Theoretical Investigation on the Cu(I)-Catalyzed *N*-Carboxamidation of Indoles with Isocyanates to form Indole-1-Carboxamides: Effects of Solvents

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Table S1. Exploring the effects of methods BHandHLYP, CAM-B3LYP, B3LYP, PBEPBE, B3P86, B3PW91 and M06 by comparing the rate-determining energy barriers from **im1+2a+DMSO** to **ts1-DMSO** (the geometric structures of **im1**, **2a**, **DMSO** and **ts1-DMSO** are optimized using BHandHLYP (CAM-B3LYP, B3LYP, PBEPBE, B3P86, B3PW91 and M06)/6-31G* in gas phase, and the single point energies are obtained at the M06-2x/6-311++G** calculated level in solution phase).

Species	**The rate-determining energy barriers (kcal/mol)**						
	BHandHLYP	CAM-B3LYP	B3LYP	PBEPBE	B3P86	B3PW91	M06
ts1-DMSO	24.3	24.3	24.1	23.3	23.6	24.0	24.7

Table S1 shows that the effects of DFT functionals BHandHLYP, CAM-B3LYP, B3LYP, PBEPBE, B3P86, B3PW91 and M06 on the rate-determining energy barriers are very small (see Figure 3).

Table S2. Exploring the effects of basis sets 6-31G*, 6-31G**, 6-31+G* and 6-311G* by comparing the rate-determining energy barriers from **im1+2a+DMSO** to **ts1-DMSO** (the geometric structures of **im1**, **2a**, **DMSO** and **ts1-DMSO** are optimized using BHandHLYP/6-31G* (6-31G**, 6-31+G* and 6-311G*) in gas phase, and the single point energies are obtained at the M06-2x/6-311++G** calculated level in solution phase).

Species	**The rate-determining energy barriers (kcal/mol)**			
	6-31G*	6-31G**	6-31+G*	6-311G*
ts1-DMSO	24.3	24.9	25.0	25.1

Table S2 shows that the effects of basis sets 6-31G*, 6-31G**, 6-31+G* and 6-311G* on the rate-determining energy barriers are very small (see Figure 3).

Table S3. Exploring the effects of basis sets LanL2DZ, SDD and QZVP by comparing the rate-determining energy barriers from **im1+2a+DMSO** to **ts1-DMSO** (the geometric structures of **im1, 2a, DMSO** and **ts1-DMSO** are optimized using BHandHLYP/6-31G* (LanL2DZ, SDD or QZVP) for Cu and I) in gas phase, and the single point energies are obtained at the M06-2x/6-311++G** (LanL2DZ, SDD or QZVP) for Cu and I) calculated level in solution phase).

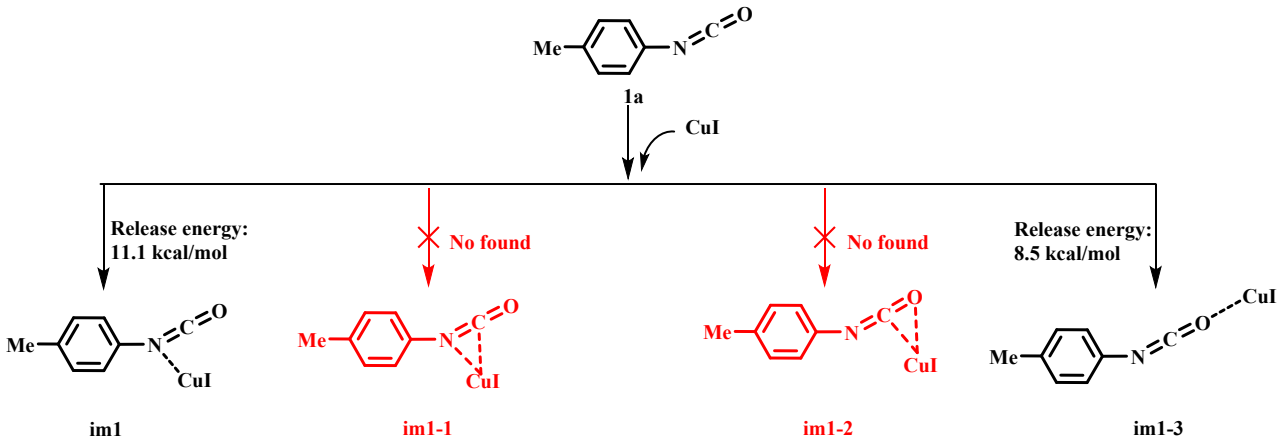
Species	**The rate-determining energy barriers (kcal/mol)**		
	LanL2DZ	SDD	QZVP
ts1-DMSO	24.3	25.2	24.9

Table S3 shows that the effects of basis sets LanL2DZ, SDD and QZVP on the rate-determining energy barriers are quit small (see Figure 3).

Table S4. The effects of solvent DMSO on the rate-determining energy barriers of Cu(I)-catalyzed reaction are explored at PCM//M06-2x/6-311++G**//BHandHLYP/6-31G* level (the rate-determining energy barriers from **im1+2a+DMSO** to **ts1-DMSO**, the geometric structures of **im1**, **2a**, **DMSO** and **ts1-DMSO** are optimized using BHandHLYP/6-31G* (LanL2DZ for Cu and I) in gas phase or in DMSO medium, and the single point energies are obtained at PCM//M06-2x/6-311++G** (LanL2DZ for Cu and I) calculated level in DMSO solution).

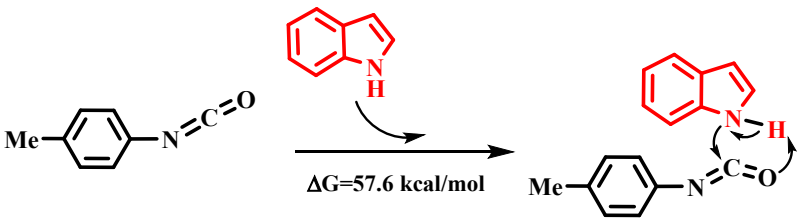
Species	**The rate-determining energy barriers (kcal/mol)**	
	in gas phase	in DMSO medium
ts1	24.3	23.3

Table S4 shows that the effects of solvent on the rate-determining energy barrier of Cu(I)-catalyzed reaction (**ts1**) are rather small (only 1.0 kcal/mol).

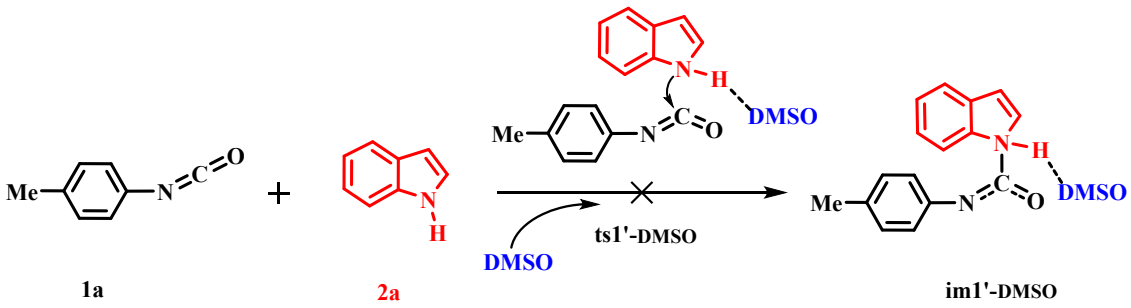


Scheme S1. Four coordination models of CuI with isocyanates (**1a**).

In principle, the four kinds of models for the coordination of CuI with **1a** (CuI/N1, CuI/N1-C1 double bond, CuI/C1-O1 double bond and CuI/O1) are proposed by us to form complexes **im1**, **im1-1**, **im1-2** and **im1-3**, respectively. According to our calculated results, the CuI/N1 coordination mode is one feasible strategy when compared with other three coordination cases.

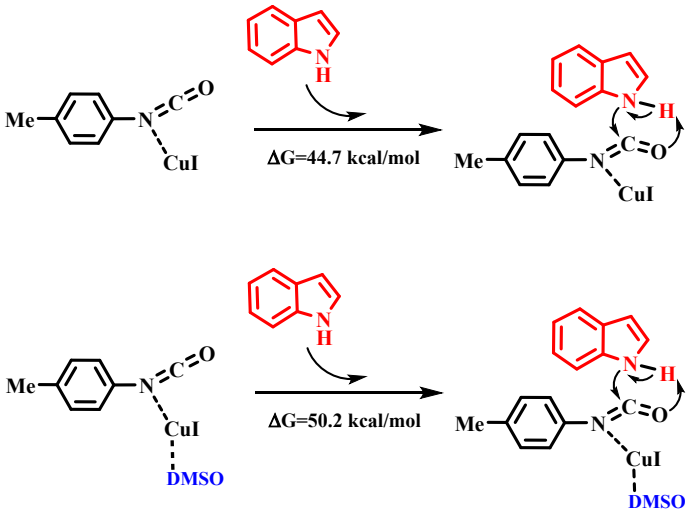


Scheme S2. The activation free energy of intermolecular nucleophilic addition without the metal-catalyst CuI.

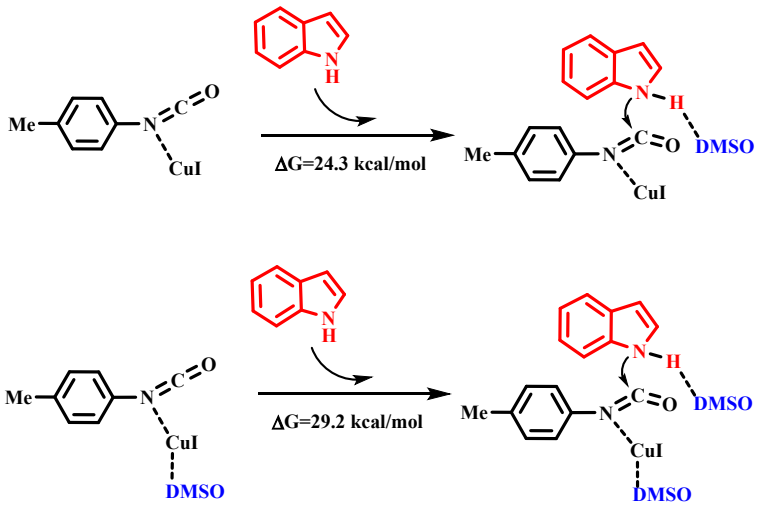


Scheme S3. The intermolecular addition cannot be carried out without the metal-catalyst CuI.

Herein, the mechanism of intermolecular addition without CuI catalyst is studied (see Scheme 3). Starting from substrates **1a** and **2a**, the intermolecular addition of C1 with N2 forms a new intermediate **im1'-DMSO** via a transition state **ts1'-DMSO** with the assistance of solvent DMSO. However, we try our best to find this process, but we failed. Furthermore, this experimental phenomenon can also be explained by the scan profile (see Figure S13 of the Supporting Information). The method using the scan to illustrate the experimental results has been adopted successfully in the previous theoretical calculations (B. Yuan, R. He, W. Shen, W. Hu and M. Li, *RSC Adv.*, 2016, **6**, 20294-20305; B. Yuan, J. Chen, X. Xie, S. He, Y. Luo, X. Guo, H. Huang and R. He, *New J. Chem.*, 2019, **43**, 9265-9273; B. Yuan, X. Guo, G. Wang, H. Huang, F. Zhang, J. Xu and R. He, *New J. Chem.*, 2019, **43**, 4291-4305; B. Yuan, J. Chen, G. Wang, F. Zhang, L. Fang, X. Guo, H. Huang and R. He, *Appl. Organomet. Chem.*, 2019, e5443. https://doi.org/10.1002/aoc.5443.). As shown in Figure S13, the energy curve is sharply rising in energy with the formation of C1-N2 bond from **1a** and **2a** to **im1'-DMSO**, which means that the intramolecular cyclization of C1 with N2 cannot be carried out without the participation of Cu(I) catalyst. Thus, CuI is essential for the process of intermolecular addition.



Scheme S4. The coordinated effect of DMSO with CuI is considered on the intermolecular nucleophilic addition.



Scheme S5. The coordinated effect of DMSO with CuI is considered on the intermolecular nucleophilic addition with DMSO as the co-catalyst.

The coordinated effects of DMSO with CuI on the catalytic reactions have been considered, as shown in Schemes S5. One DMSO molecule as the ligand coordinates with the metal catalyst CuI and another one as the co-catalyst promotes the intermolecular nucleophilic addition by the interactions of hydrogen-bond. However, the coordinated effects of DMSO with CuI do not alter the reaction mechanism of intermolecular addition process. In the present situations, the activation free energy of CuI(DMSO)-catalyzed reaction is 29.2 kcal/mol, which is 4.9 kcal/mol higher than that of CuBr-catalyzed cases without DMSO as the ligand. This means that the coordinated effects of DMSO on the process of intermolecular addition are negative.

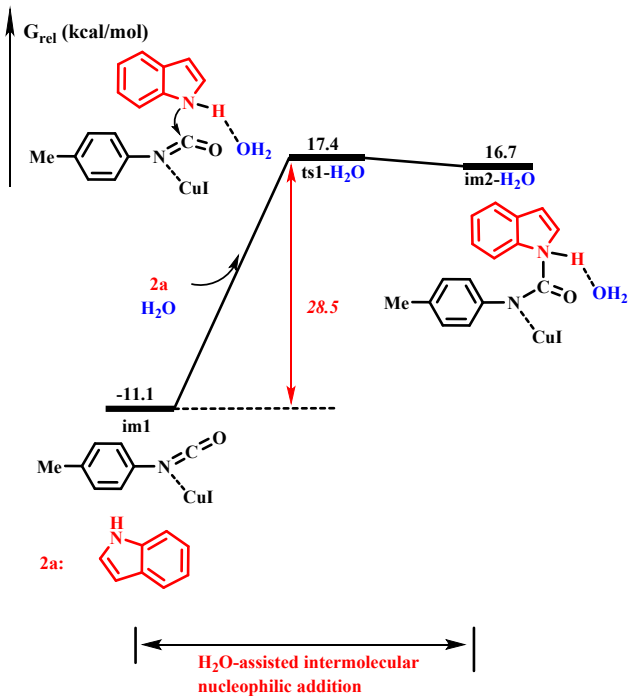


Figure S1. Energy profile of the H_2O-assisted intermolecular nucleophilic addition in DMSO medium.

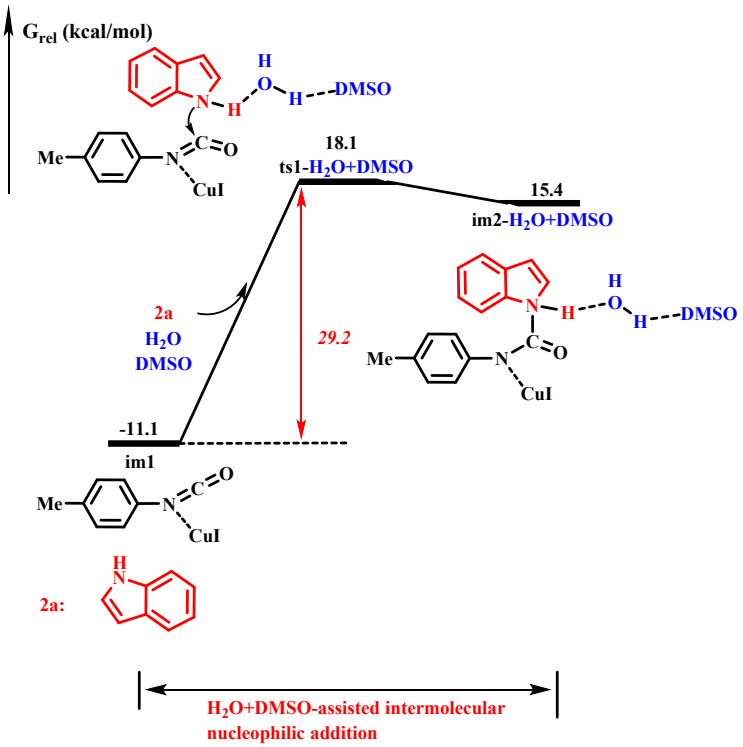


Figure S2. Energy profile of the H_2O+DMSO-assisted intermolecular nucleophilic addition in DMSO medium.

The catalysis of H_2O molecule or DMSO+H_2O (the combination of DMSO and H_2O) as the co-catalyst has been considered (see Figures S1 and S2). However, the reaction energy barriers of H_2O- and H_2O+DMSO-assisted intermolecular nucleophilic addition are 28.5 and 29.2 kcal/mol, respectively, which are far higher than the rate-determining free energy barrier (24.3 kcal/mol) of DMSO-assisted catalytic reaction (Figure 3). Thus, H_2O- and H_2O+DMSO-assisted catalytic strategies are unfavorable when compared with DMSO-assisted cases.

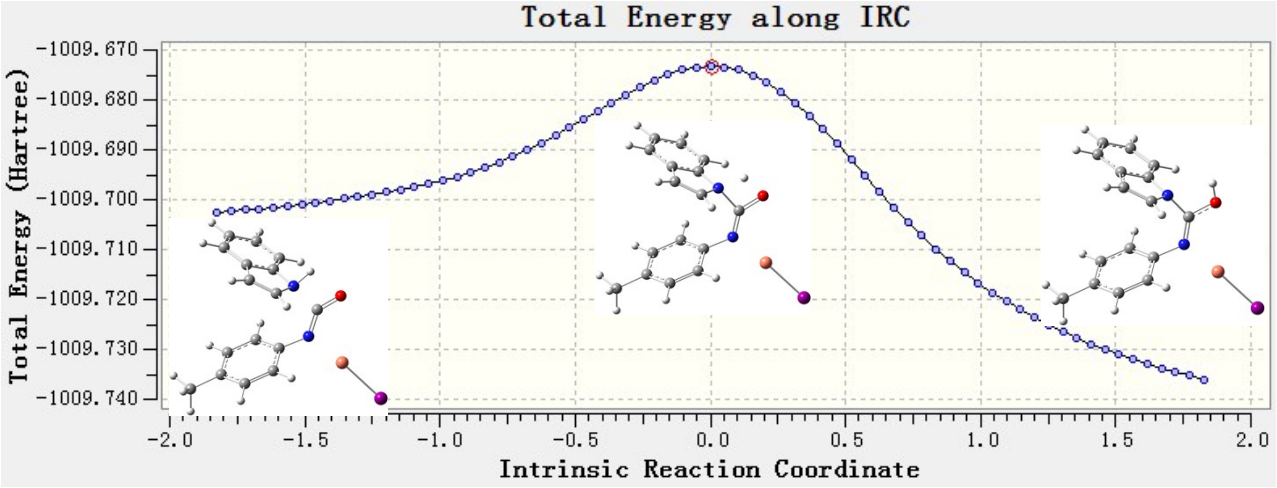


Figure S3. IRC of **ts1**.

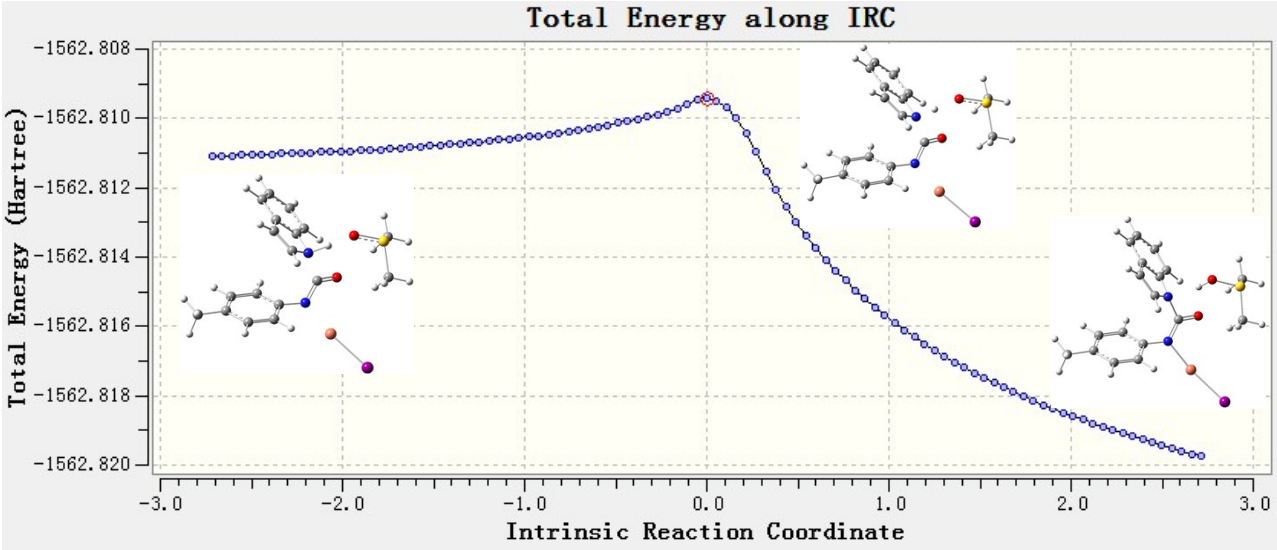


Figure S4. IRC of **ts2-DMSO**.

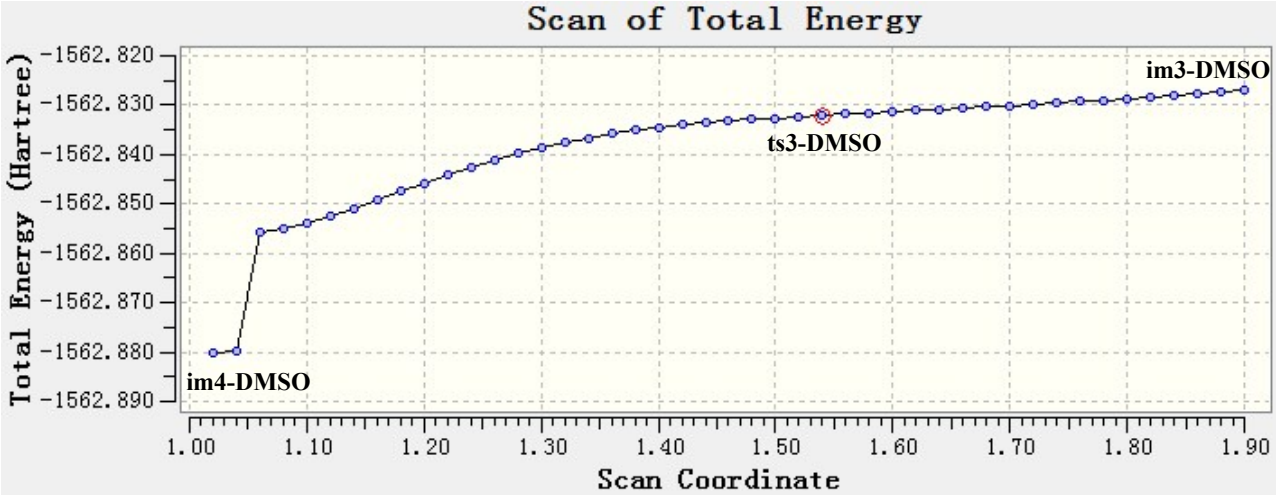
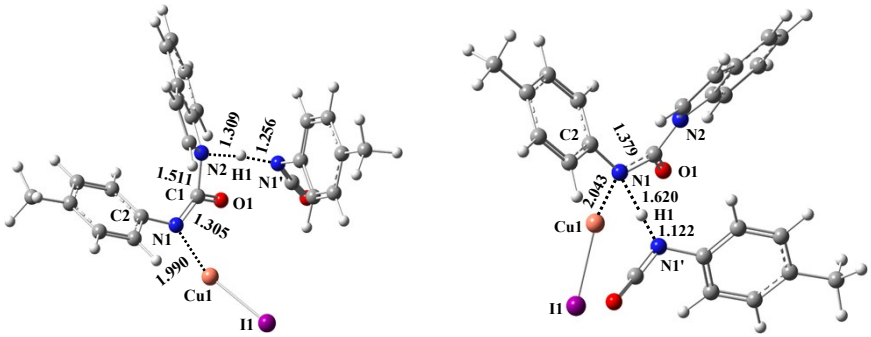


Figure S5. The scan profile from **im3-DMSO** to **im4-DMSO** along with the formation of N1-H1 bond (from 1.900 to 1.020 Å).



ts1-1a **ts2-1a**

Figure S6. The key structures of the Cu(I)-catalyzed synthesis of indole-1-carboxamides (**P**) from isocyanates (**1a**) and indoles (**2a**) with **1a** as the co-catalyst in DMSO medium (selected structural parameters are listed (bond lengths in Å)).

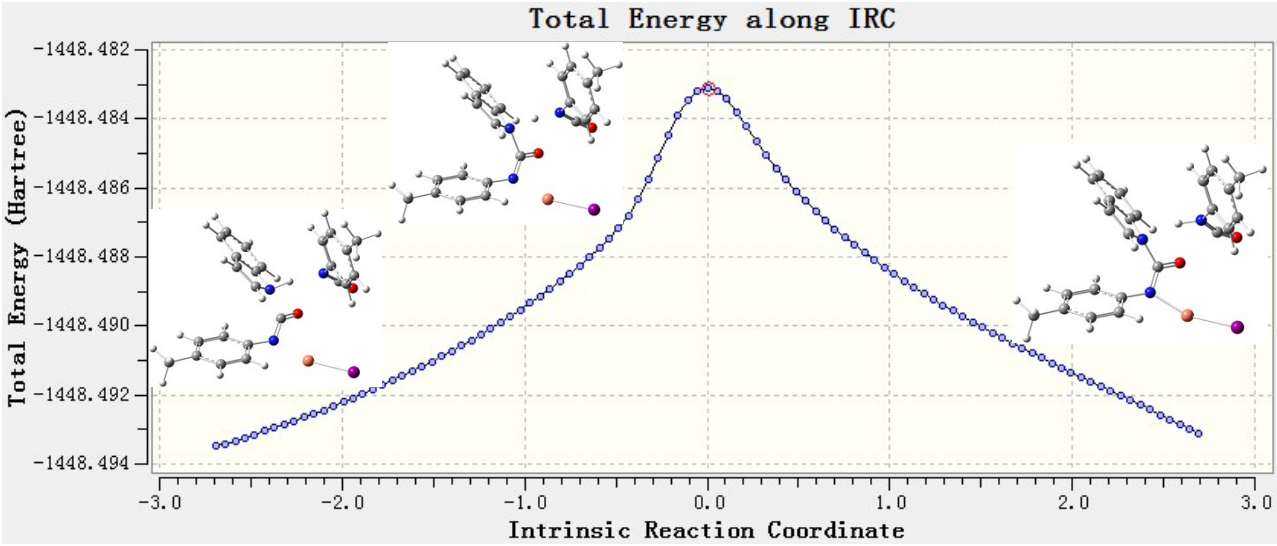


Figure S7. IRC of **ts1-1a**.

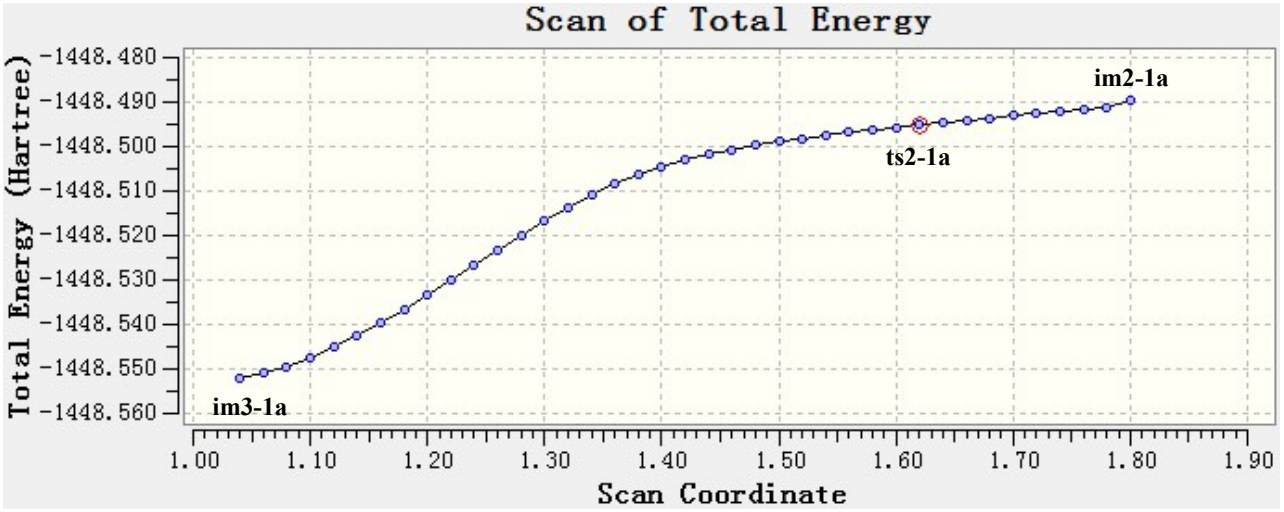
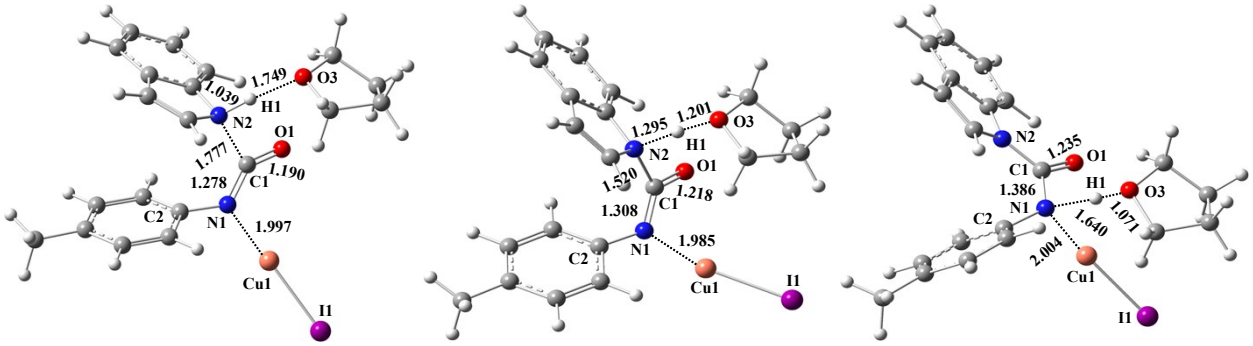
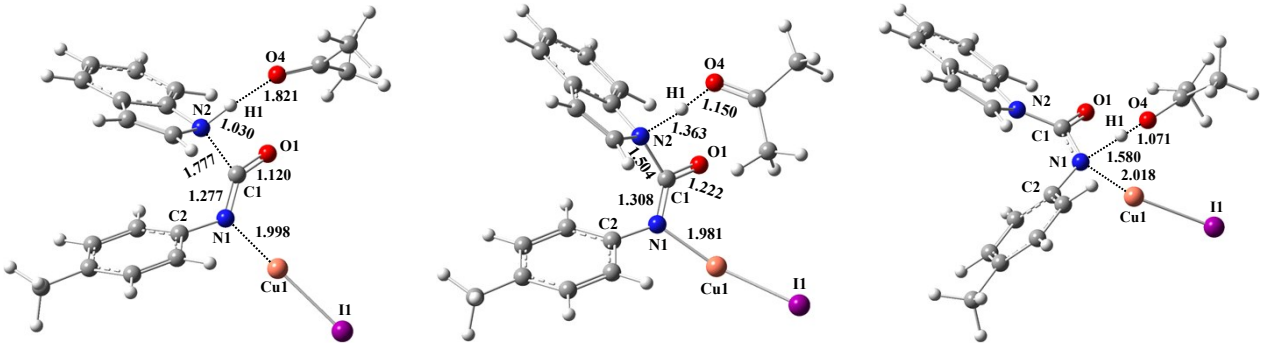


Figure S8. The scan profile from **im2-1a** to **im3-1a** along with the formation of N1-H1 bond (from 1.800 to 1.040 Å).



ts1-THF **ts2-THF** **ts3-THF**

Figure S9. The key structures of the Cu(I)-catalyzed synthesis of indole-1-carboxamides (**P**) from isocyanates (**1a**) and indoles (**2a**) with THF as the co-catalyst in THF medium (selected structural parameters are listed (bond lengths in Å)).



ts1-Acetone **ts2- Acetone** **ts3-Acetone**

Figure S10. The key structures of the Cu(I)-catalyzed synthesis of indole-1-carboxamides (**P**) from isocyanates (**1a**) and indoles (**2a**) with Acetone as the co-catalyst in Acetone medium (selected structural parameters are listed (bond lengths in Å)).

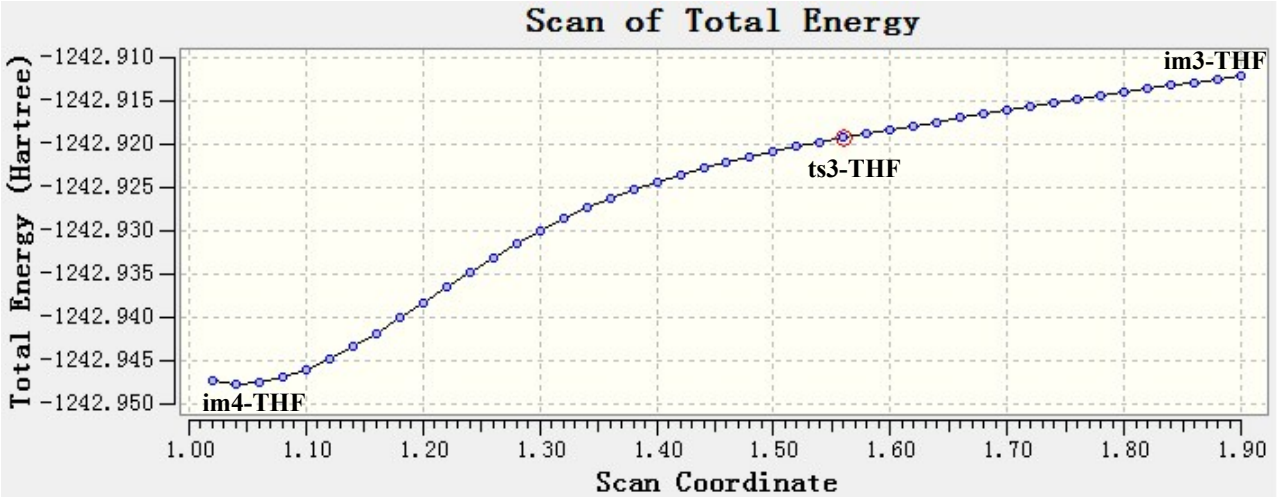


Figure S11. The scan profile from **im3-THF** to **im4-THF** along with the formation of N1-H1 bond (from 1.900 to 1.020 Å).

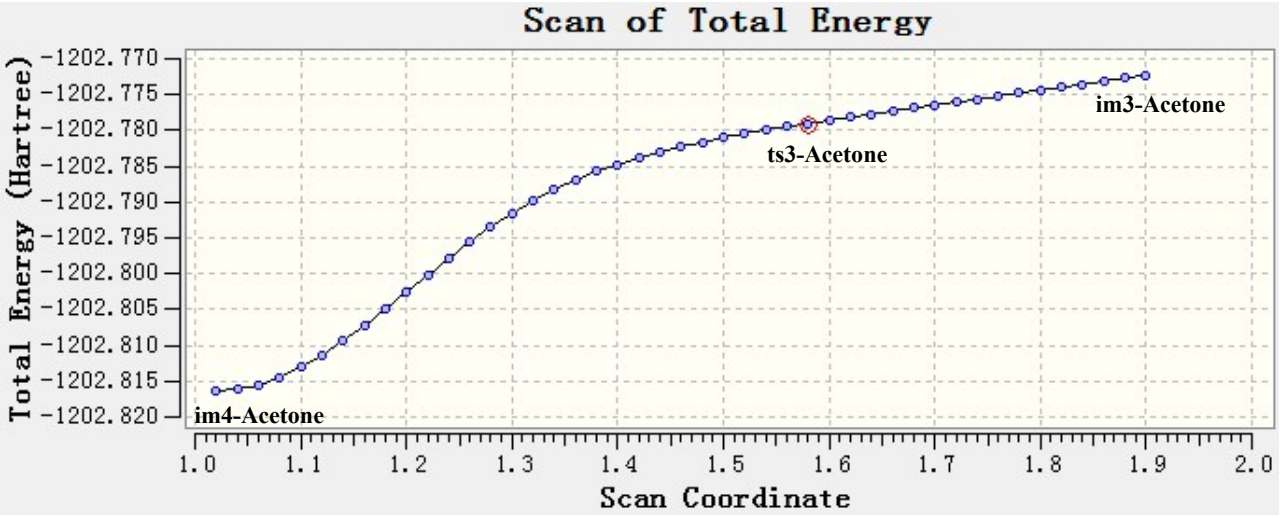


Figure S12. The scan profile from **im3-Acetone** to **im4-Acetone** along with the formation of N1-H1 bond (from 1.900 to 1.020 Å).

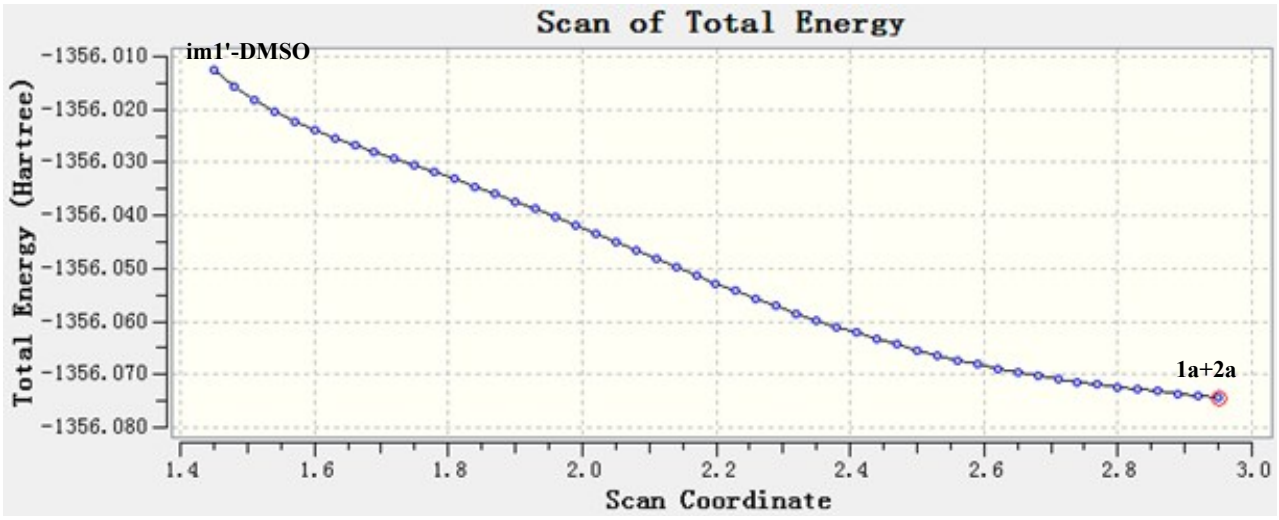
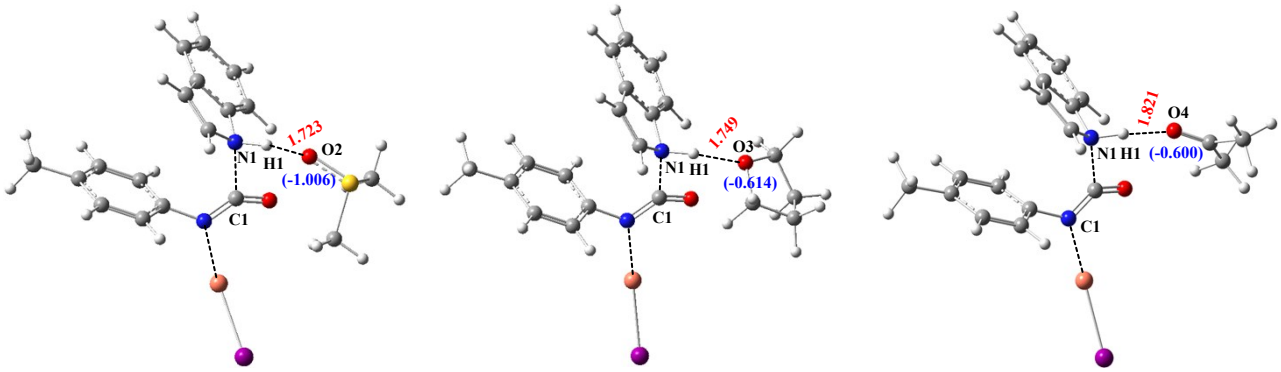
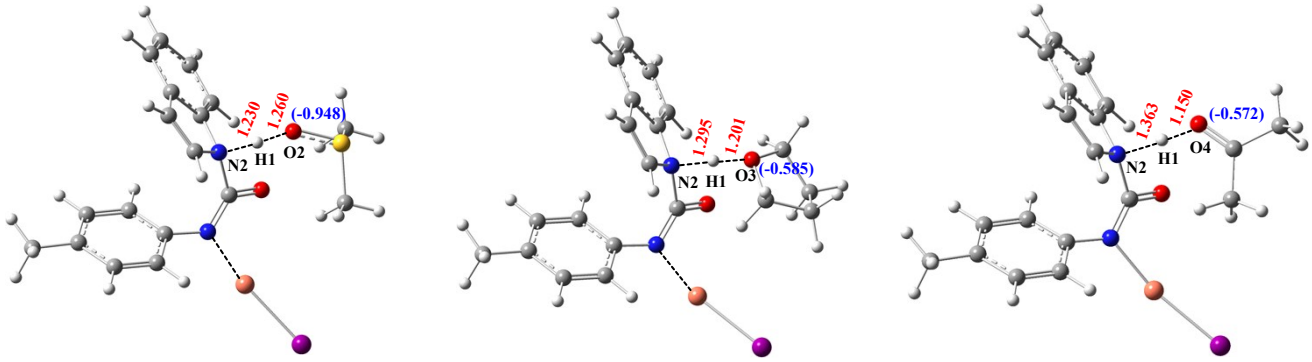


Figure S13. The scan profile from **1a** and **2a** to **im1'-DMSO** along with the formation of C1-N2 bond (from 2.950 to 1.450 Å).



ts1-DMSO **ts1-THF** **ts1-Acetone**

Figure S14. The electronic (NBO charge population) and geometric structures of **ts1-DMSO**, **ts1-THF** and **ts1-Acetone** in the solvent-assisted intermolecular addition reaction.



ts2-DMSO **ts2-THF** **ts2-Acetone**

Figure S15. The electronic (NBO charge population) and geometric structures of **ts2-DMSO**, **ts2-THF** and **ts2-Acetone** in the solvent-assisted proton-transfer reaction.

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

Direct reaction (in DMSO solution)

CuI

Cu	0.00000000	0.00000000	-1.57990200
I	0.00000000	0.00000000	0.86447500

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = -0.024808 a.u.

Sum of electronic and thermal Free Energies = 207.355590 a.u.

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

Energy = -207.5877523 a.u.

No imaginary frequency

1a

C	1.27729400	-1.19611000	-0.01093200
C	-0.09107500	-1.00101000	-0.00526700
C	2.16320400	-0.12332700	-0.00912600
C	1.62955800	1.16007800	-0.00770100
C	0.26256000	1.37275300	-0.00206700
C	-0.60504900	0.29084300	-0.00005800
C	3.64883600	-0.34746800	0.01514900
N	-1.97493200	0.53690000	0.00248100
C	-3.02967500	-0.02244300	0.00389900
O	-4.10979900	-0.45874700	0.00557400
H	1.66256300	-2.20384900	-0.01844800
H	-0.76200400	-1.84476900	-0.00891300
H	2.29274000	2.01087200	-0.01256700
H	-0.14288200	2.37015800	-0.00305400
H	4.18256700	0.49001900	-0.42531300
H	4.01260000	-0.46541500	1.03516900
H	3.92342200	-1.24524100	-0.53221300

BHandHLYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.100122 a.u.

Sum of electronic and thermal Energies= -438.685976 a.u.

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

Energy = -438.9867625 a.u.

No imaginary frequency

2a

C	-1.41418900	-1.46748200	0.00000000
C	-0.18090300	-2.08065500	0.00000000
C	1.00064400	-1.32591700	0.00000000
C	0.96854200	0.05190300	0.00000000
C	-0.27979700	0.66587200	0.00000000

C	-1.48004300	-0.07183200	0.00000000
C	-2.55080400	0.87919000	0.00000000
C	-1.98601000	2.11142200	0.00000000
N	-0.61848200	1.99419700	0.00000000
H	-2.31877400	-2.05490000	0.00000000
H	-0.11773300	-3.15676500	0.00000000
H	1.95199800	-1.83314300	0.00000000
H	1.87857300	0.63074300	0.00000000
H	-3.60268000	0.66675800	0.00000000
H	-2.44769200	3.08022800	0.00000000
H	0.02615100	2.75638200	0.00000000

BHandHLYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.104688 a.u.

Sum of electronic and thermal Free Energies = -363.487277 a.u.

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

Energy = -363.764602 a.u.

No imaginary frequency

im1

C	-4.43778400	0.25178800	-0.15258400
C	-3.31821900	1.06261300	-0.13221400
C	-4.33445100	-1.12982400	-0.02082000
C	-3.06544500	-1.67714900	0.12730000
C	-1.93349600	-0.88071400	0.15126500
C	-2.06432800	0.49060600	0.02258000
C	-5.55912600	-1.99960900	-0.01658000
N	-0.87810200	1.29229300	0.04463600
C	-0.83880000	2.51637000	0.05635200
O	-0.73168600	3.66122900	0.06850400
H	-5.40847500	0.70447700	-0.27714600
H	-3.42569400	2.13050800	-0.24359100
H	-2.95286200	-2.74489700	0.22455800
H	-0.95910300	-1.32726700	0.26800500
H	-5.33750300	-2.99555400	-0.38877300
H	-5.95596800	-2.10825900	0.99176400
H	-6.34729900	-1.57685700	-0.63315900
Cu	0.97786400	0.44028700	0.01350700
I	3.15733900	-0.66020500	-0.02652100

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.092203 a.u.

Sum of electronic and thermal Free Energies = -646.055634 a.u.

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

Energy = -646.6091116 a.u.

No imaginary frequency

ts1

C	5.24133500	-0.99110300	-0.33148600
C	5.14916000	-1.72041700	-1.50589700
C	3.97075500	-2.37326200	-1.86183800
C	2.84652900	-2.31625800	-1.05033700
C	2.95781400	-1.57079900	0.10234900
C	4.12181600	-0.91334300	0.48479900
C	3.84809200	-0.25808700	1.75196200
C	2.58632900	-0.51393900	2.09861300
N	1.97352500	-1.38305200	1.13519900
H	6.15917700	-0.49638600	-0.06066300
H	6.00552500	-1.78927400	-2.15580000
H	3.93084200	-2.93686800	-2.77866800
H	1.93441300	-2.82758000	-1.31039900
H	4.54256200	0.33177300	2.32023300
H	2.01425700	-0.20755700	2.95181300
C	2.05325900	2.41086700	-1.16046800
C	1.43599500	1.18663500	-0.95416900
C	1.82735800	3.48721500	-0.31276400
C	0.95548900	3.30289900	0.75772100
C	0.33484100	2.08767400	0.97600000
C	0.58757300	1.01457700	0.12866800
C	2.47043700	4.82285200	-0.55963800
N	-0.08792200	-0.21626100	0.35523000
C	0.51719500	-1.25537900	0.76034300
O	0.11918600	-2.42771900	1.02147400
H	2.71313000	2.52906300	-2.00545500
H	1.60366100	0.37292600	-1.63914700
H	0.75226100	4.12497300	1.42614600
H	-0.35122800	1.96150800	1.79773600
H	3.30756400	4.73830700	-1.24655500
H	1.75978800	5.52467100	-0.99321500
H	2.83659900	5.26424200	0.36420000
Cu	-2.06235800	-0.31256400	0.06978400
I	-4.49739400	-0.24277200	-0.27707000
H	1.38512900	-2.44234600	1.44282900

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.217450 a.u.

Sum of electronic and thermal Free Energies = -1009.455762 a.u.

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

Energy = -1010.3230566 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 1958.64*i*

im2

C	5.68623000	-1.45251000	0.40474400
C	5.74020500	-2.50836900	-0.48278600
C	4.58849100	-2.95964400	-1.13020900
C	3.35591600	-2.37697100	-0.89794000
C	3.30852500	-1.33167100	0.01676200
C	4.45757900	-0.84954300	0.65960100
C	4.05313600	0.25801800	1.48445200
C	2.72987600	0.42596400	1.32778700
N	2.23372600	-0.53656800	0.44055400
H	6.57966500	-1.09461500	0.88955800
H	6.68367900	-2.98568100	-0.68910600
H	4.65822300	-3.77315300	-1.83293600
H	2.48297500	-2.71331000	-1.43081000
H	4.68604100	0.84821100	2.11877900
H	2.06169200	1.13212600	1.77559900
C	1.33833500	3.37283300	-1.17705800
C	1.13490900	2.00985800	-1.05384400
C	0.68443100	4.28148700	-0.35137700
C	-0.18855000	3.77828600	0.60704700
C	-0.40692200	2.41759200	0.73767800
C	0.26684000	1.52432400	-0.08408500
C	0.88464500	5.76153500	-0.51579400
N	-0.00924600	0.13660900	0.04194300
C	0.90016200	-0.74580500	0.15868100
O	0.53519700	-2.01483800	0.01047700
H	2.01447800	3.73520000	-1.93534400
H	1.64260200	1.32524200	-1.71320300
H	-0.71575600	4.45862200	1.25697800
H	-1.09887300	2.04304300	1.47454800
H	0.15291600	6.18028100	-1.20527100
H	0.77442300	6.28382700	0.43059300
H	1.87102900	5.98666500	-0.91186200
Cu	-1.92434900	-0.45440200	-0.02851100
I	-4.30602100	-1.06323100	0.00959700
H	1.17634400	-2.61146700	0.40742600

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.223636 a.u.

Sum of electronic and thermal Free Energies = -1009.529679 a.u.

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

Energy = -1010.3931119 a.u.

No imaginary frequency

ts2

C	-3.13182400	-3.23550700	1.61576700

C	-2.76556100	-2.48540200	2.71768000
C	-1.94713900	-1.36649300	2.57943900
C	-1.48166800	-0.95829500	1.34003500
C	-1.86675100	-1.70935700	0.24423300
C	-2.67243600	-2.84752300	0.36398400
C	-2.82666500	-3.41763700	-0.95539300
C	-2.13940200	-2.66134500	-1.81743400
N	-1.54358600	-1.58448900	-1.12586700
H	-3.75234500	-4.10976500	1.72364800
H	-3.10833400	-2.77283800	3.69770800
H	-1.66343900	-0.80339700	3.45257600
H	-0.85276900	-0.09282200	1.25437900
H	-3.38674100	-4.29829300	-1.20541500
H	-1.98793200	-2.74060100	-2.87433000
C	-1.17945900	3.53917700	0.55780900
C	-0.43055100	2.49707000	0.04178200
C	-2.54847900	3.63083500	0.32900500
C	-3.14188100	2.63985300	-0.44321500
C	-2.40162500	1.59870200	-0.97691600
C	-1.03716500	1.51390100	-0.72989100
C	-3.34985600	4.77712400	0.87788300
N	-0.23123300	0.48035800	-1.29845000
C	-0.76540400	-0.69794300	-1.74629500
O	-0.36568300	-0.84730600	-2.93773700
H	-0.68713100	4.29038800	1.15503900
H	0.62883500	2.44792000	0.24074900
H	-4.20154100	2.68171500	-0.63982000
H	-2.89464200	0.85642500	-1.58399900
H	-3.01716500	5.05059900	1.87578500
H	-3.25061400	5.66126800	0.24964600
H	-4.40652000	4.53144100	0.93184900
Cu	1.61606500	0.18138600	-0.51537600
I	3.83186900	-0.12531200	0.48615500
H	0.08978600	0.28371500	-2.61682800

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.218349 a.u.

Sum of electronic and thermal Free Energies = -1009.473065 a.u.

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

Energy = -1010.3333906 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 2076.93*i*

im3

C	1.73824600	3.59860900	1.88422200
C	1.24402600	2.77961400	2.87971300

C	0.76189500	1.50960500	2.57351100
C	0.76454000	1.02704400	1.27564900
C	1.25159200	1.85547700	0.27474900
C	1.73960700	3.13834300	0.57293600
C	2.15424900	3.74790800	-0.66403800
C	1.91189100	2.87477400	-1.64900100
N	1.36649900	1.69236500	-1.12190200
H	2.11148200	4.58338900	2.11318000
H	1.22848700	3.12278200	3.90076600
H	0.37723000	0.88036700	3.35845700
H	0.41648100	0.02915900	1.09212500
H	2.57438300	4.72822800	-0.78237200
H	2.05459100	2.94386100	-2.70707300
C	1.82633700	-3.26234900	0.67174200
C	0.94908600	-2.41079000	0.02542900
C	3.20353300	-3.08107500	0.58575900
C	3.67424400	-2.02704700	-0.18658000
C	2.80793800	-1.17519800	-0.85337900
C	1.44216700	-1.36282700	-0.73649200
C	4.14666500	-3.98837500	1.32330400
N	0.48956100	-0.52250300	-1.45475500
C	0.94662400	0.71977100	-1.99425900
O	0.92943600	0.88351300	-3.18412500
H	1.42995800	-4.07613100	1.25774500
H	-0.11552100	-2.56386200	0.11451300
H	4.73658600	-1.86898800	-0.28050700
H	3.20636400	-0.37875500	-1.45934300
H	3.81636500	-5.02272700	1.27779900
H	5.14977000	-3.93643100	0.91070900
H	4.20886000	-3.71313400	2.37494200
Cu	-1.39096600	-0.30158700	-0.57942100
I	-3.67649900	-0.45045300	0.29294600
H	0.19371900	-1.02577500	-2.28383600

BHandLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.224606 a.u.

Sum of electronic and thermal Free Energies = -1009.535414 a.u.

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

Energy = -1010.3992370 a.u.

No imaginary frequency

DMSO-assisted reaction (in DMSO solution)

DMSO

S	-0.27708900	0.80871100	0.60722100
O	0.23021200	2.01673300	-0.11030400

C	-2.00052300	0.58504200	0.11560800
H	-2.38687100	-0.34660000	0.51797800
H	-2.56258200	1.41868100	0.52162600
H	-2.07223000	0.59756300	-0.96768100
C	0.37244000	-0.63543100	-0.26165900
H	-0.05484000	-1.54428300	0.15130500
H	0.15060900	-0.55061700	-1.32111600
H	1.44741500	-0.64038300	-0.11975700

BHandHLYP /6-31G*

Thermal correction to Gibbs Free Energy = 0.054836 a.u.

Sum of electronic and thermal Free Energies = -553.013381 a.u.

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

Energy = -553.1630280 a.u.

No imaginary frequency

ts1-DMSO

C	5.38783000	-0.43266100	-0.47598700
C	5.52482000	-1.09656400	-1.68387900
C	4.45347800	-1.78081800	-2.25290600
C	3.21302700	-1.81647000	-1.63159600
C	3.09139000	-1.14702300	-0.43094300
C	4.15474700	-0.46307100	0.16061200
C	3.66523900	0.08172800	1.41168100
C	2.37817200	-0.25298300	1.53027700
N	1.93462200	-1.00245400	0.39921400
H	6.22200400	0.09054900	-0.03793500
H	6.47526400	-1.08656000	-2.19168300
H	4.58752900	-2.29181200	-3.19189100
H	2.37993600	-2.33763800	-2.06933900
H	4.23413800	0.65455000	2.11948000
H	1.68098300	-0.06635900	2.32183900
H	1.50100600	-1.88979800	0.71339200
S	-0.54477500	-3.95493500	1.54455500
O	0.61295700	-2.99087400	1.69732000
C	-2.00997400	-2.97913500	1.17643000
H	-2.85137300	-3.64701100	1.01934600
H	-2.20918600	-2.35042600	2.03690800
H	-1.84616200	-2.36384600	0.29913600
C	-0.35569200	-4.73323300	-0.06674200
H	-1.21417300	-5.36855500	-0.26158000
H	-0.25993500	-3.96522700	-0.82625300
H	0.54343900	-5.33839900	-0.02962800
C	2.58655700	3.23271900	-0.40207900
C	1.84635100	2.11998900	-0.76080100
C	2.24477500	4.00387000	0.70339200

C	1.12920600	3.62351800	1.44334100
C	0.38570900	2.50889900	1.10064300
C	0.75411600	1.73758300	0.00557900
C	3.02772400	5.23491300	1.06401000
N	-0.03306000	0.62326600	-0.35916000
C	0.38687900	-0.55261500	-0.58369200
O	0.10298500	-1.55718800	-1.13918900
H	3.44051700	3.50972700	-1.00024400
H	2.11680900	1.54456600	-1.63073200
H	0.83487500	4.20809100	2.30092700
H	-0.47692600	2.22649200	1.68257100
H	2.58388800	6.12533500	0.62066700
H	3.05322800	5.38800200	2.13973300
H	4.05253000	5.17136000	0.70871700
Cu	-2.02458700	0.76999800	-0.50206200
I	-4.48384100	0.71779000	-0.40501800

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.294994 a.u.

Sum of electronic and thermal Free Energies = -1562.513074 a.u.

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

Energy = -1563.5411628 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 214.54*i*

im2-DMSO

C	-5.19702800	0.02266500	0.82503700
C	-5.23532200	-0.55552100	2.08485700
C	-4.13300900	-1.22812000	2.60295700
C	-2.95677500	-1.34853100	1.87298800
C	-2.94318000	-0.76479700	0.62755400
C	-4.02801200	-0.08303400	0.08748200
C	-3.63221800	0.39542800	-1.22642400
C	-2.36992400	0.04203900	-1.44611100
N	-1.86044400	-0.75050400	-0.34163900
H	-6.05409100	0.54320000	0.43113900
H	-6.13357200	-0.48109300	2.67519600
H	-4.18902700	-1.66344700	3.58657300
H	-2.09324700	-1.85923200	2.26050800
H	-4.25021900	0.94965800	-1.90744600
H	-1.73442400	0.18772400	-2.29485400
H	-1.71884900	-1.73760500	-0.73629600
S	-0.55710100	-4.16529700	-1.54245400
O	-1.55131700	-3.01392400	-1.62365100
C	1.09220800	-3.45377800	-1.61091100
H	1.81943600	-4.25537300	-1.52446500

H	1.19822500	-2.97775200	-2.57952500
H	1.21916000	-2.72966800	-0.81401800
C	-0.53901100	-4.70668800	0.17110200
H	0.21235900	-5.48153200	0.28804400
H	-0.32741200	-3.85529400	0.80761900
H	-1.51952000	-5.11561700	0.38898200
C	-2.06113700	3.56336300	0.36057500
C	-1.45041500	2.35853900	0.66639000
C	-1.71896400	4.27863800	-0.78062100
C	-0.73459900	3.74679900	-1.60969300
C	-0.12336500	2.54184200	-1.31802900
C	-0.49408400	1.82054700	-0.18637800
C	-2.35387200	5.60547500	-1.08954400
N	0.15991300	0.61068100	0.12223800
C	-0.42780600	-0.53146400	0.27235400
O	-0.03284500	-1.56679800	0.77048800
H	-2.80800600	3.95919400	1.03132000
H	-1.71084700	1.83246100	1.57026000
H	-0.43772200	4.28672900	-2.49559900
H	0.64439000	2.14672000	-1.96385100
H	-1.71590500	6.42950800	-0.77286800
H	-2.52751900	5.72444000	-2.15627900
H	-3.30681000	5.71719500	-0.57975400
Cu	2.12538700	0.51934900	0.39787600
I	4.58730300	0.32769000	0.46161900

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.296260 a.u.

Sum of electronic and thermal Free Energies = -1562.515280 a.u.

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

Energy = -1563.5480184 a.u.

No imaginary frequency

ts2-DMSO

C	5.29089600	-0.80385000	-0.45180900
C	5.33403200	-1.50559500	-1.64476900
C	4.16777500	-1.97158100	-2.24663400
C	2.92466700	-1.75994300	-1.66692700
C	2.90290900	-1.05983700	-0.47915500
C	4.05443700	-0.57188900	0.13518900
C	3.64046100	0.12954900	1.33444100
C	2.31125700	0.08197600	1.41077600
N	1.77077400	-0.72403800	0.34885200
H	6.19549700	-0.44018700	0.00705200
H	6.28383200	-1.69033500	-2.11896800
H	4.22850300	-2.50563800	-3.18032100

H	2.01594600	-2.10651900	-2.12489900
H	4.28887500	0.61374200	2.04007200
H	1.64004500	0.47365400	2.14711400
H	1.41329500	-1.75314200	0.91931900
S	0.02545900	-3.75666700	1.57427400
O	1.15124400	-2.70480000	1.70257000
C	-1.53016000	-2.87141900	1.44617400
H	-2.32510800	-3.60751800	1.37468000
H	-1.65342300	-2.30134100	2.36012200
H	-1.52872400	-2.22007200	0.58050800
C	0.14093700	-4.42585400	-0.08578100
H	-0.66419200	-5.14207300	-0.21737300
H	0.07018000	-3.61304000	-0.79812200
H	1.09658000	-4.93260800	-0.16049600
C	2.40341600	3.52314400	-0.47430500
C	1.75484000	2.32769200	-0.73588000
C	1.94580200	4.39659400	0.50416100
C	0.80836100	4.02954600	1.21846300
C	0.15643000	2.83608500	0.97048200
C	0.63329600	1.95883300	-0.00057200
C	2.62699500	5.71238000	0.75707700
N	-0.06837600	0.77110600	-0.27246400
C	0.46862500	-0.41040900	-0.35847300
O	-0.00782800	-1.41580700	-0.87124200
H	3.27550600	3.78443200	-1.05376700
H	2.11347000	1.67895400	-1.51882100
H	0.42279400	4.69053400	1.97945800
H	-0.72891300	2.57166500	1.52671900
H	2.12882300	6.52296200	0.22652900
H	2.61948000	5.96700100	1.81408100
H	3.66125500	5.69354700	0.42432700
Cu	-2.03572000	0.66465200	-0.50943000
I	-4.47545600	0.26586000	-0.37023100

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.294590 a.u.

Sum of electronic and thermal Free Energies = -1562.514834 a.u.

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

Energy = -1563.5511144 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 978.12*i*

im3-DMSO

C	-4.29361300	3.87540700	0.41020500
C	-3.69608800	4.76433200	-0.45813700
C	-2.50214700	4.43370200	-1.10741000

C	-1.88068600	3.21817100	-0.89799700
C	-2.48264300	2.32736700	-0.01604700
C	-3.68741600	2.64034400	0.63738800
C	-4.03137800	1.50669400	1.44730500
C	-3.07810100	0.57325900	1.25513900
N	-2.12292200	1.03733600	0.35954600
H	-5.21847500	4.12674500	0.90452500
H	-4.15387500	5.72236100	-0.64462800
H	-2.05850400	5.14180500	-1.78927000
H	-0.96421500	2.96019300	-1.39438800
H	-4.88426900	1.40996900	2.09160600
H	-2.97797200	-0.39948900	1.68937000
H	4.04171300	0.76824200	0.25523800
S	3.39048600	2.87454000	0.04948100
O	4.41376300	1.69274900	0.32815700
C	2.50474800	2.41558400	-1.44079200
H	1.94002800	3.29167000	-1.74504800
H	3.25517300	2.18254800	-2.18769200
H	1.82665400	1.59026100	-1.24898600
C	2.13287600	2.74710000	1.31930900
H	1.54197500	3.65669100	1.26382900
H	1.48804200	1.89167900	1.14390500
H	2.65783900	2.70524100	2.26700000
C	-3.85180100	-2.62958600	-1.10827300
C	-2.85751800	-1.67569500	-0.99730100
C	-3.86718600	-3.76445000	-0.30241400
C	-2.84398300	-3.90575500	0.62592500
C	-1.84567500	-2.95298300	0.74991800
C	-1.84002900	-1.81660400	-0.05296100
C	-4.93638300	-4.80991200	-0.45621100
N	-0.77993500	-0.90200800	0.05926400
C	-0.89384300	0.41293200	0.05424300
O	0.07603000	1.16165700	-0.16398400
H	-4.62950800	-2.49135600	-1.84418200
H	-2.86604500	-0.81314900	-1.64314500
H	-2.82338600	-4.77444700	1.26609700
H	-1.06013100	-3.07974000	1.47823300
H	-4.74648000	-5.44937700	-1.31772500
H	-4.99009200	-5.45160400	0.41913400
H	-5.91580800	-4.35928900	-0.59991900
Cu	1.11884500	-1.35461400	-0.01252300
I	3.62169600	-1.57131700	-0.01903500

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.296065 a.u.

Sum of electronic and thermal Free Energies = -1562.535901 a.u.

M06-2x/6-311++G** (Lanl2DZ for Cu, I)
Energy = -1563.5658561 a.u.
No imaginary frequency

ts3-DMSO

C	5.78747000	-1.54129400	-0.51413400
C	5.64673500	-2.58540500	-1.40458600
C	4.38097600	-2.98335000	-1.84235700
C	3.23098300	-2.35469400	-1.40275500
C	3.38088600	-1.30399600	-0.50647300
C	4.64401400	-0.88993600	-0.05772800
C	4.43433700	0.20858900	0.84599700
C	3.11159100	0.43922600	0.90582400
N	2.42982400	-0.45999400	0.08224500
H	6.76334000	-1.23056000	-0.17703400
H	6.52046400	-3.10128600	-1.76842900
H	4.29522100	-3.80244600	-2.53778000
H	2.25876700	-2.67066500	-1.72898500
H	5.18867800	0.75127500	1.38321100
H	2.57316100	1.16592700	1.47579500
H	-0.32069900	-0.05022400	1.72106800
S	-1.38814800	-1.53219300	3.12751100
O	-0.51539400	-0.28082100	2.74842000
C	-3.02705400	-1.23289500	2.47160400
H	-3.65537900	-2.05644800	2.79776800
H	-3.38098000	-0.30951800	2.91619100
H	-3.03350100	-1.15537000	1.38855000
C	-0.81823500	-2.88267300	2.09648300
H	-1.53119700	-3.69386600	2.20735900
H	-0.72171600	-2.57180400	1.05993400
H	0.14935700	-3.18953400	2.47674200
C	1.42374000	3.63596900	-0.99031400
C	1.14563600	2.28585100	-0.90082700
C	1.10292000	4.51521600	0.04113500
C	0.49636200	3.98544500	1.17105200
C	0.22233400	2.62986800	1.27751100
C	0.54862300	1.76091300	0.24439800
C	1.38836200	5.98562200	-0.08174300
N	0.19788200	0.38354900	0.33740900
C	1.05225500	-0.62660900	-0.02378900
O	0.60779000	-1.70911900	-0.37804400
H	1.89225700	4.01555100	-1.88529800
H	1.39507400	1.63073200	-1.71995400
H	0.23274400	4.63885800	1.98819800
H	-0.24385000	2.24622800	2.17076300

H	0.73866200	6.45395100	-0.81949400
H	1.23384700	6.49795500	0.86358700
H	2.41428600	6.16654600	-0.39525200
Cu	-1.53529400	0.01362800	-0.61484700
I	-3.85055400	-0.44218600	-1.38684800

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.296167 a.u.

Sum of electronic and thermal Free Energies = -1562.535924 a.u.

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

Energy = -1563.5712683 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 134.77*i*

im4-DMSO

C	4.07585700	4.30425700	-0.25871500
C	3.16154300	5.13808300	0.35129000
C	1.88235300	4.68006400	0.67557500
C	1.48440600	3.38500200	0.40019800
C	2.41204400	2.55315700	-0.21202400
C	3.70013300	2.99450000	-0.54555900
C	4.38517400	1.88831000	-1.16088900
C	3.54568600	0.84026200	-1.16813200
N	2.32870100	1.20197400	-0.58036500
H	5.06332800	4.65640400	-0.50990400
H	3.43342500	6.15582300	0.57902800
H	1.18272800	5.35112500	1.14611500
H	0.49418200	3.04359000	0.63479700
H	5.38212200	1.89289900	-1.55849800
H	3.68318300	-0.14538200	-1.55988600
H	0.41119800	-1.37774200	-0.61604000
S	-2.34892700	-2.93416300	-0.62684700
O	-1.39512900	-1.73992700	-0.62027300
C	-3.17077700	-2.92738000	0.97041500
H	-3.91683100	-3.71630000	0.98153200
H	-2.41448400	-3.13065600	1.72036900
H	-3.62329000	-1.95601400	1.14623500
C	-3.73666100	-2.44900500	-1.65814600
H	-4.48116700	-3.23909700	-1.63600700
H	-4.14857300	-1.51046000	-1.29930000
H	-3.35884400	-2.33123100	-2.66757900
C	4.12659300	-2.24878500	1.49023300
C	3.11480400	-1.40727900	1.06786100
C	4.42362600	-3.42797800	0.81138300
C	3.66932200	-3.73661500	-0.31288900
C	2.66554600	-2.89146600	-0.75938600

C	2.38336800	-1.72084600	-0.07213400
C	5.53456400	-4.32548300	1.27892800
N	1.30912100	-0.91327400	-0.52243600
C	1.18887500	0.43045400	-0.50097600
O	0.09093400	0.97864800	-0.44410900
H	4.68739200	-1.98944800	2.37465000
H	2.89155900	-0.51049900	1.62129100
H	3.87131400	-4.64605000	-0.85650400
H	2.09900400	-3.13601400	-1.64340400
H	5.49169300	-4.48132600	2.35427400
H	5.48644000	-5.29793600	0.79773500
H	6.50923300	-3.89506100	1.05395900
Cu	-1.83545100	0.35374100	-0.15862400
I	-4.18948300	1.02915700	0.49847700

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.298050 a.u.

Sum of electronic and thermal Free Energies = -1562.582031 a.u.

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

Energy = -1563.6035555 a.u.

No imaginary frequency

1a-assisted reaction (in DMSO solution)

ts1-1a

C	-4.67693200	2.58510700	-0.44274300
C	-4.93582100	2.79620400	-1.78568100
C	-4.07396800	2.31257000	-2.76827100
C	-2.92382700	1.61154900	-2.43751100
C	-2.68515100	1.40524900	-1.09307900
C	-3.53627800	1.87398000	-0.09181700
C	-2.97459600	1.46362700	1.17851400
C	-1.86040600	0.76851100	0.93831900
N	-1.57256300	0.75156000	-0.46296700
H	-5.34744600	2.95843200	0.31380700
H	-5.81842300	3.34073800	-2.07828200
H	-4.30208300	2.48615800	-3.80674500
H	-2.25178100	1.23300800	-3.18634300
H	-3.38298200	1.67151000	2.14955000
H	-1.17498900	0.29588600	1.61181300
H	-0.53479000	1.53284200	-0.62645800
C	-2.08218300	-3.27690600	2.39882600
C	-1.19732300	-2.71777600	1.49621900
C	-3.45862000	-3.22377700	2.19542700
C	-3.91495900	-2.59146700	1.04613800
C	-3.03808100	-2.03432600	0.13020200

C	-1.66423800	-2.07310500	0.35225800
C	-4.41038900	-3.86462200	3.16634700
N	-0.75260500	-1.54762900	-0.57465000
C	-0.89899600	-0.39842200	-1.17510000
O	-0.39720500	-0.02225800	-2.22656000
H	-1.69388900	-3.76660200	3.27874400
H	-0.13429900	-2.77385500	1.67190000
H	-4.97545600	-2.54314300	0.85198600
H	-3.41934100	-1.57823100	-0.76966400
H	-5.40724300	-3.44021100	3.08243100
H	-4.49652800	-4.93582000	2.98756900
H	-4.07705300	-3.73580000	4.19332700
Cu	1.15776800	-2.07043500	-0.77460100
I	3.62979800	-1.97669700	-0.55226100
C	1.39435000	4.37749200	1.99571700
C	0.73922400	3.83491000	0.90314500
C	2.57137700	3.81771000	2.48238100
C	3.07309300	2.68300200	1.85159300
C	2.43014400	2.11866100	0.76338700
C	1.26962500	2.71259600	0.29435000
C	3.29460000	4.42869700	3.64895500
N	0.55446700	2.12826800	-0.81827400
C	1.11607500	1.94071100	-1.91361600
O	1.65288600	1.85945700	-2.91446200
H	0.98297200	5.25183200	2.47413700
H	-0.16913400	4.27503900	0.52689500
H	3.97557100	2.22109300	2.21835000
H	2.81572200	1.22085300	0.30423600
H	3.70353600	3.66427000	4.30395000
H	4.12624200	5.04476700	3.31053400
H	2.63593700	5.06077300	4.23716400

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.337912 a.u.

Sum of electronic and thermal Free Energies = -1448.145142 a.u.

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

Energy = -1449.3376117 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 1286.64*i*

im2-1a

C	-3.07198600	4.99467200	0.43694300
C	-2.28974300	5.57297900	-0.54021500
C	-1.39415000	4.80061500	-1.28792700
C	-1.25713100	3.44290000	-1.07185800
C	-2.04266300	2.86616400	-0.07872200

C	-2.95410300	3.62551000	0.67565800
C	-3.59894200	2.72194700	1.58504800
C	-3.09425800	1.49293700	1.35267100
N	-2.15121100	1.54399700	0.33611500
H	-3.76828500	5.58875200	1.00742600
H	-2.37099700	6.63008000	-0.73640400
H	-0.80118500	5.27313700	-2.05495000
H	-0.57221600	2.84493100	-1.64363400
H	-4.34287900	2.96723500	2.31886600
H	-3.31429400	0.56263700	1.83342200
H	3.39993700	-1.45187500	0.19980800
C	-4.57081700	-2.82198000	0.97048000
C	-3.29079200	-2.29181100	0.93726300
C	-5.58284000	-2.31972500	0.16358600
C	-5.25986400	-1.26949100	-0.69170700
C	-3.98504100	-0.73823600	-0.73838300
C	-2.97508900	-1.23411100	0.08955000
C	-6.97740700	-2.87914800	0.21064000
N	-1.65368900	-0.76888900	0.03802400
C	-1.27963100	0.50127000	-0.05571700
O	-0.14979500	0.82349000	-0.43756300
H	-4.78247400	-3.64287100	1.63875400
H	-2.51761000	-2.69627800	1.57142500
H	-6.01911500	-0.86460600	-1.34398400
H	-3.76246600	0.06413600	-1.42224900
H	-7.66912600	-2.18833800	0.69175300
H	-7.36252700	-3.07423200	-0.78816700
H	-7.00919200	-3.81261500	0.76603000
Cu	-0.06082900	-1.83196700	-0.34220700
I	2.13163900	-3.08004500	-0.67672800
C	2.65338900	2.57983500	-0.12210500
C	2.72887500	1.22728000	0.16797900
C	3.79251000	3.37507300	-0.18075400
C	5.03223700	2.78068100	0.04969500
C	5.13788800	1.43026600	0.32763900
C	3.97483900	0.68290900	0.38989800
C	3.69469400	4.83625000	-0.51401800
N	4.04595300	-0.73879900	0.70580500
C	4.78170200	-1.20551000	1.59493700
O	5.45211400	-1.66886500	2.38878600
H	1.67732900	3.00260500	-0.29472800
H	1.82098500	0.64869800	0.19864800
H	5.92880600	3.37753100	0.00237300
H	6.10445300	0.97493400	0.47584400
H	2.69968900	5.21882400	-0.30997900

H	4.40991900	5.42233100	0.05692500
H	3.90243500	5.00558000	-1.56945200

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.339129 a.u.

Sum of electronic and thermal Free Energies = -1448.153482 a.u.

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

Energy = -1449.3410884 a.u.

No imaginary frequency

ts2-1a

C	5.79704900	-0.70545300	-0.39266600
C	5.91273300	-1.34672200	-1.60842800
C	4.80823300	-1.47591500	-2.45484200
C	3.56766700	-0.97233500	-2.11159900
C	3.46009400	-0.32354000	-0.88767500
C	4.55794800	-0.18647800	-0.02410100
C	4.09652500	0.52230000	1.13898300
C	2.79324400	0.79961800	0.95325500
N	2.36755700	0.30504100	-0.27996000
H	6.64824200	-0.60334900	0.26129300
H	6.86375600	-1.75367800	-1.91148800
H	4.92262300	-1.98328600	-3.39895300
H	2.71607800	-1.08433100	-2.75444800
H	4.67913100	0.79422500	1.99868900
H	2.11221400	1.32737400	1.58715400
H	-0.55199500	0.11583200	1.00134400
C	-0.19578000	4.28756300	1.64284700
C	-0.36363700	2.95786900	1.28997100
C	0.68306500	5.11210200	0.95535800
C	1.37969600	4.55399200	-0.11323200
C	1.21357900	3.23209800	-0.47918600
C	0.34166800	2.40227400	0.22789800
C	0.88073100	6.55074000	1.34273200
N	0.10174600	1.05942100	-0.14175000
C	1.05848000	0.28265700	-0.75959000
O	0.75340500	-0.48166800	-1.65376100
H	-0.76505800	4.68641700	2.46804000
H	-1.07032700	2.35438000	1.83912200
H	2.06182300	5.16891500	-0.68026600
H	1.75987000	2.84048100	-1.32157800
H	1.87215400	6.71791600	1.76146900
H	0.77907800	7.21074900	0.48390200
H	0.15332000	6.86183800	2.08712000
Cu	-1.60352600	0.57503900	-1.15695000
I	-3.95950700	-0.27273200	-1.12830300

C	-0.87909600	-4.26955000	0.82687600
C	-1.36308500	-2.97750900	0.94230600
C	0.38805800	-4.61166900	1.28772800
C	1.16880000	-3.62395000	1.88253100
C	0.70339600	-2.32884600	2.02282700
C	-0.56096200	-2.03158000	1.55172800
C	0.91873900	-6.00569000	1.11278600
N	-1.02693700	-0.65503500	1.66347900
C	-2.10151200	-0.37034800	2.22627600
O	-3.04671400	-0.07011100	2.78018100
H	-1.49520500	-5.01660900	0.35369600
H	-2.32451800	-2.70341500	0.53848200
H	2.15634300	-3.86731200	2.23910800
H	1.31432100	-1.56696300	2.47702000
H	1.44693800	-6.09826800	0.16524300
H	1.61690800	-6.26604500	1.90305200
H	0.11655000	-6.73771100	1.11317100

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.340619 a.u.

Sum of electronic and thermal Free Energies = -1448.154468 a.u.

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

Energy = -1449.3491126 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 186.53*i*

im3-1a

C	5.75924000	1.26322200	-0.25481500
C	6.08320400	0.77311400	-1.50387100
C	5.08553000	0.41504300	-2.41283300
C	3.74282200	0.53720200	-2.10314700
C	3.42968600	1.03004900	-0.84509000
C	4.41522000	1.39351200	0.08140200
C	3.73986700	1.85952200	1.26592800
C	2.41903800	1.76198200	1.05003300
N	2.18299700	1.24685900	-0.23345300
H	6.52854300	1.54096400	0.44710000
H	7.11811700	0.66657600	-1.78453800
H	5.36473300	0.03838200	-3.38298500
H	2.97678500	0.27393100	-2.80697300
H	4.20001900	2.23582900	2.15962600
H	1.60579200	2.04986300	1.68369400
H	0.07679100	0.80344500	0.98064700
C	-2.18375700	3.93295900	1.26731400
C	-1.42200100	2.77633700	1.24421800
C	-2.47107300	4.63179000	0.10198600

C	-1.97046000	4.12998400	-1.09502800
C	-1.21834100	2.96933700	-1.14142500
C	-0.93834600	2.29640000	0.03827000
C	-3.31972400	5.87142000	0.12590900
N	-0.16932200	1.06403300	0.03513000
C	0.97048500	1.03679900	-0.83367800
O	0.83507400	0.82277800	-2.00605700
H	-2.55688700	4.29323600	2.21261700
H	-1.22388100	2.25116200	2.16594000
H	-2.17855000	4.64961100	-2.01687200
H	-0.85660600	2.59143000	-2.08153400
H	-2.97163600	6.60347700	-0.59796500
H	-4.35536900	5.63976300	-0.11798600
H	-3.31133000	6.33793400	1.10677000
Cu	-1.48918900	-0.40206800	-0.63342400
I	-3.25610200	-2.05830700	-1.10417600
C	0.22248500	-3.76041900	0.94889300
C	-0.21352000	-2.67326000	1.68270100
C	1.56071600	-3.90548700	0.59188500
C	2.45434300	-2.91816900	0.98911800
C	2.03584200	-1.81843600	1.72077600
C	0.70087600	-1.70181400	2.07331500
C	2.01380100	-5.09687600	-0.20340800
N	0.29301600	-0.55481200	2.78155000
C	-0.54588300	-0.22935900	3.57580100
O	-1.30522700	0.22571400	4.32944200
H	-0.50014400	-4.49543500	0.63344800
H	-1.25776800	-2.56992700	1.92644900
H	3.49490200	-3.00181100	0.71910300
H	2.73399100	-1.05483300	2.01907200
H	3.04882700	-4.99369400	-0.51531500
H	1.93248900	-6.01226200	0.38019600
H	1.40512700	-5.22702100	-1.09504700

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.341362 a.u.

Sum of electronic and thermal Free Energies = -1448.211383 a.u.

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

Energy = -1449.3964550 a.u.

No imaginary frequency

THF-assisted reaction (in THF solution)

THF

C	0.72824600	0.98892600	0.22573500
C	-0.72862100	0.98866900	-0.22574900

C	1.15542900	-0.42948900	-0.13153600
O	0.00022700	-1.23577700	-0.00002400
C	-1.15525800	-0.42989300	0.13156500
H	0.78954000	1.14426100	1.30095000
H	1.33527200	1.74712600	-0.25968000
H	-0.78999000	1.14394600	-1.30096800
H	-1.33591500	1.74666300	0.25965700
H	1.93250600	-0.82025800	0.52023100
H	1.51904200	-0.48167700	-1.15905400
H	-1.93224100	-0.82094000	-0.52014400
H	-1.51879900	-0.48218100	1.15910700

BHandHLYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.093655 a.u.

Sum of electronic and thermal Free Energies = -232.214812 a.u.

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

Energy = -232.4095949 a.u.

No imaginary frequency

ts1-THF

C	-5.16816300	-0.60046000	-0.80379800
C	-5.28809300	-0.07011700	-2.07845100
C	-4.30732400	0.76568100	-2.60561700
C	-3.17565100	1.09641700	-1.87210500
C	-3.07447900	0.55797200	-0.60741100
C	-4.04367200	-0.27811800	-0.05805500
C	-3.59674500	-0.63349100	1.27625800
C	-2.41760500	-0.05071800	1.49058800
N	-2.01073800	0.72872100	0.35153000
H	-5.93129800	-1.24624700	-0.40184800
H	-6.15412300	-0.30846900	-2.67355700
H	-4.42461800	1.16194300	-3.60036900
H	-2.40584400	1.73178000	-2.27419000
H	-4.11703400	-1.26700700	1.96971400
H	-1.78031200	-0.06736100	2.35154000
H	-1.91126400	1.72285400	0.63639500
C	-1.78885900	-3.55575800	-0.28518100
C	-1.24707100	-2.33219500	-0.64026800
C	-1.42920900	-4.19038900	0.89825400
C	-0.49926500	-3.55886700	1.71963600
C	0.04243400	-2.33306500	1.37995800
C	-0.34781600	-1.69771600	0.20607800
C	-1.98740500	-5.53830500	1.25909700
N	0.23701700	-0.46262400	-0.14814200
C	-0.39366200	0.62459400	-0.37692800
O	-0.20478100	1.67790700	-0.89632500

H	-2.49519000	-4.03000200	-0.94867800
H	-1.52008100	-1.86621800	-1.57253700
H	-0.19029600	-4.03513600	2.63711300
H	0.76778500	-1.85766200	2.02043200
H	-1.30742200	-6.33573500	0.96253400
H	-2.14367700	-5.62989700	2.33099000
H	-2.93726600	-5.71998300	0.76385600
Cu	2.21748400	-0.36157300	-0.38361900
I	4.67794200	-0.25160400	-0.44450200
C	0.19388700	4.76642400	1.71151200
C	-0.23346800	4.92238400	0.25506200
C	-0.44369700	3.43649800	2.08437900
O	-1.61927600	3.32369300	1.27730300
C	-1.64083400	4.35364100	0.28472000
H	-0.21868300	5.56911200	2.31877200
H	1.27042300	4.75752500	1.84579900
H	0.39580700	4.31741400	-0.39106100
H	-0.20703600	5.94990500	-0.09346800
H	-0.73817900	3.37253600	3.12733200
H	0.22137700	2.60634500	1.85369500
H	-1.94680400	3.91217600	-0.65693300
H	-2.37551900	5.10078500	0.58013800

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.334797 a.u.

Sum of electronic and thermal Free Energies = -1241.703815 a.u.

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

Energy = -1242.7819552 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 135.46*i*

im2-THF

C	5.06796300	-0.70337300	0.92880300
C	5.13347500	-0.20907900	2.22257600
C	4.12885000	0.60653500	2.73484400
C	3.02645800	0.95721800	1.96538200
C	2.98365200	0.45354600	0.68532800
C	3.97215100	-0.36484700	0.14965600
C	3.57273600	-0.69589000	-1.20753600
C	2.39838600	-0.12230900	-1.45585100
N	1.95977300	0.66604400	-0.32153500
H	5.84866400	-1.33602500	0.54033900
H	5.97566100	-0.46249500	2.84490900
H	4.20319100	0.97175800	3.74534400
H	2.23612300	1.57804300	2.34998400
H	4.12144000	-1.31357400	-1.89340200

H	1.78697900	-0.12839600	-2.33499200
H	1.96261500	1.67221800	-0.61475800
C	1.63423000	-3.63096600	0.26697800
C	1.12894200	-2.38633300	0.60358300
C	1.29323500	-4.25090300	-0.92943900
C	0.41900300	-3.58226200	-1.78238300
C	-0.08520600	-2.33608900	-1.46025200
C	0.28691500	-1.71293100	-0.27257000
C	1.80880800	-5.62057300	-1.27156100
N	-0.25984600	-0.45651200	0.06192800
C	0.42122000	0.61784300	0.26602600
O	0.17592800	1.68485200	0.76278000
H	2.29458800	-4.13420300	0.95619000
H	1.38293700	-1.93423700	1.54808200
H	0.12342400	-4.04644100	-2.71055300
H	-0.77014400	-1.83339900	-2.12408000
H	1.08495900	-6.38956700	-1.00517700
H	2.00441400	-5.71746500	-2.33659700
H	2.72952000	-5.84260700	-0.73899100
Cu	-2.22297900	-0.27920000	0.33743700
I	-4.68196000	-0.11424400	0.46102900
C	0.19998100	4.80651200	-1.79573300
C	0.48867400	4.90220200	-0.30052100
C	0.79602500	3.45137000	-2.14432400
O	1.88064700	3.25220800	-1.23041100
C	1.85896700	4.25644300	-0.20842100
H	0.71342900	5.59826500	-2.33684800
H	-0.85698500	4.86221200	-2.03390900
H	-0.23163900	4.31684900	0.26280000
H	0.48359900	5.92101100	0.07355100
H	1.18842700	3.39403300	-3.15474000
H	0.06712200	2.65630700	-2.00034700
H	2.04327300	3.77425700	0.74417100
H	2.65981600	4.96527600	-0.41039800

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.335176 a.u.

Sum of electronic and thermal Free Energies = -1241.703665 a.u.

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

Energy = -1242.7838217 a.u.

No imaginary frequency

ts2-THF

C	5.18117800	-1.64538000	0.12094400
C	5.29506600	-2.40920500	-1.02696800
C	4.18304700	-2.67976100	-1.82223200

C	2.92357400	-2.20672600	-1.48568900
C	2.82783000	-1.44748800	-0.33557700
C	3.92966100	-1.15070200	0.46653600
C	3.46079600	-0.31210900	1.54961100
C	2.15356100	-0.10429800	1.38044700
N	1.66155000	-0.85751400	0.26532200
H	6.04451500	-1.43167400	0.72940000
H	6.25827000	-2.79679200	-1.31524400
H	4.30091700	-3.26714600	-2.71765300
H	2.05972800	-2.40149300	-2.09524600
H	4.05929500	0.08980000	2.34538000
H	1.46243200	0.47232300	1.96073200
H	0.99017000	-1.82515300	0.80493000
C	2.90082800	3.25373700	-0.47405700
C	2.15449300	2.13022600	-0.79008700
C	2.40972100	4.23529400	0.37648400
C	1.13477900	4.05098400	0.90601100
C	0.38387800	2.93075800	0.60461200
C	0.89012800	1.94272100	-0.23889800
C	3.20477200	5.47239300	0.68773400
N	0.09739900	0.83355300	-0.56464300
C	0.53635000	-0.39606600	-0.64598500
O	0.05286500	-1.33194700	-1.25785400
H	3.88026900	3.37186000	-0.91151200
H	2.54856100	1.39937300	-1.47837100
H	0.72005800	4.79898500	1.56440900
H	-0.60437800	2.81013900	1.02020700
H	2.85113700	6.32595900	0.11070900
H	3.12737300	5.74108700	1.73880000
H	4.25715800	5.33542900	0.45463700
Cu	-1.88151100	0.80809100	-0.71322200
I	-4.27448800	0.37592900	-0.21707400
C	-2.02013600	-3.00402000	1.65536300
C	-1.57982500	-3.63945100	0.33827600
C	-0.88643000	-2.04550700	1.96643600
O	0.29678800	-2.64202400	1.34647500
C	-0.08387500	-3.78229500	0.51643900
H	-2.11176500	-3.75294700	2.43805800
H	-2.96173400	-2.47306900	1.56468200
H	-1.78866000	-2.97299900	-0.49142900
H	-2.05749600	-4.59590000	0.15327600
H	-0.66658400	-1.93046800	3.01998700
H	-1.04496600	-1.07517500	1.50975500
H	0.48295700	-3.71014800	-0.39938200
H	0.19815700	-4.66998700	1.07207900

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.335178 a.u.

Sum of electronic and thermal Free Energies = -1241.695914 a.u.

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

Energy = -1242.7834890 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 1113.05*i*

im3-THF

C	-4.43933200	3.52378900	0.37418800
C	-3.90984400	4.43585700	-0.51421300
C	-2.69392000	4.18266300	-1.15757500
C	-1.98218400	3.02269800	-0.92113400
C	-2.51498500	2.10984700	-0.01697600
C	-3.74163700	2.34360300	0.62936900
C	-4.00043700	1.20274900	1.46039100
C	-2.97844100	0.34058300	1.28557100
N	-2.05957900	0.85965000	0.38367700
H	-5.38180000	3.71510400	0.86210400
H	-4.43903600	5.35182100	-0.72180400
H	-2.30559700	4.90617800	-1.85666500
H	-1.05035200	2.82237500	-1.41645400
H	-4.84522700	1.05344200	2.10529900
H	-2.80546300	-0.61457500	1.73614500
H	3.43592400	1.01339600	0.06849400
C	-3.54415900	-2.88430600	-1.11390600
C	-2.61235800	-1.87103800	-0.98734500
C	-3.48853400	-4.02970300	-0.32503300
C	-2.45937400	-4.11945700	0.60318700
C	-1.52400900	-3.10701500	0.74307400
C	-1.58878300	-1.96064400	-0.04322500
C	-4.48927200	-5.13834900	-0.49577600
N	-0.58823900	-0.98358800	0.08683300
C	-0.78414100	0.32413700	0.09134100
O	0.13642400	1.13344800	-0.10561500
H	-4.32853100	-2.78461700	-1.84896900
H	-2.67540500	-1.00161400	-1.62069700
H	-2.38488100	-4.99415700	1.23116300
H	-0.73355500	-3.19374700	1.47200900
H	-4.25158100	-5.75991900	-1.35860100
H	-4.51220200	-5.78746700	0.37550700
H	-5.49314400	-4.74825900	-0.64732600
Cu	1.33240300	-1.30450900	-0.01395700
I	3.85314500	-1.26408200	-0.03736200
C	2.16078800	3.89270300	-0.61950500

C	1.66767500	3.61496800	0.80773600
C	2.61916500	2.54283600	-1.11437200
O	3.25382500	2.00538300	0.10395400
C	2.50258500	2.43970200	1.30404400
H	2.99021400	4.59446900	-0.62187900
H	1.37162400	4.29107800	-1.24735700
H	0.62673200	3.32134000	0.78753200
H	1.78693600	4.48145500	1.44851300
H	3.39340600	2.55454400	-1.86831400
H	1.80111100	1.88157800	-1.36305400
H	1.90189600	1.59979400	1.61884800
H	3.26246200	2.68803300	2.03114900

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.338345 a.u.

Sum of electronic and thermal Free Energies = -1241.714703 a.u.

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

Energy = -1242.7951859 a.u.

No imaginary frequency

ts3-THF

C	5.97146900	-1.58241500	-0.17116600
C	5.87326800	-2.70057600	-0.99156100
C	4.61983200	-3.15674200	-1.43792000
C	3.43746700	-2.51372300	-1.07676700
C	3.54335000	-1.38953100	-0.25305500
C	4.79719800	-0.91427300	0.20588100
C	4.54080100	0.24736300	1.02101700
C	3.19982100	0.46218200	1.02492900
N	2.55321000	-0.51465600	0.24537600
H	6.93945800	-1.22734200	0.17275600
H	6.77345000	-3.22991600	-1.29207400
H	4.56739600	-4.03443300	-2.07629300
H	2.47281000	-2.87597800	-1.40559900
H	5.27518400	0.84508300	1.54421900
H	2.62827500	1.22408900	1.52741900
H	-0.58380200	-0.14477000	1.63122600
C	1.52887100	3.55624700	-1.09602100
C	1.25505800	2.19816800	-0.96863000
C	1.17379400	4.47466100	-0.09563300
C	0.53974600	3.97472700	1.04638800
C	0.27099300	2.61189500	1.18974100
C	0.62581900	1.70331600	0.18577400
C	1.45116500	5.95055200	-0.26211900
N	0.27650700	0.31961200	0.31448100
C	1.16687100	-0.72091400	0.10095700

O	0.74920100	-1.85332400	-0.16268200
H	2.02157800	3.91260200	-1.99796000
H	1.52947200	1.51091000	-1.76406400
H	0.25277300	4.65861200	1.84199700
H	-0.20902900	2.25065000	2.09642500
H	0.79503100	6.39738200	-1.02044300
H	1.29073800	6.49555000	0.67375300
H	2.48361500	6.13189200	-0.58372300
Cu	-1.40285700	-0.12295300	-0.68480200
I	-3.74488600	-0.49886300	-1.42181800
C	-3.34051500	-1.17013000	3.00769100
C	-2.64980200	-2.34883000	2.29763200
C	-2.49519000	0.02887900	2.60180300
O	-1.11323500	-0.53338600	2.47741800
C	-1.16862300	-2.03994600	2.45132600
H	-3.33269700	-1.30204200	4.09527800
H	-4.37509200	-1.04040200	2.67944700
H	-2.92650100	-2.36475800	1.23875400
H	-2.90273600	-3.31447000	2.74418500
H	-2.42760200	0.82727400	3.34078000
H	-2.76986800	0.41715500	1.61766400
H	-0.53300700	-2.35005600	1.62164300
H	-0.75176900	-2.34812700	3.41174300

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.342090 a.u.

Sum of electronic and thermal Free Energies = -1241.705734 a.u.

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

Energy = -1242.7994250 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 80.6*i*

im4-THF

C	5.89423100	-1.64580800	-0.17074300
C	5.70307800	-2.93511000	-0.62487700
C	4.41816800	-3.46922200	-0.73672300
C	3.29537200	-2.73544600	-0.39835300
C	3.49908300	-1.44025900	0.05470600
C	4.77979300	-0.88728200	0.17413100
C	4.62160800	0.45547800	0.66953700
C	3.30935700	0.69160200	0.81265200
N	2.57648200	-0.44452700	0.43013900
H	6.88542400	-1.23117100	-0.08440500
H	6.55358200	-3.53916300	-0.89524600
H	4.29362400	-4.47964800	-1.08975200
H	2.31069600	-3.15642300	-0.46784700

H	5.40713600	1.15072900	0.89674000
H	2.81102500	1.56427800	1.17484400
H	-0.28125100	0.36413000	1.37624400
C	1.31722100	3.36689800	-1.47693200
C	1.06963700	2.05639700	-1.11534000
C	1.10099300	4.41832500	-0.58897700
C	0.63563000	4.11094700	0.68302000
C	0.40013900	2.79927900	1.06640000
C	0.62160000	1.76972200	0.16658100
C	1.33919400	5.84069100	-1.01049300
N	0.32459300	0.42205200	0.54738900
C	1.22908900	-0.66936200	0.55143400
O	0.76360400	-1.78076200	0.63143200
H	1.67250800	3.57729300	-2.47325000
H	1.22655800	1.25821700	-1.82267000
H	0.45675600	4.90491500	1.39054700
H	0.04718700	2.57531300	2.06064300
H	0.53933800	6.19498900	-1.65870400
H	1.38526900	6.50519700	-0.15276000
H	2.27048500	5.93940300	-1.56262300
Cu	-1.27637100	-0.38990600	-0.57658100
I	-3.37172000	-0.92409200	-1.75863200
C	-3.86362100	-0.25732400	3.01704900
C	-3.12548900	-1.58206100	2.84382700
C	-2.85813500	0.75242700	2.47464000
O	-1.56632000	0.14676300	2.61777900
C	-1.69448500	-1.17725400	3.14397100
H	-4.06509100	-0.06931700	4.06940600
H	-4.80485900	-0.22114300	2.47906100
H	-3.21013500	-1.93012400	1.81745600
H	-3.48554200	-2.36411600	3.50490400
H	-2.86120700	1.69348100	3.01705900
H	-3.02679600	0.95313800	1.41984500
H	-0.94899500	-1.80075400	2.66356100
H	-1.50035900	-1.15157000	4.21585800

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.334960 a.u.

Sum of electronic and thermal Free Energies = -1241.751560 a.u.

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

Energy = -1242.8204043 a.u.

No imaginary frequency

Acetone-assisted reaction (in Acetone solution)

Acetone

C	-0.43596800	-1.17518300	0.00000000
C	-0.39061600	0.33316400	0.00000000
C	-1.71955500	1.04792200	0.00000000
O	0.65045600	0.93437600	0.00000000
H	0.57201000	-1.57220000	0.00000000
H	-0.97180400	-1.53902700	0.87504600
H	-0.97180400	-1.53902700	-0.87504600
H	-1.55935600	2.11935700	0.00000000
H	-2.30263300	0.76590900	-0.87503400
H	-2.30263300	0.76590900	0.87503400

BHandHLYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.059087 a.u.

Sum of electronic and thermal Free Energies = -192.977897 a.u.

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

Energy = -193.1261117 a.u.

No imaginary frequency

ts1-Acetone

C	5.12383800	-0.64840600	0.97710700
C	5.21728200	-0.18674900	2.28065400
C	4.24413400	0.65001800	2.81969200
C	3.14501500	1.04906200	2.07038300
C	3.06922700	0.57629500	0.77851600
C	4.03300900	-0.25667500	0.21521300
C	3.62325600	-0.52457500	-1.15164000
C	2.46826500	0.10155400	-1.37267800
N	2.03935000	0.82102400	-0.20196700
H	5.88235400	-1.29364000	0.56559400
H	6.05744500	-0.47945400	2.88854100
H	4.34182300	0.99425200	3.83570700
H	2.38257600	1.68929200	2.47802200
H	4.15284400	-1.12985600	-1.86299400
H	1.86468100	0.16363100	-2.25502000
H	1.95813100	1.82010800	-0.43998400
C	1.67920800	-3.50630800	0.09083100
C	1.16380600	-2.29864100	0.52953800
C	1.33798800	-4.03026600	-1.15095700
C	0.45444500	-3.30373800	-1.94425400
C	-0.06126600	-2.09297200	-1.52024100
C	0.31045700	-1.56894500	-0.28715800
C	1.86668900	-5.36188400	-1.60484200
N	-0.24931900	-0.34942800	0.15147500
C	0.40158300	0.69960600	0.47655400
O	0.22701400	1.71259000	1.07543800
H	2.35007700	-4.05562700	0.73290900

H	1.42267800	-1.91786700	1.50370100
H	0.16116100	-3.69285400	-2.90688300
H	-0.75087600	-1.54312400	-2.14017200
H	2.03868000	-5.37630800	-2.67809100
H	2.80289200	-5.60648100	-1.11057100
H	1.16118600	-6.16057100	-1.37980700
Cu	-2.23163000	-0.22132600	0.36481700
I	-4.69115700	-0.07596600	0.41450500
C	1.10483700	5.26760500	-2.60800700
C	1.16493900	4.35278800	-1.41782800
C	0.47187500	4.80388100	-0.16569900
O	1.76382500	3.30053000	-1.48204400
H	1.76992300	4.91549300	-3.38713300
H	0.08478900	5.29385500	-2.98869400
H	1.36358200	6.28533900	-2.32443200
H	1.09488500	5.55267100	0.32398900
H	-0.47757600	5.28061500	-0.39464000
H	0.31890900	3.96914300	0.50671300

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.298304 a.u.

Sum of electronic and thermal Free Energies = -1202.469132 a.u.

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

Energy = -1203.4956303 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 134.40*i*

im2-Acetone

C	4.93700400	-0.94938900	1.14450300
C	4.97727500	-0.49226900	2.45322900
C	4.01241100	0.38318900	2.94185200
C	2.97443000	0.83144500	2.13394600
C	2.95447300	0.36029400	0.84170700
C	3.90592100	-0.51326900	0.32698100
C	3.55148500	-0.77490700	-1.05818000
C	2.43501900	-0.11156700	-1.34412000
N	1.99240500	0.66669500	-0.20286200
H	5.68836000	-1.62679300	0.77401100
H	5.76940200	-0.82137500	3.10525100
H	4.06748900	0.71998400	3.96340900
H	2.21640300	1.50351600	2.49603700
H	4.09089100	-1.40724600	-1.73797300
H	1.87378500	-0.03689600	-2.25261300
H	2.06791200	1.66733900	-0.46688400
C	1.35088600	-3.63722900	0.13121700
C	0.91674200	-2.38176000	0.52211600

C	1.02714500	-4.15877700	-1.11600300
C	0.24392400	-3.37978500	-1.96346400
C	-0.18916100	-2.12216100	-1.58643600
C	0.16681500	-1.59914800	-0.34690900
C	1.46426800	-5.53890400	-1.51997000
N	-0.30768000	-0.32878000	0.04146700
C	0.43189400	0.68659900	0.32334300
O	0.23638600	1.73845100	0.87228500
H	1.94098800	-4.22638300	0.81608500
H	1.15621600	-2.00454700	1.50273300
H	-0.03636900	-3.76530600	-2.93153800
H	-0.80404000	-1.53274500	-2.24741400
H	0.68237700	-6.27106000	-1.32276500
H	1.69223300	-5.58897000	-2.58176000
H	2.34823900	-5.85184100	-0.97099100
Cu	-2.26378200	-0.04694900	0.28415000
I	-4.71298700	0.24185900	0.38436300
C	2.19348800	5.25003700	-2.46275400
C	1.86863200	4.26983600	-1.37197100
C	0.99899600	4.74874900	-0.24851500
O	2.31306400	3.14121100	-1.41396400
H	2.94711400	4.84104000	-3.12462500
H	1.29042500	5.46466300	-3.03234500
H	2.53421900	6.19347100	-2.04215300
H	1.59936200	5.37985600	0.40730400
H	0.18613300	5.36555600	-0.62300900
H	0.60828500	3.91212900	0.31745900

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.299317 a.u.

Sum of electronic and thermal Free Energies = -1202.468393 a.u.

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

Energy = -1203.4977310 a.u.

No imaginary frequency

ts2-Acetone

C	5.30334500	-1.16966200	-0.23577800
C	5.39119100	-1.85979400	-1.43100400
C	4.24473100	-2.23903000	-2.12892200
C	2.97823500	-1.94723100	-1.64781100
C	2.90990000	-1.24902600	-0.45761600
C	4.04191000	-0.85352400	0.25585500
C	3.58202100	-0.14476300	1.43032600
C	2.24670000	-0.10440300	1.39445000
N	1.75029100	-0.84944200	0.28386700
H	6.19196000	-0.87799200	0.29968800

H	6.36004000	-2.10847900	-1.83196700
H	4.34299400	-2.77254600	-3.05979400
H	2.08495300	-2.23982600	-2.16974000
H	4.20028100	0.28820000	2.19403600
H	1.55018400	0.35052800	2.06940900
H	1.30303000	-2.02901800	0.80114500
C	2.48972500	3.36761300	-0.41471200
C	1.83717700	2.18088100	-0.70547100
C	1.98057300	4.26746300	0.51262200
C	0.78605300	3.93480300	1.14604200
C	0.12995400	2.75000200	0.86984600
C	0.65541300	1.84559800	-0.05136200
C	2.66955800	5.57301600	0.79598100
N	-0.05031400	0.66883400	-0.34784100
C	0.49347900	-0.51466000	-0.47152000
O	0.02909700	-1.49494100	-1.03388300
H	3.40761700	3.60086100	-0.93217800
H	2.23992500	1.51452600	-1.45137400
H	0.35896400	4.61611400	1.86605000
H	-0.79903100	2.51335200	1.36446200
H	2.20628500	6.39224100	0.24733800
H	2.62251800	5.82652800	1.85245400
H	3.71639200	5.53893000	0.50661700
Cu	-2.01446500	0.55207500	-0.57806300
I	-4.43392500	0.07131100	-0.31526300
C	-0.43273600	-4.81487300	1.72232600
C	-0.14325400	-3.38393600	1.44599100
C	-1.24885300	-2.39965100	1.50886400
O	1.02428000	-3.08360800	1.16549100
H	0.43327500	-5.43138700	1.51926500
H	-0.73181300	-4.92275200	2.76371400
H	-1.27897600	-5.13389400	1.11733200
H	-0.90144800	-1.41104100	1.78520900
H	-1.67936700	-2.31642300	0.50990400
H	-2.02785600	-2.72787900	2.18748600

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.299373 a.u.

Sum of electronic and thermal Free Energies = -1202.455036 a.u.

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

Energy = -1203.4963345 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 924.86*i*

im3-Acetone

C	-5.26083200	-2.45384300	-0.32223700

C	-4.98015000	-3.47230300	0.56401600
C	-3.72742100	-3.55842600	1.18079200
C	-2.73152800	-2.63832100	0.91774300
C	-3.01501900	-1.62110100	0.01305700
C	-4.27282600	-1.51092400	-0.60510200
C	-4.22719600	-0.34433700	-1.43974600
C	-3.00353500	0.20401500	-1.29481200
N	-2.24266700	-0.54771800	-0.40942400
H	-6.23114900	-2.38197800	-0.78720100
H	-5.73493100	-4.20725200	0.79261500
H	-3.53683000	-4.35654300	1.88043000
H	-1.77208600	-2.69436200	1.39816000
H	-5.01384800	0.03146900	-2.06569200
H	-2.58494700	1.07557600	-1.75407500
H	3.11203300	-1.76406900	0.59526700
C	-2.56331000	3.43072200	1.15290200
C	-1.95436200	2.20060600	0.98963100
C	-2.22693600	4.52244900	0.35724300
C	-1.25288900	4.33321300	-0.61409500
C	-0.63984800	3.10292100	-0.79062600
C	-0.98683200	2.01433900	0.00211400
C	-2.88096800	5.86015300	0.56382600
N	-0.30115700	0.79791400	-0.16660000
C	-0.85604500	-0.40034000	-0.18073300
O	-0.19515700	-1.44436200	-0.04088200
H	-3.31174900	3.54587400	1.92239700
H	-2.22744800	1.37685100	1.62798200
H	-0.96535100	5.15926600	-1.24626100
H	0.11435400	2.97493600	-1.55093400
H	-2.54520200	6.32821300	1.48831900
H	-2.65001100	6.54191300	-0.25000500
H	-3.96348000	5.76901700	0.62462600
Cu	1.63281000	0.59737600	-0.05322000
I	4.13178100	0.33839000	0.09221300
C	0.94411200	-4.14441400	0.32981600
C	1.87942900	-3.07491800	-0.06153000
C	2.05365100	-2.70567900	-1.48180300
O	2.53428200	-2.53533900	0.86524000
H	0.95689000	-4.29908900	1.40075500
H	-0.04825000	-3.83500300	0.00731200
H	1.20360600	-5.06222000	-0.19295800
H	1.18777700	-2.09176100	-1.72612600
H	2.96465800	-2.14599000	-1.65730000
H	2.01884800	-3.60003800	-2.09665100

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.302768 a.u.
Sum of electronic and thermal Free Energies = -1202.477620 a.u.
M06-2x/6-311++G** (Lanl2DZ for Cu, I)
Energy = -1203.5098299 a.u.
No imaginary frequency

ts3-Acetone

C	5.85057900	-1.54815700	-0.16263000
C	5.77779700	-2.62761800	-1.01808600
C	4.54548700	-3.06475500	-1.51083100
C	3.36245100	-2.44055900	-1.16256800
C	3.44378600	-1.35303700	-0.30184100
C	4.67250600	-0.90032200	0.20185400
C	4.39410700	0.22725100	1.04898700
C	3.06655200	0.43659900	1.02346900
N	2.44727400	-0.50387900	0.19709600
H	6.80031500	-1.20757600	0.21757400
H	6.67892500	-3.14163400	-1.31078500
H	4.51259300	-3.91210200	-2.17626200
H	2.41561800	-2.78782000	-1.52894400
H	5.10752800	0.80304100	1.60728500
H	2.48664700	1.17666100	1.53210600
H	-0.57389200	-0.13622200	1.58922900
C	1.46881600	3.54261800	-1.04172200
C	1.20795500	2.19050800	-0.93345400
C	1.04776700	4.44627800	-0.06889200
C	0.35841500	3.93868000	1.02297800
C	0.10102000	2.58148600	1.14865600
C	0.52729200	1.68763400	0.17466600
C	1.31521900	5.91788900	-0.21526200
N	0.19234100	0.30893000	0.28112800
C	1.07928500	-0.70258500	0.01811300
O	0.67719000	-1.80688200	-0.31356400
H	2.00378700	3.90454900	-1.90626400
H	1.53688700	1.51607900	-1.70743300
H	0.01456000	4.61072200	1.79382200
H	-0.43601200	2.21831500	2.01039200
H	0.70788200	6.35285500	-1.00756100
H	1.08904800	6.45336300	0.70238400
H	2.35638900	6.10948300	-0.46555100
Cu	-1.55499600	-0.06261800	-0.65806200
I	-3.95499300	-0.56634300	-1.07576500
C	-2.46609000	-1.54814200	3.92908800
C	-1.69760200	-1.40568200	2.66986100
C	-1.70628300	-2.48727600	1.67107400

O	-1.09367600	-0.32588300	2.50640300
H	-2.43006300	-0.63911800	4.51512700
H	-3.49612900	-1.80135000	3.68442900
H	-2.06246400	-2.38177000	4.50082000
H	-2.54139200	-2.27434000	0.99121900
H	-0.80562300	-2.50417800	1.06336600
H	-1.89486400	-3.44493700	2.14332400

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.301620 a.u.

Sum of electronic and thermal Free Energies = -1202.477395 a.u.

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

Energy = -1203.5122885 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = 163.38*i*

im4-Acetone

C	5.95946900	-1.52602500	-0.04096800
C	5.87182600	-2.70912900	-0.74741100
C	4.63123500	-3.22474500	-1.12529600
C	3.44961200	-2.57776300	-0.80890600
C	3.55018100	-1.38883900	-0.10227400
C	4.78528700	-0.85626300	0.28702900
C	4.51892100	0.36735500	0.99977300
C	3.19190300	0.55738000	1.01274100
N	2.55395900	-0.49399600	0.33346800
H	6.91678400	-1.12673100	0.25212800
H	6.77009800	-3.24373700	-1.00935700
H	4.58763900	-4.15211400	-1.67228900
H	2.49645400	-2.98591600	-1.08526000
H	5.24522800	1.01610600	1.45097100
H	2.61943400	1.34385700	1.45557600
H	-0.18619200	0.19601900	1.34141800
C	1.36228700	3.43818700	-1.28682100
C	1.14320000	2.09730100	-1.02930600
C	0.99827300	4.42290500	-0.37304100
C	0.41164100	4.01682300	0.81928100
C	0.19915100	2.67679100	1.10084000
C	0.57142000	1.71441900	0.17530000
C	1.20336700	5.87875500	-0.68346000
N	0.29169500	0.33637300	0.44555600
C	1.21022500	-0.73298100	0.23231800
O	0.75935600	-1.82149600	-0.02534700
H	1.81645200	3.72327400	-2.22256700
H	1.42268300	1.35447800	-1.75901500
H	0.11488700	4.75692000	1.54551700

H	-0.26556100	2.37859200	2.02716800
H	0.37030600	6.27639000	-1.26134500
H	1.28167000	6.46994700	0.22457000
H	2.10697700	6.03627000	-1.26627900
Cu	-1.44703900	-0.30380500	-0.56157300
I	-3.77056000	-0.76041700	-1.27421400
C	-3.62563200	-0.46808000	3.40228500
C	-2.30049200	-0.83007500	2.80052500
C	-2.11223400	-2.25039100	2.35667900
O	-1.43413300	0.01008500	2.65947900
H	-3.57713400	0.51560500	3.85350300
H	-4.36776300	-0.45885400	2.60432900
H	-3.94400600	-1.20630700	4.13366200
H	-2.87821500	-2.50696200	1.62745300
H	-1.13461900	-2.39235600	1.91097400
H	-2.23050400	-2.92113000	3.20588300

BHandHLYP/6-31G* (Lanl2DZ for Cu, I)

Thermal correction to Gibbs Free Energy = 0.300880 a.u.

Sum of electronic and thermal Free Energies = -1202.515466 a.u.

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

Energy = -1203.5357817 a.u.

No imaginary frequency