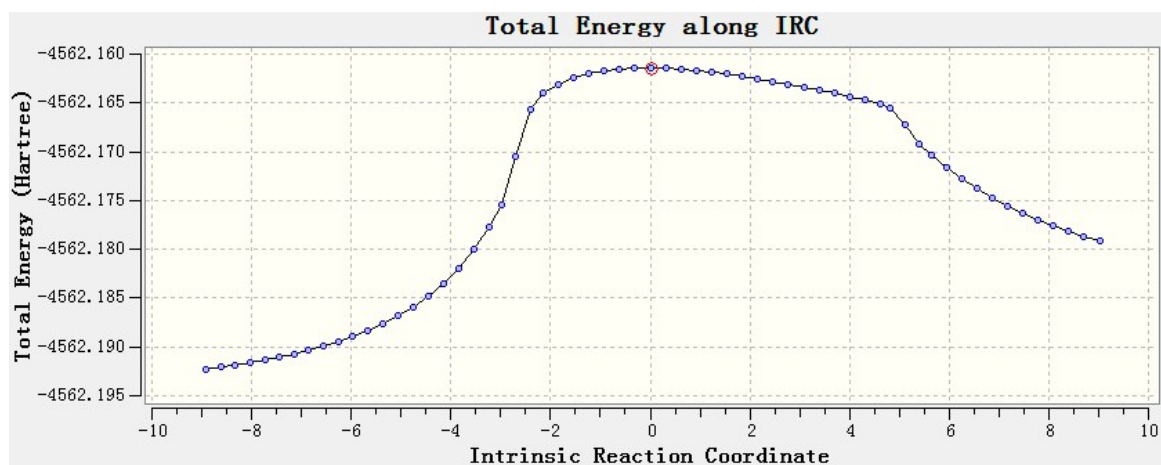


Figure S16. IRC of ts6-NH₃.

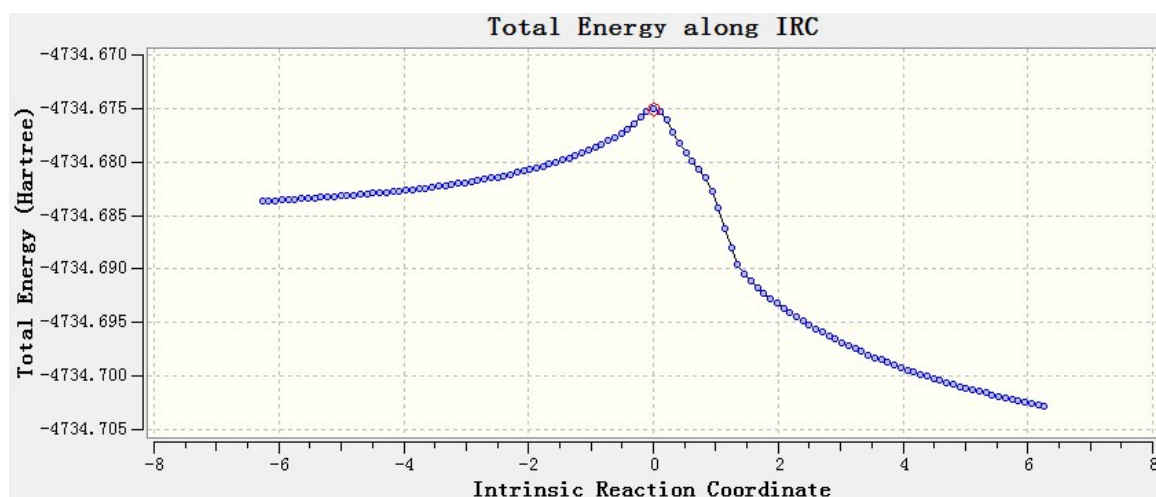


Figure S17. IRC of ts3-HOAc.

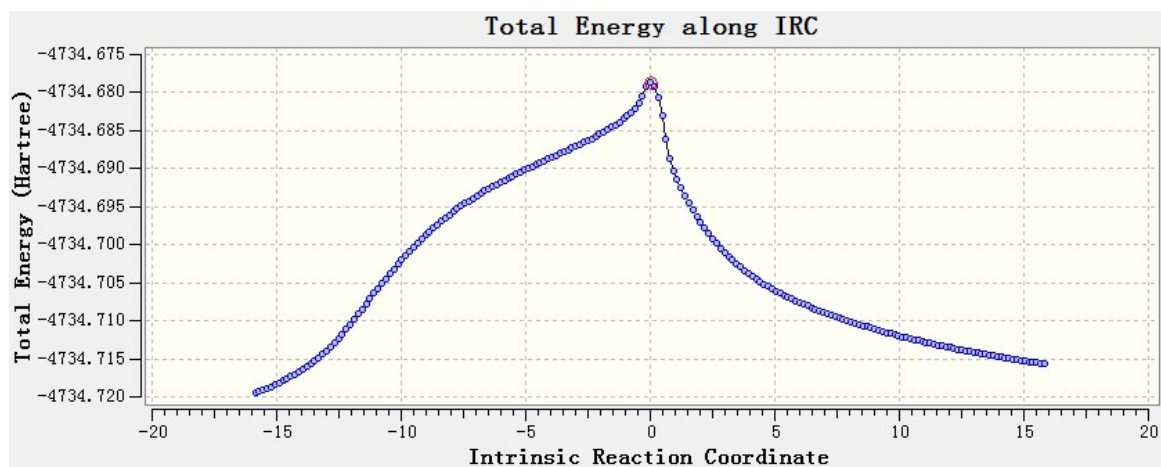


Figure S18. IRC of **ts4-HOAc**.

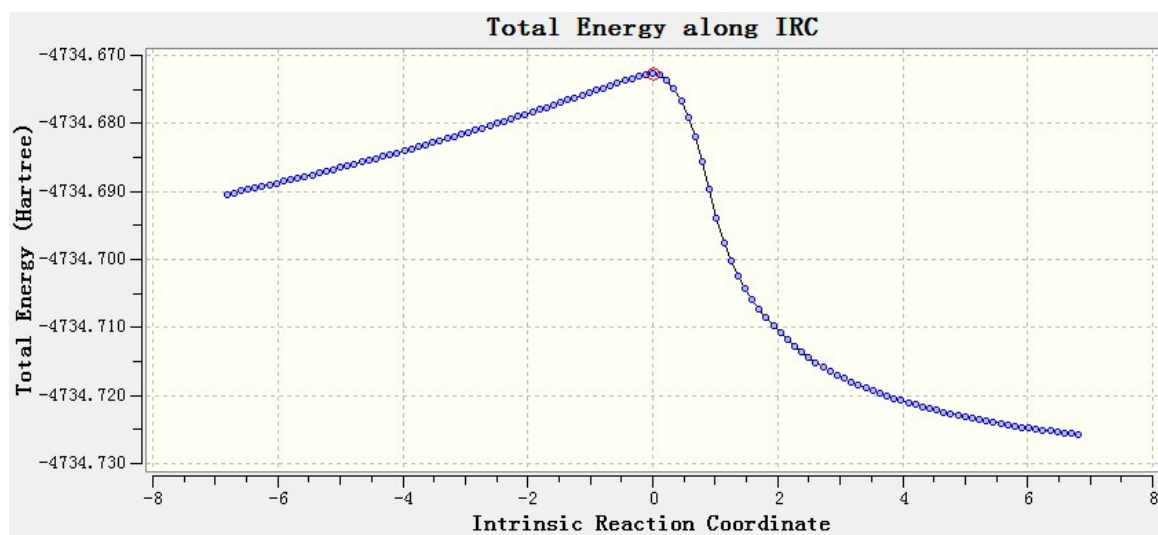


Figure S19. IRC of **ts5-HOAc**.

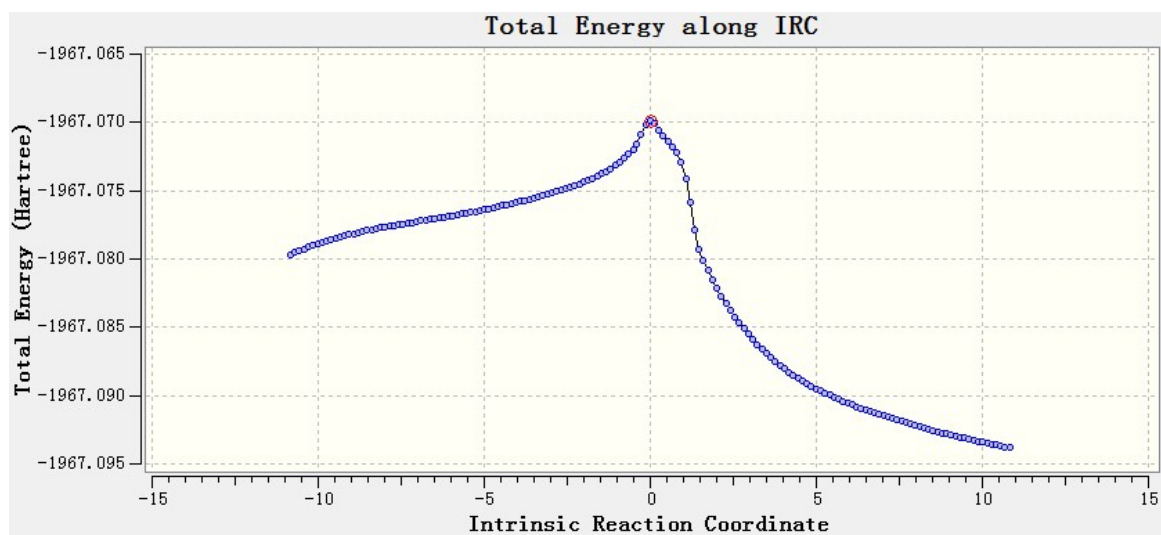


Figure S20. IRC of $ts5'-NH_3$.

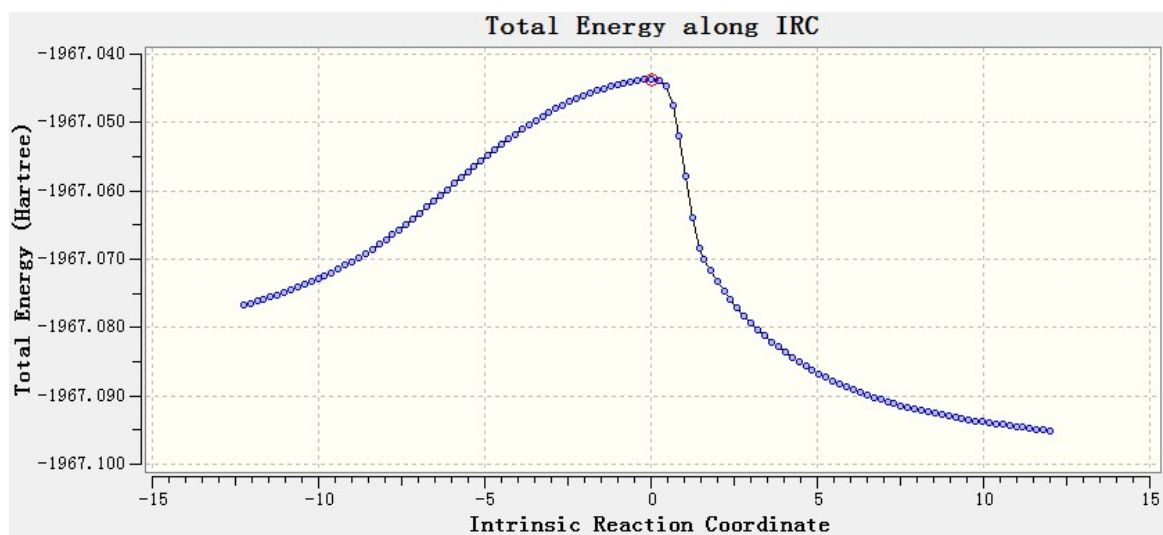


Figure S21. IRC of $\text{ts6}'\text{-NH}_3$.

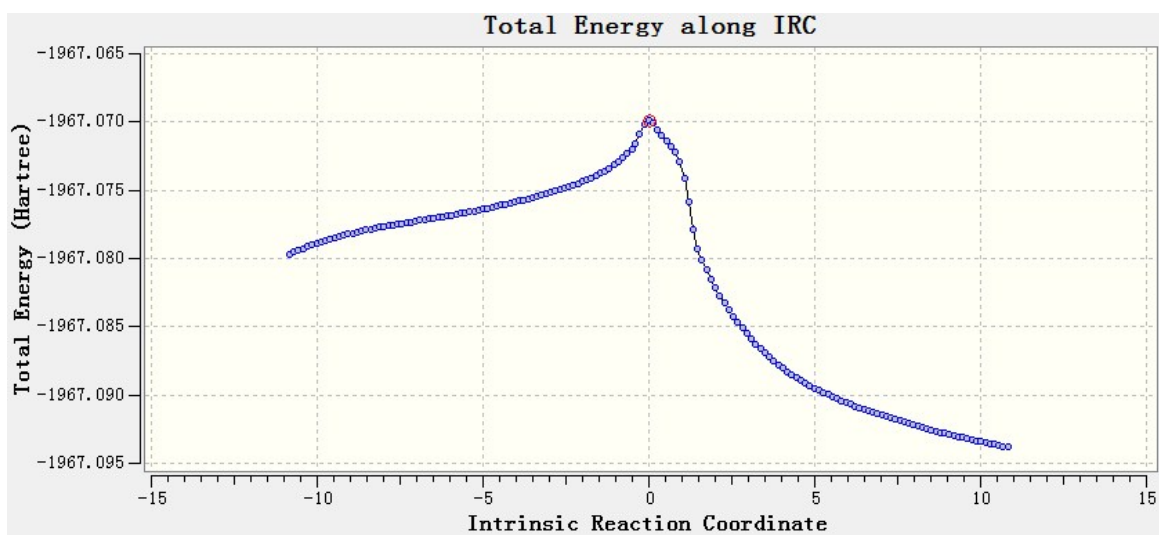


Figure S22. IRC of ts4'-HOAc.

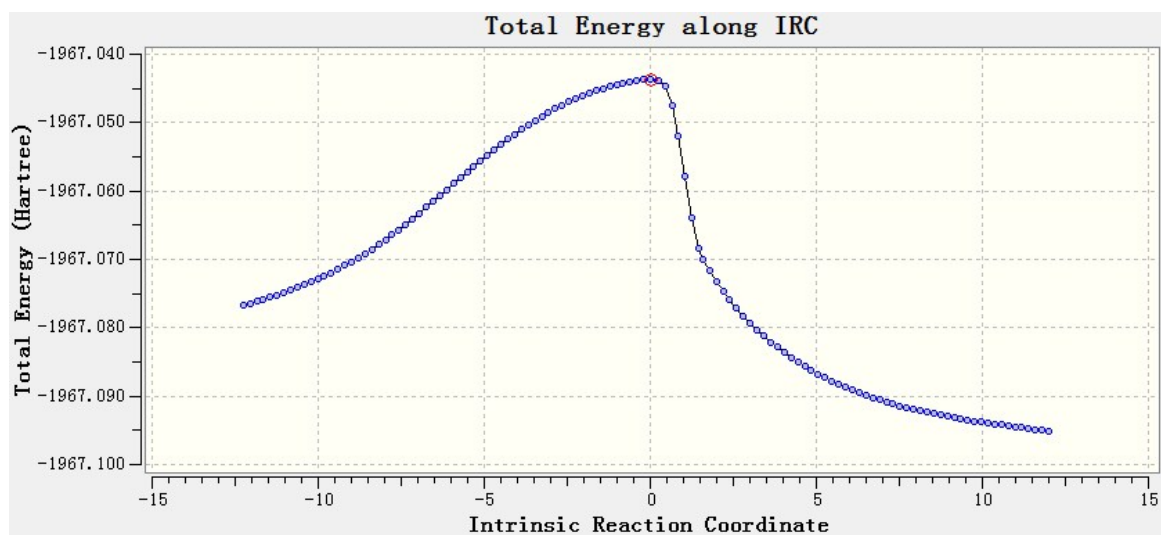


Figure S23. IRC of ts5'-HOAc.

Cartesian coordinates of the optimized stationary points on the optimal reaction channels

The solution-phase Gibbs free energy is determined by adding the solvation single-point energy (energy) and gas-phase thermal correction to the Gibbs free energy obtained from vibrational frequency calculation. Unless special emphasis, all the discussed energies are relative solution-phase Gibbs free energies (G_{rel} , kJ/mol) in this paper.

CuBr

Cu	0.00000000	0.00000000	-1.21848100
Br	0.00000000	0.00000000	1.00959800

B3LYP/6-31G* (Lanl2DZ for Cu)

Thermal correction to Gibbs Free Energy = -0.023804 a.u.

Sum of electronic and thermal Free Energies = -2767.620687 a.u.

M06-2x/6-311++G** (Lanl2DZ for Cu)

Energy = -2770.4213814 a.u.

No imaginary frequency

1a

O	-1.55681200	-2.97115600	-0.80413800
C	-0.82937900	-2.00694400	-0.53461300
C	0.63253500	-2.22983900	-0.52965100
C	1.56292500	-1.52392500	0.14346100
C	2.99896400	-1.81076800	0.21953600
C	3.60705000	-2.90945000	-0.41849000
C	4.97732100	-3.12325600	-0.31458500
C	5.77605300	-2.24727200	0.42808900
C	5.19041600	-1.15416800	1.06755700
C	3.81712400	-0.94058700	0.96385800
C	-1.45192900	-0.69183100	-0.23317000
C	-2.81612100	-0.64234800	-0.01384600
C	-0.71061200	0.51775800	-0.22347400
C	-0.11387200	1.58050900	-0.22391900
C	0.61923200	2.80114100	-0.22495000
C	1.98929100	2.81277000	-0.56048100
C	2.70473300	4.00691300	-0.55489700
C	2.07331400	5.20745100	-0.21963900
C	0.71598600	5.20663700	0.11205300
C	-0.00824100	4.01794200	0.11175400
S	-3.88225600	-2.04419800	-0.06267800
C	-5.32144800	-1.16411000	0.69042100
C	-5.31786600	0.27438700	0.20230200
S	-3.59740900	0.90037900	0.35322600

H	0.89856700	-3.14012400	-1.06154600
H	1.24613100	-0.64834400	0.70217700
H	3.00325100	-3.60134500	-0.99771600
H	5.42714200	-3.97738100	-0.81367700
H	6.84609700	-2.41886200	0.50710300
H	5.80155400	-0.46837600	1.64808800
H	3.36339600	-0.08791500	1.46371800
H	2.47804100	1.87968900	-0.82445500
H	3.75962700	4.00098900	-0.81619500
H	2.63490100	6.13759800	-0.21814200
H	0.21903000	6.13731900	0.37274500
H	-1.06279100	4.01456300	0.36974100
H	-5.24317300	-1.21213800	1.78112800
H	-6.22524300	-1.69560300	0.37615800
H	-5.95609900	0.91898200	0.81405100
H	-5.63415200	0.34523400	-0.84274800

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.252113 a.u.

Sum of electronic and thermal Free Energies = -1681.148639 a.u.

M06-2x/6-311++G**

Energy = -1681.255519 a.u.

No imaginary frequency

2a (NH₄OAc)

C	2.21572700	-0.27190900	0.00014900
C	0.75412800	0.12300700	-0.00021600
O	0.36366200	1.28324800	-0.00009500
O	-0.05532700	-0.93329200	-0.00021500
H	2.43801000	-0.88618400	-0.87890400
H	2.84634300	0.61817700	-0.00425100
H	2.43931600	-0.87787300	0.88468700
H	-1.03680400	-0.61521700	0.00009400
N	-2.59572100	-0.06736200	0.00018900
H	-3.15304500	-0.31163300	-0.81759500
H	-2.49680100	0.94723400	-0.00133700
H	-3.15278000	-0.30920700	0.81886700

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.066130 a.u.

Sum of electronic and thermal Free Energies = -285.596061 a.u.

M06-2x/6-311++G**

Energy = -285.6406062 a.u.

No imaginary frequency

NH₃

N	0.00001000	-0.00000300	-0.11941800
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H	-0.52505100	-0.77789500	0.27863600
H	-0.41124100	0.84361300	0.27862800
H	0.93622300	-0.06569600	0.27866200

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.015453 a.u.

Sum of electronic and thermal Free Energies = -56.532494 a.u.

M06-2x/6-311++G**

Energy = -56.5517822 a.u.

No imaginary frequency

HOAc

C	1.39724800	-0.11046200	-0.00003500
C	-0.09224200	0.12592600	-0.00012300
O	-0.64489100	1.20239900	0.00002100
O	-0.77916500	-1.04652700	-0.00002000
H	1.68391700	-0.69573500	-0.87991500
H	1.91786900	0.84728300	-0.00358500
H	1.68445700	-0.68904000	0.88414200
H	-1.72382600	-0.80227500	0.00029800

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.034759 a.u.

Sum of electronic and thermal Free Energies = -229.047028 a.u.

M06-2x/6-311++G**

Energy = -229.0719316 a.u.

No imaginary frequency

No cocatalysts (NH₃ and HOAc)

in1

O	0.62042900	0.94627600	-1.77343500
C	1.01752400	0.00822800	-1.09259100
C	2.45694300	-0.14200500	-0.81147900
C	2.96047300	-0.74816000	0.28535500
C	4.36254700	-0.82142900	0.69548400
C	5.42147400	-0.30979900	-0.08071700
C	6.73658500	-0.41032000	0.35994900
C	7.02669100	-1.02224600	1.58464400
C	5.98980700	-1.53552600	2.36546800
C	4.67227200	-1.43663900	1.92301900
C	0.00591500	-0.96317200	-0.50905000
C	0.12822900	-2.32688200	-0.51729200
S	1.42910600	-3.26829700	-1.26726200
C	0.67309900	-4.92436900	-0.96358000
C	-0.84186900	-4.77133200	-0.88314900
S	-1.15309600	-3.32331900	0.20134300

H	3.08840400	0.41108800	-1.50177900
H	2.26003200	-1.22768600	0.96706900
H	5.21411400	0.16540900	-1.03463300
H	7.54084300	-0.01109800	-0.25174400
H	8.05558400	-1.09737600	1.92537300
H	6.20649100	-2.01205800	3.31739700
H	3.86571700	-1.83681700	2.53273800
H	1.07814300	-5.33601800	-0.03521900
H	0.96684100	-5.56770100	-1.79842000
H	-1.31358500	-5.64123300	-0.41827500
H	-1.29049700	-4.59395400	-1.86391200
C	-1.21519900	-0.34054600	-0.10858500
C	-2.08505500	0.51606400	0.12760900
C	-2.81888900	1.73988100	0.26795300
C	-2.22831500	2.91001800	-0.25623200
C	-2.88714100	4.12939100	-0.13456300
C	-4.13130700	4.19792200	0.50018900
C	-4.72015200	3.03876500	1.01188200
C	-4.07375200	1.81011800	0.90025400
H	-1.26765400	2.83768800	-0.75673600
H	-2.43035800	5.02798300	-0.53987300
H	-4.64235000	5.15250600	0.59101400
H	-5.69000600	3.08865900	1.49844300
H	-4.53558900	0.90377100	1.28125200
Cu	-2.98501700	-1.39474200	0.36749200
Br	-5.05225500	-2.13662700	1.00017300

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.245585 a.u.

Sum of electronic and thermal Free Energies = -4448.770019 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4451.7127004 a.u.

No imaginary frequency

ts1

O	0.57782600	2.18512500	-0.63419200
C	1.20413500	1.11039600	-0.52816500
C	2.67336500	1.19716500	-0.55940100
C	3.46502400	0.59934700	0.35372500
C	4.91153100	0.75449900	0.51335300
C	5.69766000	1.57596100	-0.31844300
C	7.07110700	1.67501500	-0.12385100
C	7.69255400	0.95917300	0.90559900
C	6.92810700	0.14241800	1.74002200
C	5.55189200	0.04260800	1.54458900
C	0.39426600	-0.11705500	-0.34369200

C	0.78592900	-1.43388300	-0.50008700
S	2.36154500	-2.01165100	-1.05981700
C	2.01725100	-3.80144600	-0.81495800
C	0.53918100	-4.03837000	-1.07568700
S	-0.39522700	-2.71237500	-0.21361900
H	3.06232400	1.93675500	-1.25366300
H	2.99617400	-0.06768400	1.07462600
H	5.23241000	2.14130100	-1.12033600
H	7.66178300	2.31366600	-0.77470200
H	8.76548900	1.04129300	1.05510400
H	7.40208600	-0.41531400	2.54282700
H	4.95790100	-0.59306900	2.19685500
H	2.29367600	-4.07943800	0.20613800
H	2.65131900	-4.34839900	-1.51938200
H	0.20174500	-4.99436000	-0.66500200
H	0.30486500	-4.00351200	-2.14345600
C	-0.99724400	0.26031800	-0.15540600
C	-1.34905500	1.49176700	-0.23435000
C	-2.18271700	2.65067700	-0.18639100
C	-1.90934600	3.78238000	-0.98074300
C	-2.75273600	4.88751900	-0.93067300
C	-3.88232200	4.87998400	-0.10739300
C	-4.16090600	3.76034900	0.68050400
C	-3.31508900	2.65552200	0.65794700
H	-1.02995300	3.78279800	-1.61340200
H	-2.53036500	5.75746800	-1.54230800
H	-4.54152000	5.74310700	-0.07912600
H	-5.03664600	3.74674700	1.32284100
H	-3.52980100	1.78581100	1.27074800
Cu	-2.63202900	-0.78985800	0.19213400
Br	-4.54033900	-1.91268400	0.67713900

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.246400 a.u.

Sum of electronic and thermal Free Energies = -4448.752479 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4451.6859251 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 233.31*i*

in2

O	-1.44933100	-1.00764500	0.09113600
C	-0.84214000	0.15579200	-0.14435700
C	-1.68901000	1.29325700	0.08272000
C	-1.30977900	2.53682600	0.47158500
C	-2.18832100	3.66597000	0.74931800

C	-3.57659400	3.65197500	0.49700100
C	-4.36242500	4.76100800	0.78820600
C	-3.78630900	5.91314000	1.33588600
C	-2.41333700	5.94719600	1.58737300
C	-1.62476900	4.83728600	1.29503900
C	0.51369500	-0.13194300	-0.50457000
C	1.49555400	0.72946600	-1.02648900
S	1.20864400	2.34402600	-1.64088700
C	2.97544500	2.76770000	-1.91977300
C	3.70100800	1.49097700	-2.30681600
S	3.11936300	0.13594100	-1.19679500
H	-2.74668800	1.04685700	0.02642200
H	-0.25301200	2.73231500	0.62813200
H	-4.04086800	2.77264500	0.06093800
H	-5.42930300	4.73157400	0.58518300
H	-4.40493600	6.77718200	1.56123800
H	-1.95747900	6.83761600	2.01113000
H	-0.55632300	4.86573000	1.49528300
H	3.37794400	3.20272800	-1.00018600
H	3.00756800	3.51710100	-2.71604000
H	4.78249500	1.57958400	-2.17277200
H	3.49069700	1.19831800	-3.33970300
C	0.71411100	-1.57939000	-0.40178500
C	-0.51668600	-2.05584400	-0.04198300
C	-1.07207500	-3.38274100	0.21398600
C	-2.45638600	-3.56845100	0.39097700
C	-2.97707000	-4.83891900	0.62840100
C	-2.13169700	-5.94805500	0.69446500
C	-0.75546700	-5.77367800	0.52407300
C	-0.22861300	-4.50698500	0.29018400
H	-3.12333900	-2.71467400	0.33829400
H	-4.04900400	-4.96148800	0.76027300
H	-2.54001600	-6.93812300	0.87823600
H	-0.08510200	-6.62711000	0.57661800
H	0.84388600	-4.38406800	0.17008900
Cu	2.31317400	-2.59279000	-0.82722000
Br	4.17959400	-3.79680800	-1.33230800

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.250203 a.u.

Sum of electronic and thermal Free Energies = -4448.775965 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4451.7173251 a.u.

No imaginary frequency

in3

O	-0.81967900	2.23121400	0.15040700
C	-1.55614000	1.12023800	0.10163900
C	-2.97057400	1.35693300	0.12780600
C	-3.92083300	0.60794900	-0.48795200
C	-5.35851800	0.85217100	-0.48681400
C	-5.98137400	1.79853400	0.35334800
C	-7.35680100	1.99570500	0.30237400
C	-8.14580700	1.25219100	-0.58276900
C	-7.54690800	0.30476400	-1.41540600
C	-6.16950500	0.10574600	-1.36498500
C	-0.66254200	0.00701200	0.03845800
C	-0.94483900	-1.36185900	0.23540600
S	-2.53662000	-2.05135800	0.46909700
C	-1.93895400	-3.66528600	1.12479000
C	-0.65941700	-4.00108000	0.38609300
S	0.38242000	-2.48218000	0.34040300
H	-3.24826800	2.29134500	0.61046200
H	-3.60245800	-0.23446000	-1.09636900
H	-5.38700300	2.37099900	1.05908000
H	-7.81953300	2.72760600	0.95854400
H	-9.22023900	1.40880400	-0.61757600
H	-8.15244800	-0.27861900	-2.10329500
H	-5.70524000	-0.63035600	-2.01693900
H	-2.73055500	-4.39909900	0.94671000
H	-1.77702100	-3.56302500	2.20214500
H	-0.85197400	-4.31917900	-0.64336200
H	-0.04710500	-4.75427700	0.88416500
C	0.70267600	0.52732400	-0.03688400
C	0.54297100	1.88289600	0.05585200
C	1.44895700	3.03026200	0.06941000
C	0.95162400	4.34630100	0.01263600
C	1.82111700	5.43519100	0.01755500
C	3.20167000	5.23688500	0.07906900
C	3.70562900	3.93471000	0.13957000
C	2.84219300	2.84314100	0.13838000
H	-0.11882600	4.51242100	-0.04064500
H	1.41630700	6.44289100	-0.02935500
H	3.87825500	6.08720400	0.08166200
H	4.77761000	3.76502000	0.19190900
H	3.24689600	1.83691900	0.19799600
Cu	2.35910500	-0.45587600	-0.26472000
Br	4.32464700	-1.60219700	-0.55711700
N	2.56671300	-4.60396900	0.48338000
H	3.08669700	-3.77896900	0.16371600

H	2.81427200	-5.35036700	-0.16671200
H	2.99359300	-4.86036900	1.37383800

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.283888 a.u.

Sum of electronic and thermal Free Energies = -4505.308930 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4508.2788312 a.u.

No imaginary frequency

ts2

O	-0.47034600	2.15285200	0.11910700
C	-1.12815800	0.96983000	0.14889100
C	-2.55658700	1.11309600	0.33747700
C	-3.52895500	0.39373100	-0.26663700
C	-4.97140500	0.54470400	-0.07154200
C	-5.53578200	1.30944900	0.96926900
C	-6.91585800	1.43173900	1.09661700
C	-7.77026600	0.78826500	0.19502300
C	-7.22886800	0.01691000	-0.83495300
C	-5.84675100	-0.10495900	-0.96304500
C	-0.18725700	-0.04668900	-0.04529100
C	-0.35037000	-1.49754900	-0.00298400
S	-1.87427300	-2.28386000	0.48978000
C	-1.28362000	-3.97248500	0.07642300
C	-0.56106400	-3.89706000	-1.26216600
S	0.50560700	-2.38910100	-1.28935600
H	-2.82753700	1.95508400	0.97233200
H	-3.24016800	-0.35650100	-0.99785400
H	-4.88973900	1.79952100	1.69182200
H	-7.32949400	2.02574400	1.90721200
H	-8.84740000	0.88374300	0.29993300
H	-7.88295400	-0.49020300	-1.53916300
H	-5.43013500	-0.70320900	-1.77015700
H	-2.16467700	-4.61919500	0.02795700
H	-0.62357900	-4.34326900	0.86733400
H	-1.27150500	-3.83170200	-2.09110100
H	0.08468300	-4.76707800	-1.41317100
C	1.12425000	0.55636400	-0.22431300
C	0.87804100	1.90336800	-0.11289900
C	1.72175500	3.09522400	-0.17291400
C	1.18400000	4.37740300	0.04850000
C	1.99603200	5.50852700	-0.00833400
C	3.35907000	5.38825200	-0.28595300
C	3.90312300	4.12024600	-0.50973800
C	3.09609300	2.98766800	-0.45734700

H	0.12620600	4.48182600	0.26464900
H	1.55980700	6.48889900	0.16578400
H	3.99064600	6.27146800	-0.32881900
H	4.96205200	4.01150000	-0.72893800
H	3.52798600	2.00771700	-0.63915700
Cu	2.77838000	-0.44623900	-0.19072000
Br	4.29393600	-2.03490700	0.50258400
N	0.80689800	-1.89227500	1.63275200
H	1.78530100	-2.07708000	1.35726200
H	0.44660700	-2.66407300	2.19476900
H	0.79171500	-1.03622700	2.18633800

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.287689 a.u.

Sum of electronic and thermal Free Energies = -4505.276185 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4508.261494 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 285.75i

in4

O	0.51588800	2.12627300	-0.24248600
C	1.13528500	0.91469700	-0.29066500
C	2.57009900	1.00736800	-0.16210300
C	3.40063100	0.07820400	0.36172300
C	4.85497000	0.18489000	0.47943800
C	5.61734800	1.13536600	-0.22938700
C	6.99828600	1.20532900	-0.07140700
C	7.65926100	0.32347100	0.78979600
C	6.92211800	-0.63331000	1.49038800
C	5.53931300	-0.70242600	1.33320000
C	0.14680500	-0.06181100	-0.42584800
C	0.36416700	-1.53334900	-0.66374200
S	1.62669800	-1.86510500	-1.96446900
C	2.00124500	-3.57247700	-1.40882700
C	2.14329900	-3.54655000	0.11073000
S	0.75589100	-2.57711300	0.84087900
H	2.96965100	1.97226100	-0.46884100
H	2.96298100	-0.82269200	0.78295500
H	5.12508200	1.81103800	-0.92277000
H	7.56504800	1.94572300	-0.62987800
H	8.73793700	0.37867700	0.90722900
H	7.42421100	-1.32518800	2.16156800
H	4.97004400	-1.44207400	1.89260300
H	2.94001500	-3.86480000	-1.89024800
H	1.22568200	-4.27871400	-1.72711400

H	3.09189800	-3.08569900	0.39816200
H	2.09740100	-4.55591100	0.53156200
C	-1.15116600	0.58141300	-0.39487800
C	-0.84533100	1.92228900	-0.29294200
C	-1.65920800	3.13426200	-0.21765500
C	-1.08034300	4.37210800	0.12186600
C	-1.86013200	5.52407600	0.20140600
C	-3.23202300	5.47012400	-0.05389700
C	-3.81692700	4.24824900	-0.39795300
C	-3.04065700	3.09613000	-0.48475300
H	-0.01694200	4.42208600	0.32992100
H	-1.39285500	6.46844600	0.46870500
H	-3.83851000	6.36934300	0.01144000
H	-4.88190100	4.19268200	-0.60782500
H	-3.50162300	2.15615000	-0.77650100
Cu	-2.88096800	-0.26449300	-0.17931700
Br	-4.24589000	-2.12312100	-0.09974800
N	-0.95101000	-2.12326500	-1.21401800
H	-1.74796500	-2.12834700	-0.53036800
H	-0.80396300	-3.08548100	-1.53121900
H	-1.28254300	-1.54782600	-1.99891200

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.291373 a.u.

Sum of electronic and thermal Free Energies = -4505.286196 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4508.2821126 a.u.

No imaginary frequency

ts3

O	-0.08081700	2.06444500	0.20698500
C	-0.96414000	1.01341500	0.24571000
C	-2.33885100	1.39193400	0.04082900
C	-3.33732100	0.57203100	-0.35830500
C	-4.73791400	0.94157900	-0.55967300
C	-5.28670600	2.16480100	-0.12420200
C	-6.62430000	2.46984900	-0.35605900
C	-7.45371800	1.56114800	-1.02172900
C	-6.93028700	0.34019100	-1.45104000
C	-5.59068500	0.03534000	-1.21928600
C	-0.22879600	-0.13545100	0.47093800
C	-0.60670300	-1.55419800	0.83254600
S	-1.94811800	-1.65222700	2.09062700
C	-2.38579900	-3.38431600	1.67883900
C	-2.51449100	-3.48303300	0.16019000
S	-1.10177200	-2.60157300	-0.63536900

H	-2.52809000	2.45269000	0.18905600
H	-3.09079300	-0.46096200	-0.59063300
H	-4.66500100	2.87486900	0.41322100
H	-7.02594000	3.41851300	-0.00988000
H	-8.49833400	1.80209500	-1.19799200
H	-7.56519500	-0.37468600	-1.96765800
H	-5.18625000	-0.91383800	-1.56431200
H	-3.33621000	-3.60683200	2.17401600
H	-1.62684800	-4.07468700	2.06110500
H	-3.44810200	-3.02444800	-0.17688000
H	-2.49172400	-4.52583800	-0.17151400
C	1.17019400	0.20869400	0.52280700
C	1.19161400	1.58570100	0.38507700
C	2.25486700	2.58745100	0.38179600
C	1.99350600	3.91259200	-0.01228700
C	3.01212700	4.86297000	-0.01346100
C	4.30677300	4.51244200	0.37590700
C	4.57496100	3.20021000	0.77526700
C	3.55992800	2.24803700	0.78452600
H	0.99175800	4.18824300	-0.32354900
H	2.79405300	5.88066800	-0.32597400
H	5.10044000	5.25432000	0.36806300
H	5.57723300	2.91614200	1.08334600
H	3.77712500	1.23476200	1.11140700
Cu	2.76381200	-0.73275700	-0.28242900
Br	4.40948000	-1.98466400	-1.18563100
N	0.67978600	-2.10967900	1.41936400
H	1.01396100	-2.93957700	0.92673400
H	0.58880400	-2.30067100	2.41792500
H	1.43750800	-1.08287200	1.16513700

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.285305 a.u.

Sum of electronic and thermal Free Energies = -4505.278099 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4508.2681678 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 1272.53i

in5

O	0.00795700	1.94874600	0.21738600
C	-0.86191200	0.88398200	0.36835800
C	-2.22836900	1.25049500	0.08002000
C	-3.20108900	0.42248600	-0.35782600
C	-4.58465900	0.79427300	-0.65338700
C	-5.16186200	2.01237700	-0.24292400

C	-6.48138800	2.31834500	-0.56094200
C	-7.26091700	1.41525500	-1.29134700
C	-6.70824000	0.19939400	-1.69785900
C	-5.38723300	-0.10743900	-1.37822100
C	-0.13229200	-0.23999900	0.72558000
C	-0.54784200	-1.64413300	1.11220000
S	-1.99218200	-1.56906000	2.32020100
C	-2.55580600	-3.26004800	1.91557200
C	-2.65763400	-3.35437200	0.39488200
S	-1.12499700	-2.66359900	-0.36240700
H	-2.42120200	2.31588500	0.18383100
H	-2.94012100	-0.61297900	-0.55267200
H	-4.57913000	2.71553800	0.34493200
H	-6.90832500	3.26199400	-0.23202600
H	-8.29173400	1.65671900	-1.53527500
H	-7.30556500	-0.50999100	-2.26415900
H	-4.95777900	-1.05175000	-1.70509700
H	-3.52958600	-3.41119200	2.39182100
H	-1.85694400	-4.00339000	2.31404600
H	-3.52804400	-2.79513500	0.03931600
H	-2.74782600	-4.39430700	0.06359800
C	1.25658100	0.17139100	0.73535400
C	1.28437400	1.53262400	0.43481300
C	2.33784500	2.54768400	0.45524300
C	2.03271700	3.89511200	0.19896500
C	3.03860900	4.85857600	0.22777000
C	4.35672800	4.49492400	0.51043600
C	4.66666500	3.15571100	0.76582800
C	3.66801600	2.18782800	0.73887500
H	1.00995000	4.17893900	-0.02353400
H	2.79094500	5.89670800	0.02526400
H	5.13919100	5.24810600	0.52823800
H	5.69024800	2.86365100	0.98183600
H	3.92229600	1.14868300	0.92746400
Cu	1.82032400	-0.00052300	-1.30197600
Br	2.51120100	-0.54451100	-3.37283600
N	0.61518000	-2.33299000	1.64964500
H	0.44800300	-3.33357100	1.69536000
H	0.81640700	-1.99815800	2.59192500
H	2.06665400	-0.41949800	1.14030600

B3LYP/6-31G* (Lanl2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.288598 a.u.

Sum of electronic and thermal Free Energies = -4505.325262 a.u.

M06-2x/6-311++G** (Lanl2DZ for Cu)

Energy = -4508.3190328 a.u.

No imaginary frequency

in6

O	-0.06332700	1.94985400	0.28701900
C	-0.91121000	0.87396700	0.37127400
C	-2.27888800	1.23342700	0.08300000
C	-3.26776200	0.42659000	-0.35958700
C	-4.64459600	0.82826700	-0.64974200
C	-5.19873400	2.05355100	-0.22804900
C	-6.51137400	2.38970900	-0.54476600
C	-7.30974900	1.51048500	-1.28376900
C	-6.78126000	0.28736300	-1.70051200
C	-5.46675900	-0.04891600	-1.38347500
C	-0.16014000	-0.24917700	0.71516500
C	-0.61068200	-1.65120200	1.04692500
S	-1.94043500	-1.60628600	2.34548200
C	-2.63606900	-3.24222700	1.90692200
C	-2.80150400	-3.27645200	0.38960700
S	-1.26436700	-2.64534400	-0.40711800
H	-2.46414400	2.29982700	0.19308600
H	-3.02877100	-0.61005500	-0.57206800
H	-4.60280200	2.73944600	0.36692600
H	-6.91842100	3.33918400	-0.20726400
H	-8.33513000	1.77550500	-1.52603100
H	-7.39228700	-0.40480800	-2.27367700
H	-5.05716000	-0.99859500	-1.72100300
H	-3.60167000	-3.33153400	2.41482300
H	-1.99070300	-4.05492000	2.25833000
H	-3.65142300	-2.65806900	0.08809000
H	-2.96027500	-4.29753400	0.02814200
C	1.19779400	0.19935500	0.80937600
C	1.21251300	1.54177000	0.53685200
C	2.27254500	2.53894100	0.47597700
C	1.96744700	3.90919500	0.39175400
C	2.98826200	4.85566800	0.34077500
C	4.32567700	4.45445500	0.37315400
C	4.63692100	3.09403800	0.45183600
C	3.62239600	2.14232700	0.50017900
H	0.92947000	4.22420600	0.36841900
H	2.73744800	5.91099700	0.27605400
H	5.11978400	5.19470500	0.33203900
H	5.67412200	2.77116600	0.46611300
H	3.87783100	1.08713400	0.53647100
Cu	2.05541800	-2.86224800	0.27737800
Br	3.84012600	-3.34891200	-0.98547500

N	0.57007600	-2.42985500	1.54650200
H	0.23078900	-3.33904000	1.86231400
H	0.93478600	-1.96119000	2.38052900
H	2.06676700	-0.39580500	1.04699600

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.291225 a.u.

Sum of electronic and thermal Free Energies = -4505.341878 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4508.3372395 a.u.

No imaginary frequency

ts4

O	-0.15551300	2.40127000	0.36191400
C	0.70740300	1.37077100	0.51837500
C	2.07804600	1.71893900	0.30359100
C	3.03271400	0.85412100	-0.12980800
C	4.41446800	1.18401500	-0.44494500
C	5.03803200	2.38272100	-0.03945400
C	6.36468200	2.63629400	-0.36892500
C	7.09818900	1.70272400	-1.11059100
C	6.49613500	0.50970900	-1.51767400
C	5.16878000	0.25011000	-1.18615300
C	-0.04749900	0.17521400	0.68043300
C	0.38502100	-1.12917700	1.03280200
S	2.09662300	-2.64379000	-1.07803700
C	3.08732400	-3.02676300	0.41958300
C	2.36252600	-2.99368100	1.76644500
S	1.66107000	-1.33384400	2.19541100
H	2.28209200	2.78353400	0.38847300
H	2.74304800	-0.17630400	-0.33047200
H	4.48703900	3.10628900	0.55445000
H	6.83360500	3.56096400	-0.04403000
H	8.13435100	1.90589600	-1.36656600
H	7.06020500	-0.21686100	-2.09561700
H	4.68980300	-0.66926900	-1.51555200
H	3.93629600	-2.33063500	0.45354000
H	3.51116800	-4.03528300	0.32726300
H	3.05745400	-3.18485300	2.59292900
H	1.57632200	-3.75273500	1.82631800
C	-1.42823200	0.57231200	0.53263600
C	-1.45480600	1.92066900	0.36422400
C	-2.53540600	2.88200700	0.20700000
C	-2.30269100	4.26277100	0.32828400
C	-3.35415100	5.16479300	0.18081800
C	-4.64485700	4.70371700	-0.08779400

C	-4.88019300	3.33141900	-0.21550700
C	-3.83630900	2.42210400	-0.07390500
H	-1.30071400	4.62199100	0.53932900
H	-3.16461500	6.23028300	0.27704300
H	-5.46264000	5.40961300	-0.20297600
H	-5.87914100	2.96651900	-0.43602400
H	-4.02536000	1.35932000	-0.20271700
N	-0.32393500	-2.26317600	0.57841800
H	-0.29055600	-3.00218700	1.28308500
H	0.37605900	-2.62892000	-0.23385500
H	-2.29614000	-0.06231800	0.63828600
Cu	-2.15937400	-2.23027000	-0.18384500
Br	-4.30722600	-2.06576400	-0.82572100

B3LYP/6-31G* (Lanl2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.286425 a.u.

Sum of electronic and thermal Free Energies = -4505.294535 a.u.

M06-2x/6-311++G** (Lanl2DZ for Cu)

Energy = -4508.2711857 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 528.80i

in7

O	0.75113100	1.71804600	0.20080200
C	-0.31774100	0.87554800	0.18814500
C	-1.52877700	1.42316000	-0.36037800
C	-2.77499300	1.06635800	0.03027500
C	-4.03835400	1.56413200	-0.50996100
C	-4.12545000	2.30305300	-1.70725000
C	-5.35335200	2.76637000	-2.16813300
C	-6.52466900	2.49743200	-1.45150400
C	-6.45757400	1.75630700	-0.27011400
C	-5.22844100	1.29195300	0.19393800
C	0.04363100	-0.31187000	0.82676900
C	-0.70324700	-1.55285600	0.96428700
S	-4.06882200	-2.32751200	2.65429800
C	-3.65458100	-3.34706200	1.17706700
C	-3.28751400	-2.57712100	-0.09841800
S	-1.52601700	-2.16837100	-0.51427300
H	-1.38173600	2.21795200	-1.08789300
H	-2.87289700	0.36721500	0.85880300
H	-3.22859500	2.50099700	-2.28694700
H	-5.40110000	3.33322600	-3.09392100
H	-7.48198300	2.85861600	-1.81677500
H	-7.36238200	1.53994300	0.29108900
H	-5.17893800	0.71669600	1.11556200

H	-4.59207300	-3.87762200	0.97895800
H	-2.91924000	-4.11732700	1.42800100
H	-3.86532600	-1.65171800	-0.15542800
H	-3.55333900	-3.18694100	-0.97021600
C	1.39502200	-0.12857300	1.27735700
C	1.79368800	1.11169100	0.86391700
C	3.04324200	1.85241100	0.97198700
C	3.26174900	3.01536900	0.21286400
C	4.46565000	3.70819800	0.31991100
C	5.46677100	3.25419900	1.18135600
C	5.25405800	2.10168600	1.94319800
C	4.05261800	1.40617300	1.84448900
H	2.48672800	3.36847100	-0.45925600
H	4.62228500	4.60510000	-0.27308400
H	6.40421400	3.79703300	1.26356100
H	6.02262100	1.74822600	2.62467000
H	3.88697200	0.52667100	2.45986100
Cu	0.20397200	-1.84821100	3.74840400
Br	1.10050000	-1.39392100	5.74698800
N	-0.59237100	-2.27215100	2.04202600
H	-0.99226700	-3.20260300	1.93516900
H	-2.81402800	-1.97851400	3.01063600
H	2.00022400	-0.86655000	1.78265000

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.283499 a.u.

Sum of electronic and thermal Free Energies = -4505.343677 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4508.3159753 a.u.

No imaginary frequency

ts5

O	2.80725600	-1.28240900	0.42595200
C	1.51526100	-0.88466000	0.35869400
C	0.57968300	-1.66381400	1.10233600
C	-0.77116500	-1.64263100	0.93776700
C	-1.74872500	-2.42870700	1.67261400
C	-1.43991200	-3.11981800	2.86409000
C	-2.41237900	-3.86411600	3.51997500
C	-3.71202300	-3.93586700	3.00289300
C	-4.03354400	-3.25422600	1.82738000
C	-3.06471600	-2.50174600	1.16792600
C	1.45655700	0.24433600	-0.48987900
C	0.35067200	1.03716800	-0.74085800
S	-2.01427900	5.24884800	2.03798300
C	-0.33570500	4.70109300	2.55667100

C	0.14969300	3.40257900	1.90665600
S	0.49925200	3.57286300	0.10769500
H	1.03925000	-2.35646700	1.80211400
H	-1.19089900	-1.01376600	0.15664000
H	-0.44149300	-3.05529300	3.28703800
H	-2.16365200	-4.38559700	4.43999800
H	-4.46961400	-4.51831900	3.51988200
H	-5.03940400	-3.30634700	1.42134300
H	-3.31765500	-1.98584200	0.24395700
H	-0.42086800	4.55640800	3.64001000
H	0.37989500	5.50909600	2.38074200
H	-0.57986300	2.60382200	2.07844600
H	1.09354600	3.10910300	2.38379200
C	2.80314600	0.48889300	-0.94278300
C	3.59179100	-0.45771400	-0.36471900
C	5.01835600	-0.74962100	-0.41074900
C	5.55359800	-1.84181200	0.29400900
C	6.91981300	-2.11025100	0.24061100
C	7.76984300	-1.29840000	-0.51267000
C	7.24432500	-0.21046100	-1.21607900
C	5.88133000	0.06398500	-1.16740000
H	4.89694200	-2.47645100	0.87910400
H	7.32038600	-2.95793000	0.78932400
H	8.83436400	-1.51059600	-0.55266500
H	7.89871300	0.42657400	-1.80416100
H	5.48511100	0.91305800	-1.71664300
N	-0.76487200	1.39793500	-1.08708400
H	-0.79203400	2.49352500	-0.67857700
H	-1.71050900	5.42484300	0.73321700
H	3.10625500	1.29868200	-1.58837000
Cu	-2.21343200	0.42338900	-1.91693600
Br	-3.89993900	-0.90187700	-2.55976700

B3LYP/6-31G* (Lanl2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.272062 a.u.

Sum of electronic and thermal Free Energies = -4505.277903 a.u.

M06-2x/6-311++G** (Lanl2DZ for Cu)

Energy = -4508.2224371 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 1330.60i

in8

O	2.78943600	-1.59598600	0.24975700
C	1.46086700	-1.36663600	0.08673700
C	0.58055000	-2.12741600	0.92431800
C	-0.77337200	-2.05078300	0.91614700

C	-1.70124900	-2.80515900	1.75092300
C	-1.29047400	-3.74519500	2.71892800
C	-2.22736800	-4.43156200	3.48272200
C	-3.59570000	-4.19865200	3.30129100
C	-4.02003700	-3.27150800	2.34788500
C	-3.08255300	-2.58289900	1.58189900
C	1.31594700	-0.39736800	-0.90909800
C	0.10700100	0.13174600	-1.38935400
H	1.09604200	-2.80413300	1.59998200
H	-1.25076900	-1.36150900	0.22315500
H	-0.23364900	-3.94006400	2.87580500
H	-1.89291700	-5.15201000	4.22403100
H	-4.32367600	-4.73771000	3.90095800
H	-5.07958500	-3.08384400	2.20003200
H	-3.41724400	-1.86145500	0.84029500
C	2.63473900	-0.04358900	-1.34944700
C	3.50671100	-0.79893900	-0.61603000
C	4.95878200	-0.91110100	-0.58261600
C	5.59342600	-1.80118300	0.30139500
C	6.98305900	-1.89928100	0.32275200
C	7.76004100	-1.11547200	-0.53262600
C	7.13617000	-0.22806700	-1.41423000
C	5.74894000	-0.12471700	-1.44103500
H	4.99388800	-2.41207000	0.96757400
H	7.45994300	-2.59148000	1.01098500
H	8.84320500	-1.19439200	-0.51351100
H	7.73246800	0.38573900	-2.08335200
H	5.27652000	0.56886600	-2.13060700
N	-0.89481500	0.57274500	-1.78793300
H	2.87394100	0.68063600	-2.11348500
Cu	-2.56429000	1.20812100	-2.40122500
Br	-4.53335900	1.96348000	-3.11632100

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.209778 a.u.

Sum of electronic and thermal Free Energies = -3629.230270 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -3632.1350898 a.u.

No imaginary frequency

P

O	1.17558900	-0.33004200	-0.00005600
C	0.07077400	0.46966500	0.00003200
C	-1.19428600	-0.20919700	0.00008400
C	-2.40917200	0.38918700	-0.00014700
C	-3.70990200	-0.27565300	-0.00007000

C	-3.87102900	-1.67616100	0.00014300
C	-5.13866900	-2.24723000	0.00021700
C	-6.27996500	-1.43811200	0.00008100
C	-6.13965100	-0.04969600	-0.00013700
C	-4.86998700	0.52312100	-0.00021500
C	0.49578000	1.79454300	0.00005500
C	-0.32834100	2.94730100	0.00013400
H	-1.10789000	-1.29268400	0.00033000
H	-2.45210500	1.47606700	-0.00041400
H	-2.99912400	-2.32373800	0.00024500
H	-5.24013200	-3.32923100	0.00038000
H	-7.26854900	-1.88882700	0.00014000
H	-7.01900300	0.58857400	-0.00024700
H	-4.76498400	1.60535700	-0.00038300
C	1.92599700	1.77287000	-0.00002600
C	2.30264600	0.45640800	-0.00008800
C	3.59180500	-0.22107200	-0.00004500
C	3.66873800	-1.62505300	-0.00015700
C	4.90693300	-2.26295000	-0.00012400
C	6.08689000	-1.51685900	0.00001400
C	6.01938300	-0.12096700	0.00012400
C	4.78605100	0.52276500	0.00010100
H	2.75471500	-2.20905700	-0.00027700
H	4.94909800	-3.34875600	-0.00021000
H	7.05110800	-2.01728200	0.00003900
H	6.93171000	0.46914200	0.00023200
H	4.74768600	1.60832600	0.00020400
N	-1.00601500	3.89514100	0.00008300
H	2.57088400	2.63900100	-0.00001200

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.216870 a.u.

Sum of electronic and thermal Free Energies = -861.582536 a.u.

M06-2x/6-311++G**

Energy = -861.6690026 a.u.

No imaginary frequency

NH₃-assisted reaction

in5-NH₃

O	0.37895700	2.09846600	-0.07649600
C	1.11722200	0.95433800	-0.02041000
C	2.53178600	1.23060500	-0.03273900
C	3.57527500	0.39971000	-0.26071000
C	4.99066500	0.76919200	-0.21568200
C	5.46220000	1.97342700	0.34631900

C	6.82033800	2.27624500	0.35399400
C	7.75025400	1.38386300	-0.18956300
C	7.30407000	0.18088000	-0.73995600
C	5.94386100	-0.12117000	-0.74922900
C	0.22501300	-0.11783600	0.08879900
C	0.59041900	-1.56978600	0.27223300
S	1.41906600	-2.33729800	-1.19748600
C	2.23453200	-3.67650000	-0.24608300
C	2.86602100	-3.05855400	1.00200700
S	1.68476900	-1.87460100	1.77077700
H	2.73462300	2.28472700	0.14614600
H	3.37456300	-0.62570900	-0.55031700
H	4.76034400	2.66917900	0.79643000
H	7.15838700	3.21032400	0.79516700
H	8.81016300	1.62235600	-0.17731800
H	8.01609100	-0.52259200	-1.16386300
H	5.60312100	-1.05589200	-1.18994000
H	2.99568300	-4.11822100	-0.89745500
H	1.51705800	-4.46204900	0.01481300
H	3.78392800	-2.52158200	0.75072800
H	3.10072300	-3.82852800	1.74394700
C	-1.12827100	0.40062600	0.10168000
C	-0.95235900	1.76711400	-0.01425400
C	-1.86803900	2.90818700	-0.06253800
C	-1.39241200	4.21478200	0.16388500
C	-2.25898400	5.30502300	0.13263900
C	-3.61951100	5.12156400	-0.12431000
C	-4.10268900	3.83199000	-0.35975700
C	-3.23790300	2.74085100	-0.33780900
H	-0.33888100	4.36736900	0.37214700
H	-1.86882600	6.30319700	0.31479100
H	-4.29450100	5.97286800	-0.14516000
H	-5.15655600	3.67274700	-0.57216500
H	-3.62782500	1.74928700	-0.55342500
Cu	-2.89599500	-0.39375000	0.26775900
Br	-4.80675300	-1.67028300	0.34823900
N	-0.68334400	-2.35803500	0.51902100
H	-1.34015400	-1.77341200	1.06801400
H	-0.47009700	-3.20295800	1.05408500
H	-1.23931900	-2.63515100	-0.40254300
H	-2.11154400	-2.38067500	-2.39562100
N	-2.23917800	-3.02680900	-1.61726900
H	-3.18051100	-2.85381400	-1.24036700
H	-2.20875600	-3.97235400	-1.99732400

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.325965 a.u.

Sum of electronic and thermal Free Energies = -4561.831030 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4564.8571405 a.u.

No imaginary frequency

ts3-NH₃

O	0.36056600	2.09920000	-0.03854400
C	1.09445700	0.95207200	0.02076000
C	2.51074300	1.22407100	0.01814600
C	3.54269000	0.39904000	-0.27226900
C	4.96238900	0.75123900	-0.22379700
C	5.45545900	1.90142800	0.42585200
C	6.81639400	2.19226300	0.43133600
C	7.72744800	1.34050400	-0.20190900
C	7.25975600	0.18997300	-0.83978200
C	5.89692600	-0.10015900	-0.84661100
C	0.20158100	-0.12058500	0.11125900
C	0.56079700	-1.57601400	0.30209100
S	1.36547800	-2.34170900	-1.19521000
C	2.23154600	-3.66339500	-0.26430000
C	2.89923600	-3.02221000	0.95272500
S	1.72267700	-1.86366300	1.76156400
H	2.72351100	2.26589200	0.25090500
H	3.32565900	-0.60433100	-0.62214700
H	4.76811800	2.56188900	0.94620200
H	7.17156300	3.08413900	0.94114800
H	8.78959500	1.56902100	-0.19102400
H	7.95706600	-0.48181000	-1.33381700
H	5.53887500	-0.99302200	-1.35514200
H	2.97400400	-4.10260300	-0.93867700
H	1.53316500	-4.45327800	0.03261400
H	3.79487300	-2.46940000	0.65853800
H	3.18069000	-3.78203000	1.68904700
C	-1.15157000	0.40212000	0.09525000
C	-0.97213900	1.76913200	-0.00732100
C	-1.88340600	2.91350200	-0.06983500
C	-1.40516600	4.21899800	0.15832700
C	-2.26590700	5.31337900	0.11179600
C	-3.62373600	5.13604900	-0.16274000
C	-4.10970300	3.84774000	-0.39969000
C	-3.25065400	2.75258000	-0.36174800
H	-0.35367900	4.36749300	0.37920600
H	-1.87297900	6.31024500	0.29537200

H	-4.29419000	5.99056300	-0.19593600
H	-5.16145500	3.69274400	-0.62567900
H	-3.64300300	1.76191200	-0.57755100
Cu	-2.92023200	-0.39622000	0.17967200
Br	-4.82988000	-1.69648400	0.07990400
N	-0.68843000	-2.35931400	0.57603700
H	-1.32377500	-1.78013800	1.14345700
H	-0.45182800	-3.19036400	1.12096200
H	-1.36388300	-2.69208900	-0.47549500
H	-1.92862700	-2.36350600	-2.27368600
N	-2.13470100	-2.99592600	-1.49945100
H	-3.11103900	-2.81950800	-1.19843500
H	-2.03608100	-3.95582800	-1.83163800

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.324043 a.u.

Sum of electronic and thermal Free Energies = -4561.831407 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4564.8580988 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 827.63i

in6-NH₃

O	0.61922200	2.10797700	0.02847300
C	1.24775100	0.89814200	-0.04126800
C	2.63816200	1.00370900	0.32916900
C	3.66271500	0.16177400	0.06413100
C	5.05030700	0.33923700	0.49496900
C	5.44232500	1.25079700	1.49677400
C	6.77954300	1.38713700	1.85744700
C	7.76525100	0.61186900	1.23793900
C	7.39522900	-0.30596000	0.25304100
C	6.05650600	-0.44083200	-0.10926300
C	0.30029400	-0.05694400	-0.42207400
C	0.50359100	-1.55349300	-0.52691000
S	1.59398300	-2.02002100	-1.97922800
C	2.12894800	-3.62256900	-1.26907300
C	2.56455600	-3.36945500	0.17553300
S	1.33756200	-2.28464200	1.01111500
H	2.84763700	1.93341000	0.85527000
H	3.47776100	-0.70428600	-0.56204400
H	4.69019900	1.84340100	2.00925400
H	7.05514900	2.09575800	2.63430700
H	8.80749600	0.71811900	1.52605100
H	8.15041300	-0.91705900	-0.23481400
H	5.77747000	-1.15086600	-0.88511000

H	2.96257700	-3.99105600	-1.87585900
H	1.31880500	-4.35844800	-1.31680900
H	3.54538000	-2.88716700	0.20417200
H	2.62018700	-4.30879600	0.73550600
C	-0.96987900	0.61508500	-0.62358600
C	-0.69630600	1.93546000	-0.32268800
C	-1.49560900	3.16145600	-0.32395500
C	-0.86895400	4.42310900	-0.32030900
C	-1.62301200	5.59453000	-0.33289200
C	-3.01850100	5.53927100	-0.35035700
C	-3.65291200	4.29433200	-0.34523100
C	-2.90259100	3.12141900	-0.32376800
H	0.21450300	4.47609200	-0.31558900
H	-1.11618200	6.55633400	-0.33370600
H	-3.60477700	6.45413700	-0.36283600
H	-4.73814800	4.23393800	-0.34638200
H	-3.41172800	2.16163600	-0.28779900
Cu	-2.67733100	0.08330300	-1.36787900
Br	-4.48248800	-0.81267200	-2.53583500
N	-0.80054700	-2.22942300	-0.70779400
H	-1.51761400	-1.68941500	-0.21320200
H	-0.75792600	-3.15093200	-0.27467000
H	-1.28913700	-2.29764700	-2.28331500
N	-1.66651300	-2.25645800	-3.31756100
H	-2.65927300	-1.90608000	-3.27150700
H	-1.61330200	-3.16864700	-3.77506800
H	-1.09819100	-1.58256500	-3.83557300

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.326816 a.u.

Sum of electronic and thermal Free Energies = -4561.831194 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4564.8622557 a.u.

No imaginary frequency

ts4-NH₃

O	-0.21148400	1.99572900	0.05546700
C	-1.00087700	0.86653000	0.08131700
C	-2.38252500	1.20382500	-0.17104400
C	-3.49695600	0.45905700	-0.00071400
C	-4.86425500	0.88196400	-0.31039500
C	-5.17085100	2.01975500	-1.08397500
C	-6.49148000	2.37735400	-1.33777800
C	-7.54464100	1.60679400	-0.83426300
C	-7.26081200	0.46983800	-0.07556300
C	-5.93814900	0.11278700	0.17890700

C	-0.17277000	-0.23069300	0.29718600
C	-0.55815200	-1.69211400	0.43838700
S	-1.66490800	-1.96373100	1.91476900
C	-2.40765900	-3.50627000	1.26001900
C	-2.83750700	-3.25399900	-0.18746400
S	-1.53463600	-2.30444100	-1.07564000
H	-2.48543400	2.22671500	-0.52716600
H	-3.40474600	-0.52463400	0.44332600
H	-4.36864300	2.61772500	-1.50620500
H	-6.70231300	3.25721300	-1.94002500
H	-8.57428700	1.88705500	-1.03861000
H	-8.06989600	-0.13969600	0.31836900
H	-5.72422200	-0.77031300	0.77713000
H	-3.26765300	-3.74835500	1.89288700
H	-1.69684800	-4.33685600	1.32716300
H	-3.77289700	-2.68761200	-0.21632200
H	-2.98917600	-4.20077700	-0.71596800
C	1.20060800	0.25923700	0.39367600
C	1.08427400	1.63448200	0.25310500
C	2.04238200	2.73860400	0.32512300
C	1.59604400	4.07323300	0.27792900
C	2.50212800	5.12806500	0.36150800
C	3.86927000	4.87744900	0.49652300
C	4.32402000	3.55672600	0.54580200
C	3.42299400	2.49943900	0.46070600
H	0.53555100	4.27573300	0.17681800
H	2.13717600	6.15092300	0.32098700
H	4.57439500	5.70177500	0.55757400
H	5.38595000	3.34730800	0.64103100
H	3.79460400	1.47808700	0.48305800
Cu	2.78100600	-0.61900700	-0.45360600
Br	4.50168400	-1.87432900	-1.22218700
N	0.63703500	-2.51704600	0.64817200
H	1.26647300	-2.42472300	-0.15566700
H	0.36136500	-3.49725000	0.66993600
H	1.65268800	-1.89337600	2.21452300
H	1.90732600	-0.32727100	1.59635500
N	2.16915400	-1.05684200	2.55958500
H	3.16958400	-1.25255000	2.61335300
H	1.81362300	-0.73666400	3.46053000

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.321740 a.u.

Sum of electronic and thermal Free Energies = -4561.820721 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4564.8473144 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 892.83i

in7-NH₃

O	0.00281600	1.91413300	0.19053600
C	-0.86072100	0.83962500	0.32143800
C	-2.22747700	1.20909500	0.03947000
C	-3.21167800	0.38861100	-0.38672500
C	-4.59256400	0.77556700	-0.67637500
C	-5.15354300	2.00317600	-0.27159000
C	-6.47076300	2.32316000	-0.58562400
C	-7.26490700	1.42496800	-1.30623400
C	-6.72874200	0.19975400	-1.70669800
C	-5.41001600	-0.12097400	-1.39117600
C	-0.12239600	-0.28550300	0.66044300
C	-0.51975600	-1.69990200	1.03430600
S	-1.93624700	-1.61047200	2.31084200
C	-2.54326400	-3.28452100	1.90631100
C	-2.71551300	-3.34817700	0.39033900
S	-1.19892800	-2.68864400	-0.42141800
H	-2.41197200	2.27644200	0.13951500
H	-2.96265300	-0.64988300	-0.57905000
H	-4.55944900	2.70355500	0.30822200
H	-6.88443000	3.27441400	-0.26145800
H	-8.29377800	1.67749800	-1.54729600
H	-7.33715300	-0.50627500	-2.26542900
H	-4.99357900	-1.07256900	-1.71356700
H	-3.49672900	-3.43315100	2.42303000
H	-1.83565100	-4.04369900	2.25697100
H	-3.58727800	-2.76080700	0.08682200
H	-2.84812800	-4.37925000	0.04533300
C	1.26309500	0.13900400	0.68462000
C	1.27954500	1.50440500	0.40528000
C	2.32517000	2.52585800	0.44484100
C	1.99100700	3.88904700	0.37460900
C	2.98940300	4.85939100	0.42978900
C	4.32930900	4.48753300	0.55557100
C	4.66855500	3.13284500	0.62404500
C	3.67768900	2.15814100	0.56779500
H	0.95072400	4.18010500	0.27778400
H	2.71829100	5.90983400	0.37213400
H	5.10563000	5.24638100	0.59345600
H	5.70924700	2.83417700	0.71089200
H	3.95460500	1.10804300	0.59794400
Cu	1.80432700	-0.09428500	-1.34181600

Br	2.52020200	-0.60851500	-3.41413200
N	0.64847800	-2.39758300	1.49568500
H	0.47673800	-3.39584400	1.55620100
H	0.96598300	-2.04061400	2.40940500
H	2.07339000	-0.44272900	1.10223700
N	1.20577400	-1.25425000	4.28010100
H	0.20646000	-1.20942800	4.47830600
H	1.57734400	-0.31778100	4.43184700
H	1.62229600	-1.85180000	4.99260200

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.319924 a.u.

Sum of electronic and thermal Free Energies = -4561.852925 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4564.878582 a.u.

No imaginary frequency

in8-NH₃

O	-0.29586200	2.24530800	0.14577600
C	-1.03928400	1.08990500	0.10376900
C	-2.43327000	1.35658700	-0.15150000
C	-3.49541200	0.54611700	0.05188300
C	-4.89038800	0.86776700	-0.25367300
C	-5.27364300	1.94060800	-1.08359200
C	-6.61683900	2.20858000	-1.32970000
C	-7.61482600	1.40940900	-0.76235000
C	-7.25385200	0.33436800	0.05196900
C	-5.90883100	0.06658000	0.29885800
C	-0.17672600	0.00761400	0.27446500
C	-0.44938200	-1.47761600	0.24096500
S	-1.48571700	-2.00024900	1.71034900
C	-2.18646300	-3.47720800	0.88246200
C	-2.66059200	-3.05159300	-0.50645800
S	-1.36267300	-2.02269700	-1.30607100
H	-2.59727400	2.36615600	-0.52251800
H	-3.33088300	-0.41513000	0.52670000
H	-4.51288800	2.55546500	-1.55533500
H	-6.88842400	3.03917600	-1.97585000
H	-8.66220700	1.61931300	-0.96080600
H	-8.02024100	-0.29597000	0.49531600
H	-5.63401500	-0.76699200	0.94161500
H	-3.01874800	-3.83356800	1.49817200
H	-1.44164400	-4.27824100	0.82153700
H	-3.58983500	-2.47929900	-0.44112600
H	-2.82943500	-3.92319700	-1.14731700
C	1.13035900	0.56967600	0.43890100

C	1.01445100	1.93127500	0.34576900
C	1.97622700	3.02270200	0.42252300
C	1.54691900	4.35087300	0.59368300
C	2.47602100	5.38569000	0.67647500
C	3.84376600	5.11534400	0.59196500
C	4.27786600	3.79847900	0.41475800
C	3.35538800	2.75966300	0.32680300
H	0.48498500	4.56249300	0.66365500
H	2.12988600	6.40723900	0.80919900
H	4.56600600	5.92451600	0.65555300
H	5.33886600	3.58031100	0.33026800
H	3.70202800	1.74506300	0.15194200
N	0.84334500	-2.21474300	0.24434100
H	0.62905200	-3.21014400	0.18071600
H	1.33014100	-2.07621800	1.15905700
H	2.05167500	0.03075100	0.59391900
Cu	2.17301000	-1.88163100	-1.20041700
Br	3.87107200	-1.56197900	-2.63745700
N	2.22414600	-1.82191200	2.83966900
H	2.15679600	-0.84897700	3.13514400
H	3.21323900	-2.06712000	2.85601200
H	1.76666900	-2.37596100	3.56205800

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.319860 a.u.

Sum of electronic and thermal Free Energies = -4561.878333 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4564.9016613 a.u.

No imaginary frequency

ts5-NH₃

O	-0.28231100	2.27412500	-0.04040000
C	-1.00389500	1.10821200	-0.12218500
C	-2.40249300	1.35616000	-0.36935800
C	-3.44151600	0.58196700	0.01382000
C	-4.85617100	0.85693000	-0.23886100
C	-5.30274100	1.78640600	-1.19948600
C	-6.66160300	2.01882500	-1.38946500
C	-7.61133300	1.32522900	-0.63214800
C	-7.18726600	0.39175300	0.31571000
C	-5.82667600	0.15848200	0.50591600
C	-0.13351400	0.03065100	0.06526900
C	-0.33723500	-1.42910200	-0.06599900
S	-1.54090400	-1.95556300	1.98948600
C	-2.13605400	-3.44508500	1.11553300
C	-2.77936800	-3.01943300	-0.20105900

S	-1.62887200	-2.02677000	-1.24771200
H	-2.58795500	2.31476500	-0.85021100
H	-3.23074300	-0.29732600	0.61441600
H	-4.57998600	2.31397200	-1.81506700
H	-6.98391900	2.73722800	-2.13860800
H	-8.67150300	1.50627100	-0.78656300
H	-7.91665400	-0.15533200	0.90723500
H	-5.50025000	-0.56270800	1.25176000
H	-2.88349300	-3.95345000	1.73487000
H	-1.31647200	-4.15150200	0.93404700
H	-3.68031400	-2.43037500	-0.00859900
H	-3.05652800	-3.88939000	-0.80719800
C	1.15135000	0.61971200	0.32533300
C	1.02205400	1.97620300	0.23327200
C	1.96757100	3.07771700	0.35858600
C	1.51638800	4.40242700	0.49403800
C	2.42984200	5.44646500	0.62378300
C	3.80228700	5.18710400	0.62189300
C	4.25760800	3.87296700	0.48040400
C	3.35231900	2.82383000	0.34557400
H	0.45018400	4.60417300	0.50019500
H	2.06782200	6.46578400	0.72867000
H	4.51257000	6.00320800	0.72249500
H	5.32351200	3.66344600	0.46171400
H	3.72085700	1.81153400	0.20055500
N	0.78946600	-2.20257000	-0.08569400
H	0.54280300	-3.13166800	-0.42104800
H	1.41703100	-2.37372800	1.47027500
H	2.07779000	0.10219200	0.52732900
Cu	2.61619100	-1.78163800	-0.64008900
Br	4.82454000	-1.37277900	-0.85100500
N	1.42367500	-2.46432200	2.55697500
H	1.91804200	-1.67695500	2.98190400
H	1.84078600	-3.34571100	2.86111600
H	0.37358800	-2.41164500	2.75090000

B3LYP/6-31G* (Lanl2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.323225 a.u.

Sum of electronic and thermal Free Energies = -4561.831048 a.u.

M06-2x/6-311++G** (Lanl2DZ for Cu)

Energy = -4564.8554895 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 212.97i

in9-NH₃

O	-0.22792200	2.45852700	-0.02423000
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C	-0.90936400	1.27735700	-0.13696900
C	-2.32707200	1.45461000	0.06445800
C	-3.26377200	0.52163400	0.35003400
C	-4.68830000	0.77648300	0.56800300
C	-5.26380000	2.06410100	0.56496400
C	-6.62683300	2.23581500	0.78061600
C	-7.45335100	1.12880800	1.00407400
C	-6.90083400	-0.15283800	1.01028900
C	-5.53472600	-0.32666100	0.79622600
C	0.02775800	0.26318000	-0.36123800
C	-0.10355300	-1.16726500	-0.63543800
S	-3.04970700	-3.50649500	0.99333900
C	-1.63021600	-4.09434000	-0.01608900
C	-1.52729700	-3.50448800	-1.43179500
S	-1.47181100	-1.67205900	-1.63014700
H	-2.61076000	2.50311400	0.01639900
H	-2.97130700	-0.52137000	0.43087400
H	-4.64230900	2.93880800	0.39764600
H	-7.04936800	3.23707300	0.77616300
H	-8.51778000	1.26796700	1.17229400
H	-7.53337200	-1.01952100	1.18244100
H	-5.10623600	-1.32533700	0.79781200
H	-1.71538500	-5.17948000	-0.14119500
H	-0.72618300	-3.90845000	0.56692700
H	-2.42069700	-3.76168800	-2.01090500
H	-0.67620700	-3.95215000	-1.96111500
C	1.31732700	0.89570600	-0.35216400
C	1.11812600	2.23167100	-0.15287600
C	2.00653100	3.38343500	-0.07287500
C	1.49059800	4.68932800	0.00027600
C	2.35066000	5.78306800	0.07230600
C	3.73432200	5.59503100	0.07179100
C	4.25501200	4.29959400	0.00201100
C	3.40180600	3.20253400	-0.06772300
H	0.41626100	4.83927200	-0.00029900
H	1.93729700	6.78640200	0.12858000
H	4.40255800	6.44966800	0.12892300
H	5.33003900	4.14273800	0.00823600
H	3.81745200	2.19983700	-0.10724000
N	0.83151700	-1.97758300	-0.22412400
H	0.74946600	-2.91621600	-0.60545200
H	-0.12042500	-2.52194200	3.52635300
H	2.25780500	0.39664400	-0.53013800
Cu	1.80844900	-1.84036100	1.43453000
Br	2.57212800	-1.91146800	3.55092600

N	-1.13234100	-2.67186600	3.58113100
H	-1.51228300	-1.83275300	4.01909600
H	-1.26961200	-3.42830000	4.25130400
H	-2.28173300	-3.09625800	2.07056300

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.317367 a.u.

Sum of electronic and thermal Free Energies = -4561.880673 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4564.8805807 a.u.

No imaginary frequency

in10-NH₃

O	-2.54264900	1.49228900	-0.13096100
C	-1.34535200	0.86837900	0.09051600
C	-0.28625800	1.75606400	0.49951400
C	0.89086600	1.40053100	1.06525000
C	1.95676600	2.31301300	1.47679600
C	2.04117300	3.64864700	1.03583800
C	3.06585100	4.47918500	1.47822500
C	4.03361400	3.99780500	2.36624300
C	3.97321400	2.67242000	2.80103600
C	2.94941900	1.83874100	2.35620000
C	-1.52116200	-0.49777800	-0.11574500
C	-0.50865800	-1.56087200	-0.10683800
S	-0.01746300	-1.33371600	3.63448800
C	-1.21899900	-2.70844800	3.43296000
C	-1.96662000	-2.75557200	2.09725500
S	-0.91161100	-3.14737600	0.64205500
H	-0.52123600	2.80613800	0.34462500
H	1.07457700	0.35023900	1.27429700
H	1.31894400	4.02670400	0.31864500
H	3.11946400	5.50324800	1.11895000
H	4.83468800	4.64879500	2.70549000
H	4.72548000	2.28686000	3.48399400
H	2.90393200	0.80694300	2.69715200
H	-1.94780600	-2.66890600	4.25004200
H	-0.62621100	-3.61739700	3.57076300
H	-2.50488700	-1.82491800	1.90163800
H	-2.70845500	-3.56191500	2.13462200
C	-2.89972600	-0.68134200	-0.45726000
C	-3.48418400	0.55750800	-0.47234600
C	-4.82779500	1.03404300	-0.77134400
C	-5.13378200	2.40584500	-0.72080600
C	-6.42219300	2.85162800	-1.00756200
C	-7.42585600	1.94264800	-1.34885700

C	-7.13007200	0.57747500	-1.40227000
C	-5.84540700	0.12533700	-1.11644100
H	-4.35642400	3.11575200	-0.45975200
H	-6.64156000	3.91502900	-0.96623200
H	-8.42911900	2.29358400	-1.57346600
H	-7.90317600	-0.13781000	-1.66939100
H	-5.62796100	-0.93795900	-1.16402300
N	0.60774200	-1.45300400	-0.73616300
H	1.26803800	-2.25107400	-0.64553400
H	-0.92150900	-0.33027000	3.65554200
H	-3.36555100	-1.62257500	-0.71120700
H	2.65633100	-4.28051300	-1.35113100
Cu	1.24576300	-0.11827300	-1.97334000
Br	2.11982100	1.25279300	-3.52544200
N	2.82941200	-3.36252900	-0.94486500
H	3.44186700	-3.50440200	-0.14337100
H	3.36461000	-2.83393100	-1.63335500

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.313123 a.u.

Sum of electronic and thermal Free Energies = -4561.887252 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4564.8905953 a.u.

No imaginary frequency

ts6-NH₃

O	-2.58938800	1.51514300	-0.09027900
C	-1.34265300	0.95724400	-0.00155300
C	-0.35541600	1.84568300	0.55336200
C	0.98614800	1.66894000	0.60637500
C	1.95245500	2.59805200	1.19230600
C	1.58674700	3.62580600	2.08497900
C	2.54429600	4.49105600	2.60482900
C	3.89018600	4.34885200	2.25053000
C	4.26940100	3.33044900	1.37381400
C	3.31352400	2.46000100	0.85319000
C	-1.42828200	-0.36433100	-0.44762300
C	-0.35365400	-1.33657100	-0.52242900
S	0.44146600	-2.89761600	3.41688100
C	-1.31145700	-3.38486200	3.09165700
C	-1.98815100	-2.77057700	1.86367500
S	-1.34243900	-3.28020900	0.21787000
H	-0.78943400	2.76828000	0.93255200
H	1.41422200	0.77961600	0.15454000
H	0.54924800	3.73475800	2.38863300
H	2.24329400	5.27472700	3.29521300

H	4.63600600	5.02498700	2.65977100
H	5.31153700	3.21182200	1.09040100
H	3.61775000	1.68122700	0.15712000
H	-1.89101900	-3.13690300	3.98744800
H	-1.27990500	-4.47590000	3.01347400
H	-1.95870800	-1.67629700	1.92225600
H	-3.04592000	-3.05678600	1.90260000
C	-2.79279200	-0.58148200	-0.81911800
C	-3.46455700	0.58931000	-0.59894800
C	-4.84710000	1.00674900	-0.78958000
C	-5.25297600	2.32008300	-0.49184100
C	-6.57830300	2.70791300	-0.67752600
C	-7.52053900	1.79828700	-1.16197300
C	-7.12542300	0.49109600	-1.46109700
C	-5.80350200	0.09691100	-1.27755300
H	-4.52410500	3.03131000	-0.11825100
H	-6.87511700	3.72683400	-0.44386700
H	-8.55292900	2.10403800	-1.30661100
H	-7.85030600	-0.22439700	-1.83972300
H	-5.50894300	-0.92154600	-1.51394500
N	0.81197300	-1.41900800	-0.82863500
H	1.66226500	-2.87902300	-0.17109000
H	0.26665600	-1.56039600	3.34630600
H	-3.19301500	-1.50643400	-1.20377400
H	0.61147400	-3.98098000	0.42273800
Cu	2.43590200	-0.81131500	-1.58069900
Br	4.51007900	-0.23923000	-2.21363300
N	1.66419600	-3.79671100	0.35519500
H	2.00881000	-3.65228500	1.30917600
H	2.18396800	-4.52304600	-0.14010000

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.316201 a.u.

Sum of electronic and thermal Free Energies = -4561.845209 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4564.8491324 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 131.22i

HOAc-assisted reaction

in5-HOAc

O	-0.10846300	1.23518200	-1.15578300
C	0.96342300	0.64003600	-0.55455800
C	2.22302000	1.07234800	-1.11788300
C	3.40851900	1.17146100	-0.47825800

C	4.67432500	1.61758000	-1.06171600
C	4.89020200	1.72186900	-2.45057600
C	6.11066800	2.16382600	-2.95242000
C	7.15260700	2.50560400	-2.08412100
C	6.96089100	2.39754000	-0.70542700
C	5.73831500	1.95620300	-0.20319700
C	0.48157300	-0.19593100	0.44938500
C	1.29213200	-1.13182400	1.31432700
S	2.50769400	-2.12631100	0.34817300
C	3.60700900	-2.47146600	1.77318100
C	3.81390000	-1.16447800	2.53514300
S	2.19399400	-0.30831000	2.74058400
H	2.13788000	1.41333100	-2.14799900
H	3.43907000	0.94510700	0.58352700
H	4.10175500	1.43729600	-3.14119400
H	6.25473100	2.23425800	-4.02736900
H	8.10516000	2.84648700	-2.48014400
H	7.76325400	2.65865400	-0.02044200
H	5.59167000	1.88663400	0.87270400
H	4.55108900	-2.84536300	1.36395000
H	3.18930300	-3.25175600	2.41969300
H	4.49867400	-0.51024700	1.98945600
H	4.22032100	-1.34726800	3.53492400
C	-0.96520200	-0.05863400	0.50789200
C	-1.25067400	0.83262600	-0.50912900
C	-2.49270700	1.41722200	-1.01702000
C	-2.46288800	2.39476700	-2.02997600
C	-3.64362100	2.95604900	-2.51150000
C	-4.87882700	2.55687100	-1.99701300
C	-4.92127200	1.58490300	-0.99377200
C	-3.74448500	1.02044600	-0.51058300
H	-1.50786700	2.71463900	-2.43207800
H	-3.59685200	3.71150000	-3.29157500
H	-5.79827300	2.99748100	-2.37259200
H	-5.87518100	1.26240200	-0.58516500
H	-3.79588000	0.25853400	0.26257200
Cu	-2.11106800	-0.54967900	2.00182200
Br	-2.70004900	-1.52997000	3.97951100
N	0.34798500	-2.14211700	1.96114500
H	-0.35927400	-1.69472400	2.58366400
H	0.88295700	-2.79876700	2.53443600
H	-0.18782300	-2.69095300	1.23274600
C	-2.64852500	-4.67883300	-1.28656600
C	-1.93853000	-3.56315700	-0.56556500
O	-0.98951900	-3.75519600	0.19232300

O	-2.45293900	-2.37148800	-0.83201600
H	-2.73999100	-4.44337600	-2.35099900
H	-2.10741300	-5.61486800	-1.14684100
H	-3.66306900	-4.77732100	-0.88451900
H	-1.98115400	-1.65638200	-0.31860800

B3LYP/6-31G* (Lanl2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.346585 a.u.

Sum of electronic and thermal Free Energies = -4734.339426 a.u.

M06-2x/6-311++G** (Lanl2DZ for Cu)

Energy = -4737.3762176 a.u.

No imaginary frequency

ts3-HOAc

O	-0.57093800	2.14318800	0.05926900
C	-1.29337300	0.97229000	0.06874300
C	-2.71355400	1.23687600	0.02423400
C	-3.72021300	0.41543900	-0.34406100
C	-5.14331900	0.75857600	-0.36408300
C	-5.67757100	1.88384800	0.29511400
C	-7.03819600	2.16891600	0.23215400
C	-7.90466100	1.33628300	-0.48358300
C	-7.39511900	0.21065900	-1.13344500
C	-6.03279500	-0.07482400	-1.06956500
C	-0.39299400	-0.08308700	0.14595200
C	-0.71107600	-1.55909400	0.23137100
S	-1.77759600	-1.93925100	1.68640200
C	-2.42299300	-3.51248000	1.00484100
C	-2.83154700	-3.26699700	-0.44687100
S	-1.52947400	-2.28029900	-1.30200100
H	-2.94334100	2.26719800	0.28742300
H	-3.47478200	-0.57550200	-0.70682300
H	-5.02554600	2.52872000	0.87693500
H	-7.42807600	3.04059700	0.75105400
H	-8.96675900	1.56066600	-0.52746800
H	-8.05850100	-0.44510000	-1.69105300
H	-5.64116700	-0.94776200	-1.58747800
H	-3.28550500	-3.79719000	1.61595000
H	-1.67860700	-4.31272700	1.08427600
H	-3.78069900	-2.72562600	-0.48740600
H	-2.94067300	-4.20927400	-0.99308900
C	0.95676800	0.47618000	0.17390000
C	0.75446600	1.84928300	0.10950000
C	1.66135800	2.99719200	0.10316400
C	1.16261600	4.29553900	-0.11098000
C	2.02401100	5.39030000	-0.12740900

C	3.39454400	5.21223900	0.07142000
C	3.89758100	3.92692700	0.29248200
C	3.04382700	2.82778900	0.30897300
H	0.09942600	4.43966200	-0.26943000
H	1.62227500	6.38531500	-0.29884400
H	4.06539800	6.06676400	0.05556200
H	4.96134900	3.77827000	0.45616200
H	3.44541700	1.84041000	0.50889400
Cu	2.27027300	-0.31860200	-1.11795000
Br	3.05861100	-2.10695200	-2.29489000
N	0.57688200	-2.33959900	0.39876200
H	1.20742400	-2.22926500	-0.42313200
H	0.35667600	-3.33657000	0.45141700
H	1.13810900	-2.08318200	1.31751800
C	3.74930100	-1.08284800	3.86002500
C	2.75393700	-1.04497000	2.71921800
O	1.93740600	-1.98563800	2.57989300
O	2.83225600	-0.01498000	1.95064800
H	3.67690200	-0.16136900	4.44624300
H	3.56974600	-1.95019600	4.49701900
H	4.76500900	-1.12910400	3.45204600
H	1.96741600	0.09427200	1.07051300

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.341050 a.u.

Sum of electronic and thermal Free Energies = -4734.333926 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4737.3658895 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 1155.85i

in6-HOAc

O	-0.45811400	2.31070800	-0.09010600
C	-1.23239400	1.16898900	-0.03141000
C	-2.62505100	1.43329100	-0.30481200
C	-3.67377800	0.71232100	0.14633400
C	-5.08604000	0.97200300	-0.13544700
C	-5.52133600	1.82154500	-1.17181200
C	-6.87784700	2.04391000	-1.38755700
C	-7.83462000	1.41928700	-0.58048800
C	-7.42137500	0.56481600	0.44327900
C	-6.06291000	0.34179500	0.65930100
C	-0.41376300	0.08721100	0.25466100
C	-0.70330100	-1.39483100	0.33934700
S	-1.53148500	-1.81581700	1.95101000
C	-2.38240500	-3.30749100	1.31302700

C	-3.04326800	-2.93926200	-0.01436600
S	-1.85395400	-1.99280400	-1.04584200
H	-2.79097900	2.33985400	-0.88254800
H	-3.47434900	-0.11676700	0.81971000
H	-4.79279500	2.29272900	-1.82495500
H	-7.19280100	2.69944100	-2.19493600
H	-8.89288000	1.59246500	-0.75499600
H	-8.15677500	0.07210000	1.07355600
H	-5.74487100	-0.31738600	1.46397100
H	-3.12548500	-3.60059700	2.06195600
H	-1.67472700	-4.13446300	1.19397900
H	-3.94172000	-2.33855000	0.15315800
H	-3.32282300	-3.83705600	-0.57555000
C	0.92472000	0.62353900	0.41492300
C	0.83748100	1.99603200	0.19500900
C	1.79337500	3.09427600	0.35119800
C	1.43442000	4.40695400	0.00090200
C	2.35111500	5.44520400	0.14960300
C	3.63090500	5.18889700	0.64654400
C	3.98961600	3.88496400	1.00094600
C	3.08199300	2.83935200	0.85872900
H	0.44109400	4.60585300	-0.38724200
H	2.06500400	6.45633500	-0.12606300
H	4.34469400	6.00018300	0.75861900
H	4.98156000	3.67981200	1.39320600
H	3.36846600	1.83230400	1.14882400
Cu	1.68869700	0.68352400	-1.55637200
Br	2.44929400	-0.07939000	-3.53068300
N	0.57647500	-2.12039300	0.26356600
H	1.05396100	-1.87270100	-0.60894000
H	0.37335500	-3.11672700	0.18651900
H	1.80905500	-2.23669200	1.60773400
C	4.54882300	-2.10710000	3.34713000
C	3.45786400	-1.64707600	2.40925900
O	2.49876900	-2.56092500	2.26131600
O	3.45490100	-0.56115200	1.84771900
H	5.29175600	-1.31806500	3.46722000
H	4.11936600	-2.37061100	4.31924500
H	5.02539200	-3.00838100	2.94699900
H	1.77489900	0.11089000	0.85986700

B3LYP/6-31G* (Lanl2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.343879 a.u.

Sum of electronic and thermal Free Energies = -4734.371802 a.u.

M06-2x/6-311++G** (Lanl2DZ for Cu)

Energy = -4737.4062221 a.u.

No imaginary frequency

in7-HOAc

O	-0.36136300	2.69089900	1.35537100
C	0.71693700	1.84162400	1.38068400
C	1.88653000	2.47626300	1.93726800
C	3.00496600	1.89971300	2.43034900
C	4.16397200	2.60372800	2.98047400
C	4.38758500	3.98436400	2.80550400
C	5.50294000	4.60334300	3.36149500
C	6.43032100	3.86213500	4.10115800
C	6.23112000	2.49145800	4.27605000
C	5.11417800	1.87198100	3.71919900
C	0.32317900	0.62233600	0.82690900
C	1.12843900	-0.61616400	0.51936300
S	2.56757200	-0.14993600	-0.58811900
C	3.56908000	-1.62099300	-0.15973200
C	3.57521500	-1.72055500	1.36480800
S	1.86143100	-1.49687900	2.00966500
H	1.78166600	3.55815000	1.98310700
H	3.05086200	0.81759200	2.47683900
H	3.69197300	4.57341600	2.21501900
H	5.65552200	5.66888800	3.21148000
H	7.30132600	4.34888100	4.53100000
H	6.94502400	1.90439000	4.84765100
H	4.95920400	0.80569500	3.86932600
H	4.57768800	-1.46047600	-0.55316700
H	3.15957000	-2.52535100	-0.62212300
H	4.23028400	-0.95422700	1.78931000
H	3.92245000	-2.70453000	1.69539600
C	-1.05551900	0.77550700	0.47211600
C	-1.43453800	2.04531000	0.81752200
C	-2.68985400	2.77618100	0.71247900
C	-2.74507000	4.15668200	0.97502000
C	-3.95035400	4.84654000	0.86499100
C	-5.11697600	4.17533400	0.49187600
C	-5.07096200	2.80233700	0.23357200
C	-3.87120200	2.10571200	0.34455000
H	-1.84035900	4.68120000	1.26402900
H	-3.97783500	5.91307500	1.07160300
H	-6.05584100	4.71563500	0.40841900
H	-5.97506700	2.26887000	-0.04628700
H	-3.85327900	1.03486800	0.16365300
N	0.25571500	-1.62070000	-0.14084100
H	0.82652000	-2.43498400	-0.36817700

H	-0.09133800	-1.24815200	-1.03913400
H	-1.68960500	0.04372500	-0.00338700
C	-0.75776800	0.18562800	-5.01151800
C	-0.08701300	-0.15204400	-3.70608000
O	-0.65309200	-0.66248700	-2.75219100
O	1.21278000	0.17544800	-3.70277400
H	-0.21866400	-0.28062700	-5.84226100
H	-1.79228000	-0.15713900	-4.99273600
H	-0.72766700	1.26896900	-5.17034900
H	1.59047500	-0.03714500	-2.81831300
Cu	-1.25169600	-2.39216500	0.92109200
Br	-2.99774300	-3.31709100	1.98304100

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.344031 a.u.

Sum of electronic and thermal Free Energies = -4734.383752 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4737.4211992 a.u.

No imaginary frequency

ts4-HOAc

O	-0.37753600	2.68749600	-0.17046800
C	-1.02106400	1.51773200	-0.39833300
C	-2.43199300	1.68622100	-0.60956300
C	-3.38539100	0.76701100	-0.31914400
C	-4.82576100	0.93829200	-0.45134600
C	-5.42715200	2.05226200	-1.07395600
C	-6.81064700	2.15207300	-1.16263300
C	-7.62652800	1.14511400	-0.63262300
C	-7.04739300	0.03396500	-0.01650400
C	-5.66114600	-0.07092800	0.07054800
C	-0.08487300	0.46607400	-0.25352000
C	-0.19553000	-0.93191500	-0.53953100
S	-2.31231500	-2.45284500	1.36071200
C	-1.69807600	-3.70654500	0.17579300
C	-1.59031300	-3.28768800	-1.31615800
S	-1.34321900	-1.49908200	-1.71195500
H	-2.70237900	2.69249000	-0.91964000
H	-3.07218100	-0.19103800	0.08944800
H	-4.80865800	2.83637200	-1.50095000
H	-7.25875500	3.01453200	-1.64824200
H	-8.70749200	1.22809100	-0.70420500
H	-7.67519700	-0.75101400	0.39560700
H	-5.20668700	-0.93352600	0.55164300
H	-2.36738500	-4.57332200	0.19037500
H	-0.73156400	-4.07632700	0.53791600

H	-2.53808300	-3.47419200	-1.83113300
H	-0.82522500	-3.87942900	-1.83140200
C	1.14747700	1.09651700	0.16025000
C	0.93945800	2.43966600	0.17095700
C	1.78355300	3.59301800	0.44978500
C	1.24937800	4.89329100	0.45239300
C	2.06746200	5.98761500	0.72516300
C	3.42410500	5.80312000	0.99882700
C	3.96205400	4.51266000	0.99616600
C	3.15223000	3.41476900	0.72324200
H	0.19534000	5.04043500	0.24269000
H	1.64235700	6.98744800	0.72462900
H	4.05971900	6.65820600	1.21078100
H	5.01748600	4.36044900	1.20270200
H	3.58414100	2.41839500	0.71304600
N	0.77355600	-1.76773000	-0.03962500
H	0.56305900	-2.74658800	-0.22260100
H	0.98775700	-1.62788400	1.09130800
H	2.07597200	0.59475900	0.38702300
C	1.59080200	-2.16161700	4.66424000
C	0.87535500	-2.16469600	3.32842300
O	1.38537400	-1.48616600	2.38877100
O	-0.20164700	-2.84309300	3.26758900
H	2.64559600	-1.91085000	4.53777400
H	1.12606000	-1.40569000	5.30883900
H	1.47833500	-3.13075800	5.15612600
H	-1.09401100	-2.60525400	2.38050900
Cu	2.57920500	-1.57123400	-0.89962000
Br	4.60351200	-1.46504400	-1.85194300

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.333743 a.u.

Sum of electronic and thermal Free Energies = -4734.344966 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4737.3615073 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 1058.56i

in8-HOAc

O	-0.00392000	2.87327600	-0.23394300
C	-0.58825400	1.64092900	-0.28507000
C	-2.01899600	1.64187100	-0.10082200
C	-2.73415400	0.61939800	0.42061800
C	-4.18495000	0.56756800	0.59651700
C	-5.06697400	1.52257000	0.05154000
C	-6.43868700	1.42370900	0.25940100

C	-6.96621200	0.36598600	1.00860500
C	-6.10748200	-0.59400600	1.54670600
C	-4.73166500	-0.49642100	1.34291000
C	0.41550000	0.68633900	-0.43019000
C	0.31078200	-0.76408500	-0.61645700
S	-3.47435200	-3.65007100	-1.19528400
C	-1.67052300	-3.78726300	-0.86840800
C	-0.78384700	-3.08057600	-1.90004500
S	-0.83967800	-1.24374200	-1.87079300
H	-2.50078400	2.57940700	-0.36835800
H	-2.20177100	-0.25997600	0.77511000
H	-4.67794500	2.33875000	-0.55033900
H	-7.10264700	2.16883200	-0.17056500
H	-8.03882400	0.29001700	1.16419700
H	-6.50866000	-1.42170700	2.12531000
H	-4.06203400	-1.24071700	1.76705900
H	-1.45973700	-4.86152800	-0.91383000
H	-1.46982700	-3.44569300	0.14961500
H	-1.11364400	-3.32320500	-2.91457600
H	0.26068500	-3.41079300	-1.82657600
C	1.65860300	1.40145600	-0.43714500
C	1.35872800	2.73085600	-0.32077500
C	2.17429600	3.93676300	-0.28363400
C	1.59677800	5.20657100	-0.45784500
C	2.39250600	6.34969100	-0.42708400
C	3.77046700	6.24465000	-0.22431900
C	4.34982200	4.98536500	-0.04402100
C	3.56159700	3.83833000	-0.06835400
H	0.52700500	5.28991300	-0.61955100
H	1.93453500	7.32552600	-0.56413600
H	4.38842500	7.13792800	-0.20065300
H	5.41867900	4.89553600	0.12783300
H	4.01711200	2.86736700	0.10566300
N	1.11488900	-1.56409800	0.02899900
H	1.00976000	-2.54313800	-0.22985300
H	0.51950500	-1.65722800	2.18308400
H	2.64199200	0.97613900	-0.57612200
C	-1.54719400	-2.40988600	4.52816500
C	-1.04722400	-2.15458700	3.12991000
O	0.25515100	-1.83668900	3.11183900
O	-1.72921600	-2.21583700	2.11899200
H	-0.90761000	-3.14290100	5.02925600
H	-1.49531600	-1.48271000	5.10935000
H	-2.57691500	-2.76621500	4.49335000
H	-3.63981200	-2.40367300	-0.70525200

Cu	2.77363100	-1.12207100	0.94660900
Br	4.76309400	-0.61503100	1.84179300

B3LYP/6-31G* (Lan12DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.336551 a.u.

Sum of electronic and thermal Free Energies = -4734.392418 a.u.

M06-2x/6-311++G** (Lan12DZ for Cu)

Energy = -4737.4086095 a.u.

No imaginary frequency

in9-HOAc

O	-0.22279500	2.96601100	0.07827300
C	-0.95739100	1.81388800	0.12024600
C	-2.37119300	2.01789800	0.30761200
C	-3.25045100	1.10911100	0.79219600
C	-4.68895200	1.29539400	0.97207500
C	-5.38771500	2.43258800	0.51774900
C	-6.75649600	2.55873600	0.72938900
C	-7.46578900	1.55203700	1.39369600
C	-6.79165700	0.41536700	1.84324200
C	-5.42024900	0.28908400	1.63266700
C	-0.08484000	0.73320500	0.02443200
C	-0.34282700	-0.70981700	-0.00150500
S	-0.22015900	-1.70577800	-4.42340400
C	-0.54514300	-0.19858600	-3.42211900
C	-1.75650900	-0.26726800	-2.49002700
S	-1.61396900	-1.42435000	-1.06711200
H	-2.70057900	3.02715700	0.07170100
H	-2.87270700	0.13989400	1.10776300
H	-4.85858100	3.21982400	-0.01132400
H	-7.27604800	3.44354400	0.37170100
H	-8.53530000	1.65376900	1.55497200
H	-7.33319600	-0.37316200	2.35837500
H	-4.89875500	-0.59672200	1.98727000
H	-0.73576600	0.58280100	-4.16637700
H	0.35793300	0.09299500	-2.87981100
H	-2.63439100	-0.63962000	-3.02687900
H	-1.99782500	0.72312900	-2.09601800
C	1.23653700	1.28623400	-0.04522500
C	1.10807400	2.64869900	-0.01451700
C	2.06529800	3.74531000	-0.06552300
C	1.64379700	5.06065100	-0.32825800
C	2.57217800	6.09778800	-0.38274400
C	3.92960600	5.84076500	-0.17720900
C	4.35446800	4.53661200	0.09195600
C	3.43269600	3.49531000	0.15178600

H	0.58990500	5.26246500	-0.48969300
H	2.23404900	7.10999400	-0.58721300
H	4.65121800	6.65181400	-0.21886900
H	5.40624500	4.33054100	0.26876700
H	3.76791900	2.49133100	0.39546600
N	0.35582400	-1.51516900	0.72367400
H	2.15440700	0.72481300	-0.13882700
H	-0.87845900	-3.69651100	-1.72230400
C	0.52206800	-6.48975000	-0.96358200
C	0.04068200	-5.07273600	-0.79981200
O	-0.55702500	-4.60569900	-1.91151800
O	0.16462600	-4.40890300	0.21471200
H	1.02856000	-6.81228100	-0.05393800
H	-0.32785800	-7.14780100	-1.17323600
H	1.20360000	-6.55570900	-1.81791700
H	0.29746300	-2.46654700	-3.43627400
Cu	1.75899500	-1.11767700	1.99073200
Br	3.47748400	-0.66509100	3.35778400
H	0.17609900	-2.51412300	0.55640600

B3LYP/6-31G* (Lanl2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.334885 a.u.

Sum of electronic and thermal Free Energies = -4734.395201 a.u.

M06-2x/6-311++G** (Lanl2DZ for Cu)

Energy = -4737.4093258 a.u.

No imaginary frequency

ts5-HOAc

O	0.85099200	2.88381200	-0.46736900
C	-0.07534700	1.90854000	-0.23460100
C	-1.37905200	2.36438400	0.16076200
C	-2.24468700	1.64966400	0.91873600
C	-3.58213200	2.06883100	1.33742400
C	-4.27517900	3.13796100	0.73417700
C	-5.53607100	3.51397000	1.18613200
C	-6.14238700	2.82805900	2.24376900
C	-5.47611800	1.75824000	2.84447500
C	-4.21257700	1.38137500	2.39371700
C	0.54124400	0.67131100	-0.37240000
C	-0.02290900	-0.66982800	-0.31304800
S	-5.17700300	-1.20165600	-1.98428600
C	-4.13837800	-1.41837700	-0.48145500
C	-2.73612600	-1.96822600	-0.73861700
S	-1.63687200	-0.77075200	-1.61696300
H	-1.61964900	3.38145600	-0.14000300
H	-1.91128200	0.69013600	1.31142600

H	-3.82963600	3.66541300	-0.10429400
H	-6.05453700	4.33939000	0.70603200
H	-7.12915300	3.12174500	2.59023400
H	-5.93921000	1.21770600	3.66530200
H	-3.69207300	0.55545300	2.87347600
H	-4.68485000	-2.14863500	0.12518100
H	-4.11183400	-0.48343800	0.08297400
H	-2.79215500	-2.87192300	-1.35056200
H	-2.23288500	-2.21962400	0.20291300
C	1.91876600	0.93284200	-0.66454000
C	2.06387500	2.29335800	-0.72331900
C	3.19399800	3.17058200	-0.99845000
C	3.01034000	4.55526200	-1.15988100
C	4.09898800	5.38270400	-1.42633000
C	5.38364900	4.84613800	-1.53618000
C	5.57456200	3.47100300	-1.37344100
C	4.49213400	2.63856500	-1.10508800
H	2.01358900	4.97501800	-1.07561800
H	3.94246800	6.45098000	-1.54863900
H	6.23083500	5.49407000	-1.74272600
H	6.57139400	3.04576600	-1.44861100
H	4.65484000	1.57415300	-0.96330400
N	0.34347800	-1.74249300	0.16498900
H	2.67925500	0.18484600	-0.83336500
H	-0.85836100	-1.87861600	-2.36634200
C	0.31000600	-5.24241000	-3.00863100
C	-0.00536300	-3.95549000	-2.29801100
O	-0.29738600	-2.93076000	-2.96383200
O	0.06210700	-4.00798200	-1.00600800
H	-0.19617100	-6.07566500	-2.51330700
H	0.01942800	-5.18058900	-4.05752100
H	1.38789100	-5.42814600	-2.93767700
H	-4.51966000	-0.13099600	-2.47881500
Cu	1.82718400	-2.04694900	1.34726700
Br	3.60418900	-2.44490900	2.65977300
H	0.06135300	-3.06048500	-0.50802900

B3LYP/6-31G* (Lanl2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.328336 a.u.

Sum of electronic and thermal Free Energies = -4734.344297 a.u.

M06-2x/6-311++G** (Lanl2DZ for Cu)

Energy = -4737.3503194 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 851.72i

No metal-catalyst CuBr

ts1'

O	1.27468000	-1.28259100	-0.30337300
C	0.26653900	-0.50107400	-0.23988100
C	-1.03100600	-1.12971700	-0.45259700
C	-2.13006600	-0.88410200	0.29249200
C	-3.42535100	-1.55750700	0.20543000
C	-3.72518500	-2.54108500	-0.75805800
C	-4.97862200	-3.14174500	-0.79380500
C	-5.96422600	-2.77789300	0.13007600
C	-5.68467300	-1.80507100	1.09060300
C	-4.42917200	-1.20230700	1.12590200
C	0.65222400	0.88593500	0.02116100
C	-0.09743600	2.04864900	-0.06624100
S	-1.80165900	2.23630500	-0.47287500
C	-1.90259700	4.01307500	-0.00474000
C	-0.57297100	4.66227300	-0.35271800
S	0.78948800	3.54665500	0.19417100
H	-1.01765800	-1.94055000	-1.17677300
H	-2.06318200	-0.12342500	1.06661500
H	-2.97441300	-2.83494800	-1.48545900
H	-5.19085600	-3.89792000	-1.54469300
H	-6.94175200	-3.25109500	0.09915200
H	-6.44342900	-1.51596400	1.81261000
H	-4.21366800	-0.44507300	1.87596700
H	-2.11419600	4.07989000	1.06650500
H	-2.73678600	4.45030300	-0.56162900
H	-0.44775800	5.61842800	0.16449100
H	-0.48474800	4.82895700	-1.43071600
C	2.08386000	0.96829000	0.22521600
C	2.60726200	-0.21636800	0.06001300
C	3.84021900	-0.96420900	0.07116300
C	3.91569600	-2.34434200	-0.18916100
C	5.14525500	-3.00026400	-0.16059600
C	6.31860000	-2.30100600	0.12616500
C	6.25209600	-0.92851200	0.38613400
C	5.03111100	-0.26392000	0.35996700
H	3.00851800	-2.89369600	-0.41175100
H	5.18427900	-4.06756300	-0.36427500
H	7.27444100	-2.81769400	0.14695600
H	7.15871900	-0.37200400	0.61056600
H	4.97044700	0.80111400	0.55953100

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.253603 a.u.

Sum of electronic and thermal Free Energies = -1681.085909 a.u.

M06-2x/6-311++G**

Energy = -1681.1949005 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 367.92i

in1'

O	-0.62252000	2.21741800	0.01904100
C	-1.34532500	1.11023400	-0.11922900
C	-2.74125900	1.25685300	0.14909300
C	-3.73983600	0.46830900	-0.33020700
C	-5.16446600	0.60612700	-0.05517600
C	-5.68177300	1.46827100	0.93437500
C	-7.05208500	1.56597300	1.14707800
C	-7.94354700	0.80444300	0.38376500
C	-7.44931400	-0.06077000	-0.59418800
C	-6.07719600	-0.15982100	-0.80817300
C	-0.44197600	0.06279000	-0.50792300
C	-0.57612400	-1.32582900	-0.55856300
S	-1.98942700	-2.29995200	-0.23754700
C	-1.06410900	-3.88362400	-0.03600600
C	0.10144900	-3.84947100	-1.00765800
S	0.91030300	-2.17848300	-0.91422100
H	-2.98544400	2.13611900	0.74104800
H	-3.48548000	-0.31883800	-1.03508600
H	-5.00497700	2.05427300	1.54886600
H	-7.42964600	2.23485100	1.91573500
H	-9.01354500	0.88299600	0.55480500
H	-8.13327600	-0.65860500	-1.19042600
H	-5.69654000	-0.83244900	-1.57321800
H	-1.76425200	-4.69845900	-0.24179100
H	-0.72705000	-3.95286400	1.00254700
H	-0.22973800	-4.03063000	-2.03533200
H	0.85969200	-4.59286200	-0.74433700
C	0.90239700	0.58750800	-0.66567000
C	0.74390500	1.89523500	-0.32369300
C	1.66108100	3.02296400	-0.23659700
C	1.25448900	4.31184700	0.15201200
C	2.17714200	5.35532400	0.21582800
C	3.51787000	5.13608300	-0.10457200
C	3.93050900	3.85670300	-0.49185400
C	3.01604700	2.81134400	-0.55785500
H	0.21417400	4.49216800	0.40253500
H	1.84476900	6.34563900	0.51787100
H	4.23433300	5.95182300	-0.05353100
H	4.97249500	3.67465300	-0.74371800

H 3.32085400 1.81297800 -0.85574900

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.255564 a.u.

Sum of electronic and thermal Free Energies = -1681.091864 a.u.

M06-2x/6-311++G**

Energy = -1681.2056948 a.u.

No imaginary frequency

in2'

O	-1.27244100	-1.35718200	-0.11450700
C	-0.15516900	-0.64082800	-0.22270000
C	1.05324900	-1.36864200	0.00696900
C	2.29292900	-1.03974700	-0.44370000
C	3.52867600	-1.77542700	-0.20628300
C	3.62949100	-2.85153000	0.70040000
C	4.83449200	-3.52139400	0.87898000
C	5.97303600	-3.13505300	0.16356900
C	5.89438200	-2.06707700	-0.73213300
C	4.68813300	-1.39560400	-0.91216500
C	-0.54437400	0.70055100	-0.55294700
C	0.15806200	1.91029800	-0.55375000
S	1.83385700	2.19986700	-0.17835000
C	1.62934400	4.01097900	0.12155100
C	0.59700900	4.50843000	-0.87339200
S	-0.82858000	3.31706700	-0.88912100
H	0.90525200	-2.30340600	0.54325100
H	2.39608200	-0.17320900	-1.09106500
H	2.76128400	-3.15666400	1.27679100
H	4.89026600	-4.34695200	1.58343400
H	6.91285900	-3.66066200	0.30785400
H	6.77330300	-1.75705000	-1.29084100
H	4.63097000	-0.56594400	-1.61284800
H	2.60990700	4.47584200	-0.01727300
H	1.28088900	4.13072700	1.15435100
H	1.00503400	4.59015400	-1.88629600
H	0.19868400	5.48170800	-0.57105800
C	-1.98646900	0.78546500	-0.70563400
C	-2.38102600	-0.48577100	-0.41764900
C	-3.68369400	-1.13368800	-0.35220700
C	-3.84775500	-2.48982500	-0.01750900
C	-5.12022600	-3.05797900	0.03030800
C	-6.25051200	-2.28963100	-0.25315000
C	-6.09610500	-0.93990100	-0.58742000
C	-4.83028300	-0.36662600	-0.63710000
H	-2.97500500	-3.09572500	0.20341700

H	-5.22768600	-4.10836200	0.29046000
H	-7.24084100	-2.73593100	-0.21490800
H	-6.96955400	-0.33204800	-0.81113800
H	-4.69373600	0.67907600	-0.89476600
N	-0.30890100	3.70744000	2.85062400
H	-1.04145200	3.31950900	2.25597200
H	-0.75313300	4.44057200	3.40255600
H	-0.06345100	2.96941600	3.50968400

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.285855 a.u.

Sum of electronic and thermal Free Energies = -1737.618238 a.u.

M06-2x/6-311++G**

Energy = -1737.761671 a.u.

No imaginary frequency

ts2'

O	-1.33253900	-1.34614000	0.08503700
C	-0.22925700	-0.56203800	0.12773100
C	1.00692500	-1.29687100	0.19389400
C	2.21852800	-0.90663500	-0.27016000
C	3.46954500	-1.65548700	-0.17440100
C	3.62164900	-2.82062400	0.60544400
C	4.83512800	-3.49898300	0.64865900
C	5.93586800	-3.03234200	-0.07723900
C	5.80769800	-1.87495900	-0.84692000
C	4.59200200	-1.19667200	-0.89203400
C	-0.66068200	0.77124400	0.03205300
C	0.05371200	2.02475000	0.14675500
S	1.66913000	2.20576900	0.84939400
C	1.73765700	4.01202400	0.53637300
C	1.19241900	4.26385700	-0.86505100
S	-0.31573100	3.22733600	-1.12159800
H	0.89156100	-2.29251800	0.61867100
H	2.29107500	0.04097100	-0.79714600
H	2.78571400	-3.19060900	1.19188100
H	4.92686000	-4.39471400	1.25759900
H	6.88281800	-3.56367700	-0.03803800
H	6.65577200	-1.49987000	-1.41403300
H	4.49771700	-0.29786900	-1.49744600
H	2.78197200	4.32467100	0.62847700
H	1.14545600	4.52852400	1.29816700
H	1.93065100	3.99668900	-1.62671500
H	0.91367100	5.31382500	-0.99704900
C	-2.10481900	0.83088300	-0.09129200
C	-2.44543400	-0.49745400	-0.04931700

C	-3.73638700	-1.17255500	-0.09494700
C	-3.86361900	-2.57040200	0.00050600
C	-5.12041200	-3.17210200	-0.04377200
C	-6.27308700	-2.39683600	-0.18349200
C	-6.15596900	-1.00620300	-0.28074200
C	-4.90521300	-0.39977200	-0.23794100
H	-2.97241000	-3.18018100	0.10793200
H	-5.19862700	-4.25419000	0.03114200
H	-7.25139800	-2.86926700	-0.21796800
H	-7.04682200	-0.39244100	-0.39202800
H	-4.79924300	0.67802100	-0.31376200
N	-1.24968800	2.77366500	1.62451300
H	-2.04115100	2.31990600	1.09560600
H	-1.37592400	3.77835800	1.73509600
H	-1.12145300	2.32123500	2.52835400

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.291278 a.u.

Sum of electronic and thermal Free Energies = -1737.587901 a.u.

M06-2x/6-311++G**

Energy = -1054.7162404 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 341.59i

in3'

O	0.55037700	2.07617500	-0.25440500
C	1.18390000	0.85653400	-0.30459800
C	2.60847300	0.97168200	-0.11948100
C	3.46107200	0.00721600	0.29020900
C	4.90733100	0.15225200	0.45894100
C	5.64535100	1.22759600	-0.07488400
C	7.01829200	1.32339000	0.12917500
C	7.69592300	0.34496800	0.86343600
C	6.98375700	-0.73431800	1.38903400
C	5.60881500	-0.82929400	1.18572400
C	0.22376300	-0.12877000	-0.52325800
C	0.33687700	-1.62168100	-0.73447400
S	1.75427600	-2.05731900	-1.95661500
C	2.55437700	-3.39023300	-0.98043200
C	1.56416600	-3.92974200	0.05140800
S	0.73862400	-2.50379800	0.85409800
H	2.97839400	1.98033400	-0.29278900
H	3.05025600	-0.95798600	0.56938400
H	5.14113100	1.98312700	-0.67028800
H	7.56657200	2.16073900	-0.29477200
H	8.76894800	0.42102000	1.01666600

H	7.49944100	-1.50308000	1.95869700
H	5.05764500	-1.66756900	1.60622000
H	3.44691400	-2.99507100	-0.48648800
H	2.86194800	-4.17864400	-1.67566200
H	2.07551600	-4.49334400	0.83897400
H	0.82589900	-4.59197500	-0.41361300
C	-1.03417100	0.54959400	-0.56644700
C	-0.79322000	1.88796400	-0.40424200
C	-1.64894300	3.06520900	-0.36172200
C	-1.10389700	4.34928400	-0.18145500
C	-1.93130200	5.46907100	-0.14209800
C	-3.31400600	5.33308000	-0.28045500
C	-3.86468800	4.06100200	-0.45889400
C	-3.04379200	2.93838100	-0.49939900
H	-0.03035900	4.45995700	-0.07162800
H	-1.49245800	6.45340800	-0.00151600
H	-3.95700200	6.20828800	-0.24872300
H	-4.93968300	3.94264400	-0.56626100
H	-3.48450100	1.95512900	-0.63707400
N	-0.94181000	-2.10736200	-1.22577000
H	-1.99182600	0.06959200	-0.69324600
H	-0.90679000	-3.11894900	-1.32768000
H	-1.10698800	-1.72869900	-2.15949300

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.296220 a.u.

Sum of electronic and thermal Free Energies = -1737.702177 a.u.

M06-2x/6-311++G**

Energy = -1737.8596283 a.u.

No imaginary frequency