

# Theoretical Investigation on the Mechanism of Cu(II)-catalyzed Synthesis of 4-Quinolones: Effects of Additives HOTf vs. HOTs

Binfang Yuan,<sup>a,b</sup> Xiaogang Guo,<sup>a</sup> Guangzhao Wang,<sup>c</sup> Huisheng Huang,<sup>a</sup> Fulan Zhang,<sup>a</sup> Jianhua Xu\*,<sup>a</sup>  
Rongxing He\*<sup>b</sup>

<sup>a</sup> Chongqing Key Laboratory of Inorganic Special Functional Materials, College of Chemistry and Chemical Engineering, Yangtze Normal University, Fuling, Chongqing 408100, China.

<sup>b</sup> College of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, China.

<sup>c</sup> College of Electronic Information Engineering, Key Laboratory of Extraordinary Bond Engineering and Advanced Materials, Technology, Yangtze Normal University, Fuling, Chongqing 408100, China.

## Table-of-Contents

Table S1. Exploring the effects of methods B3LYP, CAM-B3LYP, BLYP, B3P86, B3PW91, BHandHLYP and PBE by comparing the activation free energy barriers from **in5-HOTf** to **ts4-HOTf** (the geometric structures of **in5-HOTf** and **ts4-HOTf** are optimized using B3LYP (CAM-B3LYP, BLYP, B3P86, B3PW91, BHandHLYP and PBE)/6-31G\* in gas phase, and the single point energies are obtained at the M06-2X/6-311++G\*\* calculated level in solution phase).....3

Table S2. Exploring the effects of basis sets 6-31G\*, 6-31G\*\*, 6-31+G\* and 6-311G\* by comparing the activation free energy barriers from **in5-HOTf** to **ts4-HOTf** (the geometric structures of **in5-HOTf** and **ts4-HOTf** are optimized using B3LYP/6-31G\* (6-31G\*\*, 6-31+G\* and 6-311G\*) in gas phase, and the single point energies are obtained at the M06-2X/6-311++G\*\* calculated level in solution phase).....4

Scheme S1. The possible mechanisms of Cu(OTf)<sub>2</sub>-catalyzed alkynes (**1a**) with anilines (**2a**) to form 4-quinolones (**P**).....5

Figure S1. Scan profile along with the formation of N1-Cu bond (from 3.085 to 1.885 Å).....6

Figure S2. IRC of <b>ts2-OTf</b> .....	7
Figure S3. Scan profile from <b>in8-OTf</b> to <b>in7</b> via <b>ts5-OTf</b> along with the formation of O2-H2 bond (from 1.560 to 0.980 Å).....	8
Figure S4. IRC of <b>ts5-HOTf</b> .....	9
Figure S5. Scan profile from <b>in8-HOTf</b> to <b>in7</b> via <b>ts6-HOTf</b> along with the cleavage of O10-H2 bond (from 1.591 to 0.991 Å).....	10
Figure S6. Optimized geometries involved in the Cu(OTf) <sub>2</sub> -catalyzed reaction with the participation of HOTs. Bond distances are given in Å.....	11
Table S3. The Mulliken charges of HOTf and HOTs.....	12
Table S4. Dissociation energies for H-O bonds in HOTf and HOTs at PCM//M06-2X/6-311++G**//B3LYP/6-31G* level.....	13
Figure S7. The bond lengths of O-H in HOTf and HOTs.....	14
Figure S8. Optimized geometries of the intermolecular nucleophilic addition of <b>1a</b> with <b>2a</b> ( <b>Step I</b> ) without the participation of Cu(OTf) <sub>2</sub> .....	15
Figure S9. Scan profile from <b>in5'</b> to <b>in6'</b> along with the formation of C1-C5 bond (from 3.578 to 1.578 Å).....	16
Intrinsic Reaction Coordinates.....	17
Cartesian coordinates of the optimized stationary points on the optimal reaction channels.....	20

To whom correspondence should be addressed. E-mail: herx@swu.edu.cn

Table S1. Exploring the effects of methods B3LYP, CAM-B3LYP, BLYP, B3P86, B3PW91, BHandHLYP and PBE by comparing the activation free energy barriers from **in5-HOTf** to **ts4-HOTf** (the geometric structures of **in5-HOTf** and **ts4-HOTf** are optimized using B3LYP (CAM-B3LYP, BLYP, B3P86, B3PW91, BHandHLYP and PBE)/6-31G\* in gas phase, and the single point energies are obtained at the M06-2X/6-311++G\*\* calculated level in solution phase).

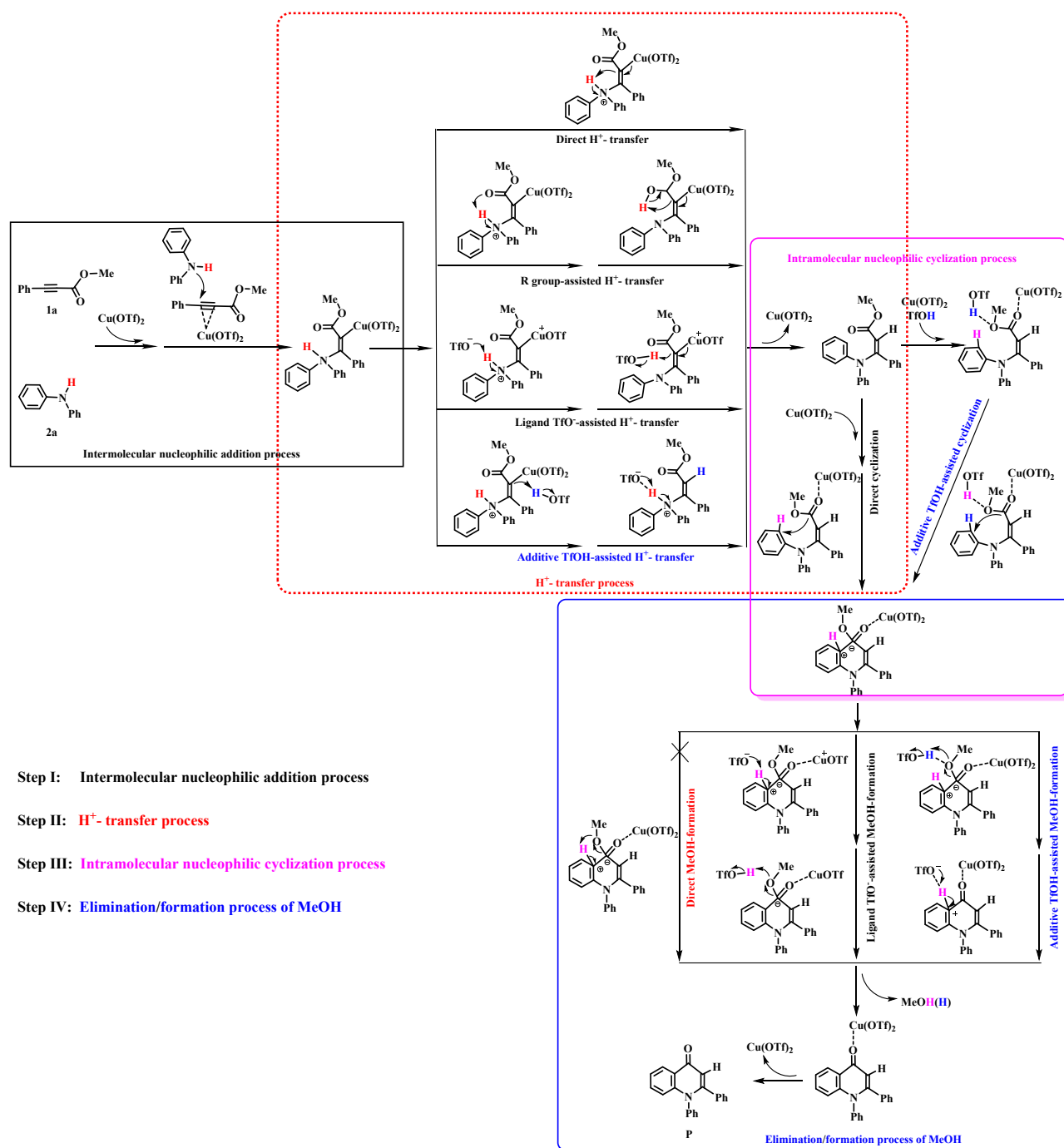
Species	Activation Free Energy Barriers (kJ/mol)						
	B3LYP	CAM-B3LYP	BLYP	B3P86	B3PW91	BHandHLYP P	PBE
<b>ts4-HOTf</b>	135.0	141.2	130.0	133.0	138.3	139.7	139.4

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

Table S2. Exploring the effects of basis sets 6-31G\*, 6-31G\*\*, 6-31+G\* and 6-311G\* by comparing the activation free energy barriers from **in5-HOTf** to **ts4-HOTf** (the geometric structures of **in5-HOTf** and **ts4-HOTf** are optimized using B3LYP/6-31G\* (6-31G\*\*, 6-31+G\* and 6-311G\*) in gas phase, and the single point energies are obtained at the M06-2X/6-311++G\*\* calculated level in solution phase).

Species	Activation Free Energy Barriers (kJ/mol)			
	6-31G*	6-31G**	6-31+G*	6-311G*
<b>ts4-HOTf</b>	135.0	134.1	136.3	143.5

Scheme S1. The possible mechanisms of  $\text{Cu}(\text{OTf})_2$ -catalyzed alkynes (**1a**) with anilines (**2a**) to form 4-quinolones (**P**).



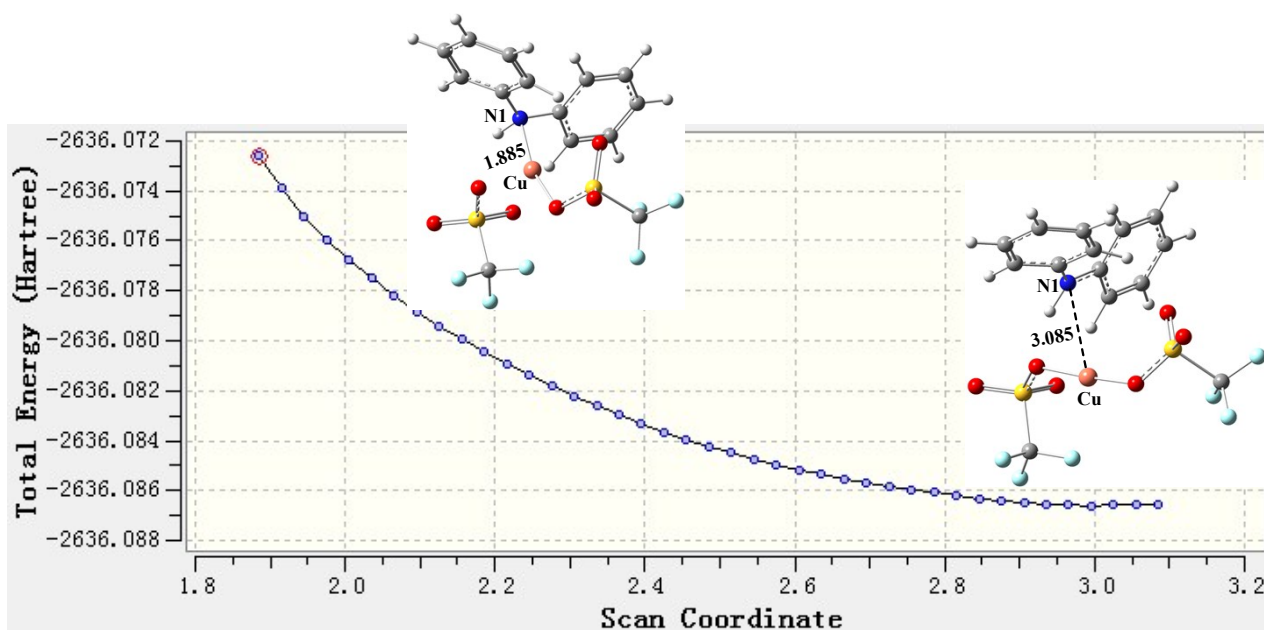


Figure S1. Scan profile along with the formation of N1-Cu bond (from 3.085 to 1.885 Å).

The coordination ability of **2a** with Cu(OTf)<sub>2</sub> is tested. The scan profile shows that the energy is rising sharply along with the formation of N1-Cu bond (from 3.085 to 1.885 Å). Obviously, the coordination of **2a** with Cu(OTf)<sub>2</sub> is unfavorable for the present catalytic reactions.

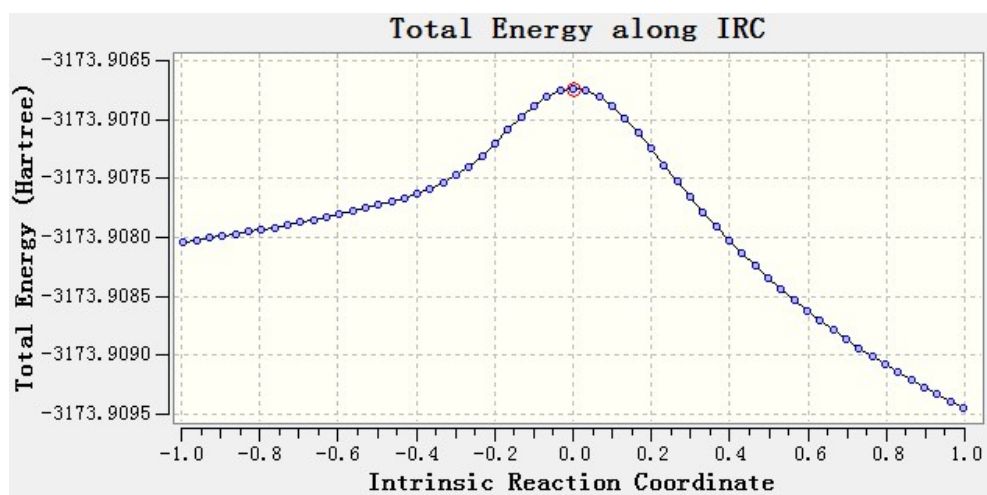


Figure S2. IRC of ts2-OTf.

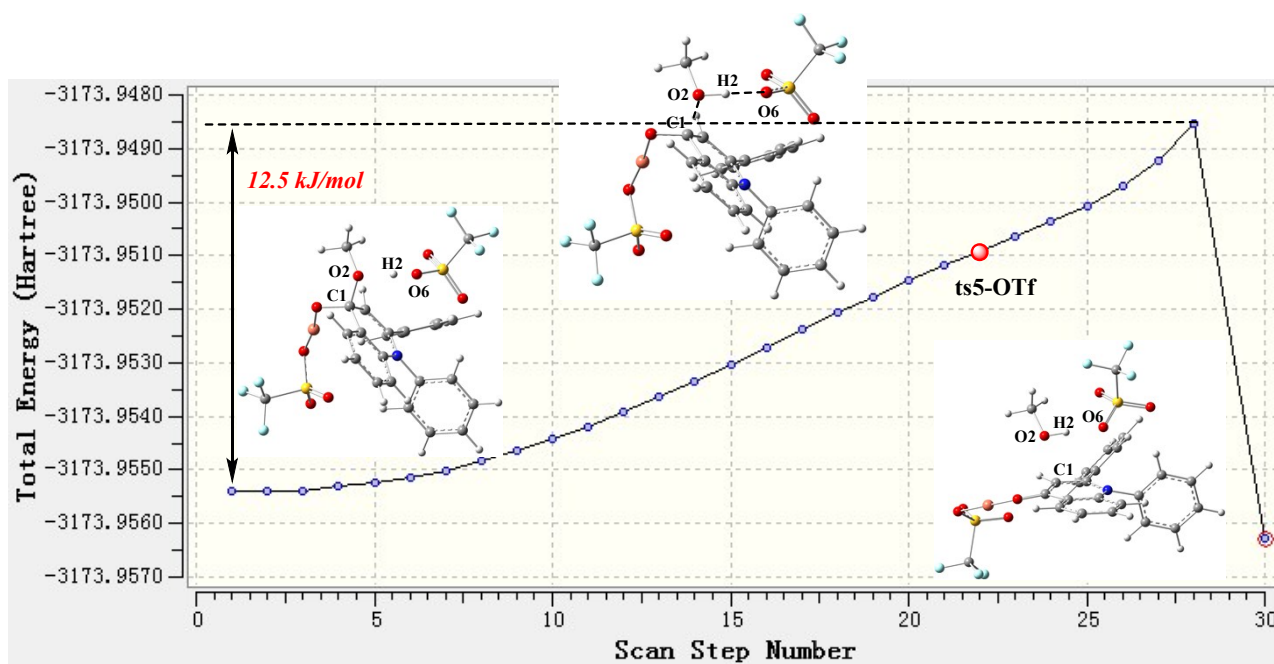


Figure S3. Scan profile from **in8-OTf** to **in7** via **ts5-OTf** along with the formation of O2-H2 bond (from 1.560 to 0.980 Å).



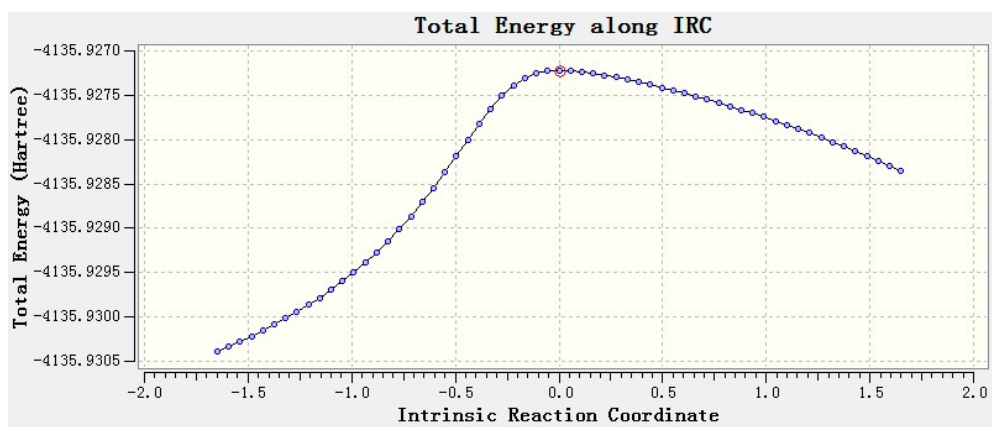


Figure S4. IRC of **ts5-HOTf**.

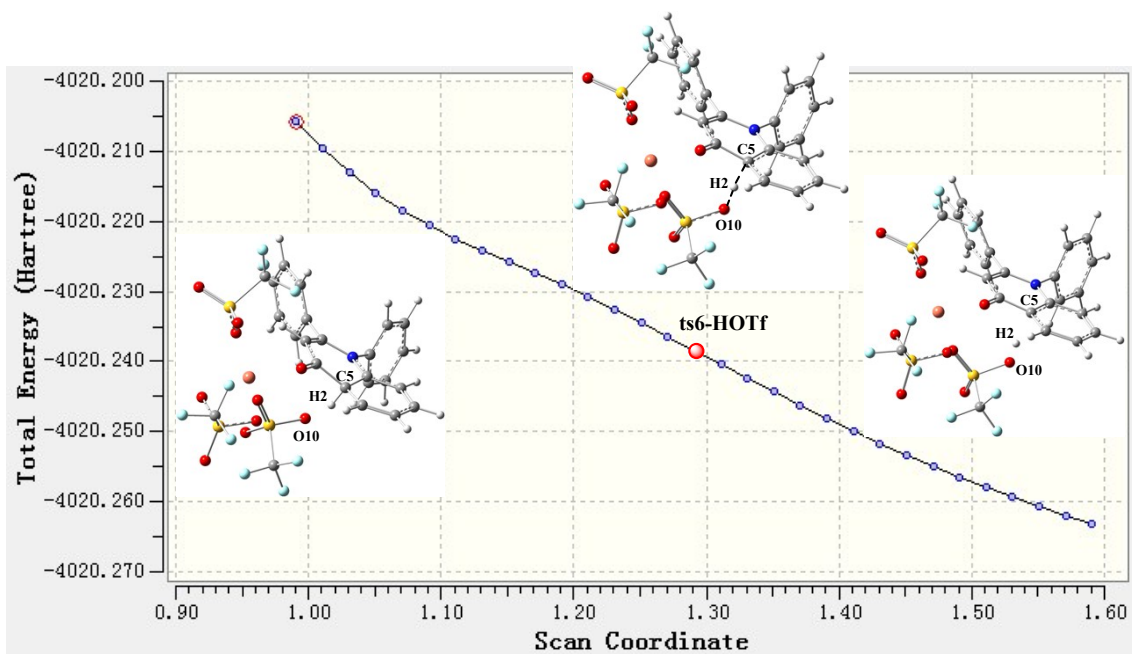


Figure S5. Scan profile from **in8-HOTf** to **in7** via **ts6-HOTf** along with the cleavage of O10-H2 bond (from 1.591 to 0.991 Å).

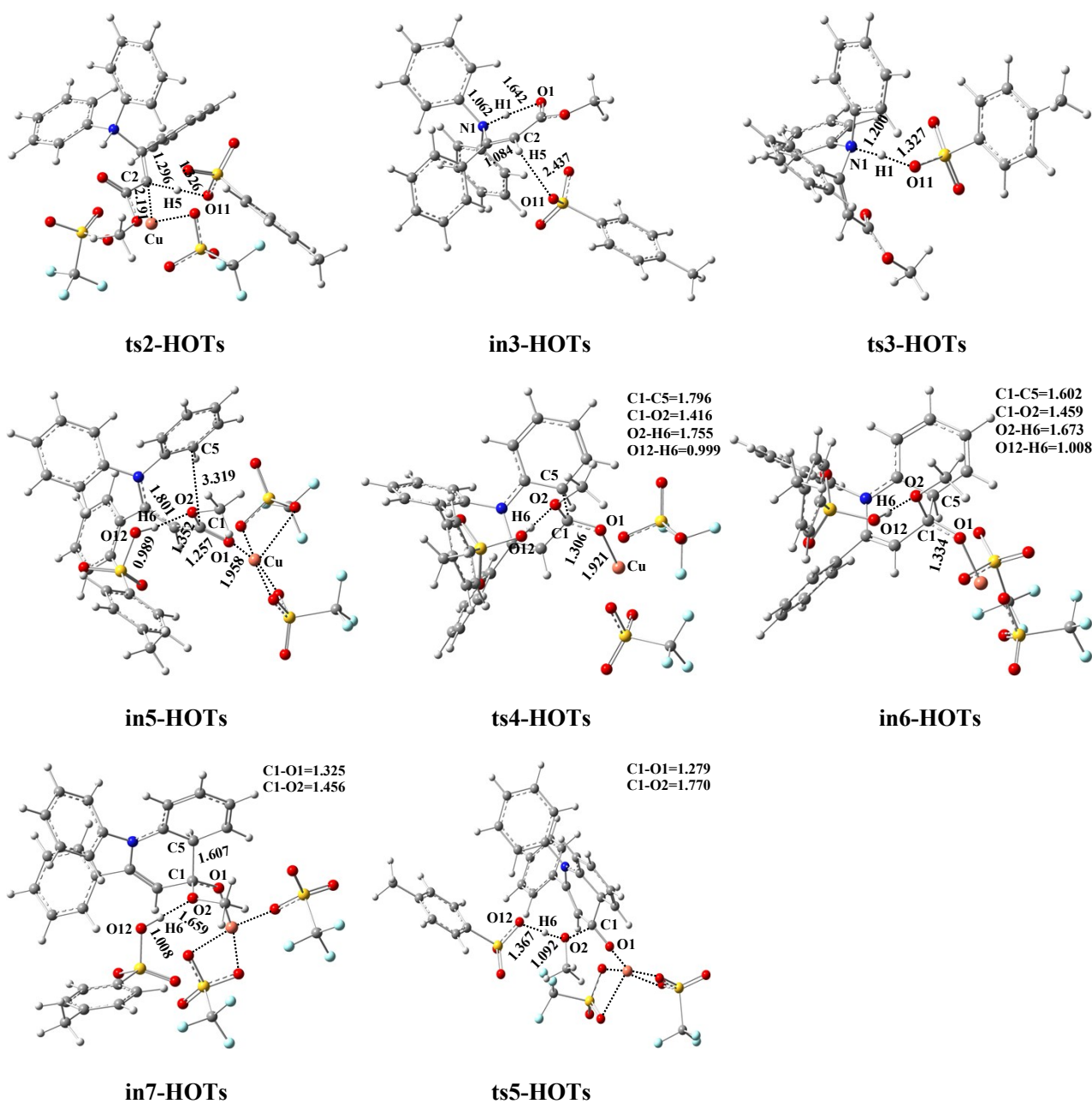


Figure S6. Optimized geometries involved in the Cu(OTf)<sub>2</sub>-catalyzed reaction with the participation of HOTs.

Bond distances are given in Å.

Table S3. The Mulliken charges of HOTf and HOTs.

Species	Mulliken Charges					
	O	O	O	S	H	total
HOTf	-0.451	-0.486	-0.620	+1.158	+0.455	+0.056
HOTs	-0.533	-0.491	-0.637	+1.194	+0.438	-0.029

Table S4. Dissociation energies for H-O bonds in HOTf and HOTs at PCM//M06-2X/6-311++G\*\*//B3LYP/6-31G\* level.

<b>Species</b>	<b>Bonds</b>	<b>Dissociation Energies (kJ/mol)</b>
<b>HOTf</b>	H-O10	638.5
<b>HOTs</b>	H-O12	701.0

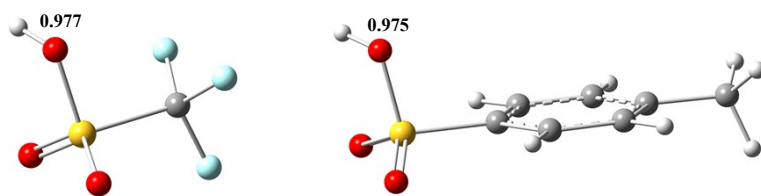


Figure S7. The bond lengths of O-H in HOTf and HOTs.

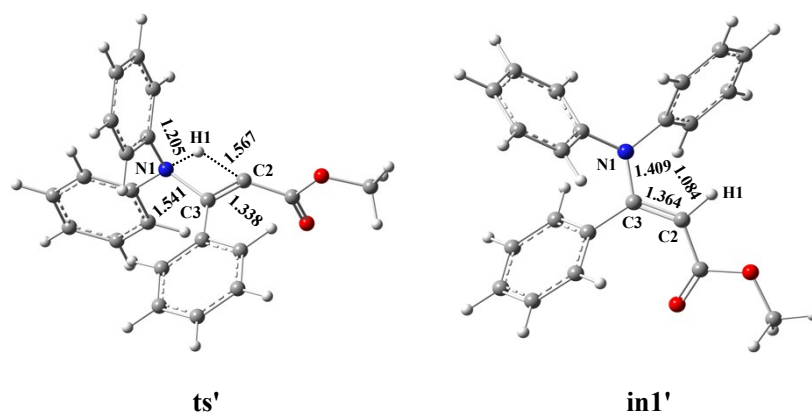


Figure S8. Optimized geometries of the intermolecular nucleophilic addition of **1a** with **2a** (**Step I**) without the participation of  $\text{Cu}(\text{OTf})_2$ .

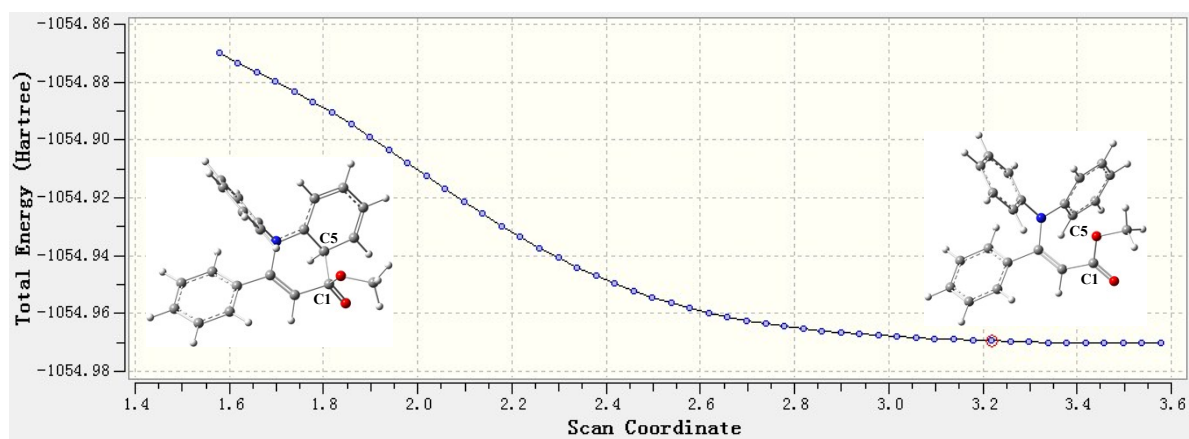


Figure S9. Scan profile from **in5'** to **in6'** along with the formation of C1-C5 bond (from 3.578 to 1.578 Å).

The scan profile of Figure S9 shows that the energy curve is sharp rising in energy with the formation of C1-C5 bond from **in5'** to **in6'**.



## Intrinsic Reaction Coordinates

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

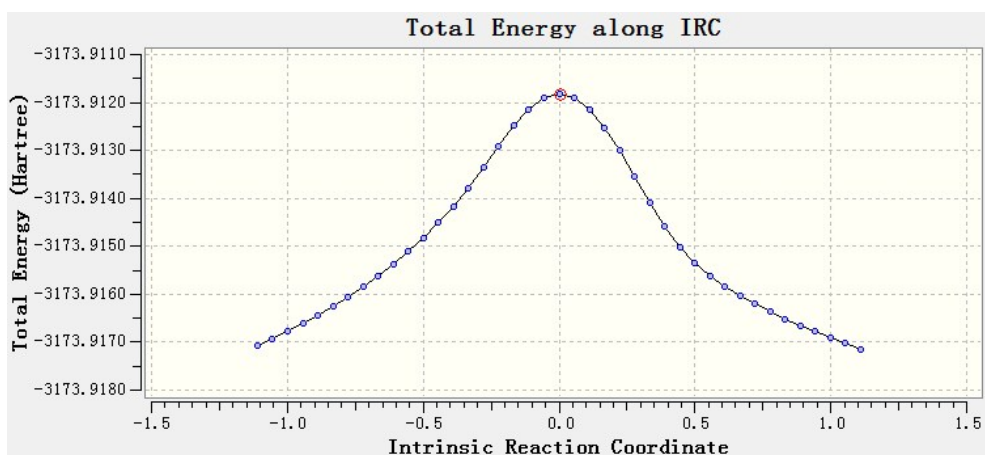


Figure S10. IRC of **ts4-OTf**.

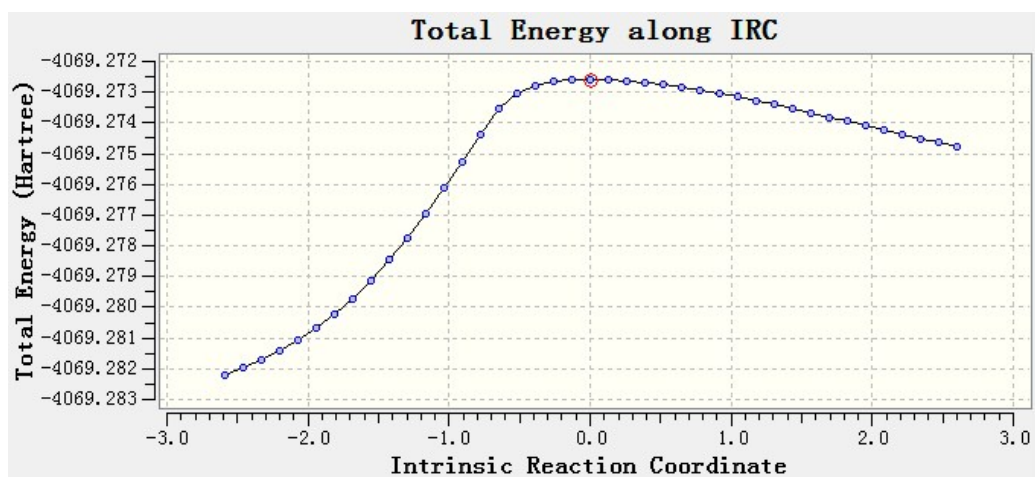


Figure S11. IRC of ts5-HOTs.

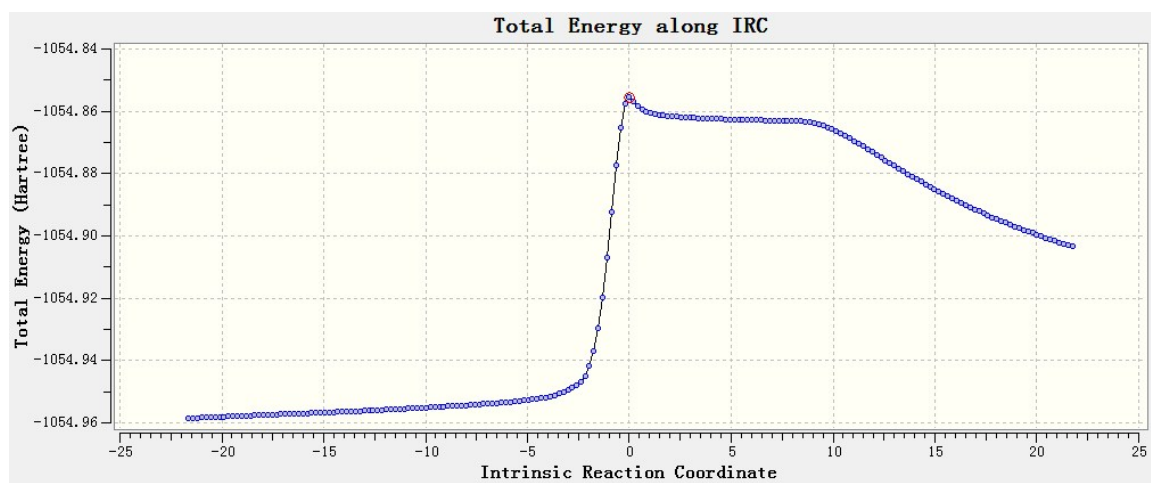


Figure S12. IRC of **ts1'**.

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

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

### Cu(OTf)<sub>2</sub>

O	1.61852100	-0.76748100	-1.18301600
C	-3.17200200	1.07994400	0.00045600
O	-1.61780000	-0.76592900	-1.18403300
O	-1.61851300	-0.76780500	1.18279700
F	-3.89941800	1.29848700	-1.08848200
F	-3.89955800	1.29678600	1.08964700
F	-2.10526100	1.88439700	0.00116100
Cu	0.00000100	-0.76063500	-0.00011200
O	1.61779300	-0.76625700	1.18381300
C	3.17200000	1.07994600	-0.00015000
F	2.10525800	1.88439600	-0.00062000
F	3.89942000	1.29817900	1.08884800
F	3.89955100	1.29709900	-1.08928300
S	2.58334500	-0.69209800	0.00066300
S	-2.58334300	-0.69209800	-0.00085700
O	3.74688800	-1.55300600	0.00147500
O	-3.74688600	-1.55300700	-0.00190000

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

Thermal correction to Gibbs Free Energy = 0.007716

Sum of electronic and thermal Free Energies = -2118.994860

### M06-2X/6-311++G\*\* (Lanl2DZ for Cu)

Energy = -2119.0429148

No imaginary frequency

### 1a

C	2.18647900	1.24786600	0.00000000
C	3.57686100	1.18348500	0.00000000
C	4.22304100	-0.05551000	0.00000000
C	3.47405300	-1.23521600	0.00000000
C	2.08322700	-1.18150600	0.00000000
C	1.42372900	0.06340000	0.00000000
C	0.00000000	0.12554100	0.00000000
C	-1.21320700	0.17402400	0.00000000
C	-2.64830900	0.31491500	0.00000000
O	-3.25633700	-0.89285200	0.00000000
O	-3.23759400	1.37710500	0.00000000
C	-4.69309200	-0.84497600	0.00000000

H	1.67623000	2.20587100	0.00000000
H	4.15827900	2.10117600	0.00000000
H	5.30859300	-0.10174700	0.00000000
H	3.97571000	-2.19886200	0.00000000
H	1.49382500	-2.09300900	0.00000000
H	-5.01636100	-1.88617800	0.00000000
H	-5.06076400	-0.32671100	0.88973200
H	-5.06076400	-0.32671100	-0.88973200

B3LYP/6-31G\*

Thermal correction to Gibbs Free Energy = 0.114859

Sum of electronic and thermal Free Energies = -536.156344

M06-2X/6-311++G\*\*

Energy = -536.2005425

No imaginary frequency

**2a**

C	1.50142800	0.85513200	-0.51800400
C	2.79557400	1.37308800	-0.53905000
C	3.88088900	0.62052800	-0.08748500
C	3.65397000	-0.67239300	0.38951800
C	2.36479300	-1.19498100	0.43161100
C	1.26724500	-0.43851600	-0.01899100
N	0.00000700	-1.03129200	-0.00003900
C	-1.26724800	-0.43845300	0.01899400
C	-2.36479500	-1.19500700	-0.43154400
C	-3.65394100	-0.67243600	-0.38945400
C	-3.88088000	0.62053800	0.08752700
C	-2.79561200	1.37311600	0.53904200
C	-1.50141500	0.85517300	0.51793800
H	0.67805800	1.44069000	-0.91085000
H	2.95447300	2.37504200	-0.92983200
H	4.88566900	1.03189000	-0.11065900
H	4.48463500	-1.27841000	0.74212700
H	2.19516400	-2.19635900	0.82220900
H	-0.00004800	-2.04136700	-0.00045800
H	-2.19514000	-2.19641300	-0.82205500
H	-4.48468000	-1.27839700	-0.74198600
H	-4.88571800	1.03176400	0.11062200
H	-2.95442900	2.37509300	0.92979600
H	-0.67807900	1.44078800	0.91075600

B3LYP/6-31G\*

Thermal correction to Gibbs Free Energy = 0.161536

Sum of electronic and thermal Free Energies = -518.490281

M06-2X/6-311++G\*\*

Energy = -518.5662263

No imaginary frequency

OTf-assisted reaction

**in1**

C	-2.00264000	3.88319500	0.31870600
C	-2.89108900	4.72144100	-0.34133900
C	-4.06647400	4.19828100	-0.89495300
C	-4.35959500	2.83405100	-0.79144900
C	-3.48603700	1.97706300	-0.13203600
C	-2.29871500	2.50427700	0.42908100
C	-1.41000600	1.64621600	1.11009200
C	-0.60453800	0.86416100	1.62422600
C	0.01368500	0.08386400	2.70940700
O	1.05698700	-0.60943000	2.21483600
O	-0.36318700	0.08419200	3.85300100
C	1.66559600	-1.56945200	3.10771800
H	-1.08549300	4.26972200	0.75142100
H	-2.67119900	5.78089800	-0.42925600
H	-4.75576200	4.85915700	-1.41308600
H	-5.27038700	2.43777800	-1.22958400
H	-3.68475800	0.91224400	-0.05418600
H	2.54611500	-1.92990000	2.57920700
H	1.94125600	-1.08548500	4.04632000
H	0.95811600	-2.38083100	3.29046500
S	-1.84859000	-1.85724100	-0.01227400
O	-0.87940800	-1.00675200	-0.86592900
C	4.14762000	0.23247700	-0.34280500
S	2.69876200	1.05783000	-1.17890500
O	1.85965100	1.59810900	-0.01948600
O	1.85180300	-0.08172000	-1.70195000
F	3.70069800	-0.71960100	0.48420800
F	4.93188000	-0.31577500	-1.26578200
F	4.83154100	1.13772400	0.35282400
Cu	0.42200000	0.20294800	-0.18854400
O	-1.26743000	-2.22255300	1.28531900
C	-1.85981800	-3.41102300	-1.03742800
F	-0.62605900	-3.91691200	-1.10728300
F	-2.66754700	-4.30349300	-0.45931700
F	-2.30085800	-3.14814800	-2.26792000
O	-3.21598400	-1.32911000	-0.04990100
O	3.24088700	2.02352000	-2.11595900

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

Thermal correction to Gibbs Free Energy = 0.141508

Sum of electronic and thermal Free Energies = -2655.132825

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

Energy = -2655.2681840

No imaginary frequency

**ts1**

C	-1.82119500	-2.04985500	1.96475500
C	-2.19537800	-2.24104900	3.29048800
C	-2.26215400	-1.15065400	4.16567300
C	-1.95495800	0.13545800	3.71541800
C	-1.58730500	0.34808800	2.38819300
C	-1.51180100	-0.75158100	1.50563200
C	-1.09871700	-0.53650100	0.14878700
C	-0.11347300	-0.31306600	-0.64400200
C	-0.01004000	-0.06427100	-2.09583700
O	1.26287800	0.04384900	-2.47180100
O	-0.95499300	0.00225600	-2.87330700
C	1.49976400	0.45475000	-3.83434000
H	-1.74969100	-2.89129800	1.28471400
H	-2.42251800	-3.24140400	3.64685400
H	-2.54583600	-1.30818900	5.20269600
H	-1.99701000	0.97860300	4.39853600
H	-1.33013600	1.34098200	2.03147200
H	2.58227600	0.44002700	-3.95148200
H	1.02071800	-0.23809300	-4.52927500
H	1.10691700	1.46405900	-3.97402700
S	0.82393500	2.80323100	0.05991700
O	1.84932900	1.73175600	0.45197300
C	4.55972200	-2.42233400	-0.39057900
S	3.38093800	-2.09723900	1.01329400
O	2.01015400	-2.21753800	0.35568700
O	3.52689300	-0.62267400	1.28876800
F	4.29712000	-1.57465500	-1.39418600
F	5.81315100	-2.24069100	0.02128300
F	4.41068900	-3.67440800	-0.82574400
Cu	1.69045000	-0.19052800	0.29743700
O	0.33678100	2.66474700	-1.32262400
C	1.94424000	4.28800300	0.04819800
F	2.91125900	4.12654600	-0.86035900
F	1.22675800	5.37154200	-0.27083000
F	2.49553300	4.46803900	1.24932700
O	-0.17190300	3.05283400	1.11009000
O	3.70175900	-3.04809000	2.06467200
C	-4.39845800	0.72447500	0.65677500
C	-5.00681700	1.90470600	1.08452600
C	-4.81757800	3.09553900	0.38170000
C	-4.00391800	3.10591900	-0.75407300

C	-3.40055900	1.93293200	-1.19914200
C	-3.61221900	0.73224300	-0.50507000
N	-2.92406300	-0.43459000	-0.95981100
C	-3.56254300	-1.72211800	-1.07210800
C	-2.75769900	-2.81231800	-1.43914500
C	-3.32107200	-4.07402100	-1.60995700
C	-4.69150700	-4.26817900	-1.41620600
C	-5.49214400	-3.18200700	-1.06519800
C	-4.93868500	-1.91107000	-0.89622600
H	-4.52578000	-0.18968300	1.22514800
H	-5.62023400	1.89130500	1.98092900
H	-5.28823800	4.01230700	0.72423900
H	-3.83064100	4.03122900	-1.29496100
H	-2.74960300	1.94664200	-2.06809200
H	-2.38435000	-0.23255000	-1.81511400
H	-1.69263600	-2.66744000	-1.58797200
H	-2.68441300	-4.90724400	-1.89328900
H	-5.12883100	-5.25395800	-1.54380100
H	-6.56191400	-3.31384100	-0.92935400
H	-5.58146500	-1.07289100	-0.65826400

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

Thermal correction to Gibbs Free Energy = 0.329445

Sum of electronic and thermal Free Energies = -3173.593559

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

Energy = -3173.8487484

Number of Imaginary Frequencies = 1

Lowest Frequency = 211.67i

## in2

C	-2.16233500	-1.74028700	2.10502200
C	-2.16331500	-1.94570200	3.48378600
C	-1.48659200	-1.06431600	4.32975600
C	-0.81559400	0.03234400	3.78808400
C	-0.81157200	0.24650700	2.40936200
C	-1.47581300	-0.64652400	1.54787700
C	-1.38817500	-0.40993800	0.08484100
C	-0.25787100	-0.19013200	-0.60187600
C	-0.25724800	0.13090700	-2.04922300
O	0.96611800	0.11185800	-2.56299300
O	-1.26004000	0.36986500	-2.73583300
C	1.10660000	0.57646500	-3.92106400
H	-2.67419000	-2.45131500	1.46661800
H	-2.68397000	-2.80592500	3.89543900
H	-1.48487100	-1.23169100	5.40317400
H	-0.29829300	0.73474600	4.43509400



H	-0.32832900	1.13146200	2.00659800
H	2.16054800	0.44247900	-4.16043000
H	0.47455200	-0.00949600	-4.59184500
H	0.82792100	1.63143100	-3.96453300
S	1.02420100	2.86901200	-0.04020400
O	1.97405200	1.70132500	0.21968300
C	4.18470700	-2.75203400	-0.39519700
S	3.07707800	-2.23740200	1.00949200
O	1.68196600	-2.31406600	0.41285800
O	3.33954900	-0.75825400	1.15829100
F	3.93088700	-1.99038100	-1.46771800
F	5.46122400	-2.60230700	-0.04385900
F	3.95715900	-4.03046400	-0.70522800
Cu	1.53544800	-0.21927700	0.23579100
O	0.31217800	2.77440800	-1.33011500
C	2.27194900	4.22989900	-0.26513100
F	3.07952900	3.95103500	-1.29391400
F	1.62945800	5.37673400	-0.51849600
F	3.00479100	4.37675000	0.84003700
O	0.22369700	3.23619800	1.13586500
O	3.38408400	-3.11602400	2.12682600
C	-4.56104800	0.43015800	0.87230100
C	-5.29263600	1.46272500	1.45991800
C	-5.02378100	2.79387400	1.13329000
C	-4.01583200	3.09846000	0.21723500
C	-3.27986400	2.07722900	-0.38509800
C	-3.57242000	0.75379800	-0.05516800
N	-2.71666500	-0.28992600	-0.67786900
C	-3.37044400	-1.57282900	-1.08068000
C	-2.62119600	-2.74844300	-1.10521200
C	-3.20911100	-3.91943700	-1.58892800
C	-4.52236300	-3.90988500	-2.05910700
C	-5.25017400	-2.71879000	-2.05383800
C	-4.67678300	-1.54159900	-1.57124800
H	-4.75795300	-0.60248200	1.13513000
H	-6.06727400	1.22205300	2.18185300
H	-5.59275600	3.59225900	1.60046000
H	-3.78757900	4.13102000	-0.02694500
H	-2.47183200	2.31375100	-1.07182600
H	-2.37427500	0.10808800	-1.60480500
H	-1.59485500	-2.75878100	-0.75485800
H	-2.62870500	-4.83696100	-1.59890700
H	-4.97421800	-4.82326000	-2.43427200
H	-6.26836600	-2.69713200	-2.43070500
H	-5.24215800	-0.61697100	-1.57895400

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

Thermal correction to Gibbs Free Energy = 0.333670

Sum of electronic and thermal Free Energies = -3173.604685

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

Energy = -3173.8794283

No imaginary frequency

**in3-OTf**

C	0.73421500	2.69350500	-1.06797000
C	1.56107500	3.12100800	-2.10456000
C	2.06345900	2.21136600	-3.04586800
C	1.71190700	0.86715500	-2.96814900
C	0.86631700	0.42572300	-1.93923800
C	0.39018500	1.33759400	-0.96041200
C	-0.31000900	0.73583400	0.20623600
C	0.32866000	-0.26882800	0.81405400
C	-0.09063300	-1.15130000	1.93093500
O	0.52380600	-2.33833000	1.79295100
O	-0.84581200	-0.86038300	2.83489800
C	0.11919200	-3.37948700	2.70911200
H	0.37814000	3.40765100	-0.33276300
H	1.83299600	4.17062700	-2.17171400
H	2.71571600	2.56026700	-3.84081700
H	2.07265000	0.15665000	-3.70535800
H	0.44186700	-0.57933600	-1.95908600
H	0.79466000	-4.21066300	2.51038000
H	0.21853700	-3.03254500	3.73996000
H	-0.91345200	-3.65823100	2.49162400
S	-2.60855200	-2.24618200	-0.39504100
O	-2.27790400	-3.45978200	0.35742900
C	5.51410000	0.42106800	-0.23266000
S	4.59498400	-1.13614400	0.21227700
O	3.67676400	-1.33982300	-0.98723700
O	3.67669800	-0.71514900	1.33251400
F	4.63090600	1.40371700	-0.46974300
F	6.30859600	0.78301300	0.77363300
F	6.24533700	0.22108400	-1.32881000
Cu	1.99873500	-0.71809200	-0.07101800
O	-3.08109200	-1.09035900	0.46352100
C	-4.14980300	-2.65337100	-1.34937800
F	-5.13685900	-3.01236000	-0.52311200
F	-4.54939400	-1.57893400	-2.05310000
F	-3.91102300	-3.65469600	-2.20212700
O	-1.64623500	-1.80467600	-1.43397700
O	5.59372800	-2.15912300	0.47048300

C	-2.65518400	3.31237700	-0.35035800
C	-3.27778700	4.02718200	-1.37569900
C	-3.62463700	3.39273600	-2.56905100
C	-3.34561200	2.03557000	-2.73894400
C	-2.72182600	1.30618700	-1.72602800
C	-2.38248800	1.95868700	-0.53955800
N	-1.72431100	1.14620000	0.53405900
C	-1.91349000	1.71691000	1.89518800
C	-0.93599200	2.51534200	2.47961100
C	-1.17968700	3.06559700	3.73992200
C	-2.38613300	2.81488300	4.39477200
C	-3.35229400	2.00559400	3.79217400
C	-3.12226300	1.45086000	2.53424200
H	-2.40381400	3.80473000	0.58125800
H	-3.49606900	5.08130900	-1.23160900
H	-4.11473200	3.95225700	-3.36057000
H	-3.61830900	1.53088100	-3.66088300
H	-2.49880400	0.25328300	-1.86290900
H	-2.26525500	0.18960300	0.52279400
H	0.01211000	2.68750700	1.98071200
H	-0.41971000	3.68356900	4.20869400
H	-2.56923700	3.24036600	5.37706500
H	-4.28554300	1.79374500	4.30510400
H	-3.85313000	0.79825200	2.06787200

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

Thermal correction to Gibbs Free Energy = 0.331058

Sum of electronic and thermal Free Energies = -3173.577471

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

Energy = -3173.8502334

No imaginary frequency

### ts2-OTf

C	0.67625600	2.76430900	-0.90126200
C	1.50244500	3.30362000	-1.88434800
C	2.03947900	2.49519500	-2.89688700
C	1.72372900	1.14126400	-2.94310600
C	0.88085300	0.58786500	-1.96634100
C	0.36920000	1.39468000	-0.91616200
C	-0.33097000	0.68436400	0.19043600
C	0.34295400	-0.35901600	0.69903700
C	-0.03641900	-1.32672100	1.75452700
O	0.61237800	-2.48628200	1.53765900
O	-0.79824900	-1.12857300	2.67886500
C	0.26839300	-3.57853900	2.41482500
H	0.28898400	3.39972100	-0.11179000

H	1.74557000	4.36204900	-1.85496600
H	2.68943100	2.93059900	-3.64993300
H	2.11057600	0.50914800	-3.73629600
H	0.48794300	-0.42265700	-2.08419400
H	0.93697400	-4.39145100	2.13364500
H	0.42409400	-3.28907700	3.45669800
H	-0.77411800	-3.85781900	2.24976700
S	-2.65633200	-2.20227900	-0.53087500
O	-2.36101400	-3.44108100	0.18327100
C	5.56337900	0.43524200	-0.09571200
S	4.61722700	-1.16183800	0.04789500
O	3.73055800	-1.14146400	-1.19116000
O	3.67454100	-0.92928300	1.20150300
F	4.69714500	1.45713800	-0.17976700
F	6.33389000	0.60508200	0.97789800
F	6.32285400	0.41870300	-1.19125000
Cu	2.02902100	-0.66826900	-0.21708200
O	-3.04556700	-1.04408300	0.41668200
C	-4.28630400	-2.46903600	-1.38570400
F	-5.22771500	-2.80098700	-0.50140900
F	-4.65652800	-1.34704200	-2.01844700
F	-4.15813500	-3.44961900	-2.28259400
O	-1.72923800	-1.74778100	-1.58313200
O	5.59948100	-2.22816700	0.14813400
C	-2.73085500	3.27343300	-0.07402800
C	-3.38619600	4.06698200	-1.01764800
C	-3.70211100	3.55461800	-2.27611700
C	-3.35898900	2.23848900	-2.58989100
C	-2.70620400	1.43333300	-1.65623600
C	-2.39240300	1.95840500	-0.39906800
N	-1.70957100	1.07104800	0.57718800
C	-1.86721800	1.51649100	1.97897200
C	-0.85042000	2.20263300	2.63957400
C	-1.05924500	2.64087800	3.94882600
C	-2.27697600	2.40008500	4.58560600
C	-3.28856000	1.71312800	3.91051300
C	-3.08923400	1.26873800	2.60461100
H	-2.49823500	3.67618600	0.90441500
H	-3.65080300	5.08858600	-0.76005200
H	-4.21588900	4.17463800	-3.00508300
H	-3.60509700	1.82566500	-3.56382200
H	-2.44120100	0.41248300	-1.90822100
H	-2.34673400	-0.03888500	0.47620900
H	0.10487100	2.37484200	2.15438100
H	-0.26404500	3.16751500	4.46845300

H	-2.43478100	2.73896300	5.60534800
H	-4.23500900	1.51093300	4.40321800
H	-3.86570400	0.71848800	2.08402400

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

Thermal correction to Gibbs Free Energy = 0.326812

Sum of electronic and thermal Free Energies = -3173.579929

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

Energy = -3173.8470250

Number of Imaginary Frequencies = 1

Lowest Frequency = 893.25i

### in4-OTf

C	-2.08983200	-2.01393200	2.43199400
C	-1.83175100	-2.40693500	3.74233400
C	-0.84363400	-1.75935600	4.49215200
C	-0.12624300	-0.70415700	3.92868800
C	-0.38460500	-0.30592600	2.61562500
C	-1.35374100	-0.97212300	1.84215400
C	-1.54264100	-0.64492800	0.40372500
C	-0.46229300	-0.44289200	-0.39705800
C	-0.49715500	-0.09331700	-1.81439700
O	-0.14716600	-1.07479500	-2.63592300
O	-0.72506900	1.05289500	-2.24779500
C	-0.05443600	-0.75504200	-4.04069400
H	-2.84810100	-2.52744700	1.84849800
H	-2.39510500	-3.22691600	4.17900600
H	-0.64373800	-2.07071400	5.51345200
H	0.62422700	-0.17674400	4.50983400
H	0.11748600	0.57461300	2.22097300
H	0.31313800	-1.66497900	-4.51323700
H	-1.03980900	-0.48786200	-4.42859900
H	0.64122600	0.07257300	-4.19564000
S	0.96889600	2.85471400	0.14238600
O	1.75243100	1.68223500	-0.29501800
C	4.74234400	-1.69378500	-0.51594100
S	3.47953400	-2.01620000	0.81334400
O	2.25706100	-2.46426100	0.04449300
O	3.14180800	-0.62711300	1.31748500
F	4.22504300	-0.85987300	-1.42999400
F	5.83211000	-1.13837800	0.01396300
F	5.07491100	-2.83976100	-1.11314400
Cu	1.34602200	-0.52732700	0.32543600
O	-0.40024400	2.93626100	-0.62701100
C	1.85385000	4.33006200	-0.57562100
F	1.98745700	4.16791500	-1.89115500

F	1.15292200	5.43354200	-0.32740100
F	3.05381300	4.42001600	-0.00857700
O	0.76852000	3.10332500	1.56096600
O	4.08454600	-2.94980100	1.75056100
C	-5.15511900	-0.32526200	0.78965300
C	-6.09449400	0.42155100	1.49612100
C	-5.74158400	1.64871400	2.06529500
C	-4.44029300	2.12979800	1.91157600
C	-3.49497800	1.39694700	1.19395400
C	-3.84637300	0.15899100	0.63835000
N	-2.87428500	-0.61077500	-0.07166500
C	-3.23099800	-1.21577800	-1.31313900
C	-2.81686400	-2.52714700	-1.59535600
C	-3.18333000	-3.13037100	-2.79653800
C	-3.97184700	-2.44222300	-3.72277000
C	-4.38504800	-1.13710700	-3.44126400
C	-4.01482300	-0.52065700	-2.24696700
H	-5.42565500	-1.28487300	0.36051800
H	-7.10393100	0.03658600	1.61221400
H	-6.47619800	2.22508300	2.62011700
H	-4.15702100	3.08770700	2.33837400
H	-2.49394900	1.79026800	1.04835900
H	-0.55032100	2.13559300	-1.30682500
H	-2.20753100	-3.06355300	-0.87466200
H	-2.85978000	-4.14680000	-3.00235600
H	-4.26325000	-2.91904800	-4.65422600
H	-4.99213800	-0.59026700	-4.15749000
H	-4.32514200	0.49659300	-2.03255000

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

Thermal correction to Gibbs Free Energy = 0.327107

Sum of electronic and thermal Free Energies = -3173.614036

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

Energy = -3173.86497430

No imaginary frequency

### ts3-OTf

C	2.16536700	-0.81228000	2.36477100
C	2.25714900	-1.38775500	3.62938800
C	1.71092800	-2.65189500	3.86630600
C	1.06499900	-3.33385200	2.83306800
C	0.95513000	-2.75355500	1.56980300
C	1.50692900	-1.48660800	1.32123500
C	1.35149900	-0.80603200	0.00136800
C	0.07296500	-0.66568500	-0.54241600
C	-0.18808000	-0.11511100	-1.89025200

O	-1.22206800	0.77766200	-1.81669400
O	0.32209300	-0.44375100	-2.94090600
C	-1.65894400	1.35961500	-3.05829500
H	2.57471200	0.17697400	2.18885500
H	2.74966000	-0.84610400	4.43177100
H	1.78622900	-3.10169600	4.85236300
H	0.64267700	-4.31910900	3.00842800
H	0.45539200	-3.29495700	0.77448700
H	-2.46455200	2.04267100	-2.79034900
H	-0.83345400	1.89958900	-3.52803700
H	-2.01914900	0.58082100	-3.73432800
S	-2.93899300	-2.48486100	0.02560700
O	-2.89515900	-1.12134800	0.63303500
C	-1.24860000	3.94204500	0.90336000
S	-1.30420000	2.49418700	2.07725700
O	-0.12699100	1.64319000	1.61820100
O	-2.52573200	1.71979800	1.66946200
F	-1.43723000	3.51893400	-0.35400100
F	-2.19452100	4.82467900	1.21585200
F	-0.04819400	4.53345200	0.97666800
Cu	-1.33021200	0.22201000	0.66342100
O	-1.54887000	-2.84100900	-0.55390800
C	-3.96183900	-2.26733800	-1.51831300
F	-3.38070700	-1.36101600	-2.31125100
F	-4.04868700	-3.42855900	-2.16120300
F	-5.17704400	-1.84623600	-1.17855400
O	-3.53470100	-3.55786400	0.79726800
O	-1.23300400	3.05173600	3.41839400
C	4.89408800	-0.19504600	0.01138900
C	6.12232700	-0.83353200	0.16968800
C	6.23655100	-2.20948100	-0.04772700
C	5.11468800	-2.94500000	-0.43409500
C	3.88249100	-2.31343200	-0.60215500
C	3.76914600	-0.93918900	-0.36497500
N	2.50203600	-0.28091000	-0.55020900
C	2.50380800	0.88954900	-1.38700600
C	1.89515200	2.06348500	-0.92825800
C	1.92323200	3.20902600	-1.72467000
C	2.56702700	3.19090400	-2.96375300
C	3.18324000	2.01722500	-3.40900400
C	3.15231100	0.86505600	-2.62734200
H	4.79998100	0.87267000	0.18223600
H	6.99108300	-0.25424300	0.46915300
H	7.19583700	-2.70319400	0.07741600
H	5.19760300	-4.01208600	-0.61919800

H	3.01343400	-2.87624600	-0.92721500
H	-0.81550300	-1.93369600	-0.48898200
H	1.41133200	2.08022700	0.04196200
H	1.44784100	4.11492100	-1.36038500
H	2.59404000	4.08646800	-3.57814900
H	3.68040500	1.99458000	-4.37449500
H	3.60893600	-0.05397000	-2.97820900

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

Thermal correction to Gibbs Free Energy = 0.327838

Sum of electronic and thermal Free Energies = -3173.606473

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

Energy = -3173.8655790

Number of Imaginary Frequencies = 1

Lowest Frequency = 999.59i

**in3**

C	2.27771600	-0.58101800	1.49010400
C	3.53864200	-0.95928200	1.94562400
C	4.19128200	-2.05608800	1.37837700
C	3.57398200	-2.77115900	0.35009100
C	2.31178700	-2.39444600	-0.10444800
C	1.64099300	-1.29918200	0.46419100
C	0.26633400	-0.93259700	0.02297900
C	-0.62129700	-1.91119100	-0.31185900
C	-1.90339300	-1.72278500	-0.99845600
O	-2.60387300	-2.89391300	-0.99883000
O	-2.31162000	-0.71670600	-1.55071800
C	-3.85096400	-2.85150000	-1.70119600
H	1.77325000	0.27105900	1.93449700
H	4.01247200	-0.39725500	2.74592100
H	5.17732200	-2.34693500	1.73049200
H	4.08057200	-3.61725400	-0.10646400
H	1.84561200	-2.93737000	-0.92149700
H	-4.27991800	-3.84952000	-1.59934600
H	-4.51693500	-2.10177500	-1.26446500
H	-3.69562300	-2.60841000	-2.75664900
C	1.01236400	2.64336700	-0.00768900
C	1.86220100	3.55053500	-0.63522300
C	2.51150700	3.21160400	-1.82545700
C	2.28975700	1.95529500	-2.39016100
C	1.42529100	1.04721500	-1.77976600
C	0.78828200	1.37901600	-0.57604000
N	-0.06633700	0.43408500	0.05962300
C	-1.27396100	0.87719400	0.68357100
C	-1.61998000	0.38663400	1.94981800



C	-2.77892900	0.83413100	2.58205100
C	-3.59257100	1.78980400	1.97022900
C	-3.24285100	2.28295400	0.71137500
C	-2.09837600	1.82358200	0.06285200
H	0.52015100	2.90839000	0.92257000
H	2.02693300	4.52515400	-0.18316300
H	3.17802400	3.92089500	-2.30781300
H	2.77740900	1.68187200	-3.32212100
H	1.22668700	0.08413300	-2.23882800
H	-0.98019400	-0.34564300	2.43333500
H	-3.03514700	0.44572600	3.56428200
H	-4.49046900	2.14489200	2.46831000
H	-3.87555100	3.01612100	0.21818400
H	-1.84543600	2.17943200	-0.92927400
H	-0.35775300	-2.93965200	-0.09475600

B3LYP/6-31G\*

Thermal correction to Gibbs Free Energy = 0.303325

Sum of electronic and thermal Free Energies = -1054.669337

M06-2X/6-311++G\*\*

Energy = -1054.82594270

No imaginary frequency

**in4**

C	2.35478000	-0.47848000	1.44964100
C	3.67051200	-0.66447800	1.86776600
C	4.52243900	-1.50903400	1.15256200
C	4.04915500	-2.16527000	0.01449700
C	2.73243400	-1.98124900	-0.40286100
C	1.86327200	-1.14215200	0.31333000
C	0.43846500	-0.98894100	-0.09510600
C	-0.23930500	-2.06250900	-0.58473300
C	-1.57059100	-2.14268400	-1.20708900
O	-2.02879900	-0.96225600	-1.69214700
O	-2.17974400	-3.19025100	-1.33603400
C	-3.32195700	-1.02297800	-2.30921400
H	1.69436800	0.17597100	2.00967100
H	4.03123300	-0.15033300	2.75455700
H	5.55029900	-1.64937600	1.47602400
H	4.70922800	-2.81346000	-0.55562600
H	2.37474000	-2.47369200	-1.30241800
H	-3.53917500	-0.00408600	-2.63168400
H	-3.31001800	-1.70335500	-3.16524600
H	-4.07478000	-1.36588200	-1.59452000
C	0.58537300	2.61566200	0.37383500
C	1.24154500	3.72950100	-0.14351000

C	1.84068700	3.67932700	-1.40551400
C	1.76511800	2.50353300	-2.15234700
C	1.09321000	1.38905000	-1.65020300
C	0.50712600	1.43272600	-0.37824900
N	-0.14427900	0.27588500	0.14096300
C	-1.39394000	0.40149800	0.81594200
C	-1.67934200	-0.41188100	1.92268200
C	-2.89059200	-0.27901400	2.59868000
C	-3.82584900	0.67793900	2.19936400
C	-3.53778600	1.49575100	1.10514400
C	-2.33782000	1.35583800	0.40988500
H	0.13230000	2.65515300	1.35941000
H	1.29663600	4.63845000	0.44982600
H	2.35782300	4.54881700	-1.80121800
H	2.21764400	2.45342500	-3.13915400
H	1.00603400	0.48416900	-2.24307900
H	0.23042400	-3.03625300	-0.50335900
H	-0.95292800	-1.15048100	2.24676800
H	-3.09526700	-0.91959100	3.45238000
H	-4.76530200	0.78493600	2.73402000
H	-4.25775000	2.24119100	0.77715700
H	-2.12880200	1.98032800	-0.45181600

B3LYP/6-31G\*

Thermal correction to Gibbs Free Energy = 0.302732

Sum of electronic and thermal Free Energies = -1054.667585

M06-2X/6-311++G\*\*

Energy = -1054.8252957

No imaginary frequency

**in5**

C	-3.92041100	2.40776500	0.51312900
C	-4.30553800	3.74573800	0.53399800
C	-3.93044500	4.60132700	-0.50538900
C	-3.16087100	4.11355200	-1.56351600
C	-2.76569400	2.77695600	-1.58104500
C	-3.14190200	1.90773700	-0.54448600
C	-2.65936200	0.49859700	-0.52905000
C	-1.33405300	0.28363100	-0.85344200
C	-0.64943700	-0.93761600	-1.16323900
O	-1.39508400	-2.00174000	-1.43961000
O	0.60267700	-1.04018200	-1.26090800
C	-0.70704000	-3.24149300	-1.70731100
H	-4.20289400	1.74920100	1.32799200
H	-4.89437200	4.12328500	1.36512900
H	-4.23624800	5.64374200	-0.48949900

H	-2.87010300	4.77247700	-2.37672700
H	-2.17631200	2.39405800	-2.40920100
H	-1.49916500	-3.97242100	-1.86386800
H	-0.08203500	-3.14406700	-2.59752400
H	-0.08912600	-3.52091100	-0.85142500
S	4.41280400	0.32015100	-1.93532100
O	3.27337400	-0.64846300	-2.22274500
C	2.76922000	1.36932500	2.96883700
S	1.60785700	0.21781500	2.07792000
O	2.40420200	-0.96981000	1.70249000
O	1.28803900	1.01199100	0.79585400
F	3.86076800	1.58112900	2.23285200
F	2.16068600	2.53409200	3.20298000
F	3.12268400	0.81499300	4.13192200
Cu	2.11567300	0.06191600	-0.69543600
O	5.02894500	1.00449100	-3.05736700
C	5.72822300	-0.73625600	-1.14137300
F	6.18360200	-1.61054900	-2.03824800
F	6.72554800	0.04279600	-0.72778300
F	5.20658700	-1.38850000	-0.10433900
O	3.85235900	1.15877400	-0.79777100
O	0.45352000	0.06249300	2.96327200
C	-5.95156500	-0.57159400	0.45397500
C	-7.28532700	-0.48973000	0.06026900
C	-7.61619400	-0.21446200	-1.26990800
C	-6.60037800	-0.03165800	-2.20905000
C	-5.26199000	-0.12561300	-1.82590300
C	-4.93289400	-0.38237400	-0.49000400
N	-3.55385000	-0.46988400	-0.10028400
C	-3.15185800	-1.58609600	0.71087200
C	-2.25208400	-1.39332600	1.76607500
C	-1.87314400	-2.47455200	2.56048500
C	-2.40770100	-3.74496800	2.33033400
C	-3.32004300	-3.92929700	1.28879800
C	-3.68660400	-2.85883900	0.47298500
H	-5.69414600	-0.77907100	1.48779300
H	-8.06938800	-0.63292900	0.79859600
H	-8.65769500	-0.14810300	-1.57086800
H	-6.84595900	0.17170400	-3.24758800
H	-4.46964300	-0.00839300	-2.55857800
H	-0.69316900	1.15473300	-0.85932600
H	-1.82675900	-0.41544900	1.96263600
H	-1.16040200	-2.30660700	3.36177000
H	-2.11758200	-4.58260700	2.95817800
H	-3.74283600	-4.91246000	1.09972700

H -4.38087800 -3.00663500 -0.34754500

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

Thermal correction to Gibbs Free Energy = 0.332679

Sum of electronic and thermal Free Energies = -3173.655642

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

Energy = -3173.9159389

No imaginary frequency

**ts3**

C	3.42676700	2.30841400	0.34347400
C	4.03687800	3.47646900	0.79786500
C	4.42251200	3.59812400	2.13533300
C	4.18761100	2.54733500	3.02315200
C	3.57716500	1.37628100	2.57221000
C	3.19598900	1.24512500	1.22948400
C	2.49718100	0.01080700	0.77590500
C	1.34109900	-0.38004800	1.33294700
C	0.53785200	-1.60628700	0.94490900
O	1.06936600	-2.67625000	1.66419900
O	-0.77313200	-1.52485900	1.00084600
C	0.20930400	-3.79604000	1.88173900
H	3.08417000	2.23497700	-0.68281700
H	4.19736600	4.30019300	0.10783400
H	4.89670800	4.51128500	2.48474200
H	4.47986900	2.63610400	4.06593200
H	3.39673000	0.55419800	3.25963000
H	0.79290200	-4.50069200	2.47757000
H	-0.70038300	-3.50451300	2.41204100
H	-0.06913700	-4.26308400	0.92784100
S	-4.66088300	-0.42888100	1.19695500
O	-3.59922900	-1.51144300	1.21998600
C	-1.90569400	3.02649400	-1.52764100
S	-0.74866500	1.64906100	-1.04496500
O	-1.22262300	0.45017100	-1.77378700
O	-1.02967200	1.48337900	0.45371800
F	-3.17066600	2.65584000	-1.32361800
F	-1.64233200	4.11826600	-0.80734600
F	-1.73366800	3.30297500	-2.82441800
Cu	-2.06441600	-0.14679700	0.82375400
O	-5.67857400	-0.43310300	2.23330500
C	-5.53572300	-0.67921600	-0.42813000
F	-6.17797900	-1.84793600	-0.40863200
F	-6.40994100	0.30664300	-0.62178000
F	-4.64000900	-0.68249700	-1.41839100
O	-3.85115500	0.84096200	0.99137900

O	0.59916300	2.14247800	-1.33216600
C	5.04468600	-0.11897600	-1.65283700
C	6.42332500	-0.02122300	-1.84464600
C	7.30224400	-0.43793700	-0.84229800
C	6.80134900	-0.95852900	0.35313000
C	5.42411900	-1.06666400	0.54950700
C	4.55173500	-0.64171200	-0.45490700
N	3.12170700	-0.75662800	-0.26935300
C	2.44492500	-1.76546600	-0.88835400
C	0.99179400	-1.79692400	-0.76034000
C	0.28774400	-2.89563000	-1.39920200
C	0.95145100	-3.89447300	-2.05320700
C	2.36848700	-3.82978000	-2.14288100
C	3.10528200	-2.80071100	-1.59008900
H	4.34947600	0.21236300	-2.41829600
H	6.80828800	0.38849400	-2.77394800
H	8.37498500	-0.35559400	-0.99162700
H	7.48194000	-1.28482600	1.13417200
H	5.02338800	-1.47627100	1.47148800
H	0.93505600	0.19650500	2.15603500
H	0.54065100	-0.83758100	-1.04043800
H	-0.79542600	-2.88423700	-1.32609500
H	0.41841600	-4.72199600	-2.51018300
H	2.89976500	-4.62454300	-2.66078700
H	4.18382300	-2.79704100	-1.68123100

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

Thermal correction to Gibbs Free Energy = 0.332497

Sum of electronic and thermal Free Energies = -3173.591476

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

Energy = -3173.8586611

Number of Imaginary Frequencies = 1

Lowest Frequency = 306.44i

**in6**

C	3.35825600	-1.42070000	2.28107000
C	3.76718300	-2.40053100	3.18374700
C	3.55184400	-3.75161300	2.90051600
C	2.92112100	-4.11821600	1.71074900
C	2.51163900	-3.13946900	0.80480300
C	2.72664500	-1.78097700	1.08013800
C	2.21488000	-0.74550100	0.14344900
C	0.94063100	-0.73980400	-0.28145000
C	0.34314600	0.32145500	-1.18978100
O	0.61598500	-0.11915600	-2.50568800
O	-0.93630500	0.63501200	-0.96250600

C	-0.25481100	0.35352600	-3.52806700
H	3.50604700	-0.37157500	2.51947600
H	4.24389200	-2.10776500	4.11502200
H	3.86994500	-4.51348500	3.60662700
H	2.74747500	-5.16633700	1.48421800
H	2.02632900	-3.42551700	-0.12402900
H	0.09682200	-0.10869600	-4.45328300
H	-1.29246400	0.06932000	-3.33500200
H	-0.19707600	1.44751800	-3.62451600
S	-3.27242900	-2.60974300	0.03790000
O	-2.01484300	-2.11585200	-0.66410100
C	-2.50939200	3.66510400	0.94930900
S	-1.73518000	2.35653300	2.02330200
O	-0.31022500	2.34802000	1.64600500
O	-2.49497100	1.11255800	1.55929500
F	-2.39662300	3.33589200	-0.35410600
F	-3.80375400	3.80336500	1.23605700
F	-1.88963000	4.83529100	1.14021900
Cu	-2.12061200	-0.23390400	0.21931400
O	-3.26623000	-3.96269100	0.56657300
C	-4.56474200	-2.54813700	-1.30115900
F	-4.26847700	-3.43367300	-2.25251100
F	-5.76020500	-2.82835600	-0.78691600
F	-4.58720300	-1.31977500	-1.83356700
O	-3.63516400	-1.46736300	0.95917900
O	-2.08061100	2.72181200	3.39231400
C	5.46648800	0.59767700	0.42336700
C	6.82061100	0.27031300	0.34000600
C	7.24781200	-0.73180700	-0.53416900
C	6.31978000	-1.40458700	-1.33223700
C	4.96514300	-1.07821800	-1.26092800
C	4.54630700	-0.08031400	-0.37872500
N	3.13950000	0.26186000	-0.31177000
C	2.68846400	1.38493000	-0.92322600
C	1.24410300	1.66828300	-0.85688700
C	0.77784900	2.87576500	-1.54761000
C	1.62950000	3.69354700	-2.22538800
C	3.01529600	3.36461900	-2.26727700
C	3.54345500	2.25656000	-1.63854600
H	5.12191400	1.36924500	1.10551500
H	7.53854600	0.79430500	0.96409500
H	8.30158400	-0.98824500	-0.59262200
H	6.64866100	-2.18236000	-2.01512900
H	4.23440200	-1.58801500	-1.88119400
H	0.28700000	-1.55930500	-0.00219700

H	0.92573900	1.76303000	0.20098700
H	-0.28015000	3.09307900	-1.45495000
H	1.27440200	4.58854700	-2.72598400
H	3.69091200	4.01274900	-2.82024100
H	4.60368900	2.05021700	-1.70513300

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

Thermal correction to Gibbs Free Energy = 0.333819

Sum of electronic and thermal Free Energies = -3173.588539

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

Energy = -3173.86105390

No imaginary frequency

**ts4-OTf**

C	3.06646000	-2.56184200	-0.22758800
C	3.66753000	-3.79858600	-0.46244000
C	4.21879800	-4.08917800	-1.71265000
C	4.16030500	-3.14003000	-2.73425600
C	3.55655000	-1.90266400	-2.50416400
C	3.01231000	-1.60076200	-1.24799700
C	2.32114900	-0.29086300	-1.04493700
C	1.10437200	-0.07100900	-1.57406500
C	0.38232000	1.24694800	-1.51660900
O	0.71462900	1.85738300	-2.77440300
O	-0.98049600	1.14929800	-1.37920000
C	-0.10548300	2.92729700	-3.22641300
H	2.61768400	-2.34827900	0.73747100
H	3.69600900	-4.54016700	0.33126200
H	4.68433100	-5.05467000	-1.89176400
H	4.57802800	-3.36281200	-3.71236800
H	3.49876800	-1.16530700	-3.30019000
H	0.23321900	3.15219700	-4.24124700
H	-1.16281200	2.64872200	-3.24254200
H	0.02441900	3.82871500	-2.60789500
S	-4.56128100	-0.78978100	-1.26960400
O	-3.74260600	0.30230900	-1.91756500
C	-1.58248200	-0.75371000	3.13014100
S	-0.24124800	-0.62292100	1.83856600
O	-0.08619800	0.89860800	1.75733500
O	-0.86483400	-1.18396700	0.59759500
F	-2.67686800	-0.13380900	2.68507800
F	-1.84744800	-2.03891800	3.34110500
F	-1.17154800	-0.18453400	4.26062100
Cu	-2.02322800	-0.24197200	-0.76690200
O	-5.45383000	-1.58478700	-2.09465900
C	-5.61682800	0.10701400	-0.02501200

F	-6.46616400	0.91781400	-0.65412800
F	-6.29834400	-0.77166200	0.70847500
F	-4.82678400	0.83309800	0.77866600
O	-3.55037400	-1.52671900	-0.40117700
O	0.93150400	-1.33769400	2.32845100
C	4.51688300	0.03091900	1.51117200
C	5.81058200	-0.18140800	1.98907700
C	6.91157400	0.04155400	1.15838800
C	6.71959400	0.47908100	-0.15378700
C	5.42843400	0.69823400	-0.63728500
C	4.33282300	0.47008800	0.19719800
N	2.99441700	0.71263400	-0.29397800
C	2.36880500	1.90218500	0.00266200
C	0.98269300	2.08429600	-0.35689500
C	0.35693000	3.33475200	-0.03333100
C	1.01204500	4.30852400	0.68526700
C	2.35596500	4.09021300	1.05280700
C	3.02337900	2.92104700	0.73313600
H	3.65060200	-0.14907200	2.14113600
H	5.95649500	-0.52636800	3.00868400
H	7.91733700	-0.12740700	1.53265900
H	7.57341200	0.65217000	-0.80256400
H	5.26434900	1.04193200	-1.65393700
H	0.63782500	-0.85396300	-2.16224800
H	0.42758200	1.40880700	0.74623900
H	-0.68305300	3.44675200	-0.32198400
H	0.51153000	5.23177200	0.95881600
H	2.88760500	4.85479100	1.61340600
H	4.05363500	2.78822800	1.03780900

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

Thermal correction to Gibbs Free Energy = 0.329632

Sum of electronic and thermal Free Energies = -3173.582202

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

Energy = -3173.8490022

Number of Imaginary Frequencies = 1

Lowest Frequency = 1178.14i

#### in7-OTf

C	0.48225300	0.87515900	2.36025200
C	0.11597400	1.42611000	3.58779400
C	0.29417900	0.70011200	4.76709100
C	0.83460700	-0.58552400	4.71619800
C	1.19326900	-1.14510100	3.48947200
C	1.02639300	-0.41501300	2.30380100
C	1.36542400	-1.07629700	1.00660800



C	0.55203400	-2.10063200	0.53492800
C	0.81338200	-2.83367400	-0.76150200
O	0.70982200	-4.23915700	-0.64303500
O	-0.15174400	-2.30258800	-1.62714700
C	-0.60196300	-4.76717900	-0.46166900
H	0.33015400	1.44057900	1.44801200
H	-0.31981800	2.42037000	3.61944000
H	0.00326900	1.13163800	5.72059500
H	0.96842500	-1.15958100	5.62870300
H	1.60016000	-2.15189100	3.44808900
H	-0.47725100	-5.85138200	-0.41394500
H	-1.06223700	-4.42653100	0.47614400
H	-1.25794300	-4.50534000	-1.29644600
S	-3.25621600	-0.31945600	1.18732600
O	-2.72263100	-1.56378400	1.74529100
C	-0.17544600	3.74442000	-1.25151000
S	-1.03062300	2.34230200	-2.13515700
O	-1.20338700	2.74605700	-3.51478900
O	-2.42487800	2.34665800	-1.38563300
F	-0.80804500	4.88683100	-1.48355700
F	-0.15547000	3.50125400	0.06295000
F	1.08283900	3.82729800	-1.70002100
Cu	-0.96963000	-0.93441500	-0.70248700
O	-3.80695300	0.71787400	2.04876300
C	-4.61210900	-0.82704200	0.01730900
F	-5.60076300	-1.41621400	0.68664400
F	-5.08404000	0.24647200	-0.62347200
F	-4.11857300	-1.68781700	-0.88836100
O	-2.24600400	0.28079100	0.15558900
O	-0.26982400	1.13144200	-1.78059100
C	2.99283400	1.66688700	0.03843000
C	3.69316300	2.81679600	0.40353700
C	4.62784600	2.76807000	1.44072300
C	4.86403600	1.56711000	2.11372600
C	4.16620200	0.41207000	1.75600800
C	3.22877900	0.47407200	0.72463500
N	2.49414600	-0.71052900	0.32900100
C	2.95913300	-1.45947700	-0.79096200
C	2.20662000	-2.54107900	-1.28362500
C	2.71785800	-3.29762700	-2.34113100
C	3.94703800	-2.99139600	-2.91710200
C	4.68676800	-1.91023600	-2.42867600
C	4.20285300	-1.14835000	-1.37233600
H	2.26686400	1.68535900	-0.76742100
H	3.50036300	3.74756300	-0.12160100

H	5.17177100	3.66450600	1.72445500
H	5.59092500	1.52665300	2.91968300
H	4.33918300	-0.52650800	2.27280300
H	-0.24274100	-2.45390200	1.18467600
H	-2.45881100	1.59426000	-0.69315700
H	2.12766500	-4.13257600	-2.70136200
H	4.32588400	-3.58701100	-3.74245100
H	5.64822200	-1.65941400	-2.86736400
H	4.79007000	-0.32240700	-0.99165800

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

Thermal correction to Gibbs Free Energy = 0.333477

Sum of electronic and thermal Free Energies = -3173.620460

M06-2X/6-311++G\*\* (LanL2DZ for Cu)

Energy = -3173.8835868

No imaginary frequency

### in8-OTf

C	1.00332700	1.96182600	-2.13941200
C	0.99481300	3.02135700	-3.04723300
C	-0.12716400	3.84391700	-3.15694100
C	-1.24607900	3.60403900	-2.35570500
C	-1.24244500	2.55671600	-1.43659800
C	-0.11081200	1.73322600	-1.31780000
C	-0.12895600	0.56081700	-0.39755200
C	-0.10089500	-0.72498400	-0.94624700
C	-0.27892300	-1.98346600	-0.14368600
O	-1.50979800	-2.70320400	-0.47532000
O	0.81401200	-2.77146100	-0.44983100
C	-1.60065400	-3.25768500	-1.79988500
H	1.87940800	1.32676000	-2.06205700
H	1.86992800	3.20016500	-3.66515300
H	-0.13284300	4.66554600	-3.86791300
H	-2.12941800	4.22934900	-2.44918300
H	-2.12285800	2.35932600	-0.83514600
H	-2.41126700	-3.98836400	-1.76494200
H	-1.84373200	-2.48227300	-2.53390700
H	-0.66199200	-3.75377300	-2.04996200
S	4.28001500	0.26134300	-0.47390800
O	3.53620000	-0.48997700	-1.59530500
C	-5.89894900	-0.67629700	-0.52163500
S	-4.07627700	-0.31849200	-0.38846400
O	-3.65088800	-1.60074700	0.44208100
O	-3.94813600	0.88741200	0.42452700
F	-6.43066400	-0.78856000	0.69305100
F	-6.47421200	0.33566600	-1.17174100

F	-6.08658800	-1.80653600	-1.20150200
Cu	2.07100900	-1.53879700	-0.98703100
O	5.06274900	1.38373600	-0.97624600
C	5.48998400	-1.04525500	0.06722300
F	6.34064900	-1.33607900	-0.91726000
F	6.17293100	-0.62629000	1.13300400
F	4.81212000	-2.16217500	0.39724400
O	3.39209900	0.45597400	0.69054800
O	-3.50896900	-0.36313100	-1.73439800
C	1.08178600	2.68686900	1.66332800
C	1.13919600	3.96253000	2.22911200
C	-0.02935000	4.60439000	2.64432600
C	-1.26702700	3.97239400	2.49661300
C	-1.34243800	2.69934800	1.93022100
C	-0.16396400	2.07656000	1.51388600
N	-0.22959600	0.73810800	0.94468500
C	-0.31630400	-0.37022100	1.83503400
C	-0.38010400	-1.68494500	1.33777800
C	-0.47272400	-2.75414500	2.23295200
C	-0.49959800	-2.53804800	3.60653200
C	-0.42370700	-1.23097100	4.09793800
C	-0.33022000	-0.15394800	3.22633000
H	1.98214200	2.16687000	1.34939400
H	2.10275900	4.44971900	2.34613300
H	0.02345400	5.59638700	3.08420500
H	-2.17752500	4.46993700	2.81789300
H	-2.29588200	2.19652300	1.79954900
H	-0.20772400	-0.80448000	-2.02273100
H	-2.80606400	-2.04247900	0.04223900
H	-0.51156200	-3.75993500	1.82833400
H	-0.56893400	-3.37879100	4.29016100
H	-0.43286200	-1.04671900	5.16804600
H	-0.26594500	0.85176400	3.61903400

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

Thermal correction to Gibbs Free Energy = 0.332510

Sum of electronic and thermal Free Energies = -3173.622892

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

Energy = -3173.8832222

No imaginary frequency

#### ts5-OTf

C	0.91539500	1.98000700	-2.13083600
C	0.88365600	3.03398200	-3.04401500
C	-0.26053400	3.82443800	-3.16335000
C	-1.37721800	3.55784500	-2.36767300

C	-1.35241900	2.51634800	-1.44199400
C	-0.19738200	1.72766800	-1.31398800
C	-0.18033300	0.56351300	-0.38544900
C	-0.12113300	-0.72661400	-0.92707900
C	-0.21467800	-1.97253000	-0.10792400
O	-1.51160900	-2.74754900	-0.40053000
O	0.81630300	-2.78182800	-0.47472800
C	-1.69122000	-3.27472200	-1.74200000
H	1.80717100	1.36846600	-2.04494000
H	1.75670900	3.23353400	-3.65844200
H	-0.28499900	4.64151700	-3.87917900
H	-2.27755500	4.15655200	-2.47151500
H	-2.23181500	2.29077000	-0.84923400
H	-2.43906700	-4.06420100	-1.65626600
H	-2.04570800	-2.48632400	-2.40946500
H	-0.73554200	-3.68865200	-2.05950700
S	4.22081400	0.30969100	-0.51762600
O	3.51415200	-0.47109400	-1.64517200
C	-5.75265800	-0.73530100	-0.50431100
S	-3.93234700	-0.38965000	-0.37073900
O	-3.46168800	-1.61202600	0.42911200
O	-3.82475600	0.85916600	0.39529100
F	-6.29898800	-0.81753700	0.71039300
F	-6.33882400	0.25419200	-1.18422700
F	-5.95085500	-1.88737700	-1.15383900
Cu	2.07157600	-1.54259500	-1.04046200
O	5.00609300	1.42912100	-1.02035600
C	5.42625500	-0.97613600	0.08166300
F	6.30857400	-1.27496800	-0.87104300
F	6.07072400	-0.53476700	1.16140600
F	4.74666600	-2.09432300	0.40824600
O	3.29694000	0.51583200	0.61648400
O	-3.40386900	-0.40323000	-1.74395200
C	0.98868500	2.73329800	1.66599400
C	1.00586500	4.01158400	2.22797100
C	-0.18353700	4.61851300	2.63711400
C	-1.40127600	3.94978100	2.48635800
C	-1.43857000	2.67281700	1.92425200
C	-0.23884800	2.08719200	1.51650300
N	-0.25940500	0.74192100	0.95488900
C	-0.28549400	-0.36061200	1.85351900
C	-0.28868400	-1.68283100	1.36970900
C	-0.30014500	-2.74966400	2.27129000
C	-0.31345200	-2.52279300	3.64354800
C	-0.30529100	-1.20924800	4.12295800

C	-0.28722800	-0.13501600	3.24282600
H	1.90410900	2.23971200	1.35335700
H	1.95358900	4.52861500	2.34609000
H	-0.16213600	5.61309900	3.07377000
H	-2.32741700	4.42174300	2.80122800
H	-2.37501300	2.14144100	1.78420200
H	-0.25068200	-0.82331500	-1.99934400
H	-2.43871300	-2.19419000	-0.03430200
H	-0.29044800	-3.75957400	1.87529900
H	-0.32281200	-3.35990400	4.33475600
H	-0.30820500	-1.01721300	5.19160900
H	-0.27352500	0.87585300	3.62677700

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

Thermal correction to Gibbs Free Energy = 0.332762

Sum of electronic and thermal Free Energies = -3173.618150

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

Energy = -3173.8864164

Number of Imaginary Frequencies = 1

Lowest Frequency = 40.14i

**in7**

C	4.39487100	1.62564500	-1.68272700
C	4.95724900	2.84342300	-2.06053700
C	4.60631900	4.01884400	-1.39228500
C	3.67881900	3.97411100	-0.35042500
C	3.10609900	2.75891900	0.02470300
C	3.46761500	1.57090500	-0.63029300
C	2.77754700	0.30664900	-0.25007800
C	1.39863000	0.26772500	-0.29204100
C	0.66924500	-0.89386000	0.06256600
O	-0.60303800	-0.97614000	0.08201900
H	4.66066800	0.72131300	-2.21951300
H	5.66484600	2.87456700	-2.88411300
H	5.04768400	4.96609200	-1.68889800
H	3.39375000	4.88462000	0.16847500
H	2.37687000	2.72648600	0.82897700
S	-2.48549800	2.75880200	-0.12018600
O	-1.29412100	1.92441600	0.34567200
C	-4.61501200	-1.89544300	0.15359400
S	-3.43896000	-2.44301500	-1.18329700
O	-2.44795600	-3.26625200	-0.48634300
O	-2.89594000	-1.07240500	-1.63943100
F	-3.95784700	-1.07108300	1.01312800
F	-5.64850000	-1.22560400	-0.35302900
F	-5.06259900	-2.94312700	0.84518900

Cu	-1.98332900	0.20277300	-0.53047600
O	-2.21117600	4.08422300	-0.64614000
C	-3.49972600	2.97678800	1.42767000
F	-2.82018300	3.72242700	2.29915200
F	-4.64814300	3.57629400	1.12454300
F	-3.74676000	1.77953500	1.96441400
O	-3.27439200	1.78352000	-0.96482300
O	-4.25792000	-3.03967100	-2.23260800
C	5.79049300	-1.29908500	-0.62894300
C	7.17224200	-1.22828000	-0.44765600
C	7.70062100	-0.56880000	0.66484400
C	6.84564800	0.01530700	1.60163400
C	5.46231800	-0.05807200	1.43105500
C	4.94301100	-0.70717500	0.31035000
N	3.50495200	-0.79427200	0.13965900
C	2.85580900	-1.99359800	0.48417300
C	1.44201800	-2.06945300	0.42449000
C	0.78508800	-3.28296500	0.72384500
C	1.51461400	-4.39168900	1.10747900
C	2.91456000	-4.30204000	1.20634700
C	3.58382800	-3.12837000	0.90019300
H	5.36767500	-1.81024600	-1.48895100
H	7.83374600	-1.68597900	-1.17730300
H	8.77652500	-0.51236700	0.80198700
H	7.25259800	0.52582200	2.46941100
H	4.78828600	0.38774900	2.15578800
H	0.86388500	1.15840700	-0.59599600
H	-0.29536500	-3.31377400	0.62357200
H	1.01033500	-5.32643300	1.33150400
H	3.49084500	-5.16736500	1.52178500
H	4.66206500	-3.08641600	0.98010100

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

Thermal correction to Gibbs Free Energy = 0.283760

Sum of electronic and thermal Free Energies = -3057.992686

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

Energy = -3058.2180259

No imaginary frequency

HOTf-assisted reaction

**ts2-HOTf**

C	-2.06398700	-1.63569200	2.49224900
C	-2.06203200	-1.64342400	3.88607100
C	-1.67327400	-0.50579000	4.59756700
C	-1.27859400	0.64302900	3.91113600

C	-1.27013700	0.66064800	2.51698600
C	-1.66448000	-0.47973100	1.79668100
C	-1.62414800	-0.45018800	0.31626900
C	-0.49406200	-0.42684800	-0.43290700
C	-0.54433000	-0.43319600	-1.92873300
O	0.66766400	-0.54392200	-2.44117200
O	-1.56747100	-0.36557700	-2.61634300
C	0.77432000	-0.58883900	-3.87908700
H	-2.33867500	-2.53332400	1.95085800
H	-2.35067500	-2.54719600	4.41473100
H	-1.67006000	-0.51940800	5.68385500
H	-0.97070100	1.53020000	4.45642600
H	-0.98551400	1.56423000	1.98720600
H	1.83211400	-0.75018200	-4.07735500
H	0.17438900	-1.41452300	-4.26629400
H	0.43445500	0.35937500	-4.30061000
S	-0.14349200	3.34113700	-0.97101500
O	0.63343900	2.09208400	-1.43147100
C	4.36346400	-0.35396000	1.24010500
S	3.13083500	0.95346100	1.74639200
O	1.79816600	0.21057500	1.81957400
O	2.96254200	1.81719000	0.51284700
F	4.00900400	-0.86162900	0.05825200
F	5.56833400	0.20666000	1.13803100
F	4.39052300	-1.31551000	2.15642100
Cu	1.09981500	0.95248400	0.08713100
O	-1.24307400	3.67658800	-1.87553300
C	1.11717200	4.69753800	-1.18370800
F	1.55069500	4.71216300	-2.44621300
F	0.54004700	5.86925500	-0.90164200
F	2.14649200	4.50420900	-0.36244100
O	-0.40377900	3.24202900	0.48041900
O	3.62348600	1.56097100	2.96898400
C	-4.34008900	1.00961000	1.14437800
C	-4.99310200	2.21727400	1.38572900
C	-5.00619800	3.22212300	0.41411300
C	-4.36341100	3.02235700	-0.80651700
C	-3.71594900	1.81387600	-1.06941000
C	-3.71827900	0.82025900	-0.09265200
N	-2.97966800	-0.43298800	-0.40339100
C	-3.74484800	-1.72683500	-0.33644000
C	-3.04084500	-2.89189000	-0.64524800
C	-3.72414900	-4.10812900	-0.66256500
C	-5.09322600	-4.15569200	-0.39288900
C	-5.78367900	-2.97631200	-0.11574700

C	-5.11539100	-1.74893100	-0.09005600
H	-4.31687800	0.23647300	1.90266900
H	-5.48303800	2.37431200	2.34187000
H	-5.50669800	4.16431700	0.61663200
H	-4.33898200	3.80693200	-1.55488000
H	-3.19217200	1.67097200	-2.00847500
H	-2.67724800	-0.35782800	-1.41624400
H	-1.98055100	-2.87988100	-0.87900400
H	-3.17219900	-5.01338800	-0.89542100
H	-5.62024800	-5.10506900	-0.40786700
H	-6.85163400	-2.99903800	0.07973200
H	-5.66632900	-0.83929900	0.10837900
S	1.05576400	-3.53864300	-0.45390200
O	1.20808500	-2.23161200	0.35754800
O	1.03658400	-4.72083000	0.39968900
C	2.67867600	-3.58831400	-1.36415300
F	3.68880400	-3.68994700	-0.49928600
F	2.69245100	-4.64277200	-2.18460300
F	2.84169800	-2.47351600	-2.09179800
O	0.02522500	-3.39939900	-1.50152900
H	0.45806100	-1.27675200	0.02550600

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

Thermal correction to Gibbs Free Energy = 0.358363

Sum of electronic and thermal Free Energies = -4135.564505

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

Energy = -4135.8790456

Number of Imaginary Frequencies = 1

Lowest Frequency = 1103.89i

### in3-HOTf

C	1.55192200	-2.38336600	-0.88423300
C	2.03647600	-3.46660400	-1.61626400
C	2.48207400	-3.29504200	-2.92819900
C	2.43536600	-2.03002000	-3.51553900
C	1.95486300	-0.94229400	-2.78940000
C	1.51337200	-1.10247600	-1.46362800
C	0.97479800	0.08957000	-0.76856100
C	-0.03617400	0.82757900	-1.25234200
C	-0.57600400	2.04854600	-0.60552100
O	-1.53600600	2.60059200	-1.32047100
O	-0.12637000	2.52580800	0.44351900
C	-2.33801100	3.60584700	-0.66391600
H	1.16767300	-2.54393300	0.11526300
H	2.04451000	-4.45350000	-1.16276900
H	2.85313500	-4.14556700	-3.49314300



H	2.77249200	-1.88726500	-4.53823700
H	1.92775700	0.04486500	-3.24105000
H	-2.98350300	4.00868400	-1.44325700
H	-2.92479700	3.11039000	0.11164000
H	-1.70473000	4.38527500	-0.23554800
C	4.00824200	0.39920300	-0.16966800
C	5.24935300	1.01780400	-0.32567100
C	5.42434600	2.35612600	0.03116100
C	4.35235100	3.08388500	0.54809000
C	3.10464900	2.47994400	0.70940200
C	2.94621700	1.14137200	0.34967800
N	1.59832800	0.54422200	0.53480700
C	1.44261500	-0.44395800	1.66068500
C	0.13370600	-0.79950900	1.98183800
C	-0.07509300	-1.72428700	3.00495000
C	1.00806000	-2.25778000	3.70656900
C	2.30768500	-1.86274700	3.38599700
C	2.53888800	-0.95002800	2.35311200
H	3.87591600	-0.63955400	-0.44478700
H	6.08029700	0.44603500	-0.72781800
H	6.39376900	2.82946800	-0.09377800
H	4.47978800	4.12568100	0.82614500
H	2.26442300	3.04624900	1.09743500
H	0.96739900	1.36341900	0.78640800
H	-0.72142100	-0.37850800	1.45488900
H	-1.09503200	-2.02013900	3.22909900
H	0.84107300	-2.97706500	4.50324300
H	3.15416900	-2.26523900	3.93481600
H	3.55035200	-0.64858800	2.11190800
S	-3.04634100	-0.58040500	-0.05243800
O	-2.75163400	-0.72276100	-1.49432500
O	-3.01458000	-1.81490600	0.75548900
C	-4.81987200	-0.01833500	-0.00568200
F	-5.61994700	-0.88458500	-0.64250200
F	-5.25342600	0.10496800	1.25876700
F	-4.94427100	1.18486600	-0.60390800
O	-2.34413300	0.57530700	0.59879900
H	-0.56848600	0.47608000	-2.12754900

B3LYP/6-31G\*

Thermal correction to Gibbs Free Energy = 0.332183

Sum of electronic and thermal Free Energies = -2016.629967

M06-2X/6-311++G\*\*

Energy = -2016.8393433

No imaginary frequency

**in4-HOTf**

C	3.78139300	-0.27321600	0.52907300
C	4.92759100	-0.98618900	0.87464400
C	4.94746400	-1.77745800	2.02454300
C	3.80984000	-1.85331500	2.82853300
C	2.66212900	-1.14051500	2.48625900
C	2.63221300	-0.33396600	1.33545100
C	1.40960600	0.46386800	1.05901900
C	0.80520400	1.17114300	2.02683500
C	-0.43331000	1.99604700	1.91750900
O	-1.09498300	1.97537600	3.08107200
O	-0.76468300	2.62923800	0.93708200
C	-2.38034600	2.64168000	3.06654600
H	3.79036800	0.33922500	-0.36529400
H	5.80873000	-0.91972400	0.24275100
H	5.84171000	-2.33512700	2.28800400
H	3.80918200	-2.47512200	3.71923500
H	1.77058000	-1.22228400	3.10069300
H	-2.77356800	2.51854200	4.07562200
H	-2.25104700	3.70031300	2.82772000
H	-3.02994800	2.16665000	2.32761000
C	1.91203600	-0.87427300	-2.16909500
C	2.16835900	-2.07912700	-2.82537300
C	1.60348100	-3.26833900	-2.36457100
C	0.77342200	-3.25201200	-1.24330100
C	0.51052800	-2.05676700	-0.57462100
C	1.08898900	-0.87925500	-1.04596900
N	0.77399800	0.39219000	-0.30838700
C	0.93432000	1.61333100	-1.15724300
C	2.01745900	2.46893200	-0.99109700
C	2.13904700	3.57504800	-1.83596000
C	1.18535900	3.81196000	-2.82510100
C	0.09976900	2.94435100	-2.96568500
C	-0.03492400	1.83430700	-2.13331000
H	2.33790400	0.04961800	-2.54129400
H	2.80716000	-2.07974800	-3.70369800
H	1.80004800	-4.20164000	-2.88423200
H	0.31190300	-4.16858900	-0.88877600
H	-0.16328500	-2.03349900	0.27267500
H	-0.28317300	0.28901000	-0.07137800
H	2.74273600	2.30624600	-0.20190900
H	2.97867800	4.25218000	-1.70882600
H	1.28075200	4.67606700	-3.47629700
H	-0.65886800	3.13371300	-3.71910200
H	-0.89612600	1.17607700	-2.21882100

S	-2.93963200	-0.08631900	-0.13524500
O	-3.92467500	0.72444300	0.59164200
O	-2.75933600	0.16723300	-1.57702700
C	-3.59471900	-1.82705900	-0.04455700
F	-4.75651300	-1.92545900	-0.69928600
F	-2.71926000	-2.68610500	-0.60187600
F	-3.78600200	-2.19642700	1.22934000
O	-1.61972700	-0.23789300	0.59847300
H	1.26613100	1.15351700	3.00922800

B3LYP/6-31G\*

Thermal correction to Gibbs Free Energy = 0.332879

Sum of electronic and thermal Free Energies = -2016.637882

M06-2X/6-311++G\*\*

Energy = -2016.8438597

No imaginary frequency

**ts3-HOTf**

C	-3.71432800	-0.23888100	-0.45544900
C	-4.88626400	-0.87822700	-0.85412100
C	-4.97031800	-1.48007500	-2.11106700
C	-3.87092400	-1.43869700	-2.96918100
C	-2.69873300	-0.79601200	-2.57465100
C	-2.60424600	-0.17922700	-1.31543800
C	-1.36475600	0.56471200	-0.96241000
C	-0.80150800	1.39462800	-1.86166300
C	0.43414900	2.20654900	-1.71139300
O	0.97192600	2.43923400	-2.92274600
O	0.89123500	2.62851100	-0.66927400
C	2.24130500	3.12737000	-2.90006800
H	-3.67016100	0.22220800	0.52465700
H	-5.73659900	-0.90504700	-0.17849500
H	-5.88374000	-1.98299000	-2.41592700
H	-3.91971200	-1.91437700	-3.94467400
H	-1.83805000	-0.78715100	-3.23682600
H	2.54333400	3.20428300	-3.94469000
H	2.12588800	4.12003800	-2.45708300
H	2.96538500	2.54893600	-2.32158200
C	-1.71936100	-1.07231300	2.19853200
C	-1.97993500	-2.33144400	2.74259300
C	-1.58054800	-3.48800200	2.07449500
C	-0.91161000	-3.38131700	0.85451200
C	-0.64287100	-2.13003900	0.30279400
C	-1.05390400	-0.97689300	0.97659000
N	-0.72701200	0.34049000	0.36332900
C	-0.84129000	1.47769600	1.30855400

C	-1.90600500	2.37347600	1.23827000
C	-1.99477400	3.40874600	2.17192300
C	-1.02974300	3.54182200	3.16883400
C	0.03328000	2.63773000	3.22487100
C	0.13456700	1.60193100	2.29794300
H	-2.02596700	-0.17994200	2.73015600
H	-2.49645700	-2.40024800	3.69572700
H	-1.78183800	-4.46501700	2.50426700
H	-0.58401200	-4.27358900	0.32926900
H	-0.10334900	-2.05180300	-0.63314100
H	0.49308400	0.16574400	0.03395500
H	-2.65143000	2.29135000	0.45493200
H	-2.82206100	4.11025500	2.11144500
H	-1.09971300	4.34929500	3.89208600
H	0.80083000	2.74154600	3.98618800
H	0.97784300	0.91933200	2.32835600
S	2.92858700	-0.14918600	0.07162400
O	3.84808500	0.64357400	-0.74307200
O	2.87568400	0.06509900	1.52235500
C	3.46130100	-1.92058300	-0.15234200
F	4.68628700	-2.08946600	0.35321400
F	2.61353700	-2.74235600	0.48412000
F	3.47694200	-2.24515500	-1.45011800
O	1.51894200	-0.23248300	-0.55801300
H	-1.30034000	1.49432800	-2.81961200

B3LYP/6-31G\*

Thermal correction to Gibbs Free Energy = 0.328227

Sum of electronic and thermal Free Energies = -2016.640068

M06-2X/6-311++G\*\*

Energy = -2016.8392407

Number of Imaginary Frequencies = 1

Lowest Frequency = 989.81i

**in5-HOTf**

C	-2.09737600	3.65512400	-0.95053600
C	-2.28502300	4.68229300	-1.87153700
C	-2.30567700	4.40362200	-3.24097800
C	-2.12547700	3.09319400	-3.68795700
C	-1.92095000	2.06490700	-2.76922800
C	-1.91224000	2.33437300	-1.39172700
C	-1.62370300	1.23976400	-0.42359100
C	-0.51647200	0.44941400	-0.70978000
C	-0.08739100	-0.79258300	-0.16369700
O	-1.02744100	-1.57703800	0.41688000
O	1.07329500	-1.26194000	-0.24749500

C	-0.56011400	-2.77143700	1.10846600
H	-2.06912600	3.87705600	0.11109200
H	-2.40911000	5.70278100	-1.52084000
H	-2.45826400	5.20660600	-3.95674100
H	-2.14248900	2.87073700	-4.75099200
H	-1.78474800	1.04346600	-3.11229100
H	-1.46486500	-3.25886300	1.46327000
H	-0.01470700	-3.41454000	0.41750500
H	0.08272300	-2.47177600	1.93702300
S	4.99623600	-2.07420800	-1.06951500
O	3.62660900	-2.48568700	-0.54397800
C	4.30835800	2.99781000	0.15004700
S	2.77777200	1.98992800	0.48353800
O	3.16900700	0.94253500	1.45336000
O	2.52830200	1.31550800	-0.87998300
F	5.30781000	2.19745600	-0.22060400
F	4.06513600	3.88306200	-0.81739100
F	4.65183700	3.64523500	1.26667900
Cu	2.87879500	-0.59122000	-0.64618800
O	5.62494800	-2.90962900	-2.07517000
C	6.09511600	-2.09083900	0.43746400
F	6.24173600	-3.34638600	0.85769900
F	7.28259200	-1.58203400	0.11751300
F	5.53486600	-1.35810900	1.39846200
O	4.79430100	-0.59784900	-1.37768600
O	1.73925100	2.95201300	0.85280100
C	-4.22514400	2.47627800	1.71179000
C	-5.55229800	2.90053400	1.71312800
C	-6.43083400	2.47703300	0.71179100
C	-5.97470900	1.61768900	-0.28854600
C	-4.64916700	1.18196600	-0.29472100
C	-3.76962000	1.62181700	0.69968800
N	-2.40153500	1.16552200	0.70927600
C	-1.89816000	0.66944700	1.96653900
C	-0.68322600	1.14938300	2.46865700
C	-0.21488000	0.67746900	3.69549500
C	-0.96055600	-0.24679400	4.43232900
C	-2.18303700	-0.70418800	3.93380600
C	-2.65238200	-0.25384600	2.69989700
H	-3.54061700	2.80474700	2.48735200
H	-5.89861000	3.56837600	2.49681600
H	-7.46467000	2.81001700	0.71658800
H	-6.65273100	1.26852400	-1.06181300
H	-4.29995000	0.49737100	-1.05931700
H	0.18319700	0.86392500	-1.42295800

H	-0.10350400	1.87780400	1.91019800
H	0.73354700	1.04684200	4.07404700
H	-0.59471300	-0.60260600	5.39124900
H	-2.77214500	-1.41958200	4.50094000
H	-3.59216500	-0.61971000	2.29950300
S	-4.02933200	-3.23983800	-1.03966700
O	-3.20088000	-1.87172100	-1.24312400
O	-4.37111400	-3.77241400	-2.34261300
C	-5.59606600	-2.53332700	-0.31740600
F	-6.13033200	-1.65445800	-1.16467800
F	-6.45121800	-3.52966800	-0.10552000
F	-5.32413900	-1.92652700	0.84201800
O	-3.39761800	-4.03786200	0.00514400
H	-2.47390500	-1.79763100	-0.56485000

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

Thermal correction to Gibbs Free Energy = 0.358380

Sum of electronic and thermal Free Energies = -4135.633579

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

Energy = -4135.9324290

No imaginary frequency

#### ts4-HOTf

C	-1.47094900	3.52246300	-1.07336500
C	-1.76504000	4.54224300	-1.97724300
C	-2.39323400	4.25073200	-3.19094400
C	-2.72117400	2.93089600	-3.50472600
C	-2.42764300	1.90512100	-2.60504800
C	-1.80528100	2.19552800	-1.38298900
C	-1.44933300	1.09008700	-0.45011800
C	-0.59712300	0.12354600	-0.83123700
C	-0.10915900	-1.03546900	0.00475600
O	-1.03148500	-2.10087400	-0.13468900
O	1.12567400	-1.41456500	-0.09714400
C	-0.53441100	-3.43638600	0.10004600
H	-0.94522800	3.74163200	-0.15004400
H	-1.49091600	5.56593800	-1.73786800
H	-2.62020800	5.04948200	-3.89182200
H	-3.20733700	2.69693200	-4.44775200
H	-2.69148700	0.87747800	-2.83992700
H	-1.38070500	-4.09451400	-0.09191800
H	0.30154100	-3.65547700	-0.56580900
H	-0.20730600	-3.52844400	1.14040100
S	5.04621200	-1.86446800	-1.05070300
O	3.72493800	-2.43987900	-0.56768200
C	3.87403100	3.15654000	0.23273800

S	2.42372400	2.01994700	0.50340500
O	2.84031300	1.05149200	1.54258200
O	2.31193700	1.29296800	-0.84399400
F	4.95900400	2.44621300	-0.07473300
F	3.60314300	4.00684400	-0.75883800
F	4.10020900	3.84482800	1.35531100
Cu	2.78694400	-0.59721900	-0.60765600
O	5.77894900	-2.58281900	-2.07717200
C	6.11649700	-1.83298900	0.47477100
F	6.36732500	-3.08349800	0.86168300
F	7.26083400	-1.21058400	0.20106200
F	5.47530500	-1.18524300	1.44915300
O	4.70198200	-0.40376600	-1.29854300
O	1.27897800	2.88759200	0.79257300
C	-3.31429200	2.88129700	1.96261900
C	-4.49851000	3.58612400	2.18066400
C	-5.65627500	3.24730900	1.47620100
C	-5.63021200	2.19856500	0.55408400
C	-4.45181100	1.48467600	0.33376500
C	-3.29790500	1.83358600	1.03816200
N	-2.06908600	1.09564900	0.84250200
C	-1.66490500	0.20721100	1.80303400
C	-0.32957400	-0.34933400	1.69819800
C	0.09007000	-1.29782600	2.70548200
C	-0.76321600	-1.72339300	3.68715200
C	-2.07156800	-1.17519900	3.74067500
C	-2.52099900	-0.22854100	2.83799700
H	-2.40341700	3.14184200	2.49333800
H	-4.51238200	4.40436000	2.89478100
H	-6.57596100	3.80022500	1.64453600
H	-6.52851700	1.92698000	0.00747800
H	-4.42478000	0.66676700	-0.37636000
H	-0.21102000	0.14280000	-1.84426600
H	0.42489000	0.41402700	1.49913800
H	1.10983600	-1.66515800	2.63968000
H	-0.45355700	-2.45624200	4.42510500
H	-2.75445800	-1.51679000	4.51446400
H	-3.52888000	0.15925100	2.91206100
S	-4.36361300	-2.95144200	-1.32593600
O	-3.34834100	-1.71410400	-1.43900100
O	-5.12167500	-3.04266000	-2.55762000
C	-5.51869300	-2.27474800	-0.02963300
F	-6.15699400	-1.20148400	-0.50260100
F	-6.40517000	-3.21191200	0.29402900
F	-4.81938400	-1.92711100	1.05671500

O	-3.69147200	-4.09733300	-0.72416000
H	-2.49162500	-1.88898600	-0.93643000

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

Thermal correction to Gibbs Free Energy = 0.357928

Sum of electronic and thermal Free Energies = -4135.577105

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

Energy = -4135.8805491

Number of Imaginary Frequencies = 1

Lowest Frequency = 413.17i

### in6-HOTf

C	-1.62521000	2.84778800	-2.01050100
C	-2.15282200	3.57972500	-3.07481700
C	-3.22225800	3.07516100	-3.81811700
C	-3.76422900	1.82869400	-3.49968500
C	-3.24084200	1.08932200	-2.43803500
C	-2.17363500	1.59890800	-1.68431300
C	-1.59042200	0.76939900	-0.58713200
C	-0.73524100	-0.23256200	-0.84493400
C	-0.14795300	-1.15961000	0.19031800
O	-1.03604700	-2.33851500	0.15190800
O	1.11893100	-1.54471200	-0.01882800
C	-0.45780100	-3.61936700	0.46852200
H	-0.78094100	3.22755500	-1.44422400
H	-1.71898000	4.54293900	-3.32886500
H	-3.62659800	3.64817700	-4.64823400
H	-4.58910600	1.42541600	-4.08044500
H	-3.65543000	0.11583600	-2.19450500
H	-1.22737100	-4.35388400	0.22930900
H	0.44955100	-3.78991000	-0.11164500
H	-0.22959400	-3.67662000	1.53884700
S	5.01736100	-1.73042400	-1.06410800
O	3.75361700	-2.43202000	-0.60783300
C	3.59794500	3.15450800	0.05186400
S	2.03678800	2.15702300	0.24476900
O	2.19580000	1.40814100	1.51285400
O	2.07953800	1.21348600	-0.95426700
F	4.66056000	2.35464500	0.14340300
F	3.60010100	3.76521200	-1.13282300
F	3.65040100	4.07119500	1.02246400
Cu	2.64898900	-0.64918500	-0.64639400
O	5.84286200	-2.36610300	-2.07501200
C	6.04441500	-1.59689800	0.48378600
F	6.40233500	-2.81571100	0.88680600
F	7.13182200	-0.86803200	0.24192400



F	5.31883100	-1.00938500	1.44192300
O	4.54642600	-0.30538900	-1.31310800
O	0.93258600	3.12273600	0.16859200
C	-2.42827400	3.37523400	1.35714800
C	-3.30508800	4.43067900	1.61114600
C	-4.68501100	4.23804500	1.51128000
C	-5.19374700	2.98768600	1.15326000
C	-4.32804500	1.92298400	0.89601900
C	-2.95310500	2.13052300	1.00210800
N	-2.01978900	1.04040800	0.75951000
C	-1.52500800	0.35255600	1.80436000
C	-0.30049100	-0.46831300	1.59917300
C	0.14023100	-1.29057300	2.74624700
C	-0.45111900	-1.19413900	3.96246800
C	-1.56028300	-0.30531800	4.13050200
C	-2.07626500	0.45548800	3.10821300
H	-1.35166500	3.51099000	1.40591200
H	-2.90643200	5.40389300	1.88177500
H	-5.36379300	5.06279200	1.70850900
H	-6.26611600	2.83689600	1.07152700
H	-4.71254700	0.95003200	0.61424000
H	-0.47649100	-0.44851800	-1.87594600
H	0.50067300	0.31238200	1.54105300
H	1.00773000	-1.91821200	2.57137200
H	-0.09633500	-1.77181000	4.80971000
H	-2.02289400	-0.23049900	5.11135700
H	-2.92510500	1.10361700	3.28419200
S	-4.23739200	-3.39300900	-0.86225200
O	-3.06829500	-2.49830700	-1.46866400
O	-5.14744000	-3.74546500	-1.93412900
C	-5.09610100	-2.10753800	0.17350400
F	-5.56001000	-1.11857100	-0.60120000
F	-6.10895500	-2.66033300	0.83439000
F	-4.22526500	-1.58562200	1.05359000
O	-3.71081700	-4.37448900	0.07863900
H	-2.26229900	-2.43478700	-0.83946500

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

Thermal correction to Gibbs Free Energy = 0.361288

Sum of electronic and thermal Free Energies = -4135.579791

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

Energy = -4135.8890350

No imaginary frequency

**in7-HOTf**

C	-4.09525700	-1.04058200	3.18669700
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C	-4.87115500	-0.43782200	4.17472900
C	-4.81220400	0.94508700	4.36654200
C	-3.97249600	1.72217500	3.56715100
C	-3.19459800	1.12289400	2.57599800
C	-3.24923700	-0.26517200	2.37798800
C	-2.35335300	-0.89262000	1.37283500
C	-1.02834100	-0.67663400	1.34858400
C	-0.10065800	-1.33895500	0.34067600
O	-0.21709000	-0.49507900	-0.85229200
O	1.14188000	-1.57043800	0.74221300
C	0.69634400	-0.75326400	-1.93685500
H	-4.12871500	-2.11895600	3.05866700
H	-5.51450800	-1.04872700	4.80182000
H	-5.41722400	1.41313500	5.13797600
H	-3.92271700	2.79772500	3.70983500
H	-2.55160600	1.72762200	1.94336500
H	0.75726500	0.16860500	-2.51626300
H	1.68176700	-1.02764900	-1.55957800
H	0.30718500	-1.56301200	-2.56446600
S	2.50517300	2.22238100	1.88094600
O	1.32252500	1.31849600	1.52815600
C	5.09472500	-1.24607000	-1.01352900
S	4.38385400	-2.53648100	0.12270700
O	3.28938000	-3.12940500	-0.66178800
O	3.90945700	-1.65047300	1.28134100
F	4.14742800	-0.30436100	-1.25958600
F	6.14875500	-0.64450600	-0.46704000
F	5.45121200	-1.79005500	-2.17900700
Cu	2.48178600	-0.34183700	1.25971200
O	2.33509600	3.13886100	2.99413700
C	2.72452500	3.24814800	0.33970800
F	1.64037300	4.00164300	0.15866800
F	3.79556000	4.02690500	0.47292900
F	2.88755900	2.43622500	-0.70656300
O	3.67433700	1.26542900	1.88916800
O	5.49564800	-3.38805000	0.53133400
C	-5.33979500	-2.40551100	0.29952500
C	-6.64694700	-2.13145900	-0.10617600
C	-6.93206600	-0.96079500	-0.81299900
C	-5.90791900	-0.06206300	-1.11963600
C	-4.59718600	-0.32868100	-0.72328900
C	-4.32570300	-1.49963500	-0.01444100
N	-2.95249000	-1.76320700	0.38324400
C	-2.20200000	-2.63655500	-0.31389800
C	-0.76266500	-2.76292300	0.05843500

C	0.06609700	-3.67142000	-0.77356100
C	-0.48729100	-4.42332600	-1.75869700
C	-1.88125900	-4.28586900	-2.04837600
C	-2.71651400	-3.42190600	-1.37464200
H	-5.10913300	-3.30938600	0.85545200
H	-7.44132900	-2.83098200	0.13660200
H	-7.95121200	-0.74961300	-1.12309200
H	-6.12046500	0.84820400	-1.67203300
H	-3.79519600	0.36218400	-0.95786500
H	-0.57667500	0.00453800	2.05945100
H	-0.73275700	-3.17814400	1.08474200
H	1.12916500	-3.69462400	-0.54174800
H	0.11825500	-5.10062400	-2.35188300
H	-2.30418900	-4.87762700	-2.85672700
H	-3.75743500	-3.33817600	-1.65808700
S	-1.08665100	2.89185900	-1.78625700
O	-1.39352900	1.84636600	-0.61617200
O	-1.50935700	4.20683200	-1.34819000
C	-2.33991900	2.30041200	-3.03179400
F	-3.57912800	2.43189000	-2.54202100
F	-2.22978700	3.00840200	-4.15131600
F	-2.11943900	1.00524100	-3.29772100
O	0.21985300	2.63219500	-2.37792500
H	-0.83203300	1.00205100	-0.69964200

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

Thermal correction to Gibbs Free Energy = 0.361550

Sum of electronic and thermal Free Energies = -4135.570864

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

Energy = -4135.8912499

No imaginary frequency

### ts5-HOTf

C	-2.53574900	-1.59279000	3.40033300
C	-3.04181900	-1.12752400	4.61187100
C	-3.25375200	0.24074200	4.80282100
C	-2.95404200	1.14139200	3.78008800
C	-2.44355000	0.68360000	2.56446000
C	-2.23393600	-0.69026900	2.36820700
C	-1.62016100	-1.15226700	1.09647400
C	-0.42728000	-0.68877500	0.67953400
C	0.23246300	-1.13501000	-0.59309000
O	-0.42996400	-0.22146700	-1.76161800
O	1.52453000	-1.08434100	-0.69321700
C	0.45613700	0.48572200	-2.66642500
H	-2.35529800	-2.65547700	3.26407200

H	-3.26198700	-1.83121100	5.40970700
H	-3.64800600	0.60183300	5.74863500
H	-3.11697200	2.20569200	3.92124600
H	-2.22321200	1.38767700	1.76793500
H	-0.12356400	1.32141700	-3.06171500
H	1.33082200	0.85295700	-2.13164700
H	0.75673200	-0.19650400	-3.46464100
S	2.55715300	2.28273000	1.04121000
O	2.16729200	0.87527300	1.55259900
C	6.60225000	-0.36908600	-0.67138300
S	5.43540600	-1.44445900	0.30730900
O	4.27550300	-1.70738200	-0.64327100
O	4.82128400	-0.51475500	1.33773000
F	5.94240200	0.68144100	-1.15239600
F	7.58964400	0.04146100	0.12115500
F	7.10532500	-1.08254400	-1.68067500
Cu	3.00542200	-0.42675700	0.35387300
O	3.16807600	3.13436300	2.05182100
C	0.87069900	3.00532100	0.71443900
F	0.13433300	2.97403000	1.82808100
F	0.98076300	4.25536400	0.28189600
F	0.25393900	2.26387500	-0.22630400
O	3.19561700	2.12307700	-0.28450800
O	6.19856700	-2.58779800	0.77755700
C	-4.26820800	-3.43626400	1.05924300
C	-5.63926900	-3.58791500	1.26968900
C	-6.51704600	-2.55248300	0.93804100
C	-6.02550800	-1.36547800	0.39058600
C	-4.65671000	-1.20073300	0.17251600
C	-3.79434500	-2.24098500	0.51506300
N	-2.36453400	-2.08268600	0.27855000
C	-1.79585600	-2.68545600	-0.77500800
C	-0.31216000	-2.56401900	-0.93321000
C	0.26861900	-3.14008500	-2.17395900
C	-0.48703400	-3.83417100	-3.05354900
C	-1.89649200	-3.97708500	-2.81407600
C	-2.53645100	-3.43796300	-1.72564700
H	-3.57475500	-4.23098800	1.31905000
H	-6.01786800	-4.51198700	1.69635700
H	-7.58332100	-2.67267000	1.10616100
H	-6.70232600	-0.55922400	0.12480400
H	-4.26005900	-0.28967500	-0.25976800
H	0.09859300	0.04804100	1.27426700
H	0.11576900	-3.14493400	-0.09021200
H	1.33361200	-2.98156400	-2.31013100

H	-0.05407600	-4.26777500	-3.94905300
H	-2.49238100	-4.52220700	-3.54160200
H	-3.60619600	-3.54923600	-1.60899900
S	-2.73666800	2.38192200	-1.41567800
O	-2.52981600	0.86061800	-1.24800800
O	-2.81347600	3.07769100	-0.12957200
C	-4.47370700	2.37102400	-2.07991700
F	-5.30258900	1.76759700	-1.20528400
F	-4.89362500	3.62194300	-2.27024900
F	-4.52912200	1.70860900	-3.23990600
O	-1.89962700	2.92991200	-2.48720100
H	-1.37137700	0.36332000	-1.50002500

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

Thermal correction to Gibbs Free Energy = 0.359756

Sum of electronic and thermal Free Energies = -4135.567467

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

Energy = -4135.8905221

Number of Imaginary Frequencies = 1

Lowest Frequency = 308.88i

### in8-HOTf

C	-4.05068000	-0.51868600	-2.31075800
C	-4.68382700	-1.03267500	-3.43944300
C	-4.55552100	-2.38573400	-3.76475800
C	-3.77732400	-3.22518700	-2.96515900
C	-3.12528300	-2.71426100	-1.84434100
C	-3.26652800	-1.35865800	-1.50097900
C	-2.49807500	-0.82734900	-0.35167600
C	-1.14652200	-1.03251000	-0.28338800
C	-0.32037800	-0.47137800	0.74465400
O	0.89459600	-0.63659100	0.85290600
H	-4.14129700	0.53699300	-2.07870800
H	-5.27297500	-0.37375900	-4.06987700
H	-5.05643600	-2.78247100	-4.64264700
H	-3.67373000	-4.27673700	-3.21434300
H	-2.52085400	-3.36889200	-1.22296700
S	4.62148000	-1.55929800	-0.08873200
O	3.55826100	-1.30632800	-1.16136100
C	2.09905100	3.89075300	-1.41636700
S	1.33519000	2.41647600	-0.55510000
O	2.23968500	2.08711100	0.61872000
O	1.51226300	1.23658600	-1.49084500
F	3.36118200	3.59781800	-1.70377600
F	1.41490600	4.13069800	-2.52704700
F	2.04047400	4.93430500	-0.59989300

Cu	2.76846300	0.25051800	-0.17723100
O	5.99461500	-1.73122500	-0.50924300
C	4.08207400	-3.13311600	0.76500500
F	4.17084500	-4.13892900	-0.09643700
F	4.87564100	-3.34489200	1.80667600
F	2.82016500	-2.99762600	1.17492200
O	4.29921300	-0.44354500	0.90938800
O	-0.04715000	2.78269300	-0.21871100
C	-5.32917900	1.05829200	0.44927300
C	-6.72398400	1.06141300	0.50084900
C	-7.41691100	-0.11305200	0.80518500
C	-6.71748700	-1.29448900	1.06374500
C	-5.32265500	-1.30965900	1.01806200
C	-4.64504200	-0.13167600	0.70328300
N	-3.18401700	-0.12957000	0.67491200
C	-2.51493600	0.39980700	1.73581500
C	-1.03911400	0.53690000	1.65427700
C	-0.32510000	0.91179700	2.89290800
C	-1.00605300	1.30585600	3.99983800
C	-2.43192300	1.27898200	3.98545400
C	-3.17217100	0.84894600	2.89976700
H	-4.78043400	1.96470900	0.20966700
H	-7.26578200	1.98046100	0.30040700
H	-8.50186200	-0.10722800	0.84209600
H	-7.25487400	-2.20641200	1.30429400
H	-4.77131600	-2.22288400	1.21878200
H	-0.66146900	-1.61527800	-1.05714700
H	-0.89392600	1.45521600	1.00529100
H	0.75833200	0.91008100	2.84090500
H	-0.48348300	1.62142500	4.89640600
H	-2.96769700	1.58827300	4.87897100
H	-4.25158100	0.81574400	2.96118200

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

Thermal correction to Gibbs Free Energy = 0.292617

Sum of electronic and thermal Free Energies = -3058.296180

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

Energy = -3058.5510466

No imaginary frequency

#### ts6-HOTf

C	4.15949000	1.06757000	-1.98906500
C	4.75457000	1.98223100	-2.85509200
C	4.64141700	3.35418300	-2.61763700
C	3.91305400	3.81163000	-1.51858400
C	3.30407800	2.90219400	-0.65489100

C	3.43608800	1.52130900	-0.87431700
C	2.71225700	0.58940700	0.02982800
C	1.36074800	0.76494400	0.21733300
C	0.58613800	-0.11452700	1.01919500
O	-0.64853600	-0.01316800	1.24143900
H	4.23267000	0.00577800	-2.19664500
H	5.29817000	1.62138300	-3.72328800
H	5.10779500	4.06360200	-3.29522900
H	3.80674800	4.87686000	-1.33637200
H	2.71563900	3.26068900	0.18333900
S	-2.01293400	3.30104600	-0.03737600
O	-1.31616100	2.11608600	-0.73899200
C	-5.71982400	-0.12124500	0.50134500
S	-4.31608600	-0.84189500	-0.49310200
O	-3.23257000	-1.12737600	0.53990300
O	-3.73816200	0.32563200	-1.27050900
F	-5.27590700	0.88300900	1.25005500
F	-6.66436700	0.31660100	-0.32961200
F	-6.22444400	-1.07608700	1.28678900
Cu	-2.06058400	0.43413400	-0.07348700
O	-2.42685800	4.35651300	-0.95243900
C	-0.59325000	4.02813700	0.92668100
F	0.39818000	4.39382300	0.09436100
F	-1.00252300	5.09860800	1.60678700
F	-0.09403100	3.12981100	1.79320300
O	-2.94602100	2.78358600	0.97920600
O	-4.86401200	-1.96473100	-1.23329400
C	5.36466400	-1.60077200	-0.21737800
C	6.74819100	-1.73778600	-0.33417400
C	7.59919900	-0.83394400	0.30737400
C	7.06777300	0.20650800	1.07243700
C	5.68501700	0.34894600	1.20042600
C	4.84580900	-0.55246200	0.54591900
N	3.40430700	-0.42737800	0.68086800
C	2.74297300	-1.30258300	1.52728200
C	1.30213200	-1.30018100	1.54871600
C	0.62373100	-2.14553000	2.49014200
C	1.32029500	-3.05968300	3.24115700
C	2.72839900	-3.09988800	3.14579700
C	3.43327600	-2.24633500	2.31440400
H	4.68836500	-2.29244700	-0.71200800
H	7.15843000	-2.54761800	-0.92997900
H	8.67563000	-0.94117700	0.21146100
H	7.72732800	0.90848600	1.57367500
H	5.26112200	1.15391500	1.79251800

H	0.85618400	1.57238300	-0.29577100
H	1.13819100	-2.01440400	0.48610200
H	-0.45566500	-2.05595400	2.54091700
H	0.80139700	-3.72687200	3.92140200
H	3.28341100	-3.81248100	3.74946600
H	4.51358300	-2.29320800	2.28325600
S	0.05778000	-2.51374800	-1.57717200
O	0.55075300	-2.94308300	-2.87528600
O	1.18263800	-2.68292600	-0.49598700
C	-1.17059600	-3.78603900	-0.98953100
F	-0.67318100	-5.01059100	-1.16905900
F	-1.40598500	-3.59749100	0.31564500
F	-2.30110800	-3.65525900	-1.67235600
O	-0.61430200	-1.21328100	-1.44053200

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

Thermal correction to Gibbs Free Energy = 0.309158

Sum of electronic and thermal Free Energies = -4019.929279

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

Energy = -4020.2022307

Number of Imaginary Frequencies = 1

Lowest Frequency = 41.34i

HOTs-assisted reaction

**ts2-HOTs**

C	0.23050200	2.19868400	2.46227400
C	0.22638500	2.15824600	3.85675400
C	1.09311900	1.30599600	4.54285000
C	1.96147700	0.47531200	3.83214000
C	1.97774000	0.50555600	2.43846800
C	1.12023000	1.37924700	1.74713400
C	1.11278000	1.38614800	0.26330800
C	0.33956600	0.58378900	-0.50605700
C	0.33545200	0.67252000	-2.00029300
O	-0.55900500	-0.13976600	-2.52851900
O	1.06607500	1.40757700	-2.67112200
C	-0.67528300	-0.13233900	-3.96543200
H	-0.48580200	2.82341000	1.94029900
H	-0.47373400	2.78377600	4.40266600
H	1.07840200	1.27486200	5.62888900
H	2.62035800	-0.20915900	4.35855600
H	2.63990600	-0.15450300	1.88656000
H	-1.44030200	-0.87335600	-4.19131700
H	-0.98242100	0.86023400	-4.30115700
H	0.28063200	-0.40689400	-4.41628600



S	2.90676100	-2.18648600	-1.19743400
O	1.42661300	-1.95173500	-1.55829300
C	-2.70838100	-3.02778400	1.40464200
S	-0.88403200	-3.00230900	1.80326500
O	-0.52209600	-1.51943400	1.82102800
O	-0.21079300	-3.49724800	0.54048900
F	-2.91157100	-2.51292800	0.19373600
F	-3.13856200	-4.28953800	1.42994800
F	-3.37201400	-2.31323100	2.31469400
Cu	0.38738300	-1.53869400	0.03701400
O	3.81962600	-1.58996200	-2.17222300
C	3.08193500	-4.03028000	-1.40612700
F	2.75309400	-4.37329800	-2.65357600
F	4.35355600	-4.37022800	-1.17590900
F	2.29222600	-4.67059600	-0.54681100
O	3.10233600	-1.91139600	0.24166000
O	-0.70742600	-3.74785200	3.03605000
C	4.06313200	2.43319400	1.04955700
C	5.40384800	2.10584900	1.24761300
C	6.12477300	1.44086600	0.25187900
C	5.50541200	1.10038000	-0.94989700
C	4.16777000	1.43335200	-1.16936600
C	3.46449500	2.10025200	-0.16824000
N	2.03325000	2.40109900	-0.43255500
C	1.58765900	3.83223800	-0.27693900
C	0.23502900	4.10140400	-0.48382600
C	-0.20896900	5.42214300	-0.41085900
C	0.68946600	6.45949400	-0.15921400
C	2.04449200	6.17343200	0.00712600
C	2.50653000	4.85641800	-0.05437100
H	3.50053000	2.93851800	1.82470400
H	5.88012700	2.36414600	2.18857400
H	7.16541900	1.17964200	0.41978100
H	6.04584200	0.55796900	-1.71809300
H	3.68224000	1.14584000	-2.09566900
H	1.86121800	2.17608800	-1.45249300
H	-0.48393200	3.32243900	-0.71827600
H	-1.26584800	5.62162700	-0.55569400
H	0.33836800	7.48569900	-0.10272400
H	2.75682700	6.97384800	0.18426900
H	3.56269400	4.65260300	0.05971500
S	-2.83256200	1.71543000	-0.18062900
O	-2.14549600	0.39308800	0.24735900
O	-2.87375900	2.68293900	0.93191900
O	-2.23494200	2.22635200	-1.44225000

H	-0.85114000	0.36826900	-0.04168300
C	-4.50215600	1.18152700	-0.54930500
C	-5.14521000	0.25897200	0.28134800
C	-5.16250700	1.73700200	-1.64355700
C	-6.46120200	-0.10029100	0.00464100
H	-4.61389500	-0.18609400	1.11540100
C	-6.48331800	1.36789200	-1.90351100
H	-4.64006400	2.43744300	-2.28634400
C	-7.15357800	0.45018400	-1.08591800
H	-6.96117500	-0.82436100	0.64411600
H	-6.99880600	1.79763100	-2.75919100
C	-8.58792500	0.06193300	-1.35912300
H	-8.92357600	0.42794000	-2.33446400
H	-8.71806600	-1.02657500	-1.34352800
H	-9.26254700	0.47712000	-0.59910200

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

Thermal correction to Gibbs Free Energy = 0.457536

Sum of electronic and thermal Free Energies = -4068.813208

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

Energy = -4069.1660838

Number of Imaginary Frequencies = 1

Lowest Frequency = 956.26i

### in3-HOTs

C	1.00909700	-2.39000700	-0.87277300
C	1.25607100	-3.68386400	-1.33443900
C	2.35305900	-3.94882100	-2.15472600
C	3.20318300	-2.90893300	-2.53689300
C	2.96669800	-1.61285800	-2.08109000
C	1.88305500	-1.34768800	-1.22643400
C	1.58399600	0.03983200	-0.78353200
C	0.67087000	0.82226800	-1.37293400
C	0.26803800	2.16644200	-0.89119700
O	-0.60160300	2.74345500	-1.69661300
O	0.74288600	2.71120700	0.11354100
C	-1.26994700	3.91294000	-1.18297800
H	0.12063600	-2.18522900	-0.28018100
H	0.57136000	-4.48155600	-1.06140800
H	2.53440300	-4.95839100	-2.51402200
H	4.04048800	-3.10153500	-3.20223600
H	3.61050200	-0.80080100	-2.40479000
H	-1.89658900	4.26576500	-2.00113000
H	-1.87787400	3.60774800	-0.32885600
H	-0.54480400	4.67470800	-0.88790700
C	4.68421700	0.00264700	0.04855100

C	5.99233100	0.41439200	-0.20955600
C	6.30019400	1.77212900	-0.31523700
C	5.29452200	2.72657500	-0.16129900
C	3.98174200	2.33003600	0.09746900
C	3.68881300	0.96964500	0.20032200
N	2.27687800	0.59393100	0.45719900
C	1.99109300	-0.19738200	1.70800900
C	0.64981700	-0.47161400	1.96348500
C	0.31710900	-1.17706100	3.11952200
C	1.30867100	-1.57070200	4.01838200
C	2.64233800	-1.25162300	3.76175500
C	2.99724100	-0.55927100	2.60134200
H	4.44725100	-1.05067100	0.13154600
H	6.77101100	-0.33352400	-0.32606500
H	7.32113300	2.08390100	-0.51518500
H	5.52551700	3.78454900	-0.24084400
H	3.19433900	3.06810500	0.21102000
H	1.75644200	1.51006500	0.58839900
H	-0.14242600	-0.15227200	1.29244600
H	-0.72777200	-1.41467800	3.29027800
H	1.04515900	-2.11965900	4.91802400
H	3.42054600	-1.53974700	4.46266500
H	4.03457900	-0.30771900	2.42411800
S	-2.36364800	-0.31362800	-0.31698000
O	-2.13530700	-0.43958900	-1.78039500
O	-1.97092500	-1.52250900	0.46739500
O	-1.77710100	0.94092700	0.27580200
H	0.10266500	0.42522600	-2.20611300
C	-4.14656500	-0.13170600	-0.10958100
C	-4.65871200	0.55046200	0.99487000
C	-5.01369400	-0.71899300	-1.03155600
C	-6.03855100	0.63873400	1.17424900
H	-3.97453700	1.01498400	1.69764400
C	-6.39171100	-0.62542800	-0.84089700
H	-4.60179900	-1.23311300	-1.89384900
C	-6.92722200	0.05380200	0.26180000
H	-6.43332100	1.17192700	2.03706400
H	-7.06387700	-1.08584100	-1.56245400
C	-8.42231200	0.17937100	0.44456900
H	-8.95061300	-0.69009200	0.03817300
H	-8.69093300	0.27385700	1.50241700
H	-8.81551800	1.06665000	-0.07050200

B3LYP/6-31G\*

Thermal correction to Gibbs Free Energy = 0.432802

Sum of electronic and thermal Free Energies = -1949.872638

M06-2X/6-311++G\*\*

Energy = -1950.1186779

No imaginary frequency

**in4-HOTs**

C	-3.64233900	1.85042000	0.62967000
C	-4.30965100	3.01216100	1.01249000
C	-3.94061100	3.68811800	2.17666700
C	-2.89417300	3.19473100	2.95651100
C	-2.22477000	2.03301200	2.57602200
C	-2.59344100	1.33709100	1.41154700
C	-1.89971300	0.06150000	1.09426200
C	-1.66823300	-0.86011100	2.04211300
C	-0.98207600	-2.17770400	1.89139200
O	-0.30839700	-2.46929200	3.01104900
O	-1.07732000	-2.90344300	0.92467400
C	0.48726900	-3.67744700	2.94549100
H	-3.95046300	1.34006500	-0.27553500
H	-5.12316800	3.38770100	0.39817300
H	-4.46090500	4.59562200	2.46974700
H	-2.58892300	3.71847000	3.85798700
H	-1.39334300	1.66748100	3.17106900
H	0.97015100	-3.74981400	3.92034700
H	-0.15862600	-4.54179200	2.77015200
H	1.22255100	-3.58618400	2.14221900
C	-1.78955700	1.50057300	-2.14157800
C	-1.46931200	2.69659300	-2.78673800
C	-0.42526200	3.49392000	-2.31882000
C	0.30763800	3.08974900	-1.20189400
C	-0.00011900	1.89766900	-0.54677500
C	-1.05375200	1.11774100	-1.02346900
N	-1.35262900	-0.15968600	-0.29362900
C	-2.10394900	-1.14858400	-1.12542900
C	-3.46257900	-1.36944400	-0.92653500
C	-4.12786400	-2.27567100	-1.75561800
C	-3.43403800	-2.94627100	-2.76225300
C	-2.06711900	-2.71734100	-2.93475200
C	-1.38785800	-1.81401300	-2.11828000
H	-2.59242800	0.87823300	-2.51776900
H	-2.03939300	2.99734900	-3.66093700
H	-0.17809100	4.42139800	-2.82743200
H	1.13319200	3.69482100	-0.83916200
H	0.58746900	1.55608400	0.29704400
H	-0.37063300	-0.56195600	-0.09297600
H	-3.99769700	-0.87575400	-0.12322300

H	-5.18748700	-2.45896900	-1.60261200
H	-3.95352900	-3.65429300	-3.40172200
H	-1.51485300	-3.25310700	-3.70105000
H	-0.31553100	-1.66079000	-2.22339200
S	2.13260200	-1.45807400	-0.26226500
O	2.54225600	-2.70266400	0.41706500
O	1.76894400	-1.55609500	-1.69689300
O	1.04609700	-0.71621600	0.52296100
H	-2.03284600	-0.64016600	3.04058500
C	3.54611100	-0.34305100	-0.17574900
C	3.73567900	0.61875100	-1.16772600
C	4.43443900	-0.43137700	0.89730500
C	4.81172700	1.50192000	-1.07382900
H	3.05608900	0.65276300	-2.01288000
C	5.50469500	0.45698800	0.97935400
H	4.29201600	-1.20511400	1.64454800
C	5.70851200	1.44075600	0.00070100
H	4.96443700	2.24349400	-1.85533500
H	6.20009800	0.38002800	1.81272900
C	6.85987500	2.41328800	0.11158500
H	7.76634300	1.92151500	0.48206100
H	7.09456300	2.86899800	-0.85595300
H	6.62796400	3.22877700	0.81011300

B3LYP/6-31G\*

Thermal correction to Gibbs Free Energy = 0.431297

Sum of electronic and thermal Free Energies = -1949.883733

M06-2X/6-311++G\*\*

Energy = -1950.1284761

No imaginary frequency

### ts3-HOTs

C	-3.54183200	1.92495300	0.60871100
C	-4.19517700	3.09473500	0.99092400
C	-3.84064400	3.74861800	2.17223200
C	-2.82324900	3.22407100	2.97002300
C	-2.16918200	2.05315000	2.59073400
C	-2.52333900	1.37957300	1.40911200
C	-1.85341800	0.09174300	1.08215800
C	-1.66133300	-0.83718900	2.03496200
C	-1.01621500	-2.17417000	1.89808900
O	-0.37155200	-2.48487100	3.03455600
O	-1.10255600	-2.90253400	0.93280300
C	0.37947400	-3.71953700	2.98607900
H	-3.83513300	1.43246700	-0.31133100
H	-4.98563900	3.49481800	0.36207300

H	-4.34908800	4.66313900	2.46447300
H	-2.52896800	3.73048100	3.88504700
H	-1.36034500	1.66330300	3.20144000
H	0.85167600	-3.80290300	3.96540200
H	-0.29337800	-4.56304300	2.81012500
H	1.12477900	-3.66452500	2.18912300
C	-1.67342200	1.47659800	-2.20463600
C	-1.32630800	2.65971300	-2.86011200
C	-0.32590100	3.48487400	-2.34825200
C	0.33525500	3.11951200	-1.17448300
C	0.00082000	1.93918000	-0.51245500
C	-1.00976700	1.12580300	-1.03054600
N	-1.32536500	-0.13493500	-0.29789800
C	-2.09525500	-1.11471100	-1.10948700
C	-3.45357700	-1.32679800	-0.88743900
C	-4.14442500	-2.23216500	-1.69585400
C	-3.47982000	-2.91355200	-2.71462700
C	-2.11598200	-2.69327500	-2.91830800
C	-1.41309300	-1.79267200	-2.11926200
H	-2.44564800	0.83710500	-2.61419700
H	-1.84384300	2.92976400	-3.77619200
H	-0.05826300	4.40300100	-2.86345700
H	1.12455700	3.74740700	-0.77160000
H	0.53263500	1.63919200	0.38235100
H	-0.22926400	-0.56933800	-0.07461100
H	-3.97060400	-0.82134900	-0.07943800
H	-5.20235800	-2.40438200	-1.51905000
H	-4.01865000	-3.62028500	-3.33944100
H	-1.58453600	-3.23404500	-3.69595200
H	-0.34503400	-1.64631700	-2.25691900
S	2.09619000	-1.50199200	-0.32476300
O	2.46484400	-2.73715000	0.38538100
O	1.76169200	-1.59779500	-1.76120000
O	0.98249700	-0.73892900	0.43910800
H	-2.02807500	-0.60522300	3.02969400
C	3.49793200	-0.38303200	-0.18845000
C	3.69236800	0.60375500	-1.15488100
C	4.37502200	-0.49954200	0.89062500
C	4.76606800	1.48478500	-1.02813500
H	3.01970200	0.66148400	-2.00414900
C	5.44307100	0.38814000	1.00428600
H	4.22581300	-1.29154200	1.61690000
C	5.65351600	1.39655000	0.05274000
H	4.92385500	2.24698200	-1.78820000
H	6.13081400	0.29097900	1.84163800

C	6.80117900	2.36842800	0.19891400
H	7.69787000	1.87455900	0.58926200
H	7.05970000	2.83088700	-0.75919100
H	6.54994100	3.17882100	0.89654300

B3LYP/6-31G\*

Thermal correction to Gibbs Free Energy = 0.427864

Sum of electronic and thermal Free Energies = -1949.887997

M06-2X/6-311++G\*\*

Energy = -1950.1287673

Number of Imaginary Frequencies = 1

Lowest Frequency = 559.22i

**in5-HOTs**

C	-1.60875800	-3.71680500	2.30706800
C	-1.75485400	-4.15460100	3.62071200
C	-1.97054400	-3.23194900	4.64844100
C	-2.03068200	-1.86753900	4.35870700
C	-1.86806600	-1.42203600	3.04726200
C	-1.66099700	-2.34494900	2.00935800
C	-1.41886900	-1.85054100	0.62433900
C	-0.46250900	-0.85016700	0.49923300
C	-0.16978700	0.04200000	-0.56699800
O	-1.11873100	0.21564000	-1.51388400
O	0.86996600	0.74098700	-0.66462000
C	-0.76063200	1.01066000	-2.67206800
H	-1.43469100	-4.43493800	1.51217800
H	-1.69656600	-5.21615300	3.84395500
H	-2.09074600	-3.57726400	5.67165100
H	-2.20561500	-1.14731200	5.15277300
H	-1.92786600	-0.36275700	2.81416900
H	-1.64188200	0.98260100	-3.31145300
H	-0.52218000	2.03204100	-2.37116700
H	0.09526800	0.55845700	-3.17499700
S	4.01025000	2.68746600	1.13821600
O	2.77036600	2.69856000	0.25341700
C	5.16763200	-2.30356900	0.08301300
S	3.58696000	-1.78339400	-0.75374700
O	3.92974800	-0.62709700	-1.60981500
O	2.74213400	-1.27504500	0.43057300
F	5.73748000	-1.25583300	0.67905700
F	4.90882400	-3.24401800	0.99408300
F	6.00352300	-2.79664800	-0.83512000
Cu	2.60419400	0.66365200	0.24084000
O	4.07410600	3.63285400	2.23774700
C	5.41157800	3.09583900	-0.02250100

F	5.26575100	4.34758100	-0.45728400
F	6.56668400	2.97971000	0.62933700
F	5.39126100	2.25725600	-1.05621000
O	4.18283800	1.20855500	1.44459000
O	3.04929200	-2.99934100	-1.36409700
C	-3.57407200	-4.41835400	-0.60756000
C	-4.81417700	-5.02247600	-0.41213700
C	-5.85167900	-4.31874000	0.20630700
C	-5.64303200	-3.00241500	0.61932300
C	-4.40763700	-2.38419800	0.41939600
C	-3.36790900	-3.09958400	-0.18265600
N	-2.08496100	-2.47399100	-0.40504900
C	-1.54993300	-2.56921000	-1.73988500
C	-0.21844100	-2.95006200	-1.93971100
C	0.28201400	-3.05839500	-3.23729200
C	-0.54492600	-2.81374600	-4.33705600
C	-1.87910600	-2.45283500	-4.13213400
C	-2.38348000	-2.32379900	-2.83803300
H	-2.76519900	-4.96230800	-1.08544100
H	-4.96700500	-6.04742900	-0.73844800
H	-6.81702200	-4.79302300	0.35875400
H	-6.44445600	-2.43934800	1.08858600
H	-4.26666200	-1.35288900	0.72221600
H	0.17422200	-0.70710700	1.36194000
H	0.43680500	-3.14602700	-1.09818400
H	1.32172900	-3.33927500	-3.37012800
H	-0.15354000	-2.90894400	-5.34598100
H	-2.53179300	-2.26457700	-4.98039100
H	-3.41551500	-2.03046300	-2.67425600
S	-3.84288900	1.75024100	0.61373100
O	-3.69176600	1.00521400	-0.83113000
O	-4.97764300	1.12461400	1.28576900
O	-2.51488600	1.76771400	1.23749200
H	-2.75587400	0.70408300	-0.94247700
C	-4.29265600	3.40768000	0.14115300
C	-3.30597000	4.39317100	0.08160500
C	-5.62590100	3.69680500	-0.15786600
C	-3.66722800	5.68562500	-0.29432600
H	-2.28152200	4.15448600	0.34708900
C	-5.96446000	4.99368300	-0.53539700
H	-6.38185600	2.92284200	-0.07885500
C	-4.99458300	6.00495900	-0.61465900
H	-2.90578500	6.46040300	-0.33161600
H	-7.00106000	5.22768400	-0.76426800
C	-5.37004300	7.40138800	-1.04959700



H	-6.39317100	7.65267200	-0.75172800
H	-4.69562800	8.14976900	-0.62143600
H	-5.31528400	7.49907800	-2.14203400

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

Thermal correction to Gibbs Free Energy = 0.455971

Sum of electronic and thermal Free Energies = -4068.892481

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

Energy = -4069.2315952

No imaginary frequency

#### ts4-HOTs

C	0.27137900	2.62560000	3.16821900
C	0.41723400	2.63129800	4.55359500
C	1.21811200	1.67149300	5.17804700
C	1.86885800	0.70580000	4.40949900
C	1.72383900	0.69147700	3.02129500
C	0.92155300	1.65326600	2.39057500
C	0.69220100	1.60061500	0.92159900
C	0.28600000	0.47171100	0.30965600
C	-0.12536900	0.34240300	-1.14504200
O	1.02476200	0.08149600	-1.92816600
O	-1.12243400	-0.46200600	-1.39955200
C	0.78976800	-0.51914700	-3.21638500
H	-0.36549400	3.36390400	2.68956300
H	-0.10064700	3.38052200	5.14595400
H	1.33190000	1.67753500	6.25862100
H	2.49757700	-0.04041300	4.88683500
H	2.25058700	-0.05029800	2.42884600
H	1.77997500	-0.67653500	-3.64646600
H	0.25434000	-1.46452900	-3.11335600
H	0.21106700	0.16490200	-3.84505700
S	-2.71167300	-2.71720900	1.72352800
O	-1.58923000	-2.50709600	0.71513000
C	-6.11884000	0.81088900	-0.73723900
S	-4.49132500	0.47778600	-1.57739800
O	-4.43996400	-0.97785100	-1.82439500
O	-3.49008900	0.82806000	-0.45909900
F	-6.23545700	0.04980900	0.35107400
F	-6.19254500	2.09806700	-0.38539100
F	-7.11501100	0.52896100	-1.58171600
Cu	-2.48192500	-0.83776900	-0.09599000
O	-2.34859600	-3.05102600	3.08929300
C	-3.67290400	-4.16051800	1.03906000
F	-2.92867600	-5.26348100	1.12372900
F	-4.78963000	-4.31962600	1.74746400

F	-3.97933300	-3.92504700	-0.23568400
O	-3.60809800	-1.51532400	1.48805600
O	-4.42819800	1.39840400	-2.71487500
C	1.51054900	5.04525400	0.99695300
C	2.46949300	5.95798700	1.43616900
C	3.80868900	5.57219100	1.53453400
C	4.18847300	4.27511800	1.18382100
C	3.23885700	3.35533300	0.73411200
C	1.90146500	3.74858700	0.65164500
N	0.89801500	2.81320400	0.18142900
C	0.40917200	2.93168900	-1.08966100
C	-0.65228200	2.02174500	-1.50415700
C	-1.17691900	2.17305500	-2.85117300
C	-0.64230100	3.07358200	-3.73098900
C	0.42280800	3.90599300	-3.29926500
C	0.93812600	3.85471900	-2.01696300
H	0.46465000	5.32922300	0.92471100
H	2.16799900	6.96538900	1.70841400
H	4.55360800	6.28202200	1.88297800
H	5.22902100	3.97172000	1.25210100
H	3.53919000	2.35342000	0.44159500
H	0.21637400	-0.44641100	0.88582800
H	-1.46838800	1.95567500	-0.77569000
H	-2.02844000	1.55706300	-3.12163300
H	-1.03177200	3.17079100	-4.73913000
H	0.85622800	4.61454900	-4.00094700
H	1.75008700	4.51068000	-1.73126000
S	4.25578500	-0.91582400	-0.16499300
O	3.17852300	-1.43507600	-1.25858500
O	4.58655900	0.48429600	-0.46097700
O	3.79000200	-1.26555000	1.17898700
H	2.40569700	-0.80391000	-1.30357300
C	5.62562100	-1.96402100	-0.59995200
C	5.75056700	-3.21196500	0.01312900
C	6.55815400	-1.51817800	-1.53690100
C	6.82617800	-4.02591700	-0.33346100
H	5.02465300	-3.52767500	0.75462200
C	7.62798100	-2.34723800	-1.86813000
H	6.45206100	-0.53513600	-1.98297700
C	7.77604200	-3.61163900	-1.27951500
H	6.93311900	-4.99729000	0.14268500
H	8.36306700	-2.00479100	-2.59202700
C	8.92147900	-4.51635300	-1.66627800
H	9.76741600	-3.94620900	-2.06291800
H	9.27502500	-5.10285500	-0.81175400

H 8.61228700 -5.22825800 -2.44302800  
 B3LYP/6-31G\* (Lan12DZ for Cu)  
 Thermal correction to Gibbs Free Energy = 0.456854  
 Sum of electronic and thermal Free Energies = -4068.835011  
 M06-2X/6-311++G\*\* (Lan12DZ for Cu)  
 Energy = -4069.1770854  
 Number of Imaginary Frequencies = 1  
 Lowest Frequency = 334.77i

**in6-HOTs**

C	0.52987800	3.41231000	2.44979700
C	0.73129800	3.88589600	3.74440700
C	1.63256500	3.23885500	4.59420200
C	2.32710700	2.11597600	4.14355500
C	2.12910700	1.63482400	2.84748200
C	1.22860000	2.28337000	1.99155700
C	0.94564900	1.74059200	0.63507900
C	0.43870400	0.51423600	0.42837100
C	0.00529300	0.00176900	-0.93643600
O	1.21836400	-0.53180600	-1.54647600
O	-0.95919900	-0.91922400	-0.92893400
C	1.02558600	-1.42843800	-2.65285000
H	-0.19114600	3.90206300	1.80104400
H	0.17659100	4.75258900	4.09305300
H	1.78857700	3.60843600	5.60408900
H	3.03128400	1.60974100	4.79781800
H	2.68747800	0.77198500	2.49743700
H	2.02344100	-1.77854500	-2.92423500
H	0.38646100	-2.26706800	-2.37083200
H	0.58183600	-0.89530700	-3.50148200
S	-3.65081000	-3.24953800	1.09054100
O	-2.44848600	-3.15873800	0.17006600
C	-5.43122500	1.68597800	0.45919800
S	-3.96479800	1.32330000	-0.62898000
O	-4.36449800	0.21931000	-1.52145100
O	-2.92029300	0.83439000	0.39024300
F	-5.83328900	0.57538700	1.07526300
F	-5.10072500	2.60372200	1.37223100
F	-6.42826900	2.15799400	-0.29591900
Cu	-2.50079800	-1.07472800	0.15368400
O	-3.60743000	-4.19130100	2.19577300
C	-5.04827000	-3.77919900	-0.02184300
F	-4.82351200	-5.02225300	-0.45098000
F	-6.19334900	-3.74377800	0.65866200
F	-5.12347600	-2.95459700	-1.06669200

O	-3.95449800	-1.79289200	1.40272600
O	-3.57533100	2.60686700	-1.22246600
C	1.87202500	4.97101400	-0.30803000
C	2.87451700	5.93532600	-0.20027800
C	4.21577400	5.54787700	-0.14893000
C	4.55582900	4.19501300	-0.21220200
C	3.56325500	3.21938800	-0.32670500
C	2.22764800	3.62208600	-0.36914500
N	1.19088100	2.61057000	-0.49203200
C	0.60538600	2.37845800	-1.68063500
C	-0.43471600	1.31765300	-1.73791300
C	-1.05021600	1.07446200	-3.06036200
C	-0.71979600	1.81117400	-4.15036700
C	0.28700200	2.82084400	-4.03180800
C	0.93643000	3.10418700	-2.85293600
H	0.82536200	5.25824800	-0.34119700
H	2.60509300	6.98625700	-0.15002000
H	4.99406100	6.30043800	-0.05978600
H	5.59733400	3.88966100	-0.17666800
H	3.82484700	2.16659800	-0.39095900
H	0.29676200	-0.15448100	1.27104800
H	-1.25851900	1.66302400	-1.08260400
H	-1.81358900	0.30378100	-3.09413400
H	-1.19932100	1.64437900	-5.10926200
H	0.55860700	3.39026300	-4.91733400
H	1.69786400	3.87226300	-2.81871800
S	4.37163400	-1.05396000	0.24321600
O	3.05886600	-1.89052400	-0.17913800
O	4.59770500	-0.00011600	-0.75695700
O	4.27406500	-0.68028700	1.65653600
H	2.37194500	-1.27978000	-0.59377200
C	5.61470300	-2.31771600	0.07463100
C	5.90691900	-3.13830500	1.16545000
C	6.28175200	-2.46481700	-1.14184600
C	6.87713000	-4.12734900	1.02294400
H	5.39079100	-2.99173100	2.10800200
C	7.25109200	-3.45852900	-1.26308800
H	6.05497500	-1.80054700	-1.96892200
C	7.55939300	-4.30688900	-0.18984300
H	7.11257000	-4.76753900	1.86941800
H	7.78064900	-3.57424100	-2.20533200
C	8.58980500	-5.40085900	-0.33870200
H	9.29582800	-5.18023300	-1.14547400
H	9.16015000	-5.54250400	0.58542100
H	8.11075300	-6.36031200	-0.57461800

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

Thermal correction to Gibbs Free Energy = 0.456803

Sum of electronic and thermal Free Energies = -4068.837437

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

Energy = -4069.1850527

No imaginary frequency

**in7-HOTs**

C	-2.91729900	-3.14043900	2.91419500
C	-3.67051600	-3.03749300	4.08180500
C	-3.97713800	-1.78036600	4.60897000
C	-3.52411500	-0.62887200	3.96355900
C	-2.77136400	-0.72504300	2.79225000
C	-2.46197000	-1.98547100	2.25774400
C	-1.58776900	-2.07974100	1.05979200
C	-0.41514400	-1.43046300	0.96886100
C	0.53252400	-1.57537100	-0.21156600
O	0.05037400	-0.60486300	-1.18348600
O	1.82904400	-1.50065200	0.05372100
C	0.91578700	-0.25596800	-2.27603900
H	-2.66291500	-4.12181600	2.52381100
H	-4.00888300	-3.93869400	4.58571000
H	-4.56282900	-1.70099700	5.52071200
H	-3.75627400	0.35204000	4.36842200
H	-2.43138000	0.17582100	2.28907800
H	0.59831100	0.73291300	-2.61184900
H	1.95614500	-0.22550000	-1.95463800
H	0.80823800	-0.98359200	-3.08977000
S	2.41881300	1.90092000	2.45341400
O	1.43156500	0.89388500	1.86567700
C	5.34175900	0.25942000	-1.56695900
S	5.13737500	-1.44058500	-0.83856200
O	4.16929500	-2.09361300	-1.73308200
O	4.57288000	-1.08387700	0.53970500
F	4.16135800	0.92670100	-1.47868200
F	6.26490100	0.96104700	-0.91259100
F	5.67802900	0.18367700	-2.85702300
Cu	2.88106300	-0.22708800	0.97032800
O	2.19968800	2.33296600	3.82242100
C	2.23073400	3.39734400	1.35718400
F	1.02446200	3.92715300	1.52610900
F	3.16357700	4.29360600	1.68403400
F	2.39467800	3.03066800	0.08490200
O	3.76145200	1.31492300	2.07628800
O	6.47940400	-2.00402500	-0.73067600

C	-4.05203100	-4.33141600	-0.09751800
C	-5.42512100	-4.47314900	-0.30162400
C	-6.20191000	-3.36107300	-0.63450300
C	-5.60417600	-2.10606000	-0.76874200
C	-4.23067500	-1.95254400	-0.57340900
C	-3.46668500	-3.07135500	-0.23647400
N	-2.03599900	-2.90895200	-0.04038100
C	-1.17154700	-3.33093700	-0.98336500
C	0.27673700	-3.06503000	-0.75733900
C	1.20845400	-3.47511500	-1.83491100
C	0.76404100	-4.12576100	-2.94066600
C	-0.63568300	-4.37422200	-3.09424100
C	-1.58095700	-3.99100700	-2.16841200
H	-3.43953700	-5.18731600	0.17044400
H	-5.88585400	-5.45056800	-0.19293700
H	-7.27128500	-3.47316200	-0.78802400
H	-6.20498400	-1.24014500	-1.03055600
H	-3.75546500	-0.98188200	-0.68283200
H	-0.10617800	-0.76151600	1.76331700
H	0.57203800	-3.62596800	0.14899400
H	2.25589100	-3.22001800	-1.68508700
H	1.45132600	-4.43399200	-3.72174600
H	-0.97862400	-4.87487800	-3.99664500
H	-2.63023800	-4.18201000	-2.35080900
S	-1.84958700	2.31993600	-0.39048600
O	-2.16126800	0.87377500	-1.07150900
O	-2.06426100	2.21901000	1.05440000
O	-0.56760500	2.79606100	-0.91408800
H	-1.31490800	0.32752800	-1.05168800
C	-3.17952000	3.27185700	-1.10039900
C	-3.01478500	3.84019600	-2.36556800
C	-4.35468200	3.45708300	-0.37301400
C	-4.05311200	4.59248200	-2.90747300
H	-2.08131500	3.70895200	-2.90250500
C	-5.38329700	4.21425400	-0.93271200
H	-4.44832700	3.03015100	0.61960400
C	-5.25277500	4.78798300	-2.20475700
H	-3.92787500	5.04428200	-3.88840300
H	-6.29852200	4.36968700	-0.36707900
C	-6.37811900	5.58981600	-2.81427700
H	-7.07745100	5.94463100	-2.05089300
H	-5.99875300	6.46046500	-3.36006400
H	-6.95029100	4.98385300	-3.52929700

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

Thermal correction to Gibbs Free Energy = 0.459928

Sum of electronic and thermal Free Energies = -4068.826531

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

Energy = -4069.1861968

No imaginary frequency

**ts5-HOTs**

C	1.90146500	2.19423200	3.37969000
C	2.39790700	1.86924400	4.63989700
C	2.71148200	0.54231700	4.94750000
C	2.52235500	-0.45712100	3.99222700
C	2.02240900	-0.14200700	2.72748200
C	1.71177100	1.19105000	2.41551900
C	1.10354000	1.49783100	1.09651800
C	-0.02067200	0.88251400	0.67848100
C	-0.67441500	1.19377500	-0.61986100
O	0.29010300	0.29133000	-1.79839900
O	-1.90381800	0.91097400	-0.82932000
C	-0.41805000	-0.59864800	-2.68514500
H	1.63963300	3.22412200	3.15362100
H	2.53031300	2.64920600	5.38449300
H	3.09714200	0.29038800	5.93159400
H	2.76248900	-1.49056100	4.22446600
H	1.89204300	-0.92386700	1.98429300
H	0.15944100	-1.52227900	-2.76340900
H	-1.40912900	-0.80651700	-2.27724600
H	-0.51509500	-0.11339000	-3.66100500
S	-2.79072100	-2.30393200	1.25001900
O	-2.53372400	-0.81872700	1.60915900
C	-6.98991500	-0.26275400	-0.89039600
S	-5.89009200	1.03962000	-0.13470500
O	-4.70401500	1.13774000	-1.08788500
O	-5.28653300	0.38362900	1.09035300
F	-6.28069800	-1.35820600	-1.14302700
F	-7.97393300	-0.54663800	-0.03930600
F	-7.50459800	0.21114000	-2.02678300
Cu	-3.41417800	0.18642400	0.18054800
O	-3.28877100	-3.10816600	2.35623600
C	-1.05332800	-2.88940000	0.90977600
F	-0.29816900	-2.69329800	1.99149000
F	-1.05975500	-4.17733000	0.58806200
F	-0.55452500	-2.17464800	-0.11117300
O	-3.49147100	-2.31343100	-0.05749500
O	-6.70350200	2.23024300	0.04720300
C	3.50784000	4.03437200	0.97440900
C	4.85118800	4.33520800	1.20222300

C	5.83533300	3.37511000	0.95218700
C	5.47858400	2.11427300	0.46893200
C	4.13890200	1.79876900	0.23360600
C	3.17035400	2.76696100	0.49605600
N	1.76935300	2.44944900	0.23903000
C	1.17903400	2.91686800	-0.86949800
C	-0.27719000	2.62616200	-1.06631400
C	-0.86132100	3.03029500	-2.37271400
C	-0.15261100	3.74945700	-3.27034800
C	1.21783400	4.07606700	-2.98867400
C	1.86809600	3.68751500	-1.84389100
H	2.73269800	4.76976500	1.17049500
H	5.12536900	5.31643500	1.57827600
H	6.87971500	3.61224700	1.13373600
H	6.23895800	1.36532100	0.26805300
H	3.83585000	0.82934500	-0.15281200
H	-0.48511000	0.12938800	1.30247500
H	-0.79574900	3.23892400	-0.29734100
H	-1.89026800	2.72900800	-2.54090200
H	-0.59005000	4.06181700	-4.21289800
H	1.77850300	4.63848800	-3.73090900
H	2.91303700	3.92724800	-1.70010200
S	2.68977200	-2.11509200	-0.89289100
O	2.41870800	-0.59190200	-0.96381500
O	2.44989100	-2.62672500	0.47091000
O	2.02771600	-2.80860700	-2.01416200
H	1.19125100	-0.17752700	-1.39864000
C	4.46259900	-2.19850200	-1.17606500
C	4.95149600	-2.38705200	-2.46906600
C	5.34157200	-2.04838600	-0.10174600
C	6.32905800	-2.41334700	-2.68402000
H	4.25377700	-2.52401000	-3.28857900
C	6.71716000	-2.07330300	-0.33222300
H	4.94606000	-1.93326400	0.90236200
C	7.23288800	-2.25709200	-1.62359400
H	6.70949700	-2.56426300	-3.69187300
H	7.40217200	-1.96502800	0.50613300
C	8.72375000	-2.32595400	-1.86074300
H	9.27791000	-1.75698000	-1.10653700
H	9.08341100	-3.36256300	-1.81464700
H	8.99220700	-1.93422100	-2.84784200

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

Thermal correction to Gibbs Free Energy = 0.460772

Sum of electronic and thermal Free Energies = -4068.811804

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



Energy = -4069.1768727

Number of Imaginary Frequencies = 1

Lowest Frequency = 211.05i

No catalyst

**ts1'**

C	0.25769400	-0.97799700	2.10221400
C	0.69869700	-1.17375900	3.41107700
C	1.95097500	-0.70674400	3.81254700
C	2.75908300	-0.03601100	2.89188000
C	2.31992000	0.16899800	1.58621100
C	1.06233800	-0.30333500	1.16516500
C	0.67846700	-0.09727800	-0.24238600
C	1.32677100	-0.02328200	-1.41095700
C	2.72877000	-0.28273200	-1.69296200
O	3.48344700	0.85978300	-1.68887400
O	3.18818800	-1.37013700	-2.00017000
C	4.84291300	0.68397400	-2.10892300
H	-0.71039200	-1.36859400	1.80599700
H	0.06181400	-1.70187500	4.11609900
H	2.29298100	-0.86234900	4.83212400
H	3.73337000	0.33943200	3.19372700
H	2.94206900	0.70778300	0.87859800
H	5.29101900	1.67864700	-2.07616700
H	5.37704600	0.00359300	-1.43901600
H	4.88710900	0.27910500	-3.12415300
C	-1.56423900	1.79920000	1.00822200
C	-2.09078700	3.06245800	1.27990900
C	-2.42705800	3.92946700	0.23832700
C	-2.23423500	3.53066900	-1.08482800
C	-1.70578900	2.27041400	-1.36645900
C	-1.37102500	1.40919100	-0.31947300
N	-0.78777500	0.11371600	-0.66835600
C	-1.68299400	-1.05392200	-0.63301800
C	-3.05123800	-0.91413000	-0.39206100
C	-3.87736900	-2.03978000	-0.43972400
C	-3.34756600	-3.29542400	-0.73181800
C	-1.97881900	-3.42286800	-0.98032700
C	-1.14178300	-2.31000200	-0.93426400
H	-1.29991200	1.13029800	1.81855300
H	-2.23681100	3.36758500	2.31224600
H	-2.83615800	4.91161200	0.45761700
H	-2.49000500	4.19935100	-1.90168600
H	-1.54862500	1.95511500	-2.39375400

H	-0.19659200	0.18316400	-1.71618500
H	-3.47395900	0.05798000	-0.16790000
H	-4.94029100	-1.92561300	-0.24574100
H	-3.99380700	-4.16782700	-0.76625700
H	-1.55385900	-4.39510400	-1.21309600
H	-0.08000500	-2.40813300	-1.13027900

B3LYP/6-31G\*

Thermal correction to Gibbs Free Energy = 0.296291

Sum of electronic and thermal Free Energies = -1054.559147

M06-2X/6-311++G\*\*

Energy = -1054.7162404

Number of Imaginary Frequencies = 1

Lowest Frequency = 1413.21i

**in1'**

C	-0.51425800	-1.85780600	1.57084200
C	-0.89577700	-3.12412000	2.01010800
C	-1.76915900	-3.89624700	1.24258500
C	-2.26463100	-3.39123000	0.03827800
C	-1.89522300	-2.12005000	-0.39310400
C	-1.01579200	-1.33761300	0.36790000
C	-0.60061400	0.02157600	-0.07782100
C	-1.44542700	0.99699800	-0.51883900
C	-2.90917100	1.00680500	-0.43755900
O	-3.37604300	2.15630700	-1.01485200
O	-3.65878300	0.18211400	0.05408000
C	-4.79860000	2.30590600	-0.99668800
H	0.17242200	-1.26155700	2.16443100
H	-0.50747400	-3.50883300	2.94932200
H	-2.06113300	-4.88735500	1.57970900
H	-2.94356200	-3.98771800	-0.56494600
H	-2.28777100	-1.72704100	-1.32467800
H	-5.00087000	3.25708100	-1.49175300
H	-5.28468000	1.48532500	-1.53300900
H	-5.17648300	2.32194900	0.02994500
C	2.93177400	-0.82050800	0.36858800
C	3.88574400	-1.76068100	-0.01250500
C	3.66752500	-2.58177100	-1.12212900
C	2.48856500	-2.44409700	-1.85522600
C	1.53604100	-1.49235400	-1.49079200
C	1.74613000	-0.68173400	-0.36789300
N	0.77790800	0.29544600	0.02312400
C	1.23894900	1.63337700	0.25257700
C	2.14435600	2.23869400	-0.62764000
C	2.61295800	3.52802500	-0.37169900

C	2.17509800	4.22857500	0.75249400
C	1.26573000	3.62696800	1.62722500
C	0.80396100	2.33559100	1.38577800
H	3.09674400	-0.18953900	1.23653900
H	4.79924600	-1.85963400	0.56781200
H	4.41067700	-3.31896400	-1.41247000
H	2.31057100	-3.06993000	-2.72561000
H	0.63039800	-1.37207200	-2.07616300
H	-1.01342300	1.91567100	-0.89821100
H	2.48120600	1.69552200	-1.50492100
H	3.31612400	3.98699700	-1.06150400
H	2.53851400	5.23351600	0.94764900
H	0.92256700	4.16089100	2.50927900
H	0.10110400	1.86436600	2.06600400

B3LYP/6-31G\*

Thermal correction to Gibbs Free Energy = 0.302469

Sum of electronic and thermal Free Energies = -1054.669625

M06-2X/6-311++G\*\*

Energy = -1054.82512870

No imaginary frequency