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Mechanistic insights into the Cu(II)/DBU-catalyzed incorporation of CO_2 into homopropargylic amines

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Table S1. Exploring the effects of methods B3LYP, CAM-B3LYP, BLYP, BHandHLYP, B3P86, and B3PW91 by comparing the energy barriers from **1a+DBU+CO_2** to **ts1-DBU** (the geometric structures of **1a**, **DBU, CO_2**, and **ts1-DBU** are optimized using B3LYP (CAM-B3LYP, BLYP, BHandHLYP, B3P86, and B3PW91)/6-31G* in MeCN solvent, and the single point energies are obtained at the M06-2x-D3/6-311++G** calculated level in solution phase).

Species	**The energy barriers (kJ/mol)**					
	B3LYP	CAM-B3LYP	BLYP	BHandHLYP	B3P86	B3PW91
ts1-DBU	74.2	73.8	74.7	74.3	71.6	71.4

Table S1 shows that the effects of DFT functionals B3LYP, CAM-B3LYP, BLYP, BHandHLYP, B3P86, and B3PW91 on the energy barriers from **1a+DBU+CO_2** to **ts1-DBU** are very small (see Figure 1).

Table S2. Exploring the effects of basis sets 6-31G*, 6-31G**, 6-31+G*, and 6-311G* by comparing the energy barriers from **1a+DBU+CO_2** to **ts1-DBU** (the geometric structures of **1a**, **DBU, CO_2**, and **ts1-DBU** are optimized using B3LYP/6-31G* (6-31G**, 6-31+G*, and 6-311G*) in MeCN solvent, and the single point energies are obtained at the M06-2x-D3/6-311++G** calculated level in solution phase).

Species	**The energy barriers (kJ/mol)**			
	6-31G*	6-31G**	6-31+G*	6-311G*
ts1-DBU	74.2	74.2	75.4	74.4

Table S2 shows that the effects of basis sets 6-31G*, 6-31G**, 6-31+G*, and 6-311G* on the energy barriers from **1a+DBU+CO_2** to **ts1-DBU** are very small (see Figure 1).

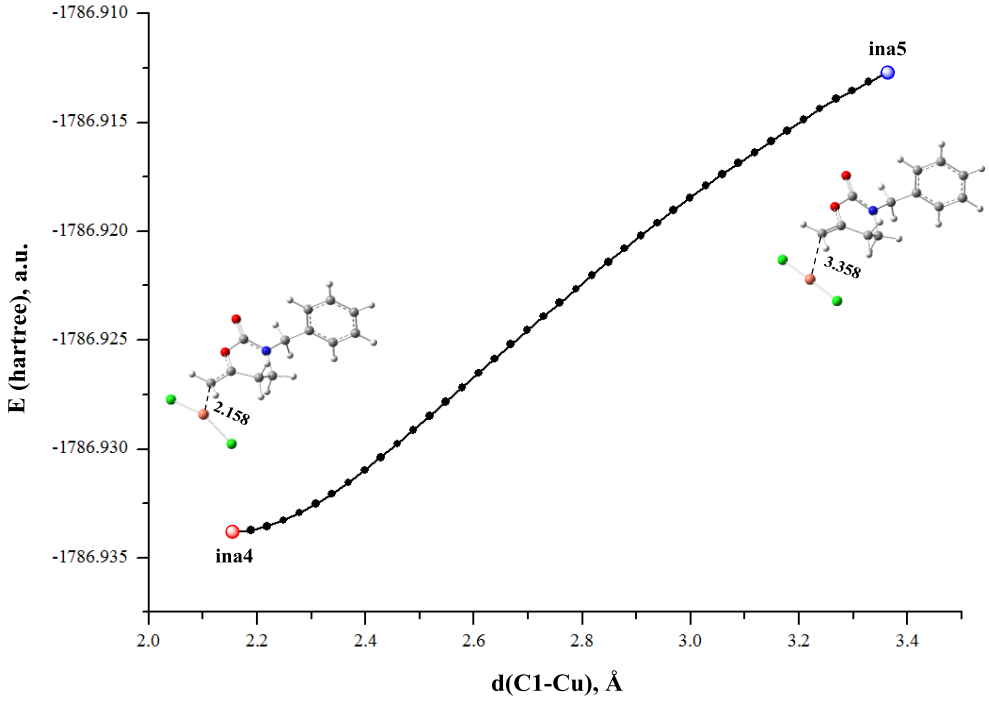


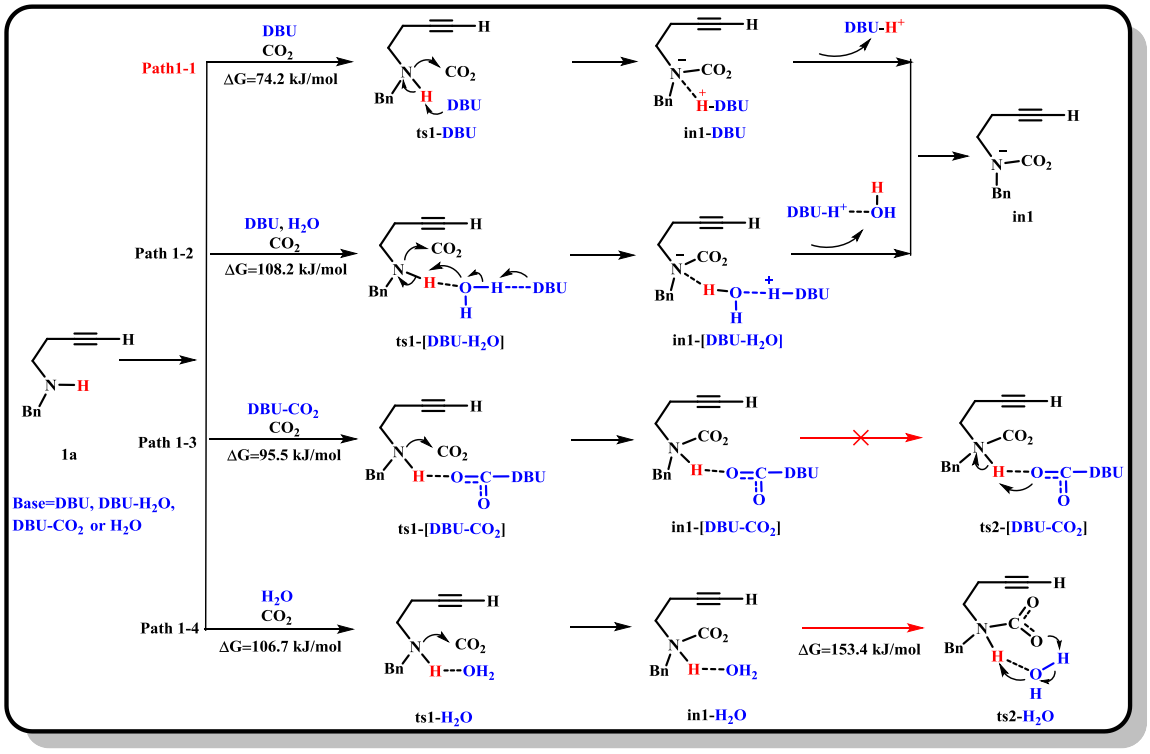
Figure S1. Scan profile from **ina4** to **ina5** along with the fracture of C1-Cu bond (from 2.158 to 3.358 Å).

Possible mechanisms for the four elementary processes

From Figure 1, the Cu(II)-catalyzed reaction is divided into four processes, including the deprotonation of **1a**, the intramolecular cyclization, the protonation of **ina3**, and the formation of **P1**. In this section, the possible mechanisms for above-mentioned processes will be discussed step by step, aiming to reduce the energy barrier (< 131.4 kJ/mol) and to further explore the role of DBU in catalytic reactions.

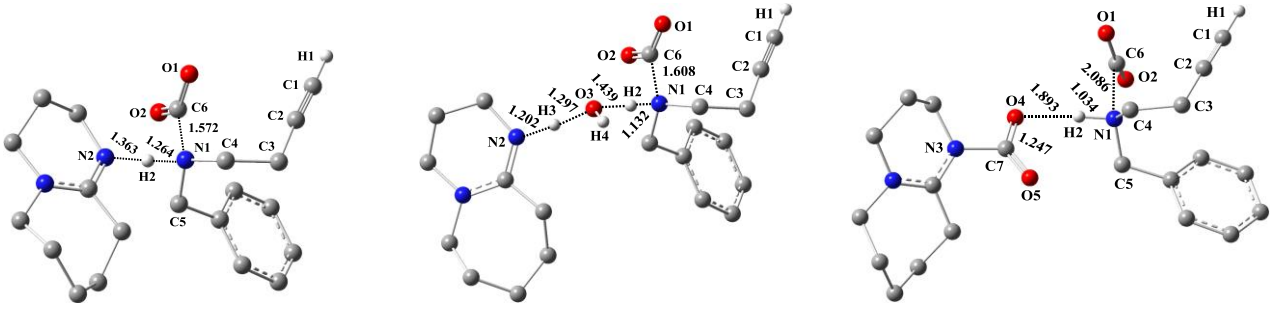
For the deprotonation of 1a

Scheme S1. Possible reaction paths for the deprotonation of **1a** with the assistance of base (Unit: kJ/mol).

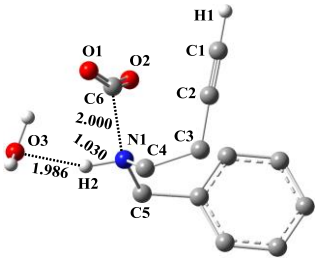


As shown in Path 1-2 of Scheme S1, the intermediate **in1** can be obtained from **1a** through a transition state **ts1-[DBU-H_2O]** and an intermediate **in1-[DBU-H_2O]**. In **ts1-[DBU-H_2O]**, DBU as a proton-acceptor captures $H3^+$ from the trace amounts H_2O (presented in solvent), and H_2O assists proton transfer as a proton-bridge ($H3^+$ of H_2O is shifted from O3 to N2; $H2^+$ of **1a** is shifted from N1 to O3, see Figure S1). In addition, DBU as a nucleophile attacks CO_2 to get DBU-CO_2, this transformation has been reported previously.[1-4] From Path 1-3 of Scheme S1, DBU-CO_2 as a

hydrogen-bond acceptor interacts with **1a** via a hydrogen-bond of O4⋯H2-N1 to promote the incorporation of CO_2 into **1a**. In **ts1-[DBU-CO_2]**, the bond lengths of H2⋯O4, N1-H2, and N1-C6 are 1.893, 1.034, and 2.086 Å, respectively (see Figure S1). Besides, H_2O, which is similar to DBU-CO_2, also serves as a hydrogen-bond acceptor to interact with **1a** via a hydrogen-bond of O3⋯H2-N1. In **ts1-H_2O**, the bond lengths of H2⋯O3, N1-H2, and N1-C6 are 1.986, 1.030, and 2.000 Å, respectively (see Figure S1). As described in Scheme S1, the energy barriers of **ts1-[DBU-H_2O]**, **ts1-[DBU-CO_2]**, and **ts1-H_2O** are 34.0, 21.3, and 32.5 kJ/mol higher than that of **ts1-DBU** (108.2, 95.5, and 106.7 *vs.* 74.2 kJ/mol), demonstrating that Paths 1-2, 1-3, and 1-4 are quite unfavorable when compared with Path 1-1. The catalytic abilities of DBU-H_2O, DBU-CO_2, and H_2O are weaker than that of DBU for assisting the incorporation of CO_2 into **1a** by the deprotonation of **1a**.



ts1-DBU **ts1-[DBU-H_2O]** **ts1-[DBU-CO_2]**

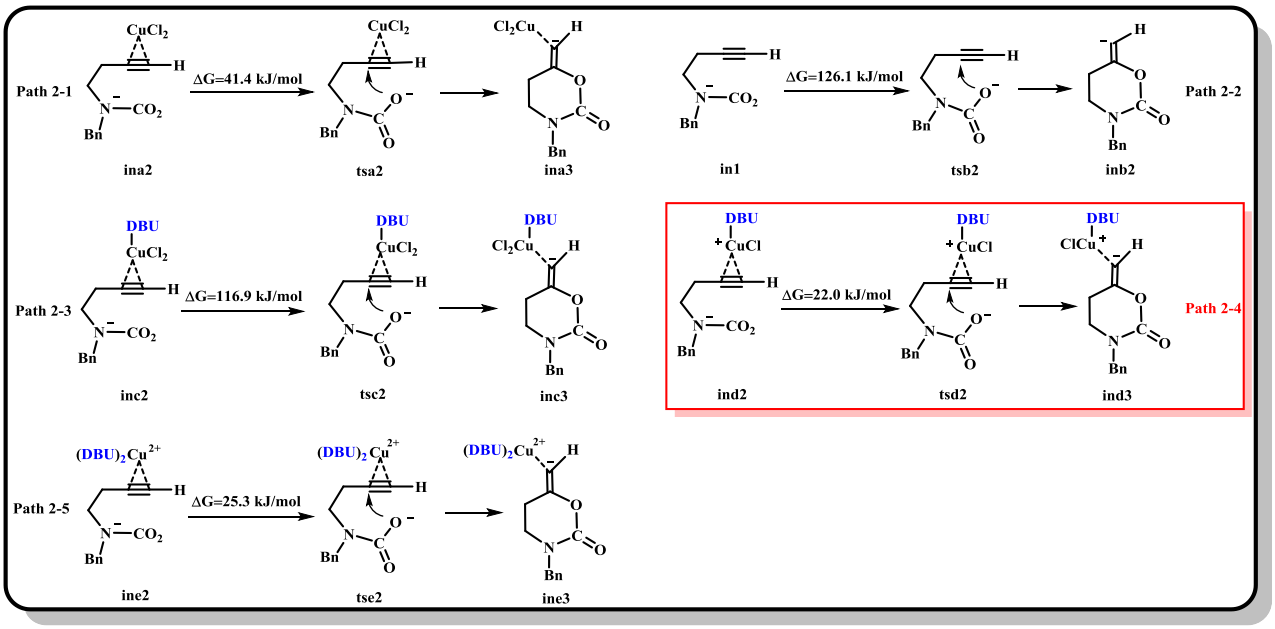


ts1-H_2O

Figure S2. Optimized structures of the deprotonation of **1a**. The H atom that does not participate in the reactions has been omitted for clarity. Bond distance is given in Å.

For the intramolecular cyclization

Scheme S2. Possible reaction paths for the intramolecular cyclization (Unit: kJ/mol).



The possible reaction paths (from Path 2-1 to Path 2-5) for the ring-closing reaction between C2 with O1 are described in Scheme S2. The geometric structures of transition states are shown in Figure S2. From Path 2-2, the mechanism of cyclization without the involvement of metal catalysts is firstly studied. The intermediate **in1** passes through a 6-membered cyclization (**tsb2**) to obtain **inb2**. The energy barrier for **tsb2** is 126.1 kJ/mol, which is higher than that of **tsa2** (41.4 kJ/mol, see Path 2-1). Obviously, the metal catalyst $CuCl_2$ is crucial for the cyclization between O1 with C2 (84% *vs.* traces for the yield of **P1**, see entries 2 and 4 of Table 1). Secondly, DBU molecule coordinates with Cu(II) to form a new catalytic species (DBU)$CuCl_2$ as a ligand, and then (DBU)$CuCl_2$ is employed to catalyze the intramolecular cyclization (see Path 2-3 of Scheme S2). However, **tsc2** has a high activation energy barrier relative to **tsa2** (116.9 *vs.* 41.4 kJ/mol), demonstrating that the catalytic effect of (DBU)$CuCl_2$ is negative on the intramolecular cyclization. Thirdly, Figure S3 shows that the formation of a new coordinated species $[(DBU)CuCl]^+$ releases the energy of 76.6 kJ/mol, in which DBU as a ligand tends to coordinate with Cu(II) by replacing Cl^- anion. The

activation energy barrier of **tsd2** is only 22.0 kJ/mol, indicating that the catalysis of $[(DBU)CuCl]^+$ is quite effective when compared with that of $CuCl_2$ for the intramolecular cyclization (see Path 2-4 *vs.* Path 2-1, see Scheme S2). Besides, two DBU molecules can also replace two Cl^- anions to coordinate with Cu(II) as the ligands, but it needs to absorb the energy of 6.7 kJ/mol for the formation of $[(DBU)_2Cu]^{2+}$ from $[(DBU)CuCl]^+$ (-69.9 *vs.* -76.6 kJ/mol, see Figure S3). What's more, the free energy barrier of **tse2** is 3.3 kJ/mol higher than that of **tsd2** (25.3 *vs.* 22.0 kJ/mol). Clearly, the catalytic activity of $[(DBU)_2Cu]^{2+}$ is also weaker than that of $[(DBU)CuCl]^+$. According to the above discussion, it can be seen that $[(DBU)CuCl]^+$ is the most effective catalyst for the cyclization reaction, and the energy barrier for $[(DBU)CuCl]^+$-catalyzed ring-closing reaction (**tsd2**) is as low as 22.0 kJ/mol. In this reaction, one molecule DBU coordinates with Cu(II) as the ligand to replace one Cl^- anion.

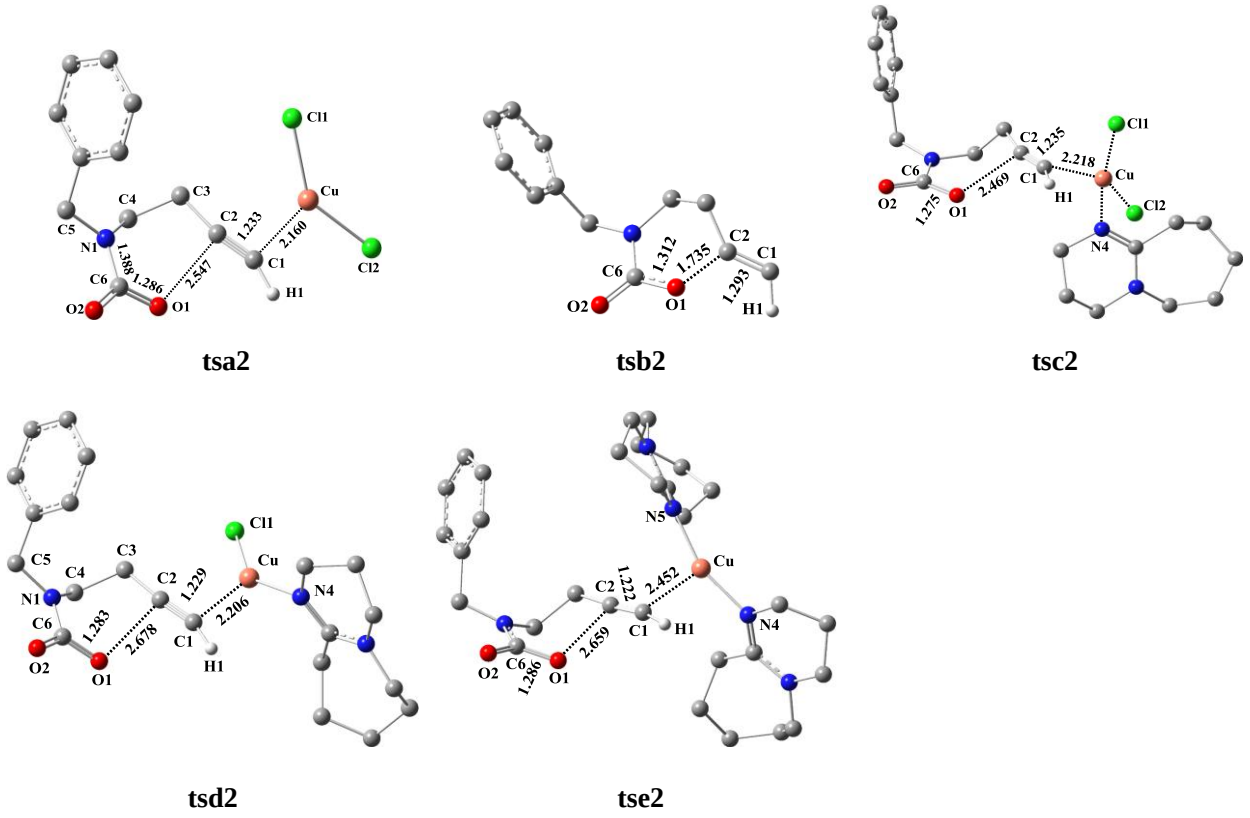


Figure S3. Optimized structures of the intramolecular cyclization. The H atom that does not participate in the reactions has been omitted for clarity. Bond distance is given in Å.

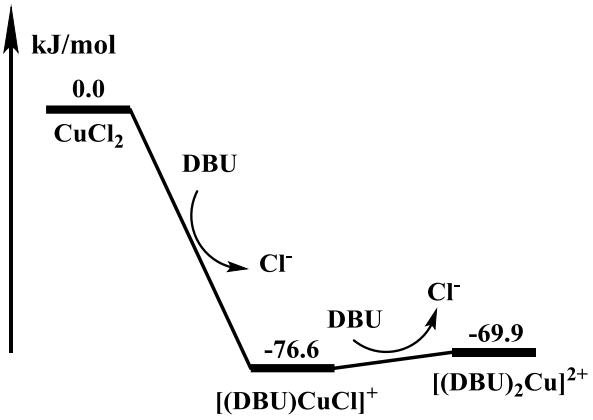
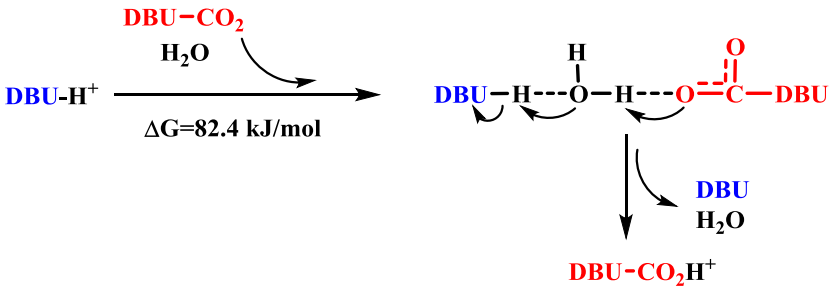


Figure S4. DBU molecule as a ligand instead of Cl^- coordinates with Cu(II) to form new catalytic species $[(DBU)CuCl]^+$ or $[(DBU)_2Cu]^{2+}$.

For the protonation of in3

Scheme S3. The mechanism of DBU-CO_2 as a proton-acceptor to get a proton from DBU-H^+ forming DBU-CO_2H^+ through the assistance of H_2O (as a proton-bridge).

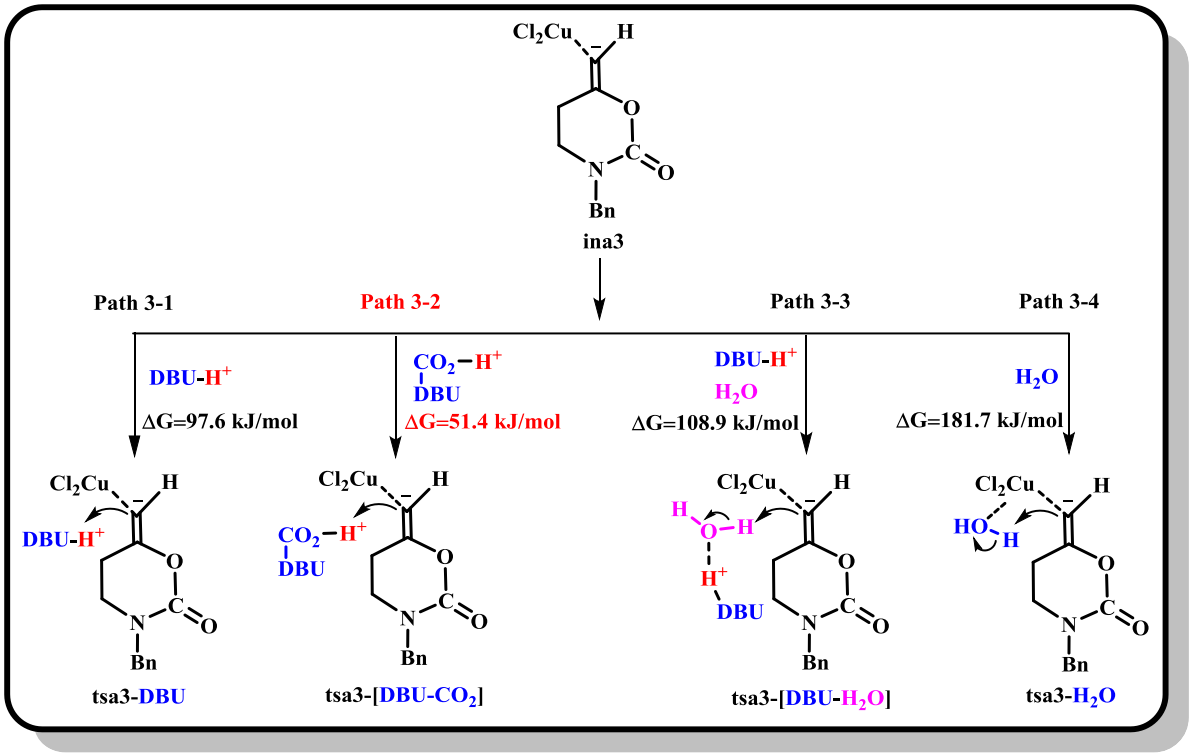


Through computation and analyzing, we are surprised to find that DBU-CO_2 can serve as a proton-acceptor to obtain a proton with the assistance of H_2O, constructing a new protonated species DBU-CO_2H^+, in which H_2O assists proton shift from DBU-H^+ to DBU-CO_2 as a proton-bridge (see Scheme S3).

Similar to DBU-H^+, DBU-CO_2H^+ can be used as a proton-donor, transmitting H^+ from O4 of DBU-CO_2H^+ to C1 of **ina3** via a transition state **tsa3-[DBU-CO_2]**, as shown in Path 3-2 of Scheme S4. The free energy barrier for **tsa3-[DBU-CO_2]** is 46.2 kJ/mol lower than that of **tsa3-DBU** (97.6 *vs.* 51.4 kJ/mol), indicating that the proton-donating ability of DBU-CO_2H^+ is relatively strong relative to DBU-H^+. Furthermore, DBU-H^+···H_2O can provide a proton to C1 via a transition state

tsa3-[DBU-H_2O] (see Path 3-3 of Scheme S4). In this transformation, DBU-H^+ plays the role of hydrogen-bond donor, and interacts with H_2O by a hydrogen-bond of N2-H2···O3 (see Figure S4). The energy barrier for **tsa3-[DBU-H_2O]** is higher than that of **tsa3-[DBU-CO_2]** (108.9 *vs.* 51.4 kJ/mol). It is mean that the proton-donating ability of DBU-H^+···H_2O is weaker than that of DBU-CO_2H^+. Besides, a proton of H_2O can also be shifted to C1 directly without the assistance of DBU-H^+ (see Path 3-4 of Scheme S4). However, the free energy barrier for **tsa3-H_2O** is as high as 181.7 kJ/mol, which is a rather high energy barrier for the protonation of **ina3**. Based on the above discussion, Path 3-2 is the most appropriate for the $CuCl_2$-catalyzed protonation of **ina3** with DBU-CO_2H^+ as the proton source.

Scheme S4. Possible reaction paths for the $CuCl_2$-catalyzed protonation of **ina3** (Unit: kJ/mol).



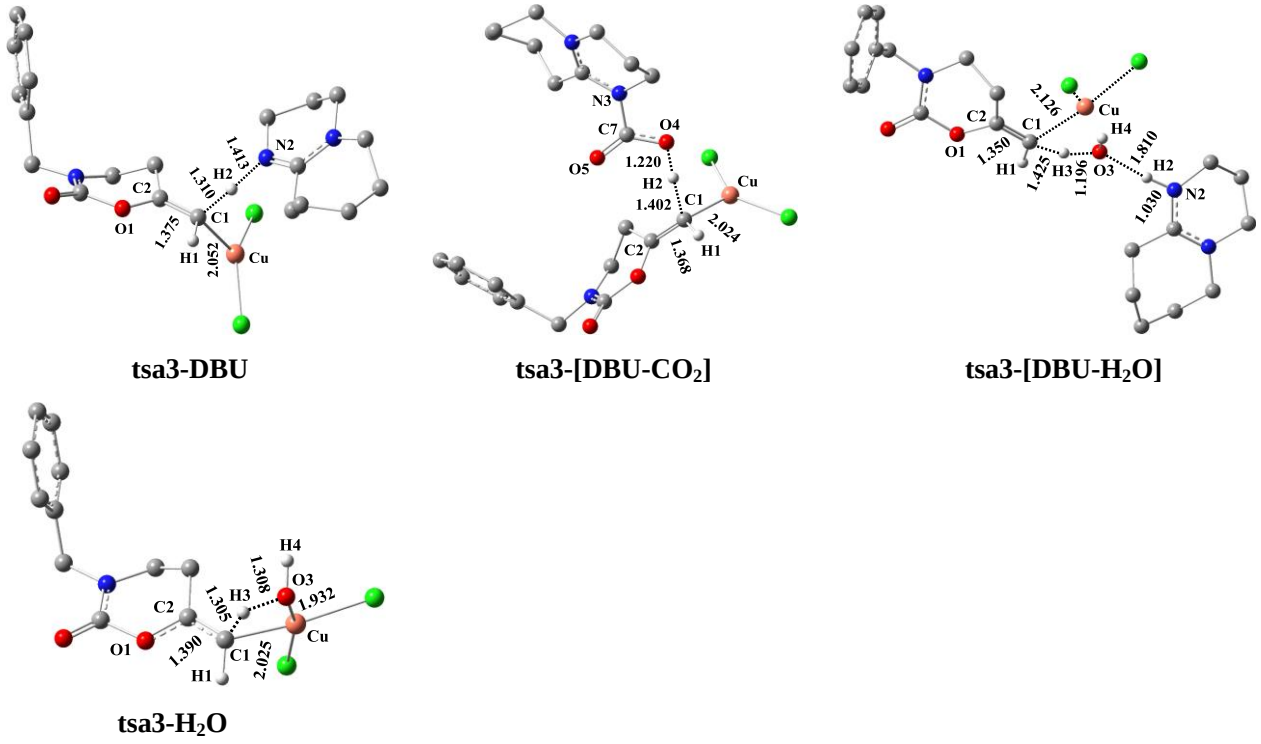
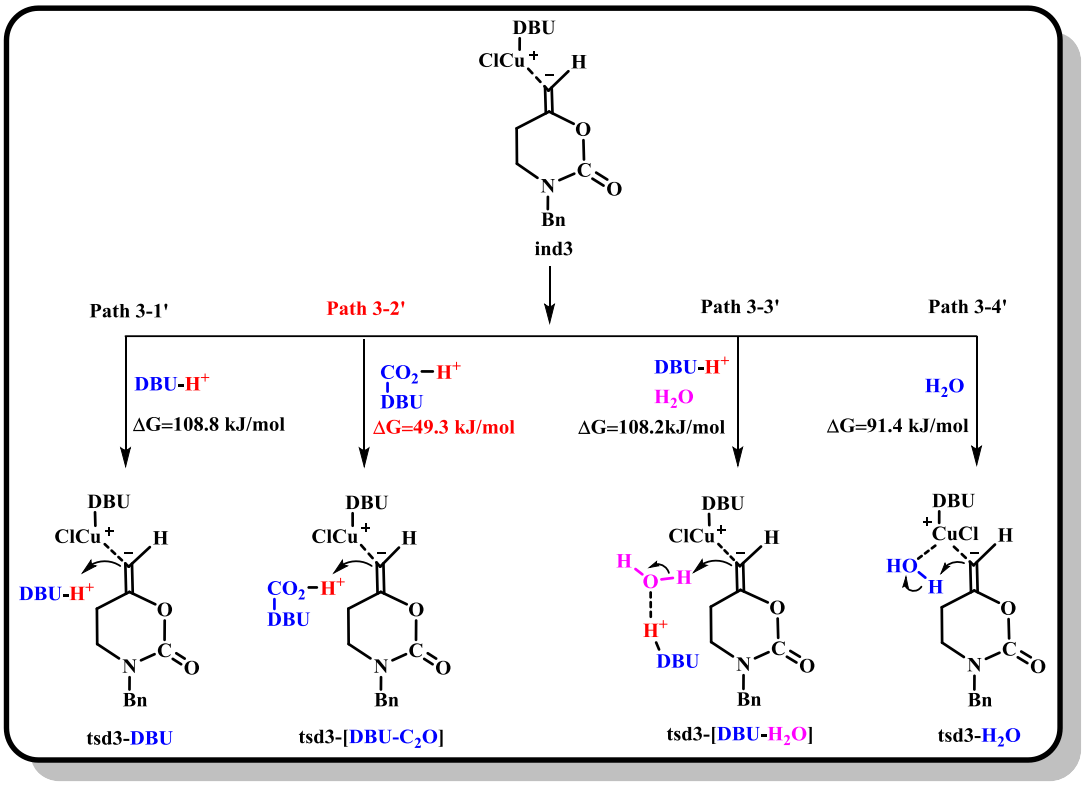
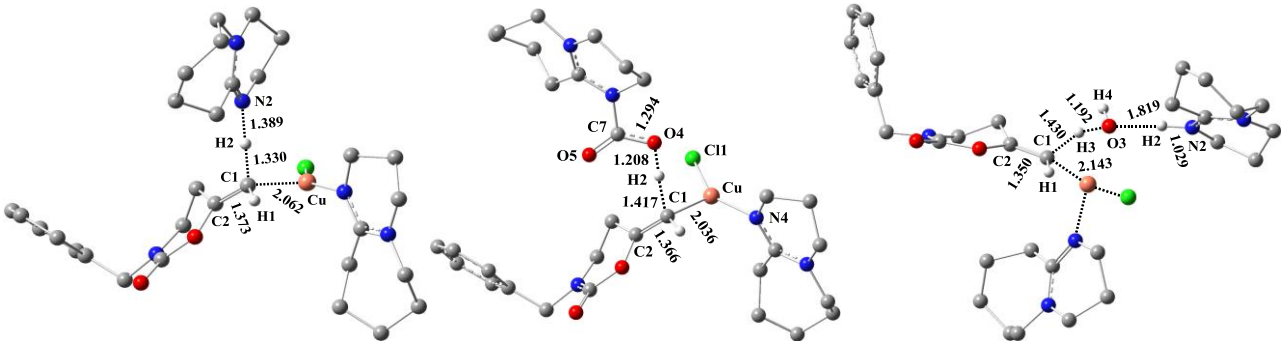


Figure S5. Optimized structures of the protonation of **ina3**. The H atom that does not participate in the reactions has been omitted for clarity. Bond distance is given in Å.

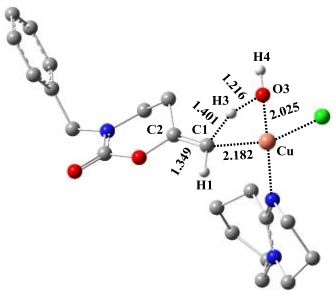
Scheme S5. Possible reaction paths for the $[(DBU)CuCl]^+$-catalyzed protonation of **ind3** (Unit: kJ/mol).



For the $[(DBU)CuCl]^+$-catalyzed reactions (see Scheme S5), $CuCl_2$ is replaced by $[(DBU)CuCl]^+$ to catalyze the protonation of **ind3**. The intermediate **ind3**, which is similar to **ina3,** captures a proton from DBU-H^+, DBU-CO_2H^+, DBU-$H^+\cdots H_2O$, or H_2O. The free energy barriers for **tsd3-DBU**, **tsd3-[DBU-CO_2]**, **tsd3-[DBU-H_2O]**, and **tsd3-H_2O** are 108.8, 49.3, 108.2, and 91.4 kJ/mol, respectively. It can be seen that 49.3 kJ/mol is the lowest in energy, which indicates that Path 3-2' is optimal path for the protonation of **ind3** in Scheme S5. More importantly, the free energy barrier for $[(DBU)CuCl]^+$-catalyzed optimal path (Path 3-2') is lower than that of $CuCl_2$-catalyzed optimal path (Path 3-2) (49.3 *vs.* 51.4 kJ/mol, see Schemes S4 and S5). Thus, the $[(DBU)CuCl]^+$-catalyzed protonation of **ind3** with DBU-CO_2H^+ as the proton source is the most effective catalytic strategy. In this reaction, DBU can not only act as the nucleophilic agent to attack CO_2 forming DBU-CO_2, but also serve as the ligand to replace Cl^- of $CuCl_2$ forming the active catalyst $[(DBU)CuCl]^+$ with the release of 76.6 kJ/mol.



tsd3-DBU **tsd3-[DBU-CO_2]** **tsd3-[DBU-H_2O]**

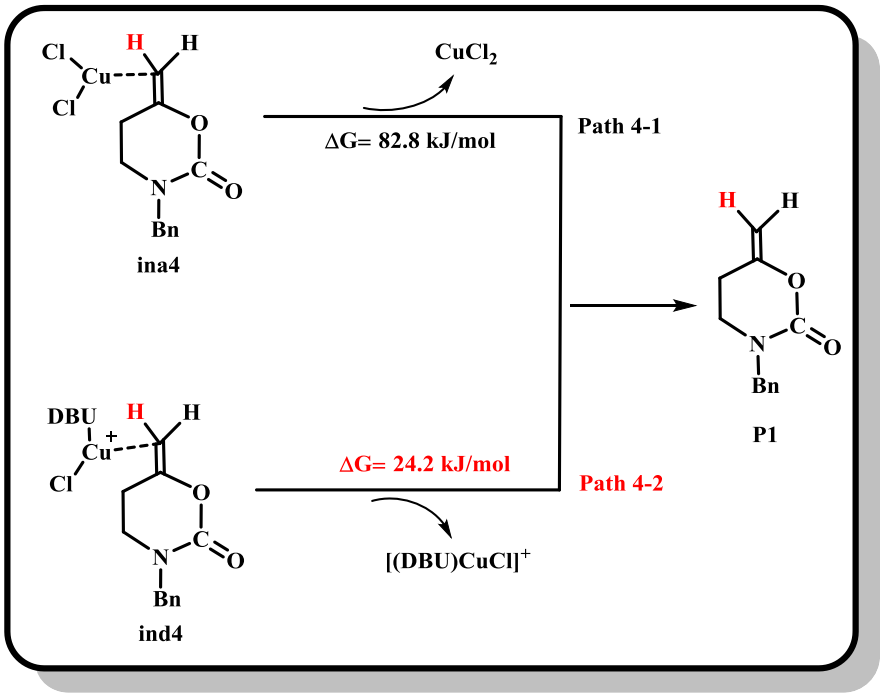


tsd3-H_2O

Figure S6. Optimized structures of the protonation of **ind3**. The H atom that does not participate in the reactions has been omitted for clarity. Bond distance is given in Å.

For the formation of P1

Scheme S6. Possible reaction paths for the formation of **P1** (Unit: kJ/mol).



Through the comprehensive analysis for the above three elementary reactions, the two possible reaction paths (Path 4-1 and Path 4-2) for the formation of **P1** are described in Scheme S6. From Path 4-1, **ina4** is directly dissociated into products **P1** and $CuCl_2$ with the absorption energy of 82.8 kJ/mol, but the formation of **P1** requires the energy of 24.2 kJ/mol from **ind4** in Path 4-2. Briefly, Path 4-2 is advantageous when compared to Path 4-1 for the synthesis of **P1** using $[(DBU)CuCl]^+$ as the catalyst and DBU-CO_2 as the assistance molecular.

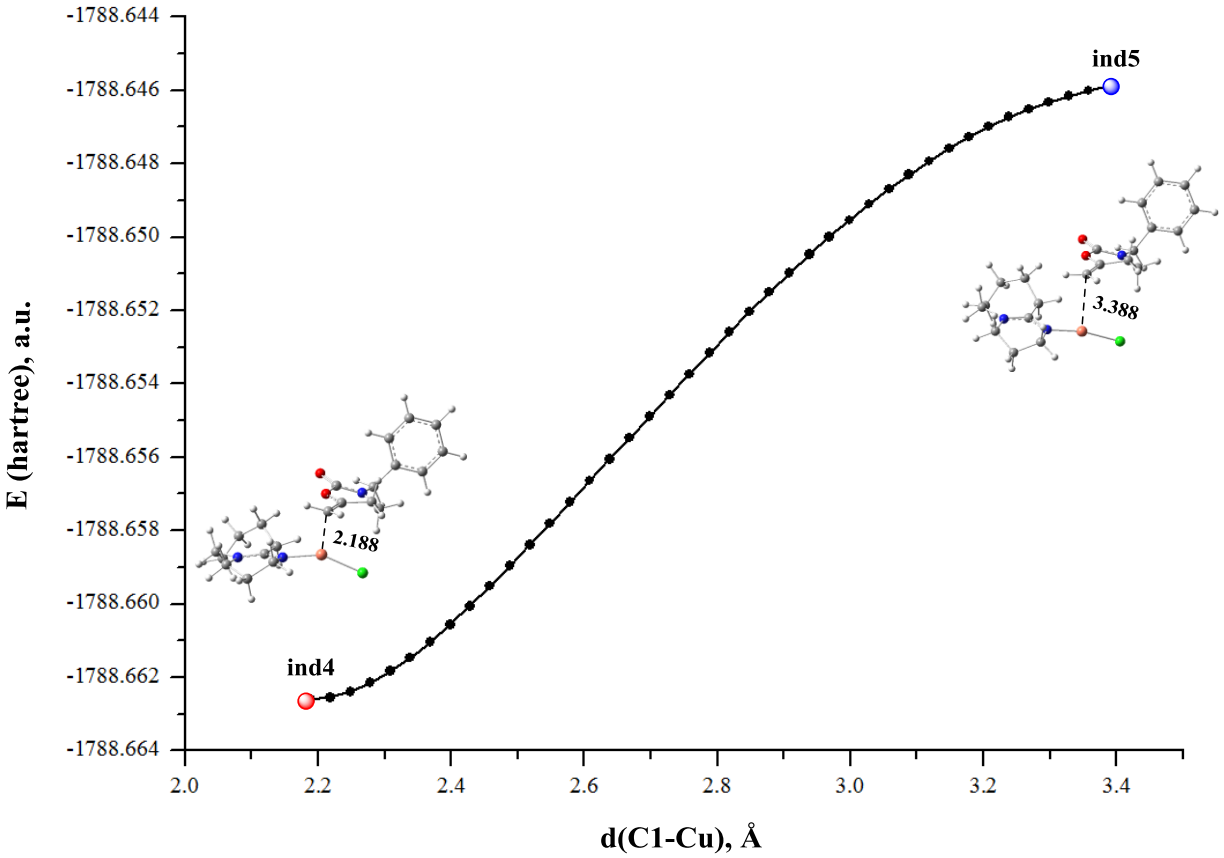


Figure S7. Scan profile from **ind4** to **ind5** along with the fracture of C1-Cu bond (from 2.188 to 3.388 Å).

Similar to the process from **ina4** to **ina5**, we tried our best to find a transition state in the formation of **P1** (from **ind4** to **ind5**), but we also failed. This experimental phenomenon can also be reasonably explained by the loose scan profile. Figures S7 shows that the energy curve is sharply rising in energy with the fracture of C1-Cu bond from **ind4** to **ind5**.

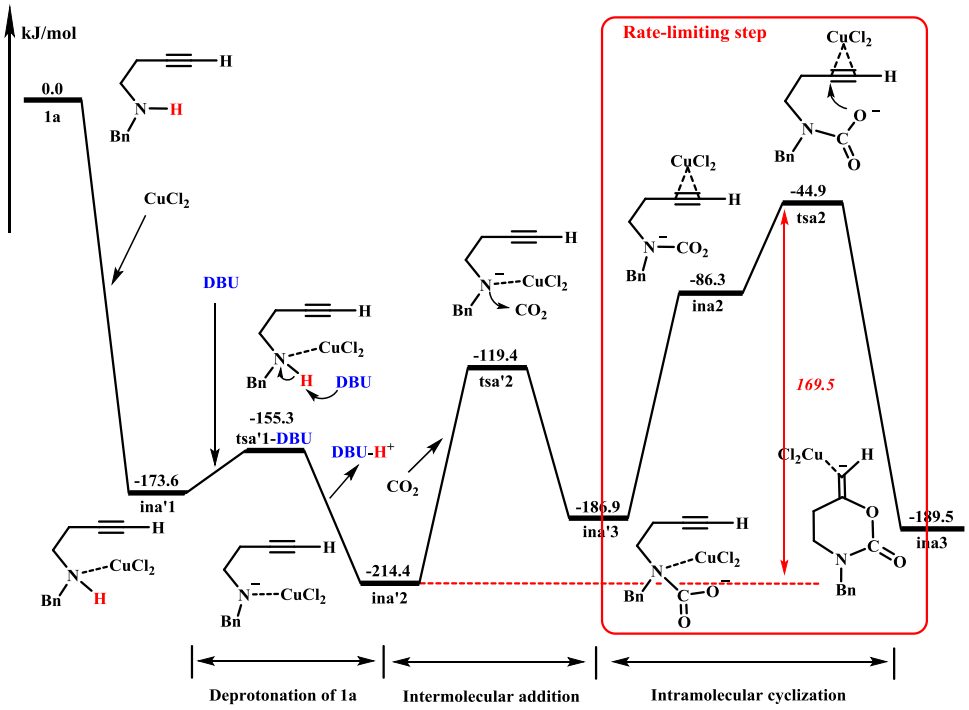


Figure S8. Energy profile of the $CuCl_2$-promoted reaction of **1a** and CO_2 with the coordination between Cu(II) and N1 of **1a** ($CuCl_2$/N1).

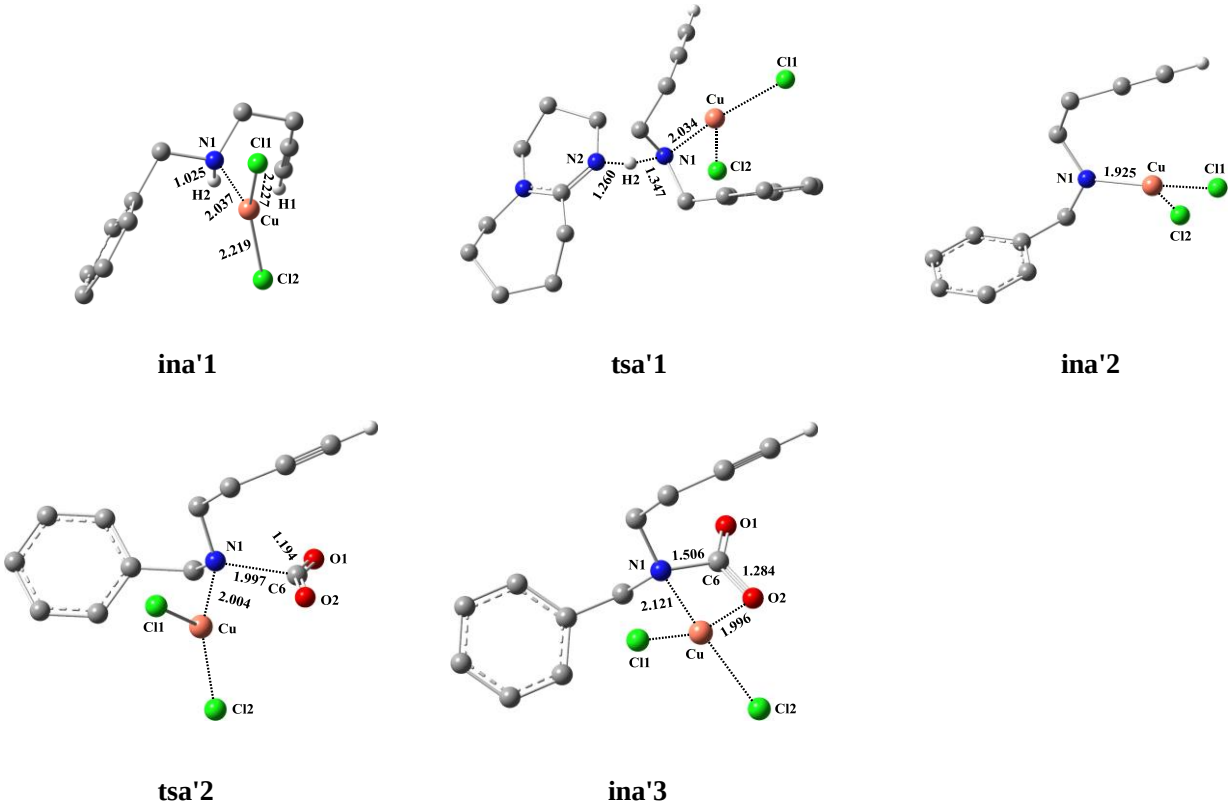


Figure S9. Optimized structures for the $CuCl_2$-promoted reaction with the coordination between Cu(II) and N1 of **1a** ($CuCl_2$/N1). The H atom that does not participate in the reactions has been omitted for clarity (bond lengths: Å).

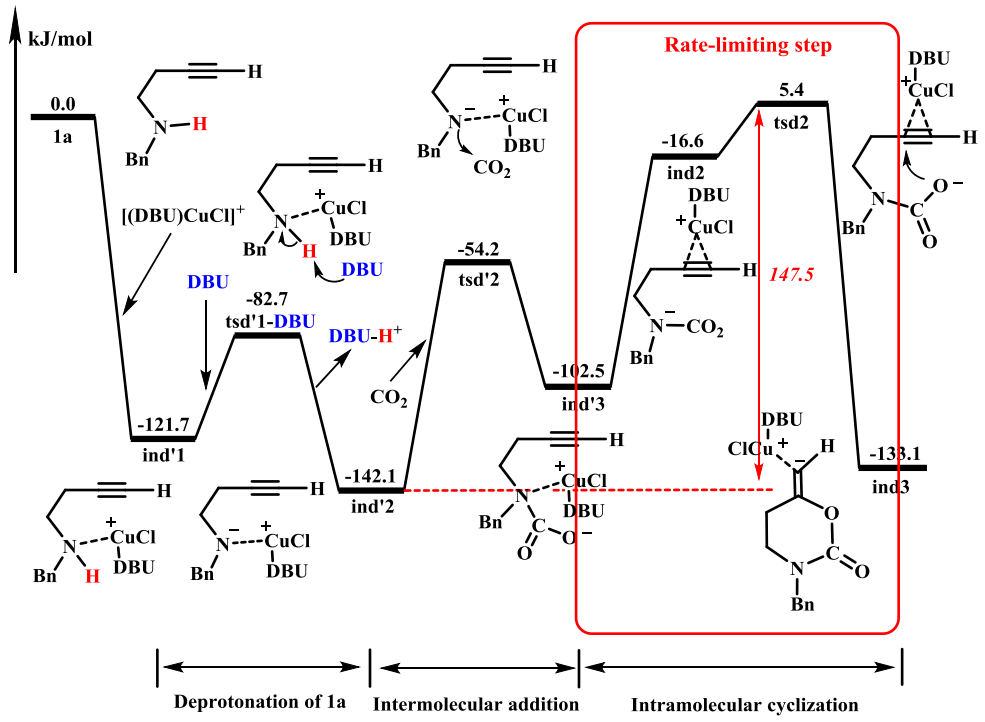
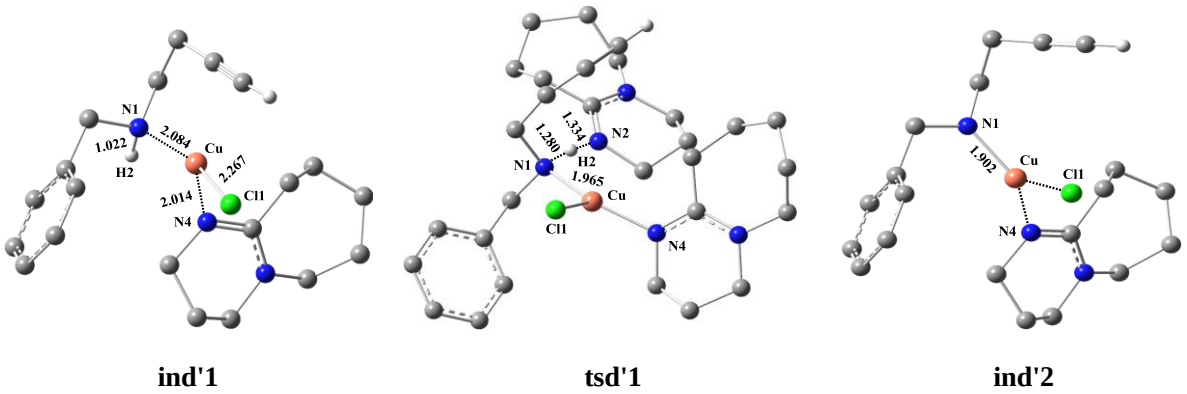


Figure S10. Energy profile of the $[(DBU)CuCl]^+$-promoted reaction of **1a** and CO_2 with the coordination between Cu(II) and N1 of **1a** ($[(DBU)CuCl]^+$/N1).



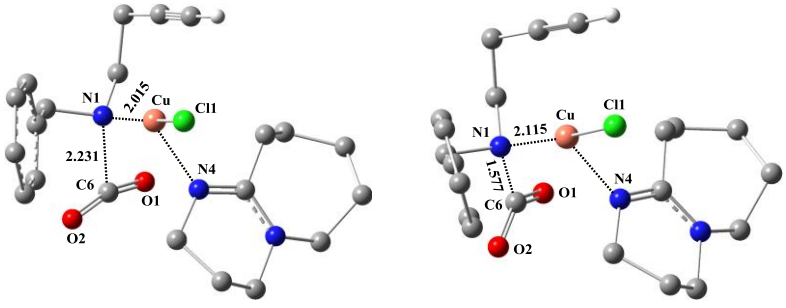


Figure S11. Optimized structures for the $[(DBU)CuCl]^+$-promoted reaction with the coordination between Cu(II) and N1 of **1a** ($[(DBU)CuCl]^+$/N1). The H atom that does not participate in the reactions has been omitted for clarity (bond lengths: Å).

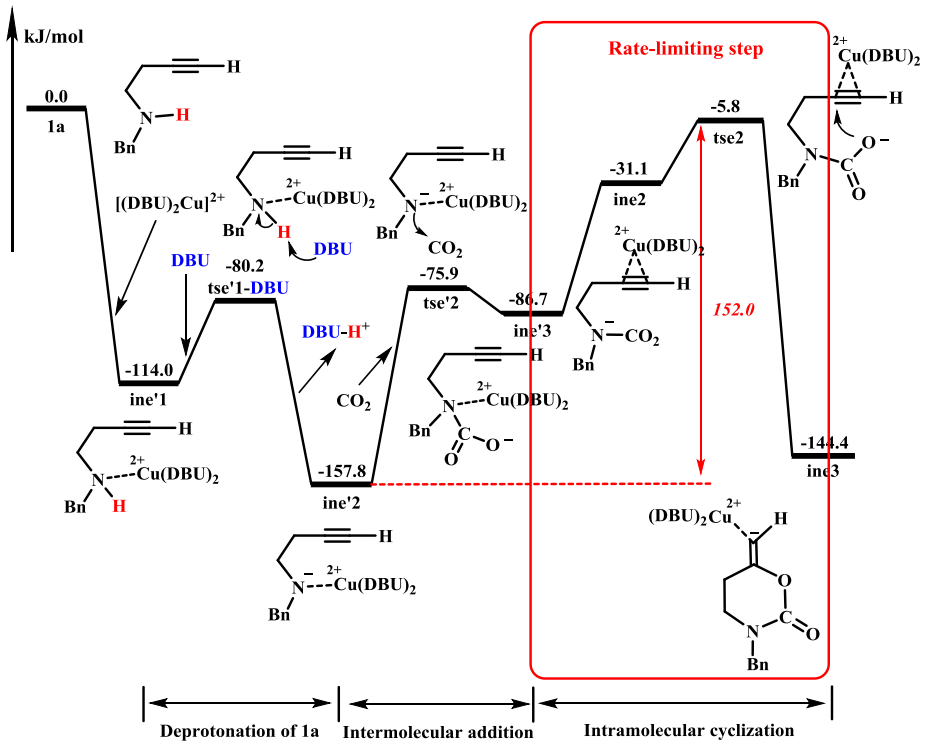
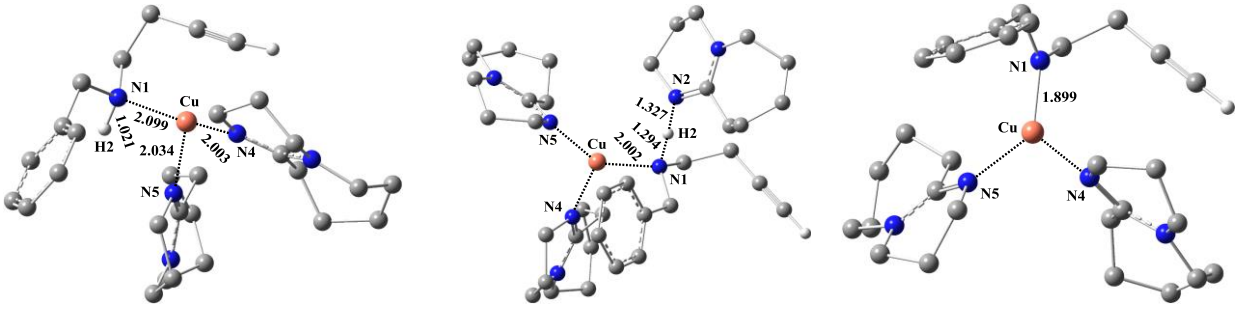
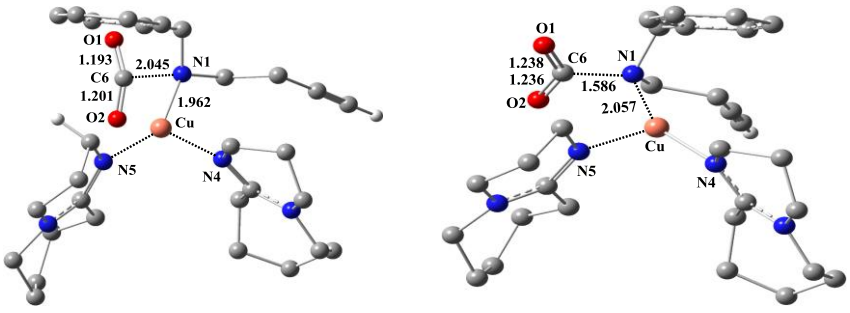


Figure S12. Energy profile of the $[(DBU)_2Cu]^{2+}$-promoted reaction of **1a** and CO_2 by the coordination between Cu(II) and N1 of **1a** ($[(DBU)_2Cu]^{2+}$/N1).



ine'1 **tse'1** **ine'2**



tse'2 **ine'3**

Figure S13. Optimized structures for the $[(DBU)_2Cu]^{2+}$-promoted reaction with the coordination between Cu(II) and N1 of **1a** ($[(DBU)_2Cu]^{2+}$/N1). The H atom that does not participate in the reactions has been omitted for clarity (bond lengths: Å).

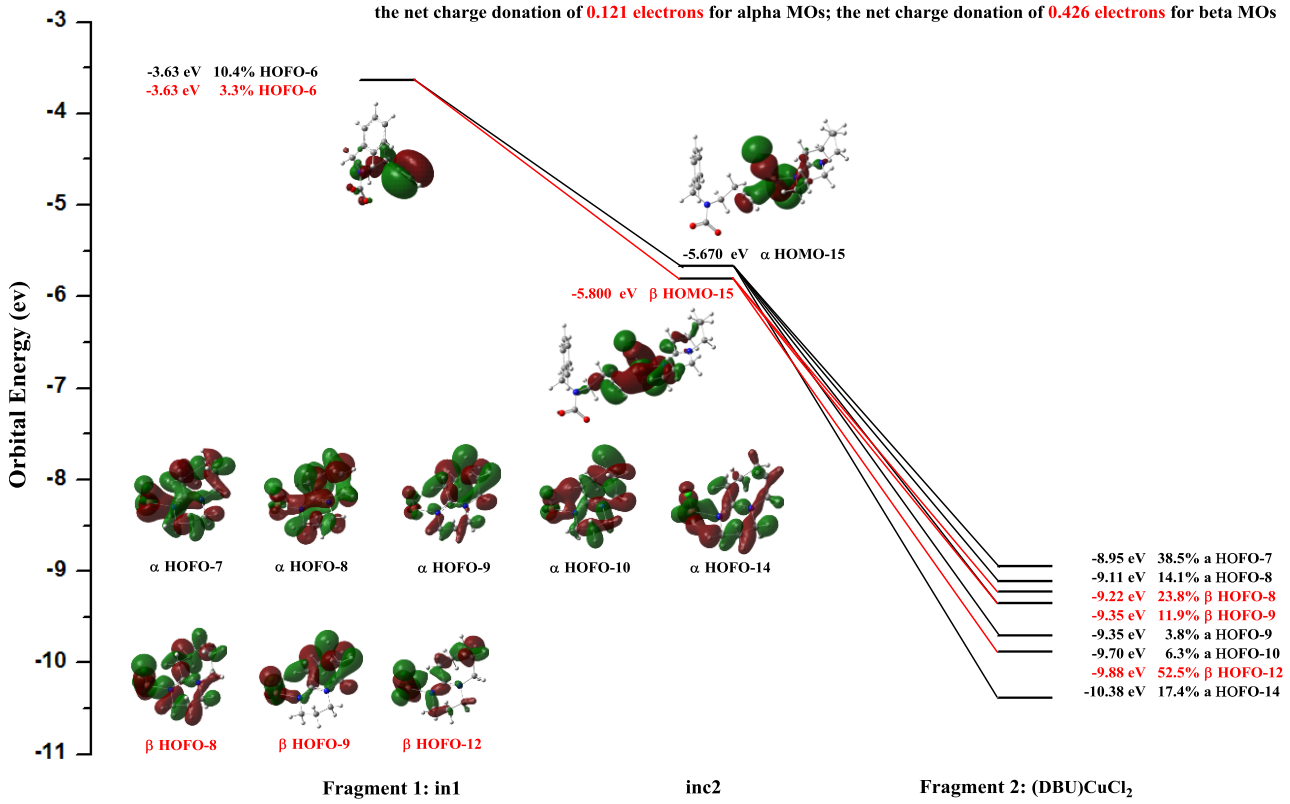


Figure S14 The orbital interaction diagram of **in1** with (DBU)$CuCl_2$ in **inc2** (α, β-MOs are described in black and red, respectively; the net charge donation is 0.547 e from **in1** to (DBU)$CuCl_2$).

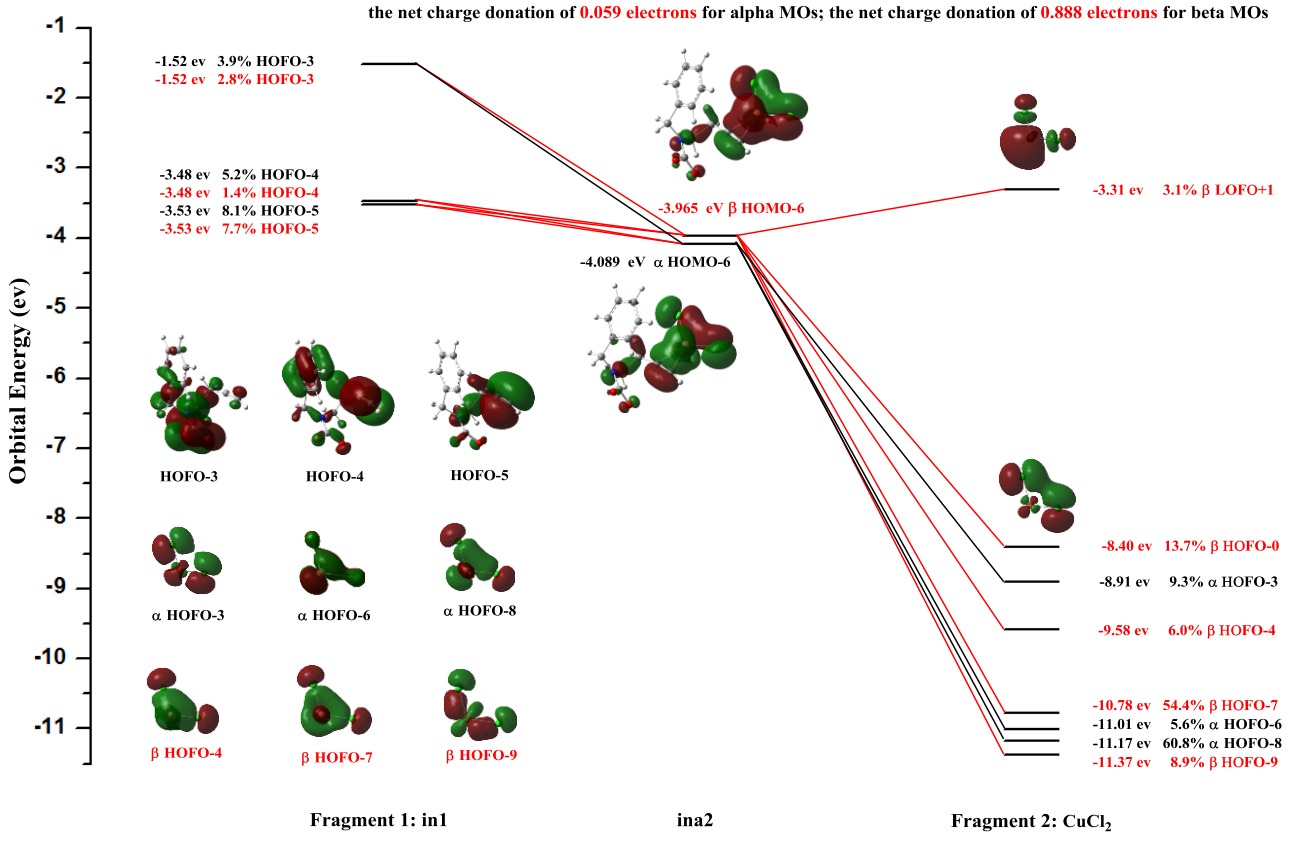


Figure S15. The orbital interaction diagram of **in1** with $CuCl_2$ in **ina2** (α, β-MOs are described in black and red, respectively; the net charge donation is 0.947 e from **in1** to $CuCl_2$).

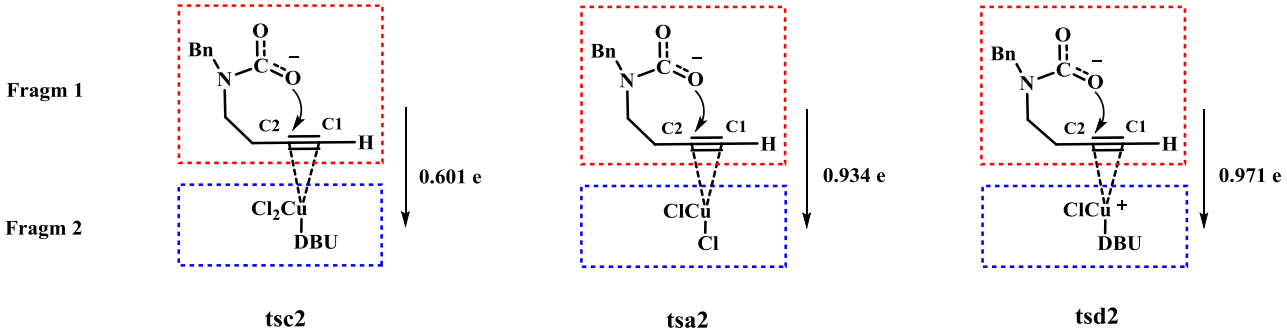


Figure S16. The donation of net Mulliken charges form fragment 1 to fragment 2 in **tsc2**, **tsa2**, and **tsd2**.

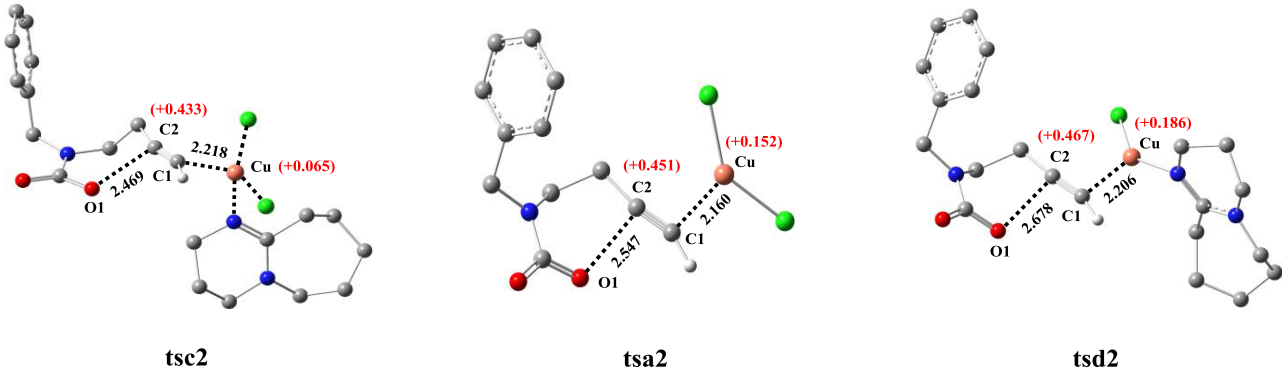


Figure S17. The bond lengths (black) and the Mulliken charges (red) of **tsc2**, **tsa2**, and **tsd2**.

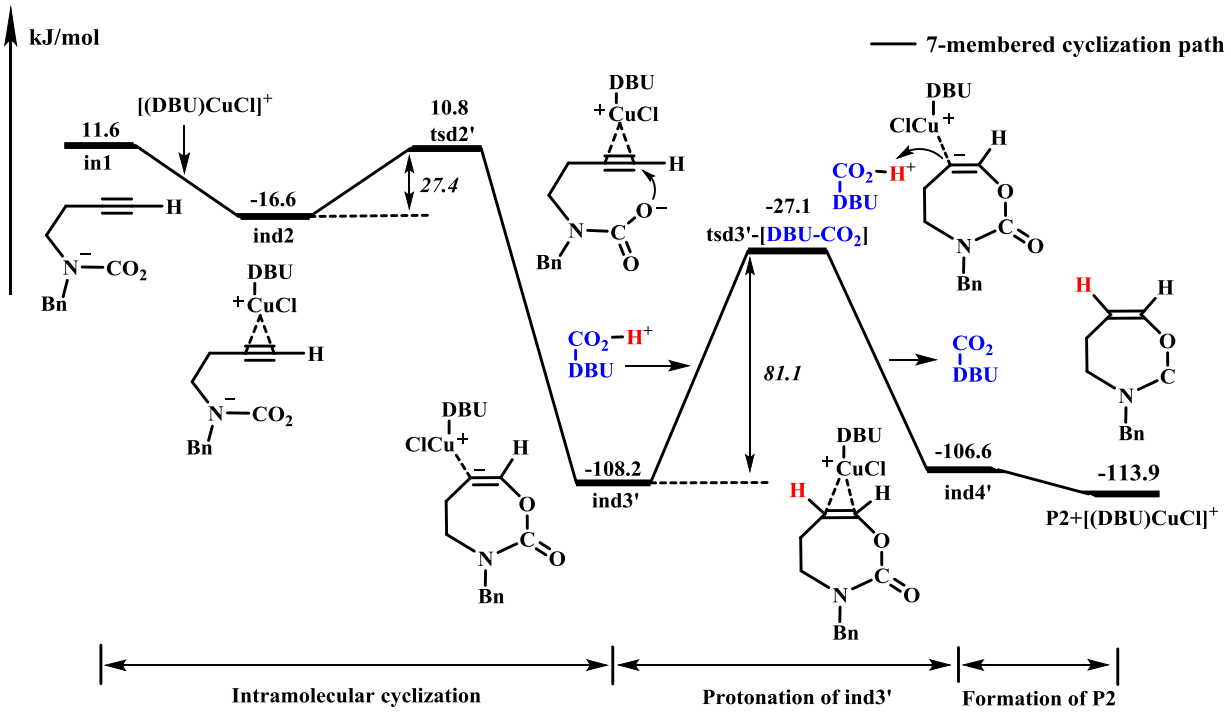


Figure S18. Energy profile for the $[(DBU)CuCl]^+$-catalyzed 7-membered cyclization reaction.

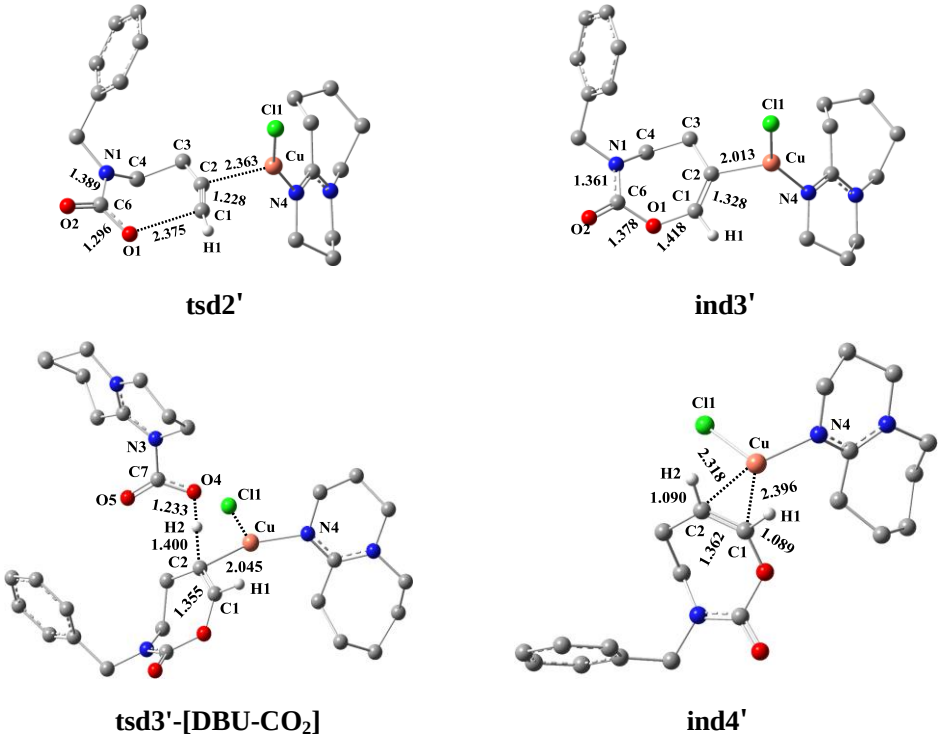


Figure S19. Optimized structures of the $[(DBU)CuCl]^+$-catalyzed 7-membered cyclization**.** The H atom that does not participate in the reactions has been omitted for clarity. Bond distance is given in Å.

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

CO_2

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16896700
O	0.00000000	0.00000000	-1.16896700

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = -0.015456 a.u.

Sum of electronic and thermal Free Energies = -188.598745 a.u.

M06-2x-D3/6-311++G**

Energy = -188.5769444 a.u.

No imaginary frequency

DBU

C	0.84642200	1.47422400	0.27323000
C	2.12524100	1.15742100	-0.51059500
N	-0.34272700	0.66677600	-0.05315000
C	2.96064700	0.00660700	0.07337400
C	2.10382900	-1.18292900	0.53466300
C	0.92353000	-1.48043600	-0.40994500
C	-0.36954900	-0.72177000	-0.12985800
C	-1.59650000	1.35812200	0.27676200
C	-2.79490200	0.60811600	-0.28939900
C	-2.72870500	-0.84295300	0.18208600
N	-1.42712400	-1.46437300	-0.04981900
H	0.55986500	2.50678800	0.04941700
H	1.05027500	1.44252600	1.35686600
H	2.73753900	2.06704500	-0.53405000
H	1.85028600	0.95029600	-1.55166600
H	3.55517600	0.37470600	0.91952400
H	3.67876000	-0.32735000	-0.68686200
H	1.71703200	-1.00151400	1.54604900
H	2.73474300	-2.07632100	0.61131600
H	0.64200700	-2.53316600	-0.34093500
H	1.23102600	-1.30752100	-1.45088800
H	-1.54238400	2.36995200	-0.14117600
H	-1.69884300	1.46734000	1.36913600
H	-2.76241500	0.64367300	-1.38569200
H	-3.72440200	1.09319600	0.02957700
H	-3.49110400	-1.44685800	-0.32762900
H	-2.96868600	-0.89802800	1.25588400

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.199777 a.u.

Sum of electronic and thermal Free Energies = -461.893220 a.u.

M06-2x-D3/6-311++G**

Energy = -462.0069823 a.u.

No imaginary frequency

H_2O

O	0.00000000	0.00000000	0.12074100
H	0.00000000	0.75867200	-0.48296600
H	0.00000000	-0.75867200	-0.48296600

B3LYP/6-31G*
Thermal correction to Gibbs Free Energy = -0.002046 a.u.
Sum of electronic and thermal Free Energies = -76.418166 a.u.
M06-2x-D3/6-311++G**
Energy = -76.4285958 a.u.
No imaginary frequency

$CuCl_2$

Cu	0.00000000	0.00038300	0.00000000
Cl	2.09882900	0.44129800	0.00000000
Cl	-2.09882900	-0.44195100	0.00000000

B3LYP/6-31G*
Thermal correction to Gibbs Free Energy = -0.028710 a.u.
Sum of electronic and thermal Free Energies = -1116.623778 a.u.
M06-2x-D3/6-311++G**
Energy = -1116.6190938 a.u.
No imaginary frequency

(DBU)$CuCl_2$

Cu	1.84976700	-0.12824000	-0.15648300
Cl	2.33496200	0.65311600	1.93513400
Cl	3.54465400	-1.34678200	-0.94058900
C	-3.54391400	0.14768400	-0.21176000
C	-3.76101200	-0.94648100	0.83893600
N	-2.19921000	0.78126900	-0.23134600
C	-3.30304500	-2.34037900	0.38386400
C	-1.97703200	-2.30119100	-0.38832100
C	-0.94709100	-1.33692300	0.23191300
C	-1.02476600	0.12183900	-0.19300400
C	-2.24457800	2.23315200	-0.51586400
C	-0.92002600	2.90559000	-0.20012700
C	0.19342300	2.11954600	-0.87317500
N	0.13268300	0.69660600	-0.50543200
H	-4.23612400	0.96809200	-0.01647000
H	-3.77253500	-0.22272400	-1.21939400
H	-4.83163400	-0.97098100	1.07069300
H	-3.25781100	-0.64858500	1.76617500
H	-4.07261000	-2.79525700	-0.25148800
H	-3.19997800	-2.98589400	1.26447900
H	-2.14689800	-2.02581300	-1.43612500

H	-1.53425000	-3.30244200	-0.40933500
H	0.05423700	-1.68479600	-0.03819100
H	-0.99937000	-1.37789000	1.32745900
H	-3.04575900	2.65499000	0.09662400
H	-2.52090100	2.37664400	-1.56841300
H	-0.75664400	2.92793600	0.88322800
H	-0.94000500	3.93859100	-0.55934800
H	1.17756200	2.50292300	-0.59000500
H	0.11994900	2.19433200	-1.96646400

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.187447 a.u.

Sum of electronic and thermal Free Energies = -1578.566256 a.u.

M06-2x-D3/6-311++G**

Energy = -1578.7134993 a.u.

No imaginary frequency

[(DBU)CuCl]$^{+}$

Cu	2.11596900	-0.03724200	-0.02011000
Cl	4.07157300	-0.91830400	0.09393600
C	-3.24390400	0.12130000	-0.29916400
C	-3.52225700	-1.06480600	0.63284400
N	-1.92221900	0.78941200	-0.11801800
C	-2.99110800	-2.40233000	0.09720600
C	-1.61782700	-2.26375100	-0.57263300
C	-0.65231800	-1.35118900	0.20660100
C	-0.75277400	0.14654400	-0.01401400
C	-2.00397500	2.27198300	-0.16518400
C	-0.76152900	2.92146400	0.40835200
C	0.45696100	2.27382300	-0.22185800
N	0.42444600	0.81261300	-0.08549600
H	-3.98009900	0.90621600	-0.13296100
H	-3.31638100	-0.16827500	-1.35400500
H	-4.60852800	-1.11859000	0.75947000
H	-3.11514700	-0.84028500	1.62505800
H	-3.69927300	-2.81905800	-0.62820800
H	-2.92942100	-3.11612000	0.92666900
H	-1.71675200	-1.89615700	-1.60050800
H	-1.14581800	-3.24786700	-0.65210500
H	0.37299300	-1.62880800	-0.05102500
H	-0.74823100	-1.52589400	1.28697300
H	-2.89437100	2.55150200	0.40104700
H	-2.17078000	2.55307800	-1.21296400
H	-0.73513100	2.79615000	1.49601100
H	-0.77931700	3.99263000	0.19276000
H	1.39012200	2.62929900	0.22126100
H	0.51308800	2.49097300	-1.29950400

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.192112 a.u.

Sum of electronic and thermal Free Energies = -1118.148131 a.u.

M06-2x-D3/6-311++G**

Energy = -1118.2785781 a.u.

No imaginary frequency

$[(DBU)_2Cu]^{2+}$

Cu	-0.00003000	-0.97092900	-0.00058700
C	5.08254400	0.80230000	-0.24221300
C	4.81806200	2.16440500	0.40865400
N	4.06224600	-0.25320500	0.01304100
C	3.92897900	3.08406700	-0.44109000
C	2.78114200	2.32352000	-1.11797500
C	2.10474500	1.29667100	-0.19047700
C	2.73514500	-0.08114500	-0.06958200
C	4.66546100	-1.58395400	0.27310200
C	3.66422500	-2.55394600	0.86965200
C	2.38615000	-2.49151300	0.05155400
N	1.87359000	-1.11242900	-0.02217500
H	6.01400300	0.39024000	0.14526000
H	5.20508400	0.89585400	-1.32782000
H	5.79138400	2.63877400	0.57333600
H	4.38887000	2.00371600	1.40439200
H	4.53358100	3.57646700	-1.21180100
H	3.52353300	3.87787500	0.19742200
H	3.12836900	1.81975600	-2.02776700
H	2.01264800	3.03173100	-1.44391000
H	1.08739900	1.12732700	-0.55112100
H	2.00785700	1.70779900	0.82346700
H	5.50437700	-1.42260100	0.95367400
H	5.07184300	-1.95594800	-0.67560100
H	3.45448200	-2.29176400	1.91259700
H	4.08242100	-3.56406100	0.85453800
H	1.60509100	-3.12381600	0.47924600
H	2.56297400	-2.84160900	-0.97529100
C	-5.08238500	0.80253800	0.24323100
C	-4.81818800	2.16450600	-0.40804400
N	-4.06228700	-0.25306100	-0.01241900
C	-3.92860900	3.08429100	0.44105200
C	-2.78048600	2.32380300	1.11752400
C	-2.10460200	1.29674200	0.18988800
C	-2.73513800	-0.08105300	0.06946500
C	-4.66571100	-1.58380600	-0.27202500
C	-3.66485700	-2.55389600	-0.86905300
C	-2.38630000	-2.49144600	-0.05170300

N	-1.87364700	-1.11237500	0.02163700
H	-6.01408600	0.39045700	-0.14363600
H	-5.20430000	0.89630100	1.32888800
H	-5.79157200	2.63889300	-0.57231000
H	-4.38952200	2.00360300	-1.40397600
H	-4.53278600	3.57691100	1.21195800
H	-3.52342200	3.87792600	-0.19784000
H	-3.12729200	1.82024600	2.02759300
H	-2.01178600	3.03203100	1.44293500
H	-1.08710000	1.12737900	0.55008600
H	-2.00814500	1.70770400	-0.82416700
H	-5.50499700	-1.42247100	-0.95214400
H	-5.07158200	-1.95569000	0.67694000
H	-3.45570600	-2.29182700	-1.91214400
H	-4.08308000	-3.56399400	-0.85359900
H	-1.60552100	-3.12380800	-0.47981800
H	-2.56254200	-2.84146600	0.97526500

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.422019 a.u.

Sum of electronic and thermal Free Energies = -1119.646476 a.u.

M06-2x-D3/6-311++G**

Energy = -1119.915404 a.u.

No imaginary frequency

1a

C	0.64532200	0.53796200	0.53789700
C	1.50313800	0.52557600	-0.31468800
C	-0.38112200	0.56637300	1.58209000
C	-1.30038400	1.80638000	1.51666900
N	-2.10693800	1.88302800	0.29664500
C	-3.37482700	1.14447400	0.33789000
C	-3.25969300	-0.32494700	-0.03638700
C	-3.93149200	-1.30361300	0.70622500
C	-3.88052700	-2.64978100	0.33206300
C	-3.15038400	-3.03505700	-0.79347600
C	-2.47245700	-2.06585600	-1.54027200
C	-2.52819300	-0.72352400	-1.16473300
H	2.25863100	0.51392800	-1.06880800
H	-0.98738100	-0.34527300	1.52717800
H	0.10359200	0.55578900	2.56793900
H	-1.92693900	1.80146500	2.42640800
H	-0.67382500	2.70331300	1.56073500
H	-3.86736300	1.22270900	1.32377300
H	-4.04621600	1.63084600	-0.38193800
H	-4.49975700	-1.00977000	1.58635300
H	-4.40670500	-3.39494700	0.92317600

H	-3.10616200	-4.08082000	-1.08601800
H	-1.90025200	-2.35781800	-2.41736400
H	-1.99455100	0.02868500	-1.73806500
H	-2.31861500	2.86048100	0.11830800

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.160501 a.u.

Sum of electronic and thermal Free Energies = -481.510959 a.u.

M06-2x-D3/6-311++G**

Energy = -481.5921997 a.u.

No imaginary frequency

ts1-DBU

C	0.69784800	-0.12303400	0.47639800
C	1.48523900	-0.58358600	-0.31703200
C	-0.23922100	0.35693900	1.49427000
C	-0.80827900	1.78260100	1.32215100
N	-1.64396000	2.09366200	0.13335500
C	-2.96732000	1.40810900	0.01484100
C	-3.01748200	-0.10731000	-0.06714500
C	-3.65320900	-0.82995900	0.95317600
C	-3.76978000	-2.22048100	0.88569900
C	-3.25231800	-2.91061600	-0.21201200
C	-2.62535500	-2.19992200	-1.23937000
C	-2.51167300	-0.81041100	-1.17197100
H	2.17533500	-0.96420500	-1.03698200
H	-1.05653200	-0.36326900	1.59552500
H	0.27585300	0.36448100	2.46529500
H	-1.41333200	1.98977900	2.21109500
H	0.01142600	2.50020500	1.29411700
H	-3.56679300	1.72702100	0.87401600
H	-3.41556400	1.83889400	-0.88197800
H	-4.06179200	-0.29869000	1.81016600
H	-4.26498000	-2.76063800	1.68825700
H	-3.34067100	-3.99222700	-0.26951000
H	-2.22726500	-2.72979600	-2.10102300
H	-2.03245500	-0.25549400	-1.97126400
H	-1.97416500	3.29842100	0.32399500
C	-4.17435700	7.27201000	2.22894600
C	-4.08283900	6.90304400	3.71237100
N	-3.25891700	6.56256100	1.30469600
C	-4.89873900	5.66044100	4.09724500
C	-4.77069100	4.53546800	3.06076600
C	-3.33419500	4.37626200	2.52883100
C	-2.95430900	5.23636300	1.33191300
C	-2.91451300	7.35515700	0.10919000
C	-1.64613100	6.82740600	-0.54329600

C	-1.81190100	5.33911300	-0.81089600
N	-2.29038500	4.62303000	0.37957900
H	-3.91560200	8.32838500	2.12400600
H	-5.20888100	7.16902700	1.87086500
H	-4.44069700	7.76488000	4.28734500
H	-3.02670000	6.77969000	3.97940600
H	-5.95610200	5.93023600	4.20974700
H	-4.56120300	5.30200100	5.07779500
H	-5.45109000	4.71105200	2.21823600
H	-5.08447800	3.58583800	3.50769900
H	-3.17957700	3.34369800	2.21831800
H	-2.61133600	4.55960400	3.33450200
H	-2.77811500	8.39206500	0.42785700
H	-3.75421700	7.33711800	-0.59984600
H	-0.79283700	6.99619000	0.12415100
H	-1.45329900	7.37008300	-1.47403300
H	-0.86161000	4.88488000	-1.10142500
H	-2.51707700	5.17233700	-1.63681100
O	-1.50554100	2.00120100	-2.22291500
O	0.30728400	2.67690000	-1.03176100
C	-0.83917600	2.24646900	-1.20811400

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.392499 a.u.

Sum of electronic and thermal Free Energies = -1131.955827 a.u.

M06-2x-D3/6-311++G**

Energy = -1132.1955429 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = -1204.94 *i*

in1

C	1.18083400	2.37985900	0.32811200
C	1.27405400	2.78379700	1.46488500
C	1.07177000	1.90078200	-1.05078400
C	1.80949000	0.56065000	-1.32118100
N	1.30894200	-0.58130700	-0.59347800
C	0.08567800	-1.21428300	-1.05843400
C	-1.20843100	-0.68330500	-0.45209700
C	-2.26265800	-0.23617200	-1.25759700
C	-3.45672900	0.22250700	-0.69059300
C	-3.61064700	0.23760100	0.69660600
C	-2.56425300	-0.21028100	1.51108300
C	-1.37537100	-0.66605000	0.94158100
H	1.35877900	3.13413000	2.46952800
H	0.01157900	1.79349700	-1.31300900
H	1.48179900	2.66048400	-1.73181800
H	1.74345800	0.38190300	-2.40732800

H	2.86118400	0.66659600	-1.05303300
H	0.02513900	-1.12368900	-2.15343800
H	0.17283900	-2.27631800	-0.81128300
H	-2.14951700	-0.24524200	-2.34033000
H	-4.26248900	0.56952700	-1.33303000
H	-4.53631100	0.59431300	1.14110300
H	-2.67896100	-0.20574600	2.59261700
H	-0.55953500	-1.02715800	1.56150400
C	2.12349900	-1.23491100	0.39676700
O	3.25345200	-0.72581700	0.62621700
O	1.61291800	-2.25430600	0.94281900

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.156386 a.u.

Sum of electronic and thermal Free Energies = -669.622633 a.u.

M06-2x-D3/6-311++G**

Energy = -669.7182608 a.u.

No imaginary frequency

ina2

C	-0.45264600	-1.20032500	0.53434400
C	-0.92611800	-1.77606000	-0.44639400
C	0.34598700	-0.69699900	1.66140800
C	1.73769700	-1.36273500	1.75273900
N	2.60478400	-1.12341200	0.59928500
C	3.34030900	0.14382200	0.45759800
C	2.52183900	1.29453800	-0.10106000
C	2.34286800	2.46588400	0.64416800
C	1.60552600	3.53420900	0.12423700
C	1.03928300	3.43850300	-1.14820600
C	1.21782900	2.27288700	-1.90152700
C	1.95622800	1.20930200	-1.38205800
H	-1.10273200	-2.41634300	-1.28683700
H	0.44966100	0.38936000	1.58306000
H	-0.18329900	-0.89081500	2.60200700
H	2.24580500	-0.98279900	2.64526300
H	1.62471600	-2.44371900	1.86714700
H	3.74066600	0.40493200	1.44260800
H	4.19517100	-0.06203800	-0.19515500
H	2.78135800	2.54387300	1.63632200
H	1.47356300	4.43668700	0.71464000
H	0.46587800	4.26713200	-1.55432000
H	0.78729600	2.19606100	-2.89623100
H	2.10085500	0.30929300	-1.97444900
Cl	-4.15185400	-0.75223800	-1.44074600
Cl	-2.83317400	1.32780300	1.56910600
Cu	-2.40010800	-0.38276500	0.05852500

O	2.26671800	-3.25790900	-0.24683400
O	3.55659800	-1.99882200	-1.32350200
C	2.80192900	-2.10115700	-0.29953800

B3LYP/6-31G* (LanL2DZ for Cu)
Thermal correction to Gibbs Free Energy = 0.141992 a.u.
Sum of electronic and thermal Free Energies = -1786.276242 a.u.
M06-2x-D3/6-311++G** (LanL2DZ for Cu)
Energy = -1786.3889776 a.u.
No imaginary frequency

tsa2

C	0.92060100	0.99197600	0.34402000
C	1.91319900	1.31862000	-0.31059600
C	-0.11667300	0.38512300	1.16903100
C	-1.27324900	1.36071400	1.52594500
N	-2.07432600	1.78823400	0.39595400
C	-3.41889200	1.24620500	0.19892200
C	-3.45205100	-0.25597300	-0.01999500
C	-4.16172000	-1.08949800	0.85200700
C	-4.21221500	-2.47069500	0.63848200
C	-3.54691200	-3.03408300	-0.45148300
C	-2.83351600	-2.20995500	-1.32896600
C	-2.78861900	-0.83208200	-1.11494500
H	2.50785800	1.97693500	-0.91206800
H	-0.52202100	-0.49334800	0.65627000
H	0.33201400	0.03986500	2.10908200
H	-1.92787700	0.84771800	2.23489800
H	-0.84724600	2.23783800	2.02173800
H	-4.04710000	1.50635300	1.06164000
H	-3.82860300	1.77442800	-0.66608300
H	-4.68091600	-0.65538800	1.70351900
H	-4.76775000	-3.10312400	1.32572100
H	-3.58257200	-4.10705600	-0.61879600
H	-2.31630900	-2.64110400	-2.18188400
H	-2.23549200	-0.19582600	-1.80198700
Cl	2.00728200	-2.51647400	-0.04161900
Cl	5.12819000	0.37285300	-0.00425700
Cu	3.04251700	-0.50122300	-0.03858000
O	-0.35511900	3.09761700	-0.31027400
O	-2.35352300	3.40212900	-1.22326500
C	-1.60171500	2.80200000	-0.42520500

B3LYP/6-31G* (LanL2DZ for Cu)
Thermal correction to Gibbs Free Energy = 0.139831 a.u.
Sum of electronic and thermal Free Energies = -1786.272733 a.u.
M06-2x-D3/6-311++G** (LanL2DZ for Cu)
Energy = -1786.3710466 a.u.

Number of Imaginary Frequencies = 1
Lowest Frequency = -80.87 *i*

ina3

C	-3.48983900	0.92102700	0.45920000
C	-4.77733300	1.20119600	0.64397900
C	-2.27195600	1.62636200	0.96834900
C	-1.37518100	0.61343200	1.67545600
N	-1.18456600	-0.56720100	0.82886500
C	-0.01595500	-1.41162200	1.10946700
C	1.28792900	-0.83038100	0.59185200
C	2.31245800	-0.46730800	1.47360800
C	3.51566800	0.05891500	0.99194800
C	3.70288900	0.22984000	-0.38052900
C	2.68373300	-0.12979800	-1.26966900
C	1.48595000	-0.65665300	-0.78716500
H	-5.54390200	0.56745700	0.19746200
H	-1.72209900	2.06482800	0.12410900
H	-2.55027000	2.43494700	1.64588700
H	-0.39033000	1.04905500	1.87319500
H	-1.81077200	0.31461500	2.63875600
H	0.04144800	-1.55219900	2.19492300
H	-0.21053000	-2.38399900	0.65400500
H	2.17091100	-0.59991800	2.54391500
H	4.30147300	0.33645000	1.68947000
H	4.63620200	0.63911900	-0.75770700
H	2.82573300	-0.00290700	-2.33967900
H	0.69673800	-0.94292000	-1.47737000
Cl	-4.56405500	4.68901600	1.31543100
Cl	-7.18121200	1.84613500	3.04367000
Cu	-5.51417600	2.66856500	1.72450800
O	-3.16915500	-0.19123000	-0.35353400
O	-1.84238600	-1.87183300	-0.93571900
C	-2.02630700	-0.92728200	-0.17741600

B3LYP/6-31G* (LanL2DZ for Cu)
Thermal correction to Gibbs Free Energy = 0.147807 a.u.
Sum of electronic and thermal Free Energies = -1786.320893 a.u.
M06-2x-D3/6-311++G** (LanL2DZ for Cu)
Energy = -1786.4340656 a.u.
No imaginary frequency

tsa3-DBU

C	-0.87381700	0.80171300	-0.57646800
C	0.48720500	0.98896800	-0.62580100
C	-1.68321400	0.25696600	0.55676300
C	-3.03652200	0.95837300	0.61430100

N	-3.67383200	0.90306800	-0.70354700
C	-5.14578900	0.90067300	-0.76717800
C	-5.75266400	-0.42227500	-0.33894200
C	-6.56914800	-0.50121200	0.79500200
C	-7.13345600	-1.72093100	1.18223700
C	-6.88133800	-2.87424200	0.43803300
C	-6.06572500	-2.80427000	-0.69698600
C	-5.50670700	-1.58655000	-1.08312900
H	0.84020300	1.40169200	-1.57182300
H	-1.84268000	-0.81587600	0.37558300
H	-1.14198400	0.36836400	1.49685400
H	-3.69017800	0.44657800	1.32413100
H	-2.93038300	2.00119700	0.94026200
H	-5.50967000	1.71123500	-0.12654400
H	-5.41506500	1.13984800	-1.79717000
H	-6.76864500	0.39569200	1.37680600
H	-7.76546900	-1.76725400	2.06483900
H	-7.31762800	-3.82323700	0.73742900
H	-5.87004800	-3.69845700	-1.28255800
H	-4.87907100	-1.53334700	-1.96929700
Cl	0.78785800	1.53145100	2.94132000
Cl	2.30630300	3.78399500	-0.32983300
Cu	1.25857700	2.19031500	0.84862300
O	-1.56666700	1.05550600	-1.71698700
O	-3.39694800	0.90521500	-2.98615800
C	-2.96666600	0.93443300	-1.85031000
C	5.42123700	-2.62791500	-0.26242300
C	6.36033500	-1.52065800	-0.75135200
N	4.13021400	-2.19397200	0.31947000
C	6.05850100	-1.02649600	-2.17459200
C	4.55370100	-0.86829600	-2.43633200
C	3.79813600	-0.25324800	-1.24291700
C	3.30889200	-1.23184700	-0.18425300
C	3.60902600	-3.12583700	1.33800300
C	2.52213500	-2.47224200	2.18077900
C	1.46497300	-1.88567200	1.25347000
N	2.07391600	-1.05456400	0.21855300
H	5.92261000	-3.17349600	0.54072700
H	5.23525700	-3.35680000	-1.06464000
H	7.38193900	-1.91644500	-0.71492000
H	6.33161400	-0.69305400	-0.03276600
H	6.48046900	-1.72577700	-2.90719500
H	6.56478600	-0.06577400	-2.33159700
H	4.10572200	-1.83769100	-2.68815600
H	4.39911600	-0.22915100	-3.31258200
H	2.91048100	0.26450100	-1.60612300

H	4.42029800	0.50995800	-0.75751600
H	4.44987800	-3.42739700	1.96926700
H	3.22734400	-4.03182100	0.84613200
H	2.95909600	-1.67607500	2.79480100
H	2.08329900	-3.21311300	2.85646800
H	0.76276800	-1.25977900	1.81420300
H	0.88156600	-2.68680800	0.77815100
H	1.25715600	0.02647800	-0.18172700

B3LYP/6-31G* (LanL2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.379188 a.u.

Sum of electronic and thermal Free Energies = -2248.631707 a.u.

M06-2x-D3/6-311++G** (LanL2DZ for Cu)

Energy = -2248.8933157 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = -1207.57 *i*

ina4

C	0.96665000	-0.26056000	1.13419800
C	2.24108600	-0.18834000	1.68796500
C	0.01536800	0.88148600	1.00718500
C	-0.74508900	0.77288800	-0.31082800
N	-1.29866900	-0.57780300	-0.45639600
C	-2.50903700	-0.74153100	-1.28871700
C	-3.75126900	-0.16487900	-0.63910000
C	-4.41090300	0.92856900	-1.21202600
C	-5.56378100	1.45356300	-0.61998900
C	-6.06371200	0.88926400	0.55437700
C	-5.40975100	-0.20365900	1.13407200
C	-4.26190700	-0.72793000	0.54057500
H	2.75248400	-1.11563500	1.92794100
H	-0.68781900	0.81836800	1.85018600
H	0.54947200	1.82996700	1.08087600
H	-1.57927600	1.47708100	-0.31486300
H	-0.09410800	1.00703300	-1.16228800
H	-2.31778400	-0.25207700	-2.24988900
H	-2.61920000	-1.81118800	-1.47193400
H	-4.02491800	1.36900600	-2.12821300
H	-6.06627700	2.30198400	-1.07607900
H	-6.95900300	1.29548500	1.01683400
H	-5.79789100	-0.64928700	2.04581800
H	-3.76017900	-1.58131100	0.99037900
Cl	3.15436500	2.56684500	-0.12203500
Cl	4.16563200	-1.58660500	-0.75047900
Cu	3.36762100	0.35969100	-0.06956700
O	0.55758500	-1.44807400	0.70274500
O	-1.03232500	-2.83092600	-0.05153300

C	-0.69097300	-1.67386100	0.02395200
H	2.49206700	0.70201500	2.25649700

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.161730 a.u.

Sum of electronic and thermal Free Energies = -1786.772063 a.u.

M06-2x-D3/6-311++G**

Energy = -1786.8872934 a.u.

No imaginary frequency

ts1-[DBU-H_2O]

C	1.31952000	1.16808900	-1.44233100
C	1.96934200	0.83980800	-2.40763800
C	0.60237600	1.62764300	-0.25121300
C	-0.69213200	0.87809600	0.13699000
N	-1.84207400	0.87808900	-0.80784300
C	-2.52777700	2.18714900	-1.03822400
C	-1.73271800	3.36179600	-1.57863400
C	-1.18872100	3.35661100	-2.87272400
C	-0.50852900	4.47404500	-3.35877700
C	-0.36716200	5.61723600	-2.56676000
C	-0.91433100	5.63716400	-1.28252600
C	-1.59279200	4.51692600	-0.79585900
H	2.52051600	0.52930100	-3.26745600
H	1.26802100	1.52633400	0.61755300
H	0.39819300	2.69742500	-0.34960500
H	-0.46350600	-0.17263900	0.31514500
H	-1.04213300	1.32242000	1.07431500
H	-3.34469000	1.95652700	-1.72418100
H	-2.97077800	2.47267100	-0.07750000
H	-1.30467400	2.46827300	-3.48414900
H	-0.09088100	4.45413900	-4.36220200
H	0.16157000	6.48613400	-2.94948300
H	-0.81552200	6.52189000	-0.65915700
H	-2.01817200	4.54009400	0.20514100
C	-1.64260600	-0.04099300	-2.06095600
O	-1.01651000	-1.07249800	-1.79754200
O	-2.22155300	0.36325300	-3.08225000
C	-6.96732300	-2.13822800	0.52169900
C	-6.96911100	-2.97683000	-0.75998900
N	-5.66513800	-1.57716000	0.95352000
C	-7.07554400	-2.14425500	-2.04583400
C	-6.20209000	-0.88381000	-1.99423400
C	-4.81899500	-1.13558900	-1.36465300
C	-4.72976000	-1.00338300	0.14833200
C	-5.56637300	-1.41006700	2.41591500
C	-4.11605600	-1.27678900	2.85265400

C	-3.45926200	-0.17089500	2.03948600
N	-3.68391300	-0.34816900	0.60074000
H	-7.28444400	-2.77792500	1.34870200
H	-7.70976000	-1.33015100	0.45311100
H	-7.81890200	-3.66667800	-0.70043800
H	-6.07014900	-3.60417500	-0.77020200
H	-8.12025100	-1.85548800	-2.21635000
H	-6.78004300	-2.76708900	-2.89952900
H	-6.71419800	-0.08653900	-1.44086900
H	-6.05503800	-0.49701200	-3.00869800
H	-4.10536400	-0.43000400	-1.78714800
H	-4.45359500	-2.13207900	-1.64602200
H	-6.02532600	-2.28700800	2.88078800
H	-6.14948300	-0.53171300	2.72694100
H	-3.59156800	-2.22496400	2.68640600
H	-4.06974700	-1.05284100	3.92293600
H	-2.37986600	-0.15731100	2.21567200
H	-3.84577400	0.81104800	2.34734400
H	-2.73043100	0.23660800	-0.18677900

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.407851 a.u.

Sum of electronic and thermal Free Energies = -1208.368906 a.u.

M06-2x-D3/6-311++G**

Energy = -1208.6286048 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = -797.56 *i*

ts1-[DBU-CO_2]

C	-4.64499900	-1.63506000	1.54460900
C	-5.53707000	-2.37343500	1.19617700
C	-3.58696300	-0.73384100	2.00622900
C	-2.21657700	-0.90292000	1.31959100
N	-2.16429900	-0.69338800	-0.14084200
C	-2.26704200	0.70447800	-0.63394100
C	-3.55537400	1.45592400	-0.36017400
C	-3.52036300	2.63800700	0.39294400
C	-4.68093700	3.38298400	0.61925600
C	-5.89927800	2.95374600	0.09024700
C	-5.94563900	1.77977200	-0.66772600
C	-4.78458300	1.03972900	-0.89497300
H	-6.31595100	-3.02978300	0.87671400
H	-3.92933300	0.30155200	1.91652300
H	-3.41901400	-0.90581500	3.07841300
H	-1.50604400	-0.22583300	1.81355300
H	-1.86392200	-1.92483500	1.48568800
H	-1.42225800	1.27524700	-0.22667500

H	-2.11655500	0.63386800	-1.71741600
H	-2.57386400	2.97899400	0.80656000
H	-4.63084500	4.29584800	1.20702400
H	-6.80459500	3.52955200	0.26324100
H	-6.88958300	1.44225200	-1.08825000
H	-4.82379800	0.13233900	-1.48822700
O	-3.46545800	-1.67305300	-2.24155900
O	-2.66565100	-3.19618100	-0.68857500
C	-2.98626500	-2.22317000	-1.29703400
H	-1.20282000	-0.97271500	-0.39867000
C	6.27314600	0.48007100	0.14109200
C	6.17021400	1.87809900	0.75499100
N	5.04932300	-0.36997600	0.19380100
C	5.60276200	2.92130400	-0.21596500
C	4.44437400	2.35130100	-1.04251800
C	3.45707800	1.51324200	-0.20518100
C	3.79534500	0.03710900	-0.05277300
C	5.40294800	-1.79267200	0.43497800
C	4.18612800	-2.67755200	0.63046300
C	3.14314800	-2.28660800	-0.40118600
N	2.81070400	-0.86201100	-0.22298400
H	7.02525400	-0.08797100	0.68997200
H	6.61636500	0.52997600	-0.89958400
H	7.17764200	2.17194600	1.07032600
H	5.57134200	1.82116600	1.67129400
H	6.39309300	3.27120600	-0.89125500
H	5.26234200	3.79607800	0.35143300
H	4.82521200	1.75242200	-1.87857600
H	3.87822800	3.17056500	-1.49846100
H	2.47155300	1.56129600	-0.65697100
H	3.33682700	1.94769200	0.79383300
H	6.04560200	-1.81421300	1.31973900
H	6.00214200	-2.13294100	-0.41795000
H	3.77259900	-2.55274200	1.63701600
H	4.47859400	-3.72541400	0.51529400
H	2.21732100	-2.84597100	-0.29856600
H	3.52133100	-2.44344000	-1.41897100
C	1.31761900	-0.53802100	-0.12351800
O	1.02035500	0.43501300	0.57995000
O	0.61724300	-1.35165500	-0.75788000

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.398456 a.u.

Sum of electronic and thermal Free Energies = -1320.540615 a.u.

M06-2x-D3/6-311++G**

Energy = -1320.7747123 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = -146.99 *i*

ts1-H_2O

C	-4.40700500	-1.73597300	1.39342500
C	-5.16218700	-2.59970600	1.01224600
C	-3.52103100	-0.67881300	1.88383900
C	-2.11566100	-0.63419700	1.25088800
N	-2.03764300	-0.46027900	-0.21958800
C	-2.28379500	0.90081300	-0.77746300
C	-3.59304000	1.57246500	-0.41516700
C	-3.58594400	2.70222800	0.41497400
C	-4.77438200	3.36068700	0.74101600
C	-5.98972500	2.89767500	0.23380700
C	-6.00697600	1.77832800	-0.60357700
C	-4.81909400	1.12270800	-0.92926000
H	-5.81937000	-3.36702200	0.66710200
H	-4.01773700	0.28908800	1.77329400
H	-3.36303200	-0.81770100	2.96204500
H	-1.55303800	0.16981900	1.74418000
H	-1.59965300	-1.57364100	1.46418600
H	-1.45673400	1.55253100	-0.46754100
H	-2.21686700	0.78092100	-1.86338000
H	-2.64195900	3.07009200	0.81055400
H	-4.74817900	4.23380400	1.38739900
H	-6.91627100	3.40730600	0.48398100
H	-6.94890400	1.41714100	-1.00808700
H	-4.83497700	0.25292900	-1.57731800
O	-3.42668500	-1.56769700	-2.14320400
O	-2.16437300	-2.95144800	-0.78987500
C	-2.72506600	-2.00852300	-1.28292700
H	-1.05854900	-0.68393800	-0.44736400
O	0.51530400	-1.87503300	-0.66460500
H	-0.15387700	-2.58415700	-0.69319000
H	0.95254800	-1.99633500	0.19322900

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.188472 a.u.

Sum of electronic and thermal Free Energies = -746.485595 a.u.

M06-2x-D3/6-311++G**

Energy = -746.6025605 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = -139.51 *i*

tsb2

C	3.34342100	-0.57272200	-0.52383400
C	4.62793700	-0.71593900	-0.51520600
C	2.13051800	-1.39316100	-0.78636200

C	1.15108900	-1.34494700	0.38691200
N	0.72277100	0.01718600	0.68634300
C	-0.50921100	0.15859600	1.45508200
C	-1.77277200	-0.00346100	0.62459800
C	-2.72498800	-0.98130900	0.93293000
C	-3.89095900	-1.11121100	0.17099400
C	-4.11486500	-0.26171700	-0.91312200
C	-3.16805800	0.71887800	-1.23049500
C	-2.00753000	0.84587200	-0.46804600
H	5.24420000	0.15525300	-0.26788900
H	1.60851000	-1.04878800	-1.69184400
H	2.43234000	-2.43258400	-0.95642100
H	0.25628700	-1.93312700	0.14586100
H	1.61361700	-1.80707100	1.27423100
H	-0.50826800	-0.58064300	2.26747200
H	-0.48568100	1.15302600	1.90551400
H	-2.55478000	-1.64663600	1.77698900
H	-4.61897200	-1.87802500	0.42333200
H	-5.01905400	-0.36075400	-1.50799700
H	-3.33817300	1.38609400	-2.07181500
H	-1.27234300	1.61016600	-0.70590000
O	2.63513000	0.97699300	-0.19940100
O	1.03395500	2.27960700	0.65534300
C	1.47194200	1.14590600	0.38433400

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.157586 a.u.

Sum of electronic and thermal Free Energies = -669.583381 a.u.

M06-2x-D3/6-311++G**

Energy = -669.6714265 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = -299.16 *i*

tsc2

C	1.31538800	-0.46269900	1.18694800
C	0.50602800	-0.54719100	2.11550100
C	2.10913100	-0.70329000	-0.01219000
C	2.36858500	0.54911100	-0.88544400
N	3.43241500	1.41381300	-0.42179700
C	4.66032100	1.53982600	-1.18699100
C	5.64495200	0.39193800	-1.00877300
C	6.01914400	-0.42978300	-2.07691100
C	6.92433500	-1.48018900	-1.89355400
C	7.46686200	-1.71958700	-0.63129800
C	7.10009900	-0.90246100	0.44420400
C	6.19814100	0.14387700	0.25871700
H	0.12892100	-0.26209900	3.07617100

H	3.07116600	-1.14865100	0.27195500
H	1.56008100	-1.45737100	-0.59491200
H	2.63668600	0.19946400	-1.88860300
H	1.42873400	1.10988600	-0.97196300
H	4.41992900	1.64806000	-2.25497900
H	5.12413000	2.46934200	-0.84561100
H	5.59648000	-0.24711200	-3.06370400
H	7.19913300	-2.11223700	-2.73538000
H	8.16845600	-2.53743900	-0.48325200
H	7.52100200	-1.08278800	1.43087000
H	5.90930100	0.79018800	1.08384500
Cl	-2.65467900	-0.91256500	2.92340000
Cl	-0.80018400	-2.75008100	-0.56041800
Cu	-1.33225900	-1.15603800	1.03312100
O	2.25539900	1.80001100	1.48736500
O	4.25406500	2.80586000	1.20837000
C	3.32347500	2.05649100	0.83950100
C	-5.56831500	1.43964700	-1.52040700
C	-6.62480200	0.42723900	-1.05533900
N	-4.30313000	1.44638500	-0.77282800
C	-6.46613600	-0.96799300	-1.67970300
C	-4.99732000	-1.40622700	-1.77113600
C	-4.16691400	-1.05926100	-0.52294400
C	-3.54142900	0.32695800	-0.48086300
C	-3.70296500	2.78305000	-0.66013700
C	-2.55215900	2.79192800	0.33578400
C	-1.59704400	1.66027700	-0.02033800
N	-2.29954700	0.37700400	-0.10461200
H	-5.98163700	2.44534500	-1.39099500
H	-5.38415700	1.32506600	-2.60209200
H	-7.61611800	0.82831800	-1.30426000
H	-6.58156300	0.36953700	0.03829700
H	-6.91542100	-0.97932000	-2.68266400
H	-7.03363400	-1.69120100	-1.07925500
H	-4.52332300	-0.96255100	-2.65668200
H	-4.94992100	-2.49028600	-1.92603500
H	-3.32745300	-1.75430400	-0.46257100
H	-4.75423700	-1.20357500	0.39367400
H	-4.49286600	3.47581600	-0.34202700
H	-3.35313200	3.12692800	-1.64789000
H	-2.93444900	2.63708400	1.35127400
H	-2.04423000	3.76262400	0.31048200
H	-0.79239200	1.57498500	0.71422400
H	-1.11146900	1.85901200	-0.98809800

B3LYP/6-31G* (LanL2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.393850 a.u.

Sum of electronic and thermal Free Energies = -2248.028209 a.u.
M06-2x-D3/6-311++G** (LanL2DZ for Cu)
Energy = -2248.4304749 a.u.
Number of Imaginary Frequencies = 1
Lowest Frequency = 93.79 *i*

tsd2

C	0.32816700	0.44952900	-0.86685100
C	1.09247500	0.39256800	-1.82708000
C	-0.48801400	0.41693500	0.33847800
C	-1.46087600	1.62467900	0.45741000
N	-2.52841100	1.65417000	-0.52459300
C	-3.87588200	1.21003400	-0.16307200
C	-3.96002900	-0.25804400	0.21620200
C	-4.37870900	-0.64406700	1.49462700
C	-4.47246000	-1.99648800	1.83803500
C	-4.14345600	-2.97931800	0.90317100
C	-3.72450000	-2.60420800	-0.37830500
C	-3.63575300	-1.25421500	-0.71856900
H	1.48573300	0.60151800	-2.80066900
H	-1.06108300	-0.51562400	0.37317200
H	0.17666500	0.42281700	1.21101400
H	-1.91437000	1.58430600	1.45136400
H	-0.87981800	2.54791400	0.37887800
H	-4.24935900	1.82830100	0.66387200
H	-4.50425900	1.42355900	-1.03180100
H	-4.63480000	0.11791900	2.22721600
H	-4.79877600	-2.27876000	2.83533400
H	-4.21384800	-4.03079700	1.16766700
H	-3.47291900	-3.36420900	-1.11319000
H	-3.31412000	-0.96857400	-1.71747800
Cl	2.47484100	-1.47848300	1.31605100
Cu	2.42627000	-1.10771000	-0.91231700
O	-1.06157200	2.37131700	-2.11140800
O	-3.22250000	2.50971300	-2.54779400
C	-2.28792500	2.19477000	-1.77687000
C	5.95316800	-1.03197600	-5.09810100
C	7.10517000	-0.37660800	-4.32990400
N	4.89996700	-1.69910300	-4.29569100
C	6.79773200	1.04435800	-3.83446400
C	5.37995400	1.16776200	-3.25824100
C	4.97291500	-0.05188700	-2.41018400
C	4.33456400	-1.21513700	-3.15733500
C	4.27560700	-2.83475400	-5.00248800
C	3.49977400	-3.72165400	-4.04167800
C	2.54716600	-2.85118900	-3.23496100

N	3.25433200	-1.72775000	-2.60293400
H	6.36889600	-1.82267600	-5.72696900
H	5.48471600	-0.30750800	-5.77972300
H	7.97004200	-0.34656400	-5.00264600
H	7.39309700	-1.03088700	-3.49869400
H	6.91627800	1.75873600	-4.65850100
H	7.53469100	1.32208900	-3.07065300
H	4.64960800	1.30775400	-4.06487000
H	5.31311900	2.06448000	-2.63263700
H	4.24266700	0.26170400	-1.65934500
H	5.83761700	-0.42888700	-1.84872700
H	5.07695900	-3.40307500	-5.48324000
H	3.62018400	-2.45452000	-5.79856000
H	4.19414700	-4.23716900	-3.36778300
H	2.94982500	-4.48358100	-4.60276300
H	2.06270300	-3.43496900	-2.44646600
H	1.74909500	-2.45648600	-3.87903200

B3LYP/6-31G* (LanL2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.368193 a.u.

Sum of electronic and thermal Free Energies = -1787.772531 a.u.

M06-2x-D3/6-311++G** (LanL2DZ for Cu)

Energy = -1788.0188828 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = -32.73 *i*

tse2

C	0.39216600	-1.54494000	-0.31954600
C	-0.48720500	-1.65066600	-1.16197800
C	1.38133000	-1.26199500	0.71337300
C	1.96104600	-2.54066100	1.37762300
N	2.83591100	-3.32746600	0.52509900
C	4.28497300	-3.30088500	0.74448200
C	4.91556600	-1.94025300	0.51030800
C	5.51018400	-1.23445100	1.56268900
C	6.10724800	0.01082100	1.34115100
C	6.11531700	0.56354500	0.05970700
C	5.52502400	-0.13466900	-1.00013200
C	4.92937600	-1.37620500	-0.77507600
H	-1.15360200	-2.01713400	-1.91346700
H	2.19988000	-0.66716400	0.29434100
H	0.91069900	-0.65888200	1.50075500
H	2.53709800	-2.22965500	2.25276600
H	1.13052600	-3.16588800	1.71912100
H	4.50124500	-3.63967700	1.76622600
H	4.70612500	-4.04478600	0.06364400
H	5.51106600	-1.66338800	2.56213300

H	6.56485700	0.54508700	2.16932800
H	6.58148700	1.52909100	-0.11626900
H	5.53703600	0.28496700	-2.00238100
H	4.47680100	-1.91719500	-1.60289600
Cu	-1.41971500	0.60778100	-0.95419300
O	1.04025700	-4.10273700	-0.64995200
O	2.97197400	-5.12054300	-0.91616400
C	2.29155300	-4.21721900	-0.37770600
C	-6.07492300	-1.62070200	0.80652100
C	-5.92390900	-1.19217500	2.26959500
N	-5.28212000	-0.86535700	-0.19384500
C	-4.72505600	-1.83717300	2.98117600
C	-3.48041300	-1.89489100	2.08510200
C	-3.26633300	-0.60521700	1.27125600
C	-3.97645700	-0.51131700	-0.07295100
C	-5.96918600	-0.73996200	-1.49515200
C	-5.33621600	0.34532700	-2.35004300
C	-3.83666600	0.09804500	-2.41446100
N	-3.25464700	-0.02783000	-1.06698600
H	-7.11506600	-1.47114300	0.50972100
H	-5.87188400	-2.69498600	0.69566500
H	-6.84811300	-1.46608800	2.79120900
H	-5.86617100	-0.09801800	2.31143400
H	-4.98560600	-2.85355000	3.30128100
H	-4.50080500	-1.26900900	3.89254600
H	-3.53974700	-2.74979400	1.40030500
H	-2.59115500	-2.06540100	2.70177100
H	-2.20142500	-0.50091200	1.05073100
H	-3.54176200	0.27121100	1.87307800
H	-7.01709800	-0.50220300	-1.29150600
H	-5.94697600	-1.70807000	-2.01422500
H	-5.53349000	1.33046600	-1.91081400
H	-5.77622500	0.33071500	-3.35192400
H	-3.33000400	0.91877500	-2.93057300
H	-3.62691400	-0.81853900	-2.98349800
C	1.85204100	4.70158400	0.47529500
C	1.63573300	4.57333700	1.98661500
N	1.55344900	3.50505800	-0.34864600
C	0.18753300	4.82660500	2.43081200
C	-0.83304300	4.17749700	1.48547300
C	-0.40848900	2.77096200	1.02299900
C	0.46816300	2.69738600	-0.22040100
C	2.39767700	3.42244800	-1.55724100
C	2.34862000	2.03297900	-2.17082700
C	0.89365000	1.63024500	-2.35591100
N	0.11998200	1.78994400	-1.11305800

H	2.90969000	4.90696600	0.29622900
H	1.29638000	5.56316000	0.07838800
H	2.29789100	5.29729200	2.47522500
H	1.98057500	3.58373800	2.30916400
H	-0.00245900	5.90581100	2.48067100
H	0.05244300	4.43722500	3.44756300
H	-0.99964200	4.81248300	0.60646500
H	-1.80308500	4.09934700	1.98842900
H	-1.30496300	2.18841300	0.79155200
H	0.09415600	2.23902800	1.84133200
H	3.42052100	3.67198700	-1.26082600
H	2.07142500	4.18144100	-2.28192700
H	2.85899000	1.31748800	-1.51570500
H	2.87404300	2.03564600	-3.13101900
H	0.81670300	0.58520500	-2.66818000
H	0.42624200	2.23800600	-3.14301800

B3LYP/6-31G* (LanL2DZ for Cu)
Thermal correction to Gibbs Free Energy = 0.601200 a.u.
Sum of electronic and thermal Free Energies = -1789.264811 a.u.
M06-2x-D3/6-311++G** (LanL2DZ for Cu)
Energy = -1789.6630822 a.u.
Number of Imaginary Frequencies = 1
Lowest Frequency = -59.64 *i*

tsa3-[DBU-CO_2]

C	-3.60013000	1.31595600	0.26868900
C	-4.70784400	2.04909200	-0.05716300
C	-2.37910100	1.78652400	0.99008600
C	-1.78425700	0.65806100	1.82299500
N	-1.61638200	-0.53505200	0.98910700
C	-0.53570400	-1.47528900	1.32750900
C	0.83853700	-0.95827900	0.94463100
C	1.81022000	-0.71416600	1.92176000
C	3.07869100	-0.24649000	1.56319600
C	3.38381500	-0.01528600	0.22118600
C	2.41772700	-0.25612900	-0.76224900
C	1.15475500	-0.72528000	-0.40275000
H	-5.48479600	1.49847700	-0.58968600
H	-1.66064000	2.10831800	0.22281700
H	-2.61724500	2.65294000	1.60817000
H	-0.79813500	0.94816300	2.19340700
H	-2.41635100	0.42543800	2.69027500
H	-0.58290500	-1.66670100	2.40506000
H	-0.75899900	-2.40989000	0.81033000
H	1.57636100	-0.89421300	2.96855100
H	3.82313900	-0.06127900	2.33270600

H	4.36815000	0.34901200	-0.05989900
H	2.65155800	-0.08200000	-1.80907500
H	0.40772700	-0.91800700	-1.16873800
Cl	-4.22032500	4.58315100	2.50730700
Cu	-5.58401300	3.23509600	1.32904800
O	-3.53603000	0.04365900	-0.22120400
O	-2.41027700	-1.80715200	-0.75189900
C	-2.45965900	-0.83714000	-0.01913900
C	-0.39982500	7.35218000	-4.83604900
C	0.94995700	6.64843900	-4.67913900
N	-1.60581600	6.58556900	-4.39514300
C	1.55863800	6.82867300	-3.28231400
C	0.49060100	6.73466000	-2.18762700
C	-0.49577300	5.56871400	-2.39949500
C	-1.69553900	5.84755600	-3.29360100
C	-2.75049500	6.82844700	-5.31685800
C	-3.96637400	5.97847400	-4.99995300
C	-4.14441600	5.93575100	-3.49342200
N	-2.91018000	5.37509900	-2.89861000
H	-0.57537800	7.55185900	-5.89311600
H	-0.40927000	8.32129200	-4.32484200
H	1.62347100	7.06122500	-5.43808500
H	0.82905600	5.58747100	-4.92688400
H	2.05936900	7.80202300	-3.21563100
H	2.32848900	6.06459900	-3.12104400
H	-0.06115000	7.67808900	-2.10001700
H	0.96973500	6.58017400	-1.21517100
H	-0.89076000	5.26816600	-1.43272100
H	0.02611100	4.68670800	-2.78681500
H	-2.38683900	6.62481700	-6.32711000
H	-2.98679400	7.89635700	-5.25475900
H	-3.84181000	4.96056100	-5.38332200
H	-4.84569600	6.41456300	-5.48235100
H	-4.97113400	5.29948200	-3.19210100
H	-4.31161000	6.93681100	-3.08106000
C	-3.04667100	4.23491400	-1.99808500
O	-2.14427200	3.41440900	-1.89871700
O	-4.19392900	4.23438200	-1.40318900
H	-4.36501300	3.22863400	-0.73328000
Cl	-7.76018800	2.68910700	1.14961600

B3LYP/6-31G* (LanL2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.390648 a.u.

Sum of electronic and thermal Free Energies = -2437.197525 a.u.

M06-2x-D3/6-311++G** (LanL2DZ for Cu)

Energy = -2437.471704 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = -1229.48 *i*

tsa3-[DBU-H_2O]

C	-0.20728900	0.35806100	0.96331200
C	0.97502600	0.50944000	0.32880800
C	-1.25825100	1.39717100	1.21341500
C	-2.63741100	0.80560800	0.93618600
N	-2.79012400	-0.44908000	1.67509300
C	-4.15164100	-0.87286400	2.03657500
C	-4.71834500	-0.11432900	3.22269600
C	-5.83750600	0.71338600	3.07748200
C	-6.36107700	1.40314800	4.17594900
C	-5.76503000	1.27249200	5.43103800
C	-4.64525800	0.44731100	5.58518500
C	-4.12654900	-0.24145900	4.48925800
H	1.59487600	-0.38353500	0.24225500
H	-1.21005700	1.71006800	2.26578300
H	-1.08826200	2.27882900	0.59249200
H	-3.41583600	1.49392400	1.27629200
H	-2.78320600	0.63303700	-0.13852800
H	-4.78926000	-0.73118200	1.15711500
H	-4.10346700	-1.94224600	2.24833600
H	-6.30619300	0.81642600	2.10139300
H	-7.23077800	2.04187300	4.04783200
H	-6.16950000	1.80743000	6.28598500
H	-4.18018900	0.33803600	6.56128500
H	-3.26145100	-0.88828800	4.61123000
C	-1.74620200	-1.25303800	1.98865900
O	-0.49332700	-0.87507100	1.52545400
O	-1.81074700	-2.29772300	2.61618600
Cu	1.05173600	1.77182900	-1.38062800
Cl	0.71496400	0.08868500	-2.92393400
Cl	0.64174000	3.66952600	-2.68057300
H	3.76547100	3.18689000	-0.59712300
C	8.25389200	2.60597600	-0.86307400
C	8.29989600	1.16760000	-0.34086200
N	6.92383100	3.11444800	-1.29030200
C	7.90882800	1.01897900	1.13700100
C	6.68113200	1.86143400	1.51122800
C	5.58930500	1.84061500	0.42652300
C	5.75672200	2.84780900	-0.69616200
C	6.98503300	4.14813400	-2.35214900
C	5.67766800	4.22617200	-3.13198200
C	4.52326800	4.42932300	-2.16295400
N	4.63749700	3.45436500	-1.07450300
H	8.87760700	2.67116900	-1.75653300

H	8.67675300	3.30471700	-0.12956500
H	9.32492700	0.80727300	-0.48279200
H	7.66978600	0.53945500	-0.98162000
H	8.75221300	1.30915800	1.77510100
H	7.70866200	-0.03954000	1.34321000
H	6.97275900	2.89960300	1.71162900
H	6.24444300	1.48611000	2.44252200
H	4.61575500	2.04473300	0.87815700
H	5.51228900	0.84074000	-0.01943700
H	7.80810800	3.88082500	-3.01765200
H	7.22821100	5.11330500	-1.89073700
H	5.53191000	3.30234000	-3.70249900
H	5.72854400	5.05540000	-3.84268300
H	3.55122700	4.27595900	-2.63907800
H	4.53700900	5.44129500	-1.74015000
O	2.15883100	2.75433300	0.11632800
H	1.65712400	1.74572400	0.51737100
H	1.64819500	3.52266100	0.43184700

B3LYP/6-31G* (LanL2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.402861 a.u.

Sum of electronic and thermal Free Energies = -2325.050097 a.u.

M06-2x-D3/6-311++G** (LanL2DZ for Cu)

Energy = -2325.3432679 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = -1317.60 *i*

tsa3-H_2O

C	-0.39345100	0.26602400	0.72452200
C	0.88662800	0.56184000	0.27060800
C	-1.52080300	1.23134600	0.89206600
C	-2.85124600	0.50174200	0.73672900
N	-2.87234200	-0.67422800	1.61287600
C	-4.16602000	-1.09781700	2.19245500
C	-4.64524900	-0.16098300	3.28327700
C	-5.78522400	0.62939000	3.09652200
C	-6.22391200	1.49257500	4.10556300
C	-5.52253000	1.57245000	5.30936600
C	-4.38259200	0.78450100	5.50427900
C	-3.94764700	-0.07724400	4.49819100
H	1.54534300	-0.25189600	-0.02549100
H	-1.44316500	1.65769400	1.90311400
H	-1.43912200	2.05364500	0.17965300
H	-3.66737300	1.15947100	1.03979500
H	-3.01938400	0.20066600	-0.30393500
H	-4.89287500	-1.14451300	1.37534700
H	-4.02117000	-2.10977100	2.57322600

H	-6.33645100	0.56616600	2.16127300
H	-7.11048400	2.10039100	3.94806000
H	-5.86136000	2.24252600	6.09459700
H	-3.83664800	0.83926800	6.44203600
H	-3.06576400	-0.69358300	4.65519000
C	-1.78506200	-1.42416300	1.83054500
O	-0.58683800	-0.97398100	1.14371300
O	-1.65379700	-2.42878200	2.48560500
Cu	1.17062100	2.12480600	-0.98475900
Cl	0.14419800	0.94736700	-2.55529200
Cl	1.52654900	4.05628300	-2.15712500
O	2.07496300	2.66052900	0.63685900
H	1.48868700	1.52442000	0.91446300
H	1.54905500	3.39404400	1.01385000

B3LYP/6-31G* (LanL2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.170455 a.u.

Sum of electronic and thermal Free Energies = -1862.495755 a.u.

M06-2x-D3/6-311++G** (LanL2DZ for Cu)

Energy = -1862.8181347 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = -1327.55 *i*

tsd3-DBU

C	0.15143500	0.84804500	0.71259100
C	1.38569400	0.39091000	1.10299100
C	-0.68576900	0.33245200	-0.41334100
C	-2.16567100	0.43453000	-0.06111200
N	-2.47088000	1.79043000	0.40294900
C	-3.84045300	2.29745200	0.20968800
C	-4.13431500	2.67416400	-1.23010900
C	-5.10996000	1.98897400	-1.96311800
C	-5.38636100	2.34464500	-3.28714100
C	-4.68413900	3.38883800	-3.89045600
C	-3.70642500	4.07884800	-3.16485900
C	-3.43461200	3.72459600	-1.84376900
H	1.83709700	0.97142400	1.90937200
H	-0.48009700	0.95698200	-1.29529100
H	-0.41055700	-0.69509400	-0.65020100
H	-2.77394400	0.23903300	-0.94735800
H	-2.44132200	-0.29922300	0.70737800
H	-4.53446400	1.52028000	0.54789500
H	-3.95262000	3.15889200	0.86996000
H	-5.66034900	1.17579100	-1.49552000
H	-6.14685700	1.80395000	-3.84381300
H	-4.89634000	3.66669600	-4.91920000
H	-3.15992700	4.89574300	-3.62832700

H	-2.68011400	4.26725200	-1.27956700
C	-1.57814200	2.55099900	1.06791400
O	-0.32445300	1.96376800	1.32957500
O	-1.74393900	3.67618800	1.49750800
Cu	1.43927800	-1.55826700	1.77452200
Cl	0.14621200	-3.01303400	0.67749300
H	2.22796800	0.12082300	0.11022500
C	6.26167300	1.29063800	-2.43061200
C	6.86529600	2.25424300	-1.40339900
N	5.21558100	0.36403000	-1.93808800
C	6.04435500	3.53348200	-1.18366200
C	4.53523000	3.26002900	-1.10786700
C	4.19457600	1.98543400	-0.31182100
C	4.18771400	0.68694500	-1.10720200
C	5.18322400	-0.91497100	-2.67549200
C	4.36527000	-1.96510700	-1.93597100
C	3.00481300	-1.37206800	-1.59208000
N	3.15158600	-0.09162000	-0.90537000
H	7.05888600	0.64230800	-2.80218800
H	5.88002300	1.84376800	-3.30091600
H	7.86762400	2.52361900	-1.75612300
H	7.01197000	1.71449400	-0.46034300
H	6.24176500	4.24511000	-1.99497500
H	6.38100900	4.01498000	-0.25698900
H	4.11028900	3.18074200	-2.11632200
H	4.03127500	4.11053000	-0.63582700
H	3.19509900	2.08195600	0.11366200
H	4.88259500	1.87706900	0.53685800
H	6.21727600	-1.25216600	-2.79343000
H	4.77738200	-0.74586500	-3.68266300
H	4.88501500	-2.26133500	-1.01702100
H	4.25957900	-2.85633700	-2.56236300
H	2.42987300	-2.04208300	-0.94307300
H	2.40842300	-1.22742200	-2.50393500
C	3.15536900	-0.81201800	6.87665900
C	1.93462400	-1.48208600	7.51428200
N	3.40331400	-1.10148200	5.44032900
C	0.62358700	-0.71361200	7.29459000
C	0.50943300	-0.16594900	5.86597700
C	0.97921100	-1.17419100	4.80201500
C	2.46682000	-1.19486700	4.47267200
C	4.84210300	-1.11554200	5.09250300
C	5.09446800	-1.86576700	3.79475900
C	4.15775300	-1.32309100	2.72562400
N	2.76403900	-1.35612700	3.18993900
H	4.05105600	-1.16431800	7.39152700

H	3.12085600	0.27637500	7.01870600
H	2.13325400	-1.56779000	8.58851400
H	1.85884300	-2.50942500	7.13889700
H	0.55530600	0.11826400	8.00610100
H	-0.22199400	-1.37937100	7.50658800
H	1.08148900	0.76417300	5.76304900
H	-0.53240700	0.09597400	5.65274600
H	0.46429200	-0.95092800	3.86342800
H	0.67241500	-2.19128500	5.07892500
H	5.37317400	-1.59590500	5.91781400
H	5.20220700	-0.08070300	5.02546300
H	4.91464000	-2.93705000	3.94028300
H	6.13848800	-1.73842200	3.49310300
H	4.22937900	-1.91447800	1.80858500
H	4.42677800	-0.28946100	2.46913300

B3LYP/6-31G* (LanL2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.727104 a.u.

Sum of electronic and thermal Free Energies = -2250.125022 a.u.

M06-2x-D3/6-311++G** (LanL2DZ for Cu)

Energy = -2250.5402602 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = -1288.57 *i*

tsd3-[DBU-CO_2]

C	-3.59352700	1.31872300	0.25352500
C	-4.70495800	2.04532400	-0.06669700
C	-2.37036200	1.79343900	0.96960500
C	-1.77815100	0.67225500	1.81434400
N	-1.61358000	-0.53002200	0.99341100
C	-0.53872900	-1.47141800	1.34585100
C	0.83969300	-0.96491000	0.96382900
C	1.81019900	-0.72103400	1.94217800
C	3.08254500	-0.26335200	1.58444500
C	3.39282200	-0.04190000	0.24197100
C	2.42797300	-0.28258700	-0.74271300
C	1.16117200	-0.74192000	-0.38400500
H	-5.47046700	1.48664100	-0.60863800
H	-1.64973500	2.10469200	0.20030000
H	-2.60545600	2.66718300	1.57873700
H	-0.79120200	0.96355500	2.18190000
H	-2.41059100	0.45049500	2.68438700
H	-0.59103400	-1.65194800	2.42510300
H	-0.76397800	-2.41015000	0.83706000
H	1.57226900	-0.89329200	2.98937800
H	3.82599200	-0.07820300	2.35493500
H	4.38015700	0.31466900	-0.03847400

H	2.66577000	-0.11611500	-1.78989300
H	0.41513400	-0.93475400	-1.15092300
Cl	-4.23477200	4.62167300	2.44634400
Cu	-5.58911700	3.21323100	1.34761700
O	-3.52362200	0.04201300	-0.23450600
O	-2.40198700	-1.81752600	-0.73805100
C	-2.45365500	-0.83835000	-0.01666100
C	-0.40634100	7.36013000	-4.83502500
C	0.93982700	6.64756900	-4.68771000
N	-1.61513400	6.59810100	-4.39303100
C	1.55541900	6.81612700	-3.29247200
C	0.49135700	6.72247400	-2.19392500
C	-0.50262700	5.56342600	-2.40801700
C	-1.70419500	5.85418100	-3.29587000
C	-2.76243700	6.85314200	-5.30822600
C	-3.98164200	6.00792300	-4.99150200
C	-4.15392900	5.95685000	-3.48449100
N	-2.92025700	5.38587500	-2.89838600
H	-0.58537200	7.56675200	-5.89016500
H	-0.40814600	8.32633100	-4.31826200
H	1.61251200	7.06080300	-5.44712400
H	0.81177500	5.58877300	-4.94107800
H	2.06239800	7.78597300	-3.22227900
H	2.32115900	6.04641200	-3.13876000
H	-0.05463500	7.66853500	-2.09921400
H	0.97346600	6.56003700	-1.22425000
H	-0.89558700	5.26028000	-1.44114100
H	0.01244500	4.68042800	-2.80207100
H	-2.40425900	6.65379500	-6.32122900
H	-2.99228000	7.92195300	-5.23834600
H	-3.86404500	4.99170600	-5.38154000
H	-4.86042100	6.45181900	-5.46772300
H	-4.98285700	5.32291800	-3.18425500
H	-4.31424500	6.95614800	-3.06525900
C	-3.05707600	4.24003600	-2.00721000
O	-2.16026900	3.41285000	-1.92037400
O	-4.20100300	4.24208200	-1.40265700
H	-4.36890300	3.24720700	-0.73785600
C	-10.08251200	0.38121000	2.51870900
C	-9.78417600	0.30248800	4.01863300
N	-9.34982000	1.41150900	1.73858000
C	-8.53935500	-0.52737000	4.36190400
C	-7.37666300	-0.24567300	3.40120400
C	-7.22949700	1.24986500	3.06842300
C	-8.06056600	1.77993300	1.90672200
C	-10.11473700	1.90832700	0.57342100

C	-9.61194900	3.27048600	0.12267500
C	-8.10556100	3.19391300	-0.07707900
N	-7.44370500	2.64370300	1.11385600
H	-11.13744400	0.63307100	2.39239800
H	-9.93542900	-0.59715300	2.04114400
H	-10.66309800	-0.13979100	4.50120600
H	-9.70281300	1.32079100	4.41684900
H	-8.78353500	-1.59620000	4.33055800
H	-8.23376400	-0.30446700	5.39159700
H	-7.49988500	-0.81397000	2.47105400
H	-6.43767900	-0.59349000	3.84495400
H	-6.18544000	1.44783600	2.80963700
H	-7.43988500	1.86101500	3.95559000
H	-11.16414900	1.96925400	0.87120000
H	-10.04477600	1.17456600	-0.24040900
H	-9.85245300	4.02630100	0.87916100
H	-10.10927100	3.55770100	-0.80866500
H	-7.68856800	4.18568500	-0.27448700
H	-7.86652500	2.56219700	-0.94325700

B3LYP/6-31G* (LanL2DZ for Cu)
Thermal correction to Gibbs Free Energy = 0.619978 a.u.
Sum of electronic and thermal Free Energies = -2438.695967 a.u.
M06-2x-D3/6-311++G** (LanL2DZ for Cu)
Energy = -2439.1190327 a.u.
Number of Imaginary Frequencies = 1
Lowest Frequency = -1201.33 *i*

tsd3-[DBU-H_2O]

C	-1.54734400	-0.05771400	0.84072600
C	-0.22462800	-0.15392400	1.09378200
C	-2.28723400	-0.50318100	-0.38563900
C	-3.62282200	-1.12655900	0.00812600
N	-4.34770400	-0.21383000	0.89249000
C	-5.81587000	-0.30180300	0.91689200
C	-6.46994400	0.32143700	-0.30242100
C	-7.19374800	-0.46292000	-1.20767800
C	-7.80004600	0.11683300	-2.32693400
C	-7.68373900	1.48935100	-2.55120000
C	-6.96165000	2.28126300	-1.65117700
C	-6.35989600	1.70134000	-0.53478000
H	0.10783600	0.27839700	2.03891800
H	-2.48114100	0.37326500	-1.01976400
H	-1.68993600	-1.20939600	-0.96543800
H	-4.23616700	-1.29076500	-0.88188400
H	-3.47850400	-2.09672800	0.50188600
H	-6.08665000	-1.36093100	0.99096200

H	-6.14567800	0.19439700	1.83097300
H	-7.28833900	-1.53259700	-1.03483300
H	-8.35911200	-0.50486400	-3.02095800
H	-8.15348700	1.94233500	-3.41998700
H	-6.87224000	3.35129100	-1.81845200
H	-5.80494500	2.31822700	0.16760900
C	-3.72509400	0.65096700	1.72894600
O	-2.33819400	0.61687400	1.75897400
O	-4.27483100	1.43833700	2.48206200
Cu	0.94329300	-1.87809000	0.58652500
Cl	1.93286600	-3.67135500	-0.55010700
H	3.21087100	-0.18140900	-1.00647200
C	6.95170300	2.33198500	-0.48995000
C	6.43257500	3.22249600	0.64154700
N	6.17223200	1.09894200	-0.77696000
C	5.30208600	4.17565700	0.22768100
C	4.24946600	3.49390700	-0.65804900
C	3.91689500	2.06343100	-0.19664600
C	4.84285500	0.97739500	-0.71311400
C	6.97921600	-0.00149900	-1.35768500
C	6.33831800	-1.36031600	-1.09993100
C	4.90254700	-1.34343400	-1.60159600
N	4.23516100	-0.13849700	-1.10008100
H	7.94825900	1.97564600	-0.22185200
H	7.05872100	2.90308900	-1.42139800
H	7.28492400	3.80711600	1.00545700
H	6.12573700	2.58611800	1.48020400
H	5.71983200	5.03654000	-0.30795800
H	4.82530200	4.57019200	1.13324600
H	4.58248100	3.46856100	-1.70278500
H	3.32412600	4.07914600	-0.65108700
H	2.91190700	1.79185000	-0.52817700
H	3.89998100	2.00907000	0.89936800
H	7.96879500	0.04466700	-0.89914200
H	7.10054800	0.18039000	-2.43265000
H	6.36055800	-1.58192500	-0.02716500
H	6.91228800	-2.13552400	-1.61468800
H	4.32949800	-2.20511500	-1.24936500
H	4.86895300	-1.33998700	-2.69799400
O	1.41547100	-0.41969200	-0.84274900
H	0.59628300	-0.02669100	-0.07078300
H	0.98769200	-0.61765000	-1.69616000
C	-0.64399700	-5.10866200	4.76402100
C	-1.19072700	-6.24758300	3.89729400
N	0.31040400	-4.17746700	4.11629600
C	-2.40747800	-5.85131800	3.04812000

C	-2.25250700	-4.45729400	2.42411300
C	-0.83348800	-4.19554900	1.88611100
C	0.17840700	-3.63559100	2.87482300
C	1.29552100	-3.61598700	5.06045200
C	2.47379800	-2.99977100	4.32329100
C	1.94340700	-2.01882200	3.28752500
N	0.92219600	-2.64417600	2.43685600
H	-0.08605900	-5.54766100	5.59425200
H	-1.46778900	-4.53508200	5.21229900
H	-1.46807100	-7.06843000	4.56866100
H	-0.37889300	-6.63250200	3.26893800
H	-3.31412300	-5.87166400	3.66532200
H	-2.54956600	-6.59820200	2.25714800
H	-2.51685600	-3.67928900	3.15116200
H	-2.96120700	-4.34826200	1.59535500
H	-0.88710300	-3.47231700	1.07059300
H	-0.41898400	-5.11052700	1.44495800
H	1.63548300	-4.43092800	5.70567100
H	0.80509200	-2.87138800	5.70304900
H	3.05630300	-3.78597200	3.82924200
H	3.13184700	-2.49157000	5.03496200
H	2.75637900	-1.66244300	2.64625000
H	1.51066700	-1.13608700	3.77752200

B3LYP/6-31G* (LanL2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.633545 a.u.

Sum of electronic and thermal Free Energies = -2326.546256 a.u.

M06-2x-D3/6-311++G** (LanL2DZ for Cu)

Energy = -2326.9914547 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = -1284.38 *i*

tsd3-H_2O

C	-1.81864800	0.22249300	0.84741700
C	-0.49333400	0.28454200	1.08915900
C	-2.50076000	-0.20395800	-0.41841600
C	-3.73888900	-1.03305800	-0.09287500
N	-4.57268400	-0.31098200	0.86878000
C	-6.01438600	-0.59789200	0.87648100
C	-6.75118600	0.02050200	-0.29762800
C	-7.40871200	-0.78363100	-1.23541900
C	-8.09637900	-0.20897200	-2.30931300
C	-8.12810600	1.17852900	-2.45571300
C	-7.47219100	1.99026200	-1.52329300
C	-6.78952200	1.41494500	-0.45193400
H	-0.20030600	0.67692700	2.06390800
H	-2.81271800	0.69235200	-0.97256500

H	-1.81545600	-0.76770700	-1.05400300
H	-4.33141000	-1.19471300	-0.99736700
H	-3.46396100	-2.01761300	0.30897300
H	-6.14176800	-1.68632700	0.87054000
H	-6.40522400	-0.21936600	1.82236000
H	-7.38638400	-1.86536300	-1.12433000
H	-8.60208600	-0.84615300	-3.02975800
H	-8.66062800	1.62748700	-3.28969400
H	-7.49682500	3.07138500	-1.63041600
H	-6.28561000	2.04651300	0.27548300
C	-4.06381200	0.54279400	1.79071400
O	-2.68728900	0.69605600	1.82303400
O	-4.71014900	1.17012600	2.61487100
Cu	0.86857800	-1.29833300	0.45602200
Cl	1.82487000	-2.98513000	-0.88712700
O	1.16993000	0.23369400	-0.83346200
H	0.29064300	0.52675000	-0.04693400
H	0.77538600	0.00360400	-1.69437100
C	-0.19896900	-4.87995800	4.52794100
C	-0.73070400	-5.99597500	3.62308600
N	0.62413000	-3.83257500	3.87872500
C	-2.03876100	-5.63879500	2.90270300
C	-2.03153200	-4.20054900	2.36630800
C	-0.68343600	-3.80235000	1.73852900
C	0.36776200	-3.23584700	2.68194800
C	1.62670700	-3.24311800	4.78610000
C	2.72052400	-2.53298600	4.00439100
C	2.07107500	-1.54210800	3.04878400
N	1.01563100	-2.17833200	2.24756100
H	0.45974100	-5.32935800	5.27465200
H	-1.02228600	-4.40863900	5.08410700
H	-0.88931600	-6.88145100	4.24932600
H	0.05214200	-6.26819000	2.90542200
H	-2.88715600	-5.76604200	3.58646800
H	-2.19412000	-6.34257600	2.07548200
H	-2.28677800	-3.49168200	3.16373200
H	-2.81331000	-4.09138000	1.60601100
H	-0.85074500	-3.03208300	0.98389100
H	-0.24668200	-4.65310400	1.20071100
H	2.05138300	-4.05549700	5.38217500
H	1.13236000	-2.54984500	5.48110700
H	3.30946300	-3.26581200	3.44072400
H	3.39645200	-2.01801100	4.69414100
H	2.81797800	-1.12537500	2.36421900
H	1.63931700	-0.69756600	3.60294400

B3LYP/6-31G* (LanL2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.395943 a.u.
Sum of electronic and thermal Free Energies = -1864.204923 a.u.
M06-2x-D3/6-311++G** (LanL2DZ for Cu)
Energy = -1864.4952105 a.u.
Number of Imaginary Frequencies = 1
Lowest Frequency = -1365.52 *i*

ind2

C	-1.16867300	0.97332900	0.72408500
C	-0.42205100	1.21375600	-0.22878100
C	-2.26507000	0.90312000	1.70235600
C	-3.37154400	1.94912200	1.44069000
N	-4.04848600	1.81311000	0.15137600
C	-5.08570200	0.78874600	-0.05416800
C	-4.55776300	-0.59287200	-0.40073300
C	-4.85128700	-1.69027400	0.41745800
C	-4.38655600	-2.96758800	0.08896400
C	-3.62209800	-3.15789200	-1.06367700
C	-3.32797200	-2.06679800	-1.88910200
C	-3.79470700	-0.79369300	-1.56071100
H	0.02120100	1.61912200	-1.11656700
H	-2.68857100	-0.10616400	1.69979100
H	-1.87252000	1.06962500	2.71178200
H	-4.12361900	1.86283400	2.23215500
H	-2.94898600	2.95569300	1.49045400
H	-5.69138200	0.74702400	0.85665800
H	-5.73396000	1.15576000	-0.85704700
H	-5.44673600	-1.54702100	1.31620700
H	-4.62199300	-3.80976000	0.73381000
H	-3.26131900	-4.14961500	-1.32216600
H	-2.74157900	-2.21001100	-2.79271100
H	-3.57328800	0.04940300	-2.21009900
Cl	0.27954400	-1.56258000	2.75575300
Cu	0.57493500	-0.25829200	0.83655900
O	-2.95418300	3.65168600	-0.74734000
O	-4.34171900	2.67162000	-1.98081000
C	-3.78670200	2.68866900	-0.83181300
C	5.74295100	0.19324600	-1.08376800
C	6.26424000	1.12076300	0.01940200
N	4.54895100	-0.61867400	-0.76064900
C	5.55887400	2.48497600	0.07244000
C	4.04162900	2.36825300	-0.13395200
C	3.42687200	1.16263900	0.60130900
C	3.41274900	-0.16191000	-0.15086400
C	4.51753400	-1.90372000	-1.48143200
C	3.49673500	-2.84900000	-0.86733100

C	2.15867300	-2.12851400	-0.77729900
N	2.28032800	-0.82264200	-0.11532900
H	6.52409900	-0.53524600	-1.31467100
H	5.56688200	0.76136500	-2.00953200
H	7.33575700	1.27348600	-0.15468500
H	6.18485100	0.59999700	0.98098800
H	5.97771800	3.14967600	-0.69352600
H	5.76609600	2.95581300	1.04174800
H	3.80602800	2.29855200	-1.20356400
H	3.55201700	3.28146500	0.22261400
H	2.38188300	1.37840600	0.83783300
H	3.93115500	1.01411900	1.56564300
H	5.52087000	-2.33748200	-1.42819200
H	4.29313900	-1.72967100	-2.54415900
H	3.82666300	-3.15032500	0.13424500
H	3.41407100	-3.75399100	-1.47777900
H	1.43483800	-2.72439700	-0.21232300
H	1.73676400	-1.98242000	-1.78216000

B3LYP/6-31G* (LanL2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.371282 a.u.

Sum of electronic and thermal Free Energies = -1787.774895 a.u.

M06-2x-D3/6-311++G** (LanL2DZ for Cu)

Energy = -1788.0303794 a.u.

No imaginary frequency

ind3

C	-3.61512700	0.95542100	0.15198100
C	-4.90123700	1.28354800	0.26819800
C	-2.38806000	1.64687500	0.65606100
C	-1.54115500	0.64596000	1.43757900
N	-1.35792300	-0.57860500	0.65471700
C	-0.21488400	-1.43356200	1.00064800
C	1.11373200	-0.89761800	0.49724600
C	2.12477700	-0.52882900	1.39200100
C	3.35080700	-0.04494900	0.92368600
C	3.57465900	0.07737900	-0.44839800
C	2.56926700	-0.28854500	-1.35056400
C	1.34865100	-0.77317500	-0.88116300
H	-5.64959800	0.62762500	-0.17719500
H	-1.80306700	2.02018500	-0.19618700
H	-2.65916600	2.49790900	1.28196300
H	-0.55107800	1.06502200	1.64404400
H	-2.01232300	0.40603200	2.40073300
H	-0.18913400	-1.53324800	2.09193200
H	-0.41663300	-2.41891600	0.57724200
H	1.95453600	-0.62343000	2.46214800

H	4.12574800	0.23771600	1.63115700
H	4.52576200	0.45379500	-0.81524700
H	2.73989600	-0.19968900	-2.42021700
H	0.57010300	-1.06453700	-1.58134200
Cl	-4.39154000	4.56338300	1.82779700
Cu	-5.70624400	2.84178000	1.17035400
O	-3.31090000	-0.21562100	-0.58235900
O	-2.01780200	-1.95661200	-1.05267800
C	-2.18996600	-0.96932600	-0.34778400
C	-10.40655800	0.62074500	2.88869200
C	-10.07922400	0.74062600	4.38038100
N	-9.63223600	1.48243400	1.96178300
C	-8.88724100	-0.11994500	4.82324600
C	-7.73253300	-0.06997900	3.81341800
C	-7.48788900	1.34407800	3.25577600
C	-8.30561100	1.75379900	2.03702200
C	-10.39600000	1.86878600	0.75702600
C	-9.78936300	3.09260900	0.08867100
C	-8.30543200	2.84090600	-0.13595500
N	-7.64420000	2.41678600	1.10572100
H	-11.44788400	0.91526500	2.74133200
H	-10.32868100	-0.42476700	2.55940300
H	-10.97383900	0.43964100	4.93743100
H	-9.91450600	1.79735800	4.62156600
H	-9.20822200	-1.16062900	4.95506400
H	-8.53926100	0.22811500	5.80374700
H	-7.91951500	-0.76006100	2.98118600
H	-6.80970500	-0.41729100	4.29066600
H	-6.44015800	1.42467300	2.95451800
H	-7.63578100	2.09435700	4.04359000
H	-11.42255100	2.07613600	1.07041000
H	-10.42930000	1.01932700	0.06139000
H	-9.92683200	3.97234500	0.72828900
H	-10.29774400	3.28601200	-0.86095300
H	-7.80841500	3.74677600	-0.49662300
H	-8.15964000	2.06670300	-0.90182700

B3LYP/6-31G* (LanL2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.375368 a.u.

Sum of electronic and thermal Free Energies = -1787.821187 a.u.

M06-2x-D3/6-311++G** (LanL2DZ for Cu)

Energy = -1788.0788423 a.u.

No imaginary frequency

ind4

C	0.72173700	-0.97182500	1.08189400
C	-0.43697300	-1.52672400	1.60012400

C	1.94647000	-1.72735400	0.69103300
C	2.60192900	-1.08469300	-0.52610600
N	2.72882100	0.36339900	-0.32449500
C	3.81988000	1.06389800	-1.03357600
C	5.18080300	0.79588600	-0.42175600
C	6.16059700	0.09800400	-1.13716200
C	7.41850400	-0.13847300	-0.57367000
C	7.70411600	0.31894400	0.71345900
C	6.72942300	1.01639200	1.43576300
C	5.47687400	1.25422000	0.87111300
H	-1.13586300	-0.87331700	2.11302700
H	2.63331600	-1.68929700	1.54886100
H	1.69958200	-2.77231700	0.50070800
H	3.60620800	-1.49066000	-0.66231800
H	2.02170600	-1.28866600	-1.43345700
H	3.79758300	0.73612500	-2.07798600
H	3.57844300	2.12728600	-1.00928500
H	5.94218000	-0.25743700	-2.14145700
H	8.17041700	-0.68042300	-1.14051000
H	8.68060300	0.13598200	1.15321200
H	6.94834800	1.37853700	2.43647100
H	4.72430600	1.80306200	1.43199100
Cl	-0.47064100	-3.24309200	-1.46865900
Cu	-1.62227700	-1.83184400	-0.21380500
O	0.75506900	0.35719500	0.95811200
O	1.81933000	2.28338300	0.56642800
C	1.84209600	1.08761400	0.37420900
H	-0.41000000	-2.57419000	1.88711900
C	-4.87152500	2.50114100	0.05689500
C	-4.24706400	3.19597600	-1.15580900
N	-4.59240500	1.04831000	0.22808500
C	-2.79281000	3.63790800	-0.93970200
C	-1.96887600	2.56662500	-0.21412700
C	-2.27870300	1.14547800	-0.72073900
C	-3.43273400	0.42443200	-0.04057200
C	-5.70732800	0.32937600	0.89062900
C	-5.62081200	-1.17169400	0.67009600
C	-4.21055000	-1.63539900	1.00585000
N	-3.22505400	-0.86435600	0.23175400
H	-5.95754400	2.56755700	-0.02740200
H	-4.59565600	3.01469800	0.98727100
H	-4.86705400	4.07213100	-1.37639500
H	-4.33751200	2.53828800	-2.02810500
H	-2.76813400	4.56806200	-0.35945000
H	-2.33945700	3.86118600	-1.91312100
H	-2.14725000	2.61129200	0.86712600

H	-0.89905400	2.75627500	-0.34726900
H	-1.39452700	0.52166900	-0.56931800
H	-2.45967000	1.15261500	-1.80294900
H	-6.63820300	0.72194200	0.47488500
H	-5.69201800	0.57437700	1.96008900
H	-5.85536100	-1.41523300	-0.37212500
H	-6.35157600	-1.67854400	1.30705700
H	-4.08169400	-2.69529800	0.77245000
H	-4.01024700	-1.50415700	2.07763500

B3LYP/6-31G* (LanL2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.392961 a.u.

Sum of electronic and thermal Free Energies = -1788.269644 a.u.

M06-2x-D3/6-311++G** (LanL2DZ for Cu)

Energy = -1788.5348574 a.u.

No imaginary frequency

tsd2'

C	-0.94911000	-1.91494200	-0.23069400
C	-1.19367900	-3.01839500	0.25072600
C	-1.07212800	-0.82820300	-1.20367900
C	-2.00419100	-1.27798700	-2.36762600
N	-3.37194700	-1.57686000	-1.98149100
C	-4.40288300	-0.55350600	-2.17467700
C	-4.22341400	0.67215000	-1.29618000
C	-3.99074800	1.93142900	-1.86123600
C	-3.83822200	3.06189800	-1.05182500
C	-3.91597300	2.94261200	0.33664700
C	-4.15069400	1.68850800	0.91201600
C	-4.30435000	0.56370900	0.10126100
H	-1.28144500	-3.91995200	0.81697000
H	-1.47414000	0.07076500	-0.72635200
H	-0.09053500	-0.57238000	-1.61879700
H	-2.02394100	-0.47248600	-3.10874200
H	-1.56662100	-2.16529100	-2.83171700
H	-4.42007900	-0.25095400	-3.23041900
H	-5.35636000	-1.04322100	-1.96395800
H	-3.93015000	2.02994400	-2.94279600
H	-3.65755500	4.03179900	-1.50744600
H	-3.79801200	3.81882500	0.96827500
H	-4.21981900	1.58945200	1.99200800
H	-4.48975100	-0.40752200	0.55410100
Cl	-0.55749100	-1.12380000	3.37236100
Cu	0.59384400	-1.44340500	1.49550500
O	-2.81949100	-3.71251400	-1.33477200
O	-4.94854800	-3.22297500	-1.66585800
C	-3.75289200	-2.87005700	-1.64769600

C	4.82363900	0.50714900	-1.33331000
C	5.01548800	1.77221600	-0.49016900
N	4.08653200	-0.61477400	-0.70376700
C	3.82258300	2.73880200	-0.53690700
C	2.47408800	2.00841900	-0.45834000
C	2.48417700	0.84287600	0.54883100
C	2.94044900	-0.51018200	0.01936200
C	4.54496300	-1.93568700	-1.17821500
C	4.03722700	-3.05098100	-0.27885600
C	2.53320800	-2.89372200	-0.11279000
N	2.18634000	-1.54072000	0.34915700
H	5.80933000	0.09830100	-1.56663700
H	4.35394200	0.75451700	-2.29601400
H	5.91047800	2.28238800	-0.86453700
H	5.24529600	1.47786500	0.54070500
H	3.85972100	3.32999500	-1.46028000
H	3.90783000	3.45008700	0.29404100
H	2.18349400	1.63109600	-1.44684600
H	1.69017600	2.71451300	-0.16370200
H	1.47067300	0.69259300	0.93088900
H	3.09871100	1.10228000	1.42079300
H	5.63871800	-1.91968300	-1.18690000
H	4.21067000	-2.08801300	-2.21387600
H	4.52860700	-2.99523300	0.69977200
H	4.28097100	-4.02200000	-0.72102400
H	2.14458300	-3.61324800	0.61367400
H	2.02042600	-3.09126300	-1.06389500

B3LYP/6-31G* (LanL2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.371251 a.u.

Sum of electronic and thermal Free Energies = -1787.766006 a.u.

M06-2x-D3/6-311++G** (LanL2DZ for Cu)

Energy = -1788.019887 a.u.

Number of Imaginary Frequencies = 1

Lowest Frequency = -165.95 *i*

ind3'

C	-0.52936200	-0.94903000	0.05431700
C	-0.78875300	-2.25148400	0.02843600
C	-1.19605800	0.13101300	-0.74287800
C	-2.13361500	-0.43227600	-1.82273800
N	-3.24264000	-1.21868400	-1.27201100
C	-4.60879300	-0.69916400	-1.43415100
C	-4.85212600	0.59715300	-0.68336000
C	-5.22987700	1.75674700	-1.36993600
C	-5.47956500	2.94715900	-0.67951900
C	-5.34876800	2.98945300	0.70923600

C	-4.97092900	1.83548400	1.40509300
C	-4.72638800	0.64895900	0.71355000
H	-0.23445300	-2.99495600	0.59260300
H	-1.76195700	0.80187800	-0.08412700
H	-0.43890000	0.75391400	-1.23971100
H	-2.57366600	0.39270200	-2.38857700
H	-1.56450300	-1.04929900	-2.52622300
H	-4.80976700	-0.55092500	-2.50262500
H	-5.27886400	-1.48420100	-1.07951200
H	-5.33266900	1.72853800	-2.45238000
H	-5.77198300	3.83836000	-1.22825400
H	-5.54031400	3.91303200	1.24863100
H	-4.87207300	1.85997200	2.48699700
H	-4.43626100	-0.24542700	1.25975000
Cl	-0.08668200	0.42568200	3.23569100
Cu	0.89251500	-0.34691000	1.34614100
O	-1.77632300	-2.93489000	-0.72473000
O	-3.98108400	-3.29520900	-0.62908000
C	-3.07802600	-2.50169900	-0.85002300
C	5.44345600	0.83642800	-1.42492600
C	5.61650900	2.24703600	-0.85385000
N	4.60855200	-0.10946300	-0.64445800
C	4.47002700	3.20684600	-1.20449300
C	3.09241600	2.54111300	-1.07521400
C	2.98926700	1.62298900	0.15681200
C	3.43301100	0.17828700	-0.02979800
C	5.02670500	-1.51613300	-0.81192800
C	4.45745000	-2.39323300	0.29182900
C	2.95492500	-2.16689200	0.36984000
N	2.63377700	-0.73736800	0.48538000
H	6.42745100	0.36496500	-1.47556500
H	5.06649800	0.88223600	-2.45645800
H	6.55780800	2.64592300	-1.24907200
H	5.75232900	2.17374500	0.23155700
H	4.59718400	3.57919100	-2.22848300
H	4.52349200	4.08123500	-0.54404500
H	2.85837900	1.96376000	-1.97828000
H	2.31652900	3.31065200	-1.00031900
H	1.94682300	1.58264300	0.48386600
H	3.54799800	2.05326400	0.99801400
H	6.11970500	-1.53879100	-0.79099900
H	4.70940800	-1.87540500	-1.80059400
H	4.92497000	-2.13562200	1.24946600
H	4.68085900	-3.44386900	0.08211700
H	2.53156000	-2.68196500	1.23771500
H	2.45747100	-2.57489300	-0.51999500

B3LYP/6-31G* (LanL2DZ for Cu)
Thermal correction to Gibbs Free Energy = 0.377281 a.u.
Sum of electronic and thermal Free Energies = -1787.807972 a.u.
M06-2x-D3/6-311++G** (LanL2DZ for Cu)
Energy = -1788.0712685 a.u.
No imaginary frequency

tsd3'-[DBU-CO_2]

C	1.97917500	0.14804200	-0.11240500
C	1.77404700	0.29440200	1.21871300
C	3.34263600	0.24077500	-0.75814500
C	4.34942400	1.04133000	0.07439800
N	4.78985100	0.33986300	1.28720100
C	6.19959100	-0.08775800	1.36478000
C	6.52821200	-1.24684100	0.44141600
C	7.45291500	-1.09326800	-0.59773500
C	7.76422500	-2.16602600	-1.43929800
C	7.14737500	-3.40353800	-1.25065400
C	6.22136600	-3.56651000	-0.21419400
C	5.91658500	-2.49654900	0.62680000
H	0.77519900	0.25397100	1.65085800
H	3.73537100	-0.76623600	-0.94049300
H	3.24398900	0.71508400	-1.74023700
H	5.24879600	1.22628400	-0.51631200
H	3.93288400	2.01779600	0.34830400
H	6.82701200	0.77631800	1.12265300
H	6.38635200	-0.35646400	2.40544000
H	7.93647800	-0.13077500	-0.74824300
H	8.48459600	-2.03128100	-2.24156300
H	7.38594700	-4.23792000	-1.90447600
H	5.74111100	-4.52887000	-0.05937500
H	5.20344900	-2.62943100	1.43672200
Cl	0.86896100	1.27525300	-3.13768400
Cu	0.42020900	1.22254400	-0.88401900
O	2.65281300	0.50026000	2.25182800
O	4.31947000	-0.44570500	3.38964500
C	3.98768000	0.07505300	2.33942000
C	0.31790800	-7.33642200	-3.35883400
C	1.75618700	-7.62255900	-3.79569300
N	0.12793300	-6.20507100	-2.39908000
C	2.20117300	-6.76411400	-4.98697500
C	1.68643800	-5.32592800	-4.86746600
C	1.85554900	-4.73621600	-3.45284200
C	0.74059100	-5.02736600	-2.45841400
C	-0.91776200	-6.53832600	-1.39130400
C	-1.07881600	-5.47696100	-0.31937000

C	-0.99243400	-4.11225100	-0.97821600
N	0.31907400	-4.01078000	-1.65598400
H	-0.07512800	-8.20773600	-2.83480600
H	-0.33704300	-7.16296200	-4.21992600
H	1.81365200	-8.68493200	-4.05640100
H	2.42224100	-7.48555400	-2.93589600
H	1.83296600	-7.20278400	-5.92213900
H	3.29613200	-6.76568300	-5.04587100
H	0.63611200	-5.26139400	-5.17523000
H	2.23757500	-4.67712400	-5.55618700
H	1.92717800	-3.65456100	-3.53249800
H	2.80503700	-5.05959600	-3.01213500
H	-0.63123700	-7.49637300	-0.95011600
H	-1.85235300	-6.68924200	-1.94234100
H	-0.29603600	-5.56728800	0.44073900
H	-2.04509900	-5.60947000	0.17545900
H	-1.05292900	-3.30068500	-0.25940500
H	-1.78528800	-3.97563200	-1.72193400
C	1.17869300	-2.88034200	-1.31721500
O	2.39440900	-2.98836200	-1.38302900
O	0.48551000	-1.85433400	-0.94266600
H	1.17929700	-0.90483400	-0.57360600
C	-2.72559300	5.49615500	0.29962700
C	-1.65502300	6.55643100	0.02225800
N	-2.51148900	4.15772300	-0.31040500
C	-0.45625300	6.49343100	0.97990700
C	-0.00813900	5.05243400	1.26342000
C	-0.03033600	4.16056800	0.00738100
C	-1.34775600	3.47448000	-0.32354400
C	-3.77220700	3.50976400	-0.73483400
C	-3.50836200	2.34052300	-1.66714300
C	-2.47023700	1.43562600	-1.02424200
N	-1.26273400	2.18786200	-0.64696100
H	-3.67490800	5.84259500	-0.11227400
H	-2.88068500	5.36920400	1.37916100
H	-2.13796500	7.53643900	0.10612700
H	-1.33285300	6.46746200	-1.02178300
H	-0.71200000	6.98232300	1.92779500
H	0.37547200	7.06232500	0.54685200
H	-0.63562800	4.59941300	2.04068400
H	1.01110100	5.05602600	1.66384000
H	0.70818100	3.36401100	0.13420100
H	0.29079400	4.73367800	-0.87188800
H	-4.37477400	4.27235400	-1.23503300
H	-4.32196700	3.18690000	0.15908400
H	-3.13932600	2.70558300	-2.63263700

H	-4.44085900	1.79764700	-1.84749000
H	-2.17103000	0.63352400	-1.70492200
H	-2.87930400	0.95824600	-0.12336400

B3LYP/6-31G* (LanL2DZ for Cu)
Thermal correction to Gibbs Free Energy = 0.622158 a.u.
Sum of electronic and thermal Free Energies = -2438.670430 a.u.
M06-2x-D3/6-311++G** (LanL2DZ for Cu)
Energy = -2439.0996329 a.u.
Number of Imaginary Frequencies = 1
Lowest Frequency = -1350.34 *i*

ind4'

C	-1.21428400	-1.38370000	-0.87914400
C	-0.71275500	-0.38270700	-1.65404900
C	-2.15527200	-1.22560900	0.28216800
C	-2.22671200	0.20439800	0.81733200
N	-2.77632900	1.16077500	-0.15423200
C	-4.05796100	1.81792300	0.17682200
C	-5.21476200	0.84255100	0.28130800
C	-5.91031300	0.69339900	1.48678500
C	-6.99266700	-0.18705400	1.58108100
C	-7.38646500	-0.93111700	0.46806000
C	-6.69667000	-0.78933700	-0.74108100
C	-5.61998900	0.09262700	-0.83369700
H	-0.11763900	-0.60280500	-2.53892000
H	-3.15653800	-1.54466400	-0.03460600
H	-1.84605200	-1.89952100	1.08797600
H	-2.88767200	0.22637500	1.68498300
H	-1.24392200	0.55049300	1.15563300
H	-3.93583900	2.35832300	1.12254500
H	-4.23798600	2.55606200	-0.60596500
H	-5.60690700	1.27171500	2.35649000
H	-7.52282900	-0.29142700	2.52370000
H	-8.22603100	-1.61706900	0.53893400
H	-7.00143600	-1.36267500	-1.61230700
H	-5.09119800	0.20292500	-1.77744900
Cl	0.92556400	-2.49593000	1.64405200
Cu	1.01671200	-1.28086900	-0.25948000
O	-0.85625500	0.96530200	-1.49246000
O	-2.37004900	2.55286900	-1.93794000
C	-2.08351200	1.62046500	-1.21680000
H	-1.06313700	-2.38931100	-1.27089200
C	5.60897200	1.49682000	0.24109400
C	5.12133000	2.32045100	1.43918600
N	4.84675500	0.24721800	-0.03567300
C	3.99753400	3.30698700	1.08747100

C	2.98381000	2.71383800	0.10057700
C	2.59735300	1.25856500	0.42804800
C	3.50989400	0.15508000	-0.08309300
C	5.71830800	-0.90131300	-0.38720100
C	4.96896900	-2.21899200	-0.33082300
C	3.66563700	-2.06181000	-1.09361600
N	2.88760700	-0.92104500	-0.59272200
H	6.63291800	1.16802100	0.41769200
H	5.62192200	2.09532200	-0.67731300
H	5.98624000	2.86779500	1.82896700
H	4.81330500	1.63495600	2.23735000
H	4.42583600	4.21760600	0.65219500
H	3.48587600	3.60738100	2.00939700
H	3.36198700	2.76727200	-0.92715200
H	2.06674200	3.31148400	0.11276700
H	1.61374200	1.06447200	-0.00895200
H	2.48784700	1.12968400	1.51305000
H	6.54914400	-0.89344400	0.32195100
H	6.13053000	-0.71309900	-1.38640300
H	4.76122300	-2.49434600	0.70904300
H	5.58621800	-3.00627800	-0.77197500
H	3.04291100	-2.95690900	-1.02318100
H	3.85303500	-1.88513500	-2.16251400

B3LYP/6-31G* (LanL2DZ for Cu)

Thermal correction to Gibbs Free Energy = 0.394147 a.u.

Sum of electronic and thermal Free Energies = -1788.244867 a.u.

M06-2x-D3/6-311++G** (LanL2DZ for Cu)

Energy = -1788.5133977 a.u.

No imaginary frequency

P1

C	3.14125300	-0.49867800	-0.51718500
C	4.44906500	-0.71366900	-0.64496300
C	2.03451000	-1.49980200	-0.61470800
C	1.10024800	-1.32266000	0.57907700
N	0.72963300	0.08850000	0.71359200
C	-0.52601200	0.39193000	1.41451900
C	-1.76021600	0.15510700	0.56297800
C	-2.71368800	-0.80070600	0.93057800
C	-3.85361300	-1.00865700	0.14768300
C	-4.04778600	-0.26199000	-1.01483900
C	-3.09909500	0.69536400	-1.39064800
C	-1.96470000	0.90279800	-0.60708500
H	5.16516200	0.09664200	-0.55897000
H	1.46759700	-1.33433700	-1.54075500
H	2.43768400	-2.51453400	-0.64066700

H	0.18211100	-1.89895700	0.43141800
H	1.57566200	-1.67604400	1.50384200
H	-0.56425600	-0.23106600	2.31502900
H	-0.46891200	1.43492600	1.73026700
H	-2.56692300	-1.38465300	1.83642500
H	-4.58488100	-1.75500500	0.44623200
H	-4.93218400	-0.42208300	-1.62555900
H	-3.24703100	1.28285000	-2.29292100
H	-1.23116300	1.65146800	-0.89484300
O	2.71093700	0.81101500	-0.30223000
O	1.19262600	2.29984900	0.33229400
C	1.49458100	1.11682700	0.26359500
H	4.81917300	-1.71094600	-0.85186200

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.175331 a.u.

Sum of electronic and thermal Free Energies = -670.138200 a.u.

M06-2x-D3/6-311++G**

Energy = -670.2215536 a.u.

No imaginary frequency

P2

C	-2.31325800	1.98184300	-0.14193500
C	-3.14923200	1.02679700	-0.54758500
C	-1.13343200	1.83013400	0.77216400
C	-1.07233900	0.45215300	1.42977000
N	-0.93112600	-0.64636900	0.46193700
C	0.30241500	-1.44592600	0.50241100
C	1.54371500	-0.65889000	0.12420000
C	2.64442100	-0.61557700	0.98704500
C	3.80677100	0.07384200	0.62866000
C	3.87689100	0.73409000	-0.59855900
C	2.78028400	0.70002000	-1.46641700
C	1.62412400	0.00710900	-1.10800700
H	-4.01141400	1.24059800	-1.17090000
H	-0.19865800	2.01922400	0.22761600
H	-1.18742300	2.59476400	1.55959100
H	-0.20978100	0.39877300	2.09712900
H	-1.96802200	0.28369500	2.03761900
H	0.42312600	-1.86600600	1.50872000
H	0.15028300	-2.28068600	-0.18410200
H	2.59382700	-1.12668300	1.94581800
H	4.65226200	0.09720200	1.31090000
H	4.77769300	1.27315000	-0.87889400
H	2.82809700	1.21099700	-2.42433500
H	0.77487400	-0.01584600	-1.78658500
O	-3.12498300	-0.33483700	-0.25326700

O	-2.01753000	-2.17756300	-0.86011700
C	-1.98238600	-1.11665600	-0.25824600
H	-2.53471300	2.98097600	-0.51007000

B3LYP/6-31G*

Thermal correction to Gibbs Free Energy = 0.175531 a.u.

Sum of electronic and thermal Free Energies = -670.124741 a.u.

M06-2x-D3/6-311++G**

Energy = -670.2110852 a.u.

No imaginary frequency

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3. C. Villiers, J. P. Dognon, R. Pollet, P. Thuéry and M. Ephritikhine, *Angew. Chem. Int. Edit.*, 2010, **122,** 3543-3546.

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