

## Electronic Supplementary Information

### DFT study on *E*-stereoselective reductive A<sup>3</sup>-coupling reaction of terminal alkynes with aldehydes and 3-pyrroline

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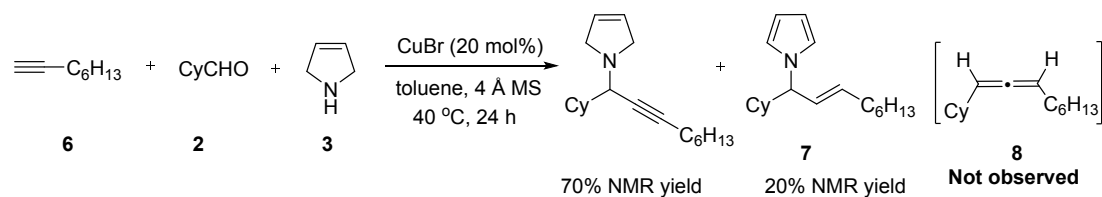
E-mail: [masm@sioc.ac.cn](mailto:masm@sioc.ac.cn)

[xzhang@sioc.ac.cn](mailto:xzhang@sioc.ac.cn)

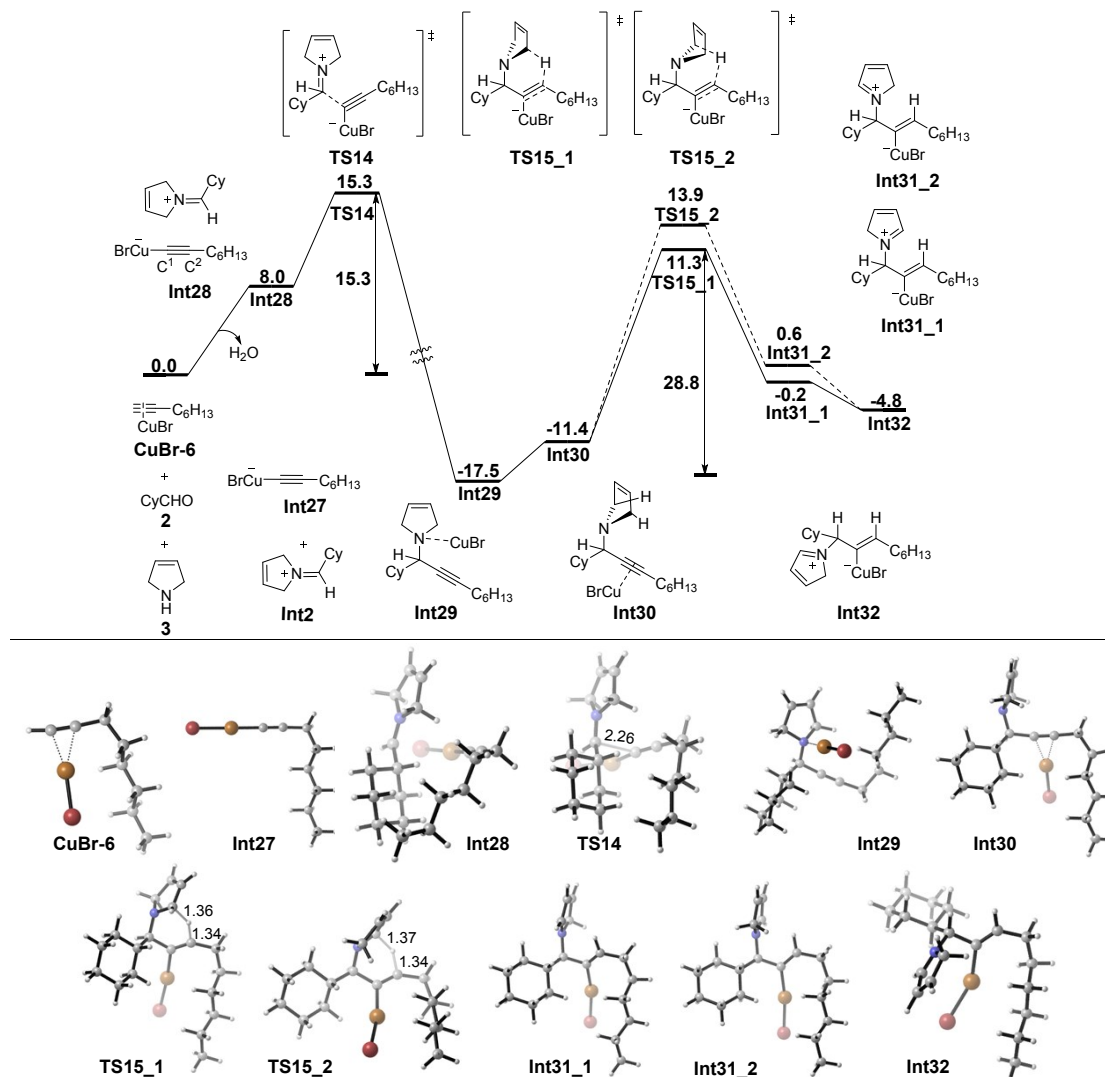
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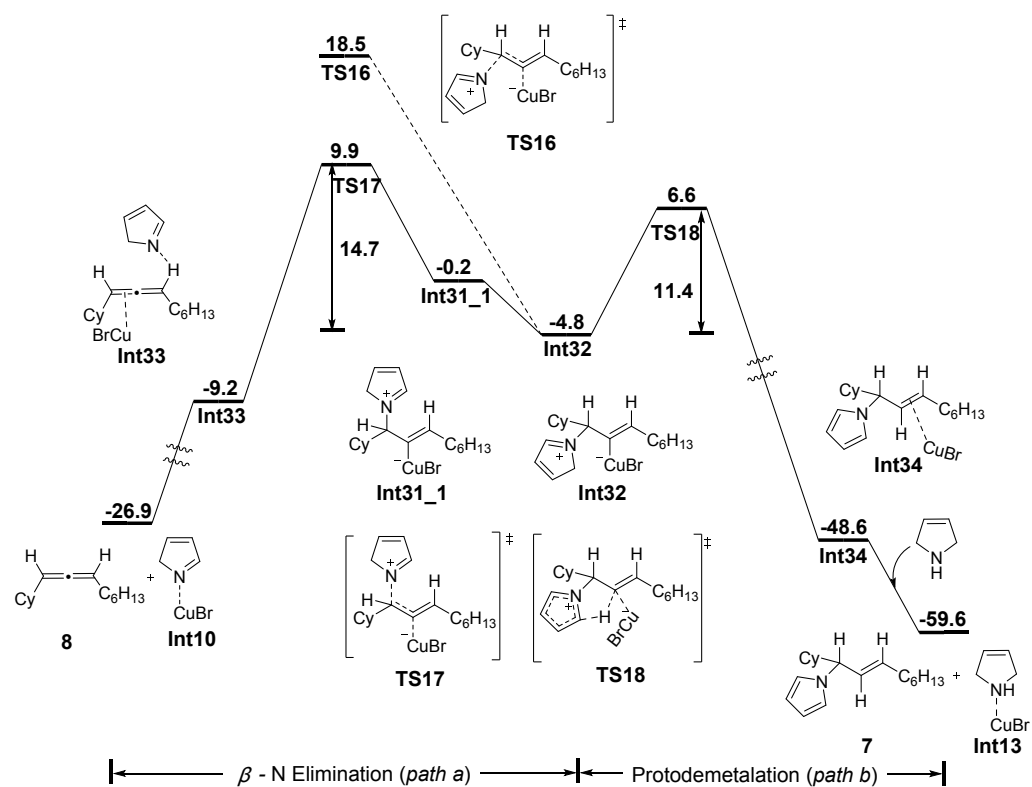
## 1. Energy profiles for the 1-octyne participated system



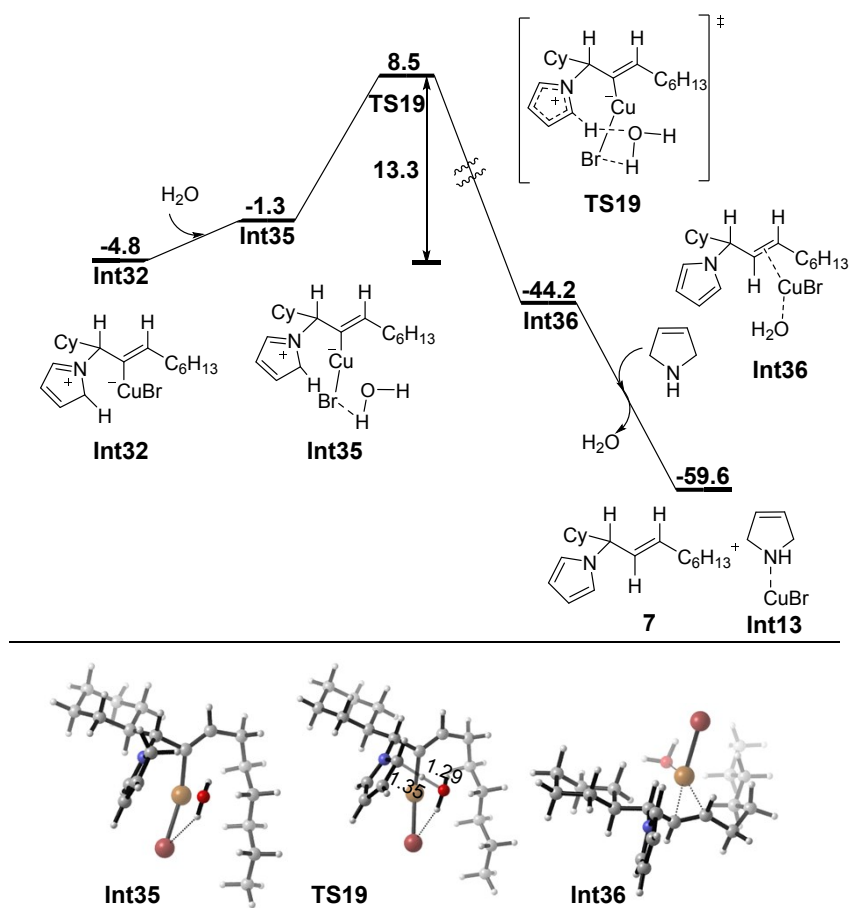
**Scheme S1** Reductive  $\text{A}^3$ -coupling reaction of 1-octyne with cyclohexanal and 3-pyrroline



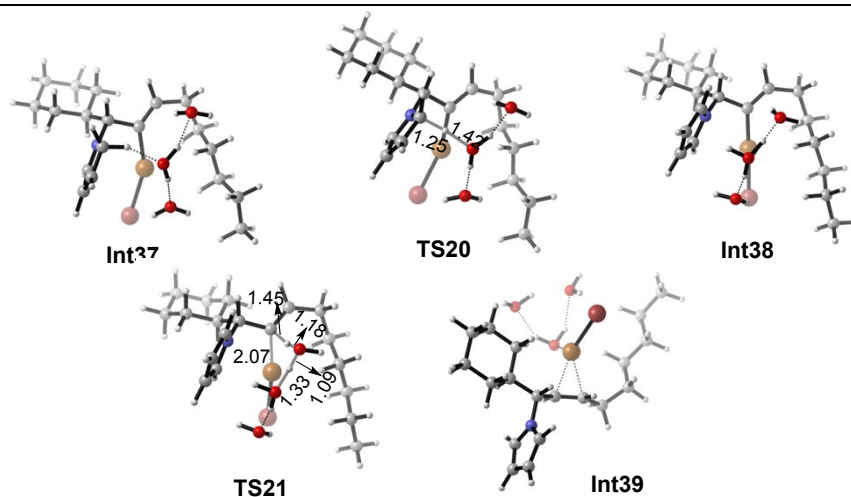
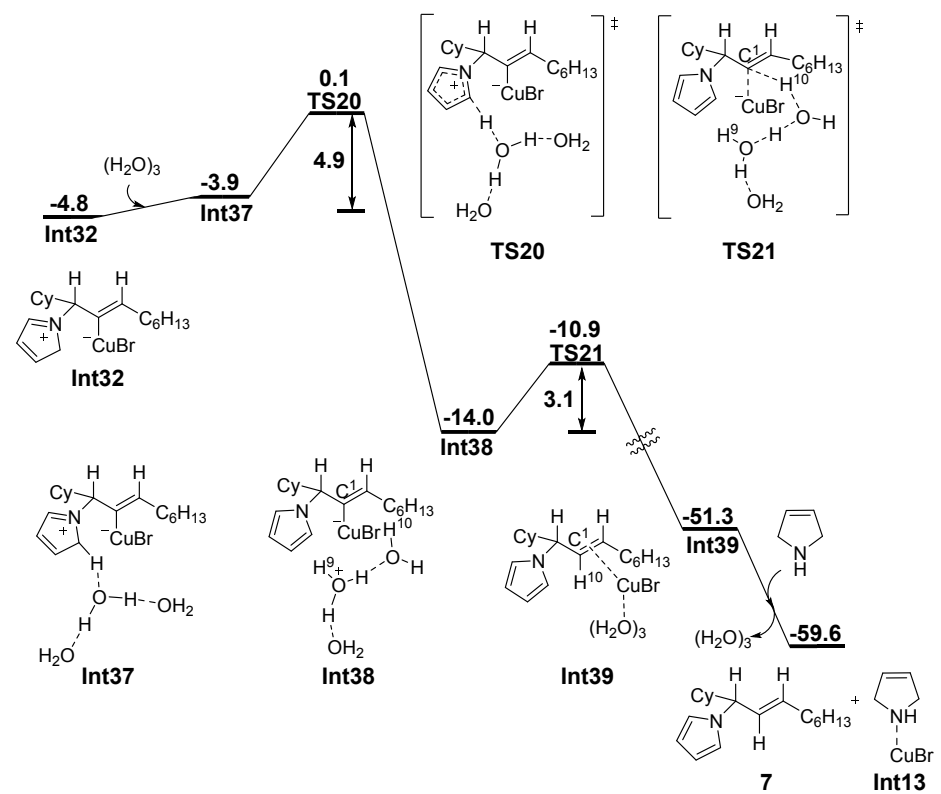
**Figure S1.** Free energy profile ( $\Delta G$  in  $\text{kcal mol}^{-1}$ ) for the formation of propargylic amine and the subsequent 1,5-H transfer for 1-octyne participated system. Bond lengths are given in angstroms.



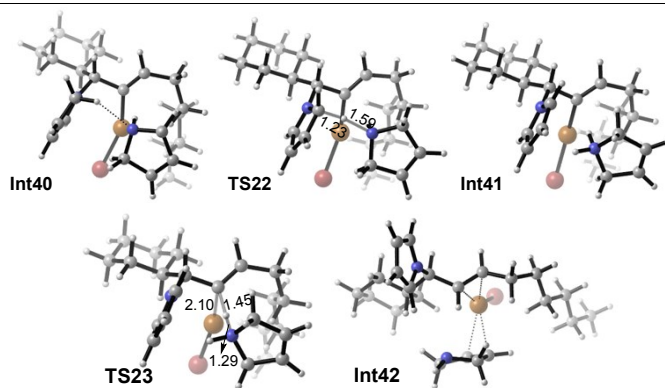
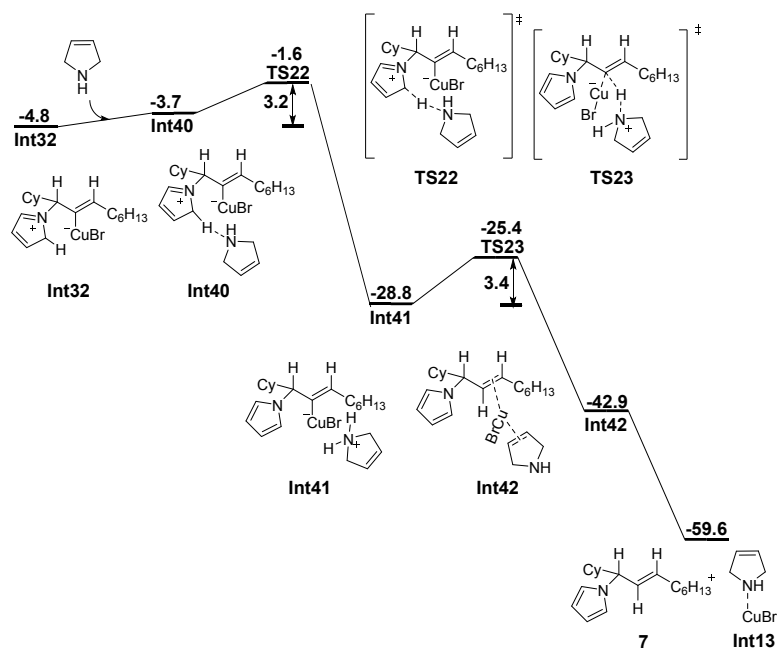
**Figure S2.** Free energy profile ( $\Delta G$  in kcal mol<sup>-1</sup>) for either intramolecular protodemetalation or  $\beta$ -N elimination for 1-octyne participated system. Bond lengths are given in angstroms.



**Figure S3.** Free energy profile ( $\Delta G$  in kcal mol<sup>-1</sup>) for H<sub>2</sub>O assisted protodemetalation of **Int32**. Bond lengths are given in angstroms.




**Figure S4.** Free energy profile ( $\Delta G$  in kcal mol<sup>-1</sup>) for water cluster assisted stepwise protodemetalation of **Int32**. Bond lengths are given in angstroms.



**Figure S5.** Free energy profile ( $\Delta G$  in kcal mol<sup>-1</sup>) for 3-pyrroline assisted stepwise protodemetalation of **Int32**. Bond lengths are given in angstroms.

**Table S1.** The summary of activation energies ( $\Delta G$  in kcal mol<sup>-1</sup>) for the processes from **Int32**.

Assisted species	Protodemetalation				$\beta$ -N elimination
	none <sup>a</sup>	H <sub>2</sub> O <sup>a</sup>	(H <sub>2</sub> O) <sub>3</sub>		
Deprotonation	11.4	13.3	4.9	3.2	14.7
Protodemetalation			3.1	3.4	

a: the protodemetalation proceeds in the concerted manner.

## 2. 3D optimized structures of intermediates and transition states

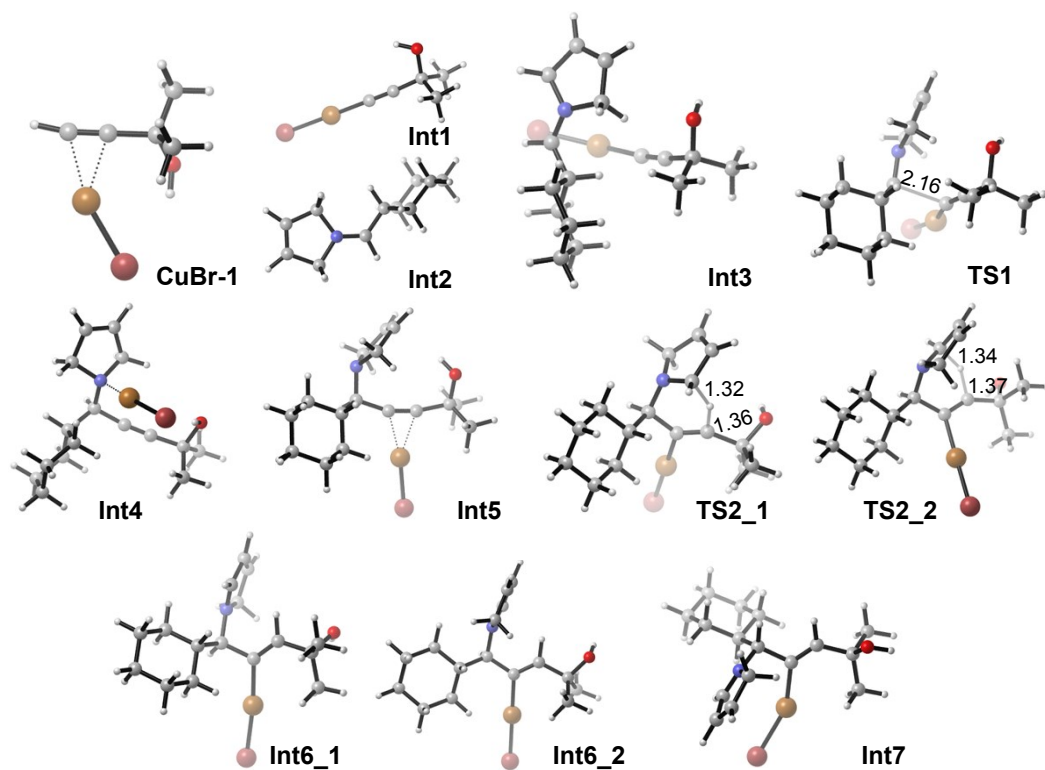


Figure S6 3D-structures for the stationary points showed in Figure 1.

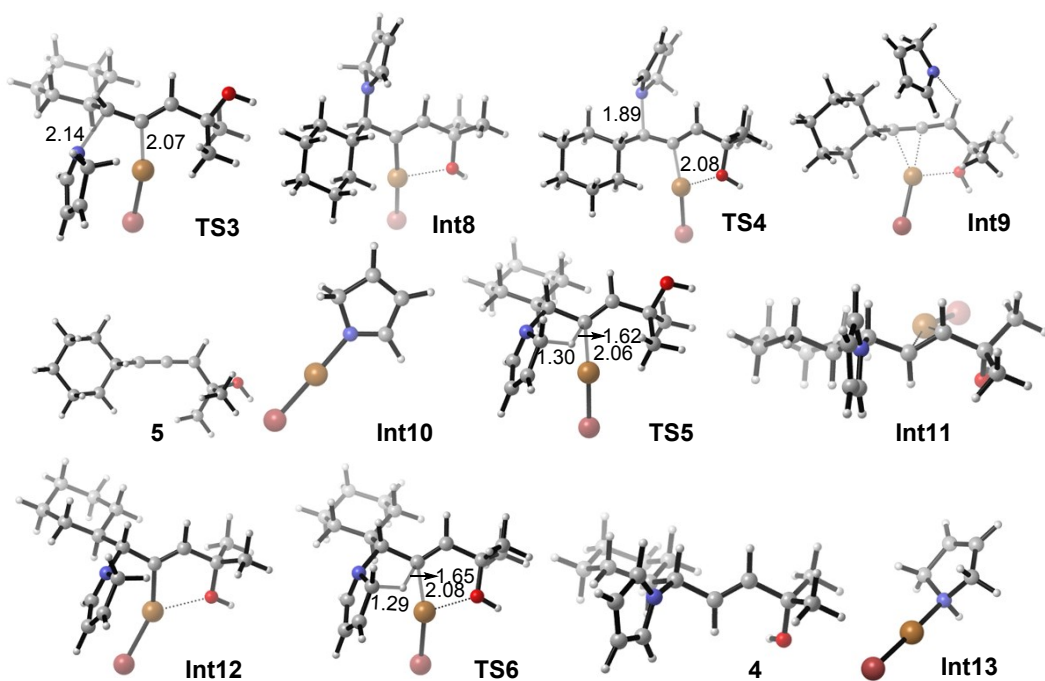
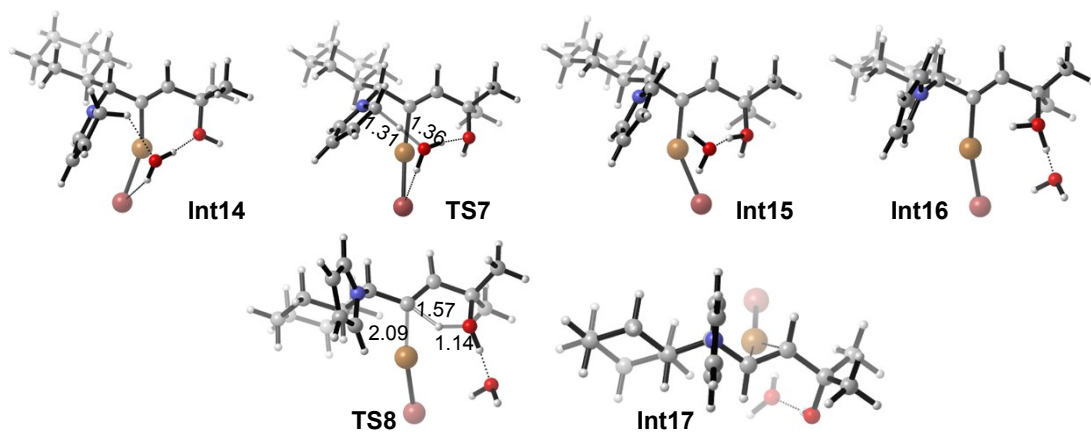
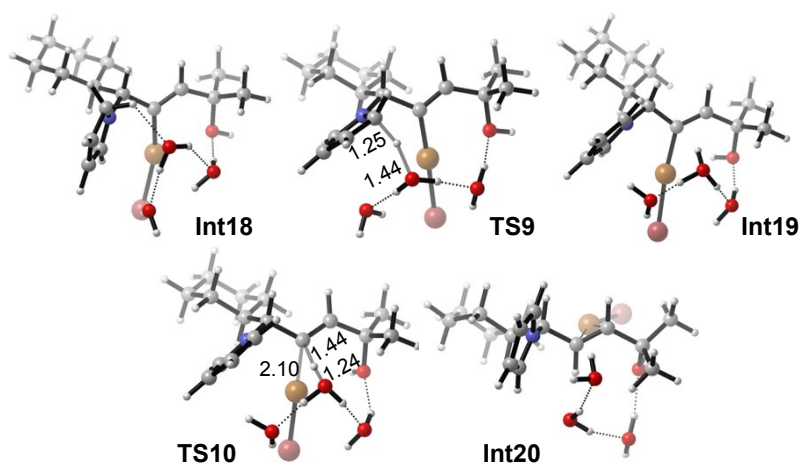


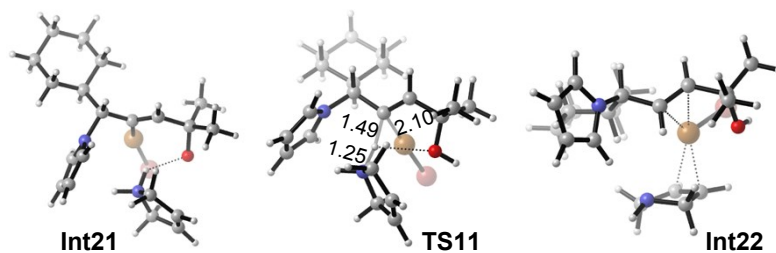
Figure S7 3D-structures for the stationary points showed in Figure 2.



**Figure S8** 3D-structures for the stationary points showed in Figure 3.

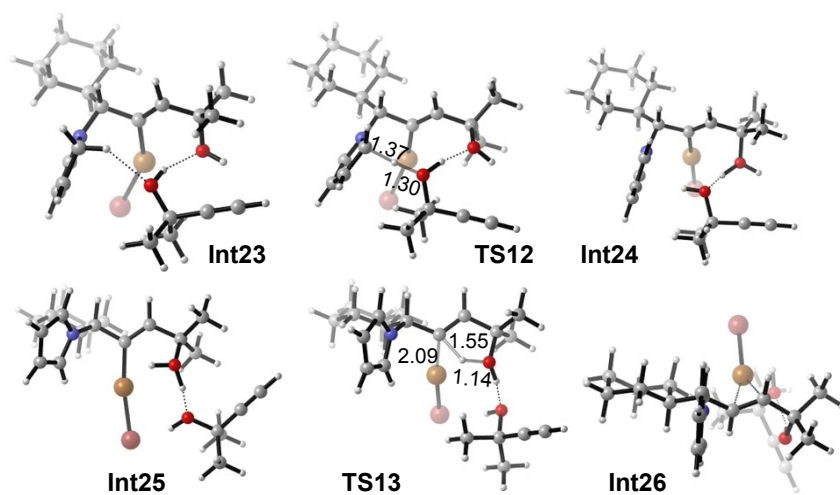


**Figure S9** 3D-structures for the stationary points showed in Figure 4.



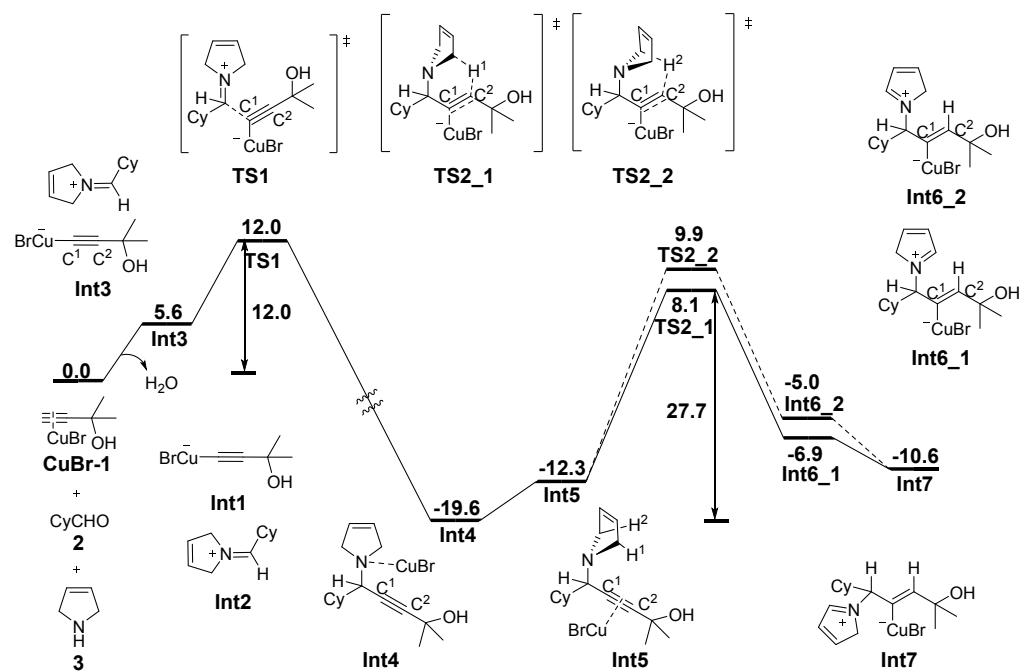
**Figure S10** 3D-structures for the stationary points showed in Figure 5.



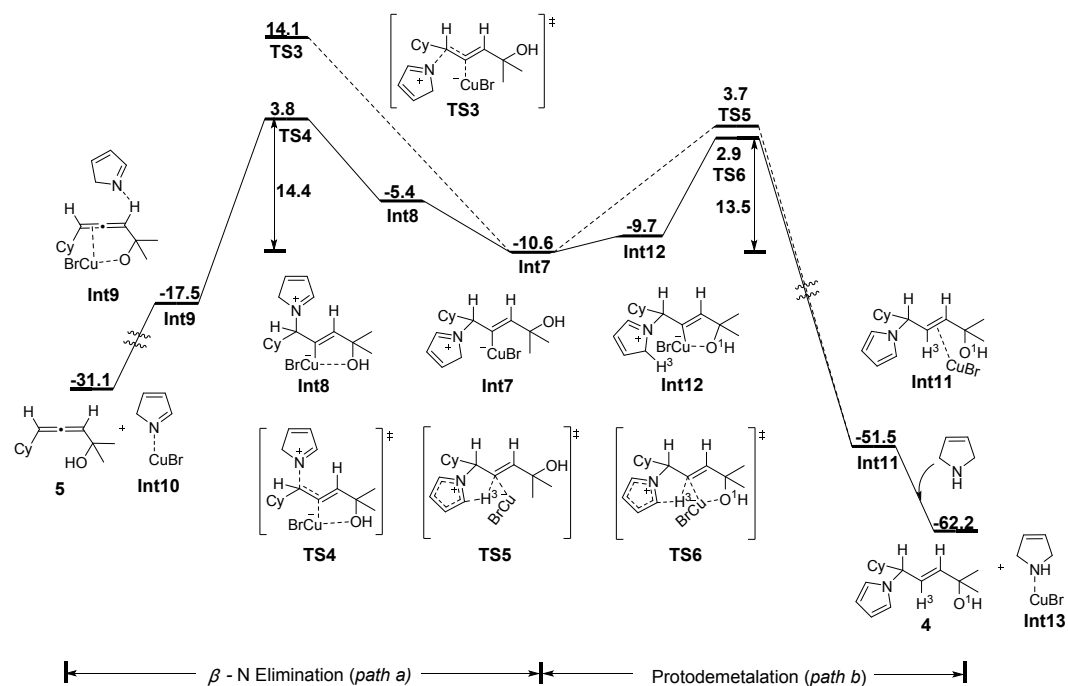


**Figure S11** 3D-structures for the stationary points showed in Figure 6

### 3. M06-2X free energy profile without the Grimme's dispersion corrections

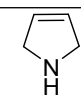
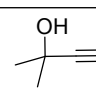


**Figure S12** Free energy profile (ΔG in kcal mol<sup>-1</sup>) without the Grimme's dispersion corrections for Figure 1 in main article. Calculations were performed at M06-2X/SDD,6-311++G(d,p)/SMD(toluene)//M06-2X/LANL2DZ,6-31G(d,p) level.



**Figure S13** Free energy profile ( $\Delta G$  in kcal mol<sup>-1</sup>) without the Grimme's dispersion corrections for Figure 1 in main article. Calculations were performed at M06-2X/SDD,6-311++G(d,p)/SMD(toluene)//M06-2X/LANL2DZ,6-31G(d,p) level.

**Table S2.** Activation energies ( $\Delta G$  in kcal mol<sup>-1</sup>) without the Grimme's dispersion corrections for Table 1 in main article.

Assisted species	Protodemetalation					$\beta$ -N elimination
	none	H <sub>2</sub> O	(H <sub>2</sub> O) <sub>3</sub>			
Deprotonation	13.5	8.3	5.3	No barrier	11.4	14.4
Protodemetalation		No barrier	4.1	2.2	1.8	

Calculations were performed at M06-2X/SDD,6-311++G(d,p)/SMD(toluene)//M06-2X/LANL2DZ,6-31G(d,p) level.

#### 4. Energies of intermediates and transition states

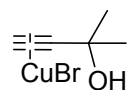
**Table S2.** Electronic energies ( $E_{elec}$ ), enthalpies ( $H_{298}$ ), Gibbs free energies ( $G_{298}$ ), thermal correction to Gibbs free energy ( $cor G_{gas}$ ), solvation energies ( $E_{sol}$ ), solvation free energies ( $G_{sol}$ ) in toluene ( $\epsilon = 2.37$ ) for all stationary points of the this process.

species	$E_{elec}$ (a.u.)	$H_{298}$ (a.u.)	$G_{298}$ (a.u.)	$cor G_{gas}$ (a.u.)	$E_{sol}$ (a.u.)	$G_{sol}$ (a.u.)
<b>CuBr-1</b>	-479.7791386	-479.646625	-479.696582	0.082556	-481.2811356	-481.1985796
<b>2</b>	-349.0432804	-348.853524	-348.894219	0.149062	-349.1412618	-348.9921998
<b>3</b>	-211.2556428	-211.143394	-211.176077	0.079566	-211.3174237	-211.2378577
<b>H<sub>2</sub>O</b>	-76.3839203	-76.358422	-76.379845	0.004075	-76.4253775	-76.4213025
<b>Int1</b>	-479.2536709	-479.132801	-479.184228	0.069443	-480.7977360	-480.7282930
<b>Int2</b>	-484.3067794	-484.017345	-484.067232	0.239548	-484.4718018	-484.2322538
<b>Int3</b>	-963.7032963	-963.290874	-963.371129	0.332168	-965.3331822	-965.0010142
<b>TS1</b>	-963.6933220	-963.281914	-963.362210	0.331112	-965.3222830	-964.9911710
<b>Int4</b>	-963.7563649	-963.342799	-963.419051	0.337314	-965.3782817	-965.0409677
<b>Int5</b>	-963.7358294	-963.323182	-963.402812	0.333018	-965.3622228	-965.0292048
<b>TS2_1</b>	-963.7005654	-963.292660	-963.369365	0.331200	-965.3280312	-964.9968312
<b>TS2_2</b>	-963.6991230	-963.291655	-963.367854	0.331269	-965.3251987	-964.9939297
<b>Int6_1</b>	-963.7179924	-963.306095	-963.384424	0.333569	-965.3546697	-965.0211007
<b>Int6_2</b>	-963.7142135	-963.302602	-963.380381	0.333832	-965.3514906	-965.0176586
<b>Int7</b>	-963.7322855	-963.320623	-963.398750	0.333535	-965.3603749	-965.0268399
<b>TS3</b>	-963.6917308	-963.283306	-963.362375	0.329356	-965.3165227	-964.9871667
<b>Int8</b>	-963.7180759	-963.306637	-963.385510	0.332566	-965.3510209	-965.0184549
<b>TS4</b>	-963.7061612	-963.296990	-963.375887	0.330275	-965.3341946	-965.0039196
<b>Int9</b>	-963.7413028	-963.331017	-963.413536	0.327767	-965.3648707	-965.0371037
<b>5</b>	-544.2644001	-543.949973	-544.007130	0.257270	-544.4142385	-544.1569685
<b>Int10</b>	-419.4674925	-419.373440	-419.417790	0.049702	-420.9501783	-420.9004763
<b>TS5</b>	-963.7101408	-963.303173	-963.379344	0.330797	-965.3349642	-965.0041672
<b>Int11</b>	-963.8032436	-963.390367	-963.468367	0.334877	-965.4267139	-965.0918369
<b>Int12</b>	-963.7337181	-963.322195	-963.400837	0.332881	-965.3581232	-965.0252422
<b>TS6</b>	-963.7157662	-963.308690	-963.384407	0.331359	-965.3366252	-965.0052662
<b>4</b>	-754.4043592	-753.997510	-754.063854	0.340505	-754.6078245	-754.2673195
<b>Int13</b>	-420.6686271	-420.549443	-420.595268	0.073359	-422.1522483	-422.0788893
<b>Int14</b>	-1040.1505309	-1039.710374	-1039.792561	0.357970	-1041.8047408	-1041.4467708
<b>TS7</b>	-1040.1424673	-1039.707213	-1039.786245	0.356222	-1041.7914407	-1041.4352187
<b>Int15</b>	-1040.1656538	-1039.726993	-1039.805943	0.359711	-1041.8132459	-1041.4535349
<b>Int16</b>	-1040.1559669	-1039.718411	-1039.798311	0.357537	-1041.8103901	-1041.4528531
<b>TS8</b>	-1040.1530425	-1039.718417	-1039.801222	0.351820	-1041.8053794	-1041.4535594
<b>Int17</b>	-1040.2182178	-1039.777445	-1039.861750	0.356468	-1041.8715172	-1041.5150492
<b>water cluster</b>	-229.1920818	-229.108922	-229.145114	0.046968	-229.3002131	-229.2532451
<b>Int18</b>	-1192.9654637	-1192.468408	-1192.561454	0.404009	-1194.6881463	-1194.2841373
<b>TS9</b>	-1192.9635742	-1192.470685	-1192.561215	0.402359	-1194.6783027	-1194.2759437
<b>Int19</b>	-1193.0081258	-1192.512644	-1192.600662	0.407464	-1194.7132409	-1194.3057769

<b>TS10</b>	-1192.9935419	-1192.501466	-1192.591352	0.402190	-1194.7013957	-1194.2992057
<b>Int20</b>	-1193.0164403	-1192.518268	-1192.612240	0.404201	-1194.7403028	-1194.3361018
<b>Int21</b>	-1175.0644907	-1174.535778	-1174.624929	0.439562	-1176.7431713	-1176.3036093
<b>TS11</b>	-1175.0568324	-1174.534376	-1174.623277	0.433555	-1176.7336432	-1176.3000882
<b>Int22</b>	-1175.0908807	-1174.563566	-1174.652566	0.438315	-1176.7638585	-1176.3255435
<b>1</b>	-270.3790451	-270.252577	-270.290855	0.088190	-270.4642800	-270.3760900
<b>Int23</b>	-1234.1466015	-1233.605314	-1233.699804	0.446797	-1235.8457766	-1235.3989796
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<b>Int24</b>	-1234.1476311	-1233.609718	-1233.704664	0.442967	-1235.8483701	-1235.4054031
<b>Int25</b>	-1234.1514502	-1233.611951	-1233.707068	0.444382	-1235.8531315	-1235.4087495
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<b>Int26</b>	-1234.2123876	-1233.670457	-1233.767631	0.444756	-1235.9117979	-1235.4670419
<b>CuBr-6</b>	-522.4717156	-522.254245	-522.313188	0.158527	-523.9754899	-523.8169629
<b>Int27</b>	-521.9394542	-521.733207	-521.792548	0.146906	-523.4844656	-523.3375596
<b>Int28</b>	-1006.3928606	-1005.895474	-1005.982275	0.410586	-1008.0235561	-1007.6129700
<b>TS14</b>	-1006.3831805	-1005.886586	-1005.971621	0.411559	-1008.0128929	-1007.6013339
<b>Int29</b>	-1006.4425947	-1005.944350	-1006.030396	0.412198	-1008.0658065	-1007.6536085
<b>Int30</b>	-1006.4301647	-1005.932180	-1006.018894	0.411270	-1008.0551238	-1007.6438538
<b>TS15_1</b>	-1006.3928694	-1005.900119	-1005.983634	0.409236	-1008.0170254	-1007.6077894
<b>TS15_2</b>	-1006.3917906	-1005.899112	-1005.981182	0.410609	-1008.0142517	-1007.6036427
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<b>Int32</b>	-1006.4248198	-1005.927411	-1006.010692	0.414128	-1008.0474465	-1007.6333185
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<b>TS17</b>	-1006.3930884	-1005.898585	-1005.983684	0.409404	-1008.0193946	-1007.6099906
<b>Int33</b>	-1006.4208263	-1005.925595	-1006.015112	0.405715	-1008.0460476	-1007.6403326
<b>8</b>	-586.9580189	-586.558213	-586.621629	0.336390	-587.1044743	-586.7680843
<b>TS18</b>	-1006.4021529	-1005.909671	-1005.993213	0.408940	-1008.0241459	-1007.6152059
<b>Int34</b>	-1006.4875866	-1005.989835	-1006.078022	0.409565	-1008.1126696	-1007.7031046
<b>7</b>	-797.0931543	-796.601192	-796.677211	0.415943	-797.2956076	-796.8796646
<b>Int35</b>	-1082.8340903	-1082.30815	-1082.395261	0.438829	-1084.4878463	-1084.0490173
<b>TS19</b>	-1082.8199966	-1082.299902	-1082.385913	0.434083	-1084.4676040	-1084.0335210
<b>Int36</b>	-1082.9007971	-1082.374401	-1082.465975	0.434822	-1084.5523472	-1084.1175252
<b>Int37</b>	-1235.6430952	-1235.061037	-1235.163757	0.479339	-1237.3645144	-1236.8851754
<b>TS20</b>	-1235.6410725	-1235.063727	-1235.161871	0.479202	-1237.3579900	-1236.8787880
<b>Int38</b>	-1235.6742052	-1235.093668	-1235.189988	0.484217	-1237.3854793	-1236.9012623
<b>TS21</b>	-1235.6624164	-1235.086779	-1235.184448	0.477969	-1237.3743100	-1236.8963410
<b>Int39</b>	-1235.7232878	-1235.140034	-1235.245388	0.477900	-1237.4386031	-1236.9607031
<b>Int40</b>	-1217.7043261	-1217.092773	-1217.191494	0.512832	-1219.3822585	-1218.8694265
<b>TS22</b>	-1217.7022504	-1217.094470	-1217.190496	0.511755	-1219.3779356	-1218.8661806
<b>Int41</b>	-1217.7458666	-1217.132939	-1217.229909	0.515957	-1219.4254475	-1218.9094905
<b>TS23</b>	-1217.7408001	-1217.132641	-1217.227667	0.513133	-1219.4172381	-1218.9041051
<b>Int42</b>	-1217.7663667	-1217.153904	-1217.252793	0.513573	-1219.4455510	-1218.9319780

## 5. Cartesian coordinates for the optimized structures

### CuBr-1



C	-1.43383600	2.10426100	-0.13185800
C	-1.68717300	0.91145200	-0.07602000
C	-2.01214300	-0.55235900	0.02046200
Cu	0.49953600	1.05762800	0.01209200
Br	2.16836300	-0.58331300	0.01429500
C	-1.72460500	-1.23118800	-1.32048900
H	-2.00527700	-2.28404200	-1.23884800
H	-2.29637200	-0.76805600	-2.12818400
H	-0.65791700	-1.17193900	-1.56176700
O	-1.26448000	-1.13224100	1.06378500
H	-0.35991000	-1.32195100	0.75992700
C	-3.48341700	-0.67681400	0.41516900
H	-4.12917300	-0.20292200	-0.32729900
H	-3.72715000	-1.73907500	0.48437300
H	-3.64706400	-0.21393100	1.38986200
H	-1.39351600	3.17248500	-0.18290600

### 2

### CyCHO

C	2.11099400	0.42144600	0.16166500
H	2.49879500	1.42195400	0.45856900
C	0.64470300	0.20004500	0.44216800
C	-0.18135000	1.33661000	-0.18442300
C	0.16484600	-1.16924500	-0.03183000
H	0.52562500	0.27547700	1.53665900
C	-1.67166700	1.14479000	0.10417900
H	-0.01841900	1.33312300	-1.27108700
H	0.16413200	2.30789700	0.18840100
C	-1.32757100	-1.35352400	0.24913200
H	0.35588900	-1.24841200	-1.10978700
H	0.75911000	-1.95559500	0.44293000
C	-2.15305600	-0.22644900	-0.37653000
H	-2.25119100	1.94278200	-0.37102600
H	-1.84017400	1.22894900	1.18644800
H	-1.66405200	-2.32512100	-0.12616900
H	-1.49349700	-1.35963600	1.33532400
H	-3.21501300	-0.35739100	-0.14494100
H	-2.05746600	-0.27602900	-1.46973700
O	2.83935800	-0.38875500	-0.35521900

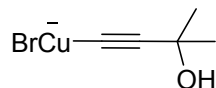
3



N	0.00002600	-1.21996200	-0.06186500
C	1.18098400	-0.35452900	0.11620600
H	1.59931300	-0.47949700	1.12502800
H	1.97233500	-0.62790000	-0.58938900
C	-1.18096700	-0.35457700	0.11621500
H	-1.59928800	-0.47955200	1.12504100
H	-1.97230900	-0.62798600	-0.58937300
C	-0.66462000	1.05699200	-0.06407000
C	0.66457400	1.05702100	-0.06405200
H	1.30575700	1.92953600	-0.11856200
H	-1.30584200	1.92947700	-0.11859100
H	0.00003200	-1.53378400	-1.02689100

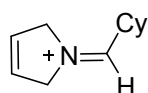
**H<sub>2</sub>O**

O	0.00000000	0.00000000	0.11779300
H	0.00000000	0.76021000	-0.47117300
H	0.00000000	-0.76021000	-0.47117300

**Int1**

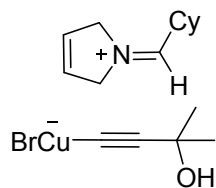
C	-2.12688300	0.01343500	-0.04322200
C	-0.90067300	0.01095200	-0.04139100
Cu	1.06097100	0.00630800	-0.02606000
Br	3.44176800	-0.00307000	0.00583300
C	-4.19345100	1.25430800	-0.61758200
H	-5.28180600	1.24850800	-0.49350000
H	-3.78509400	2.14171200	-0.13005100
H	-3.95090900	1.29344600	-1.68274000
C	-4.16180600	-1.26109800	-0.63672000
H	-3.73926800	-2.14576400	-0.15536400
H	-5.25104800	-1.27979200	-0.52259200
H	-3.90772600	-1.28688100	-1.69984500
O	-4.02727100	-0.00357600	1.39984800
H	-3.22158500	-0.12373800	1.91375900
C	-3.59626300	0.00000800	0.02610300

**Int2**



C	-0.49194300	-0.60891600	-0.52736800
H	-0.42548400	-1.31568300	-1.35808500
C	0.76875500	-0.11905100	0.07141200
C	1.70634700	-1.30598200	0.38202600
C	1.43527600	0.84994200	-0.94289000
H	0.56250300	0.43073400	0.99695000
C	3.04549300	-0.79668300	0.92023300
H	1.87438200	-1.87489400	-0.54255900
H	1.23308800	-1.98245200	1.10066800
C	2.77630900	1.34113000	-0.39128300
H	1.59923100	0.31695100	-1.88868800
H	0.76801000	1.69266600	-1.15307500
C	3.70624700	0.17323800	-0.05999200
H	3.69873800	-1.65028400	1.11897100
H	2.87964600	-0.29425800	1.88181700
H	3.23787200	2.00691100	-1.12549300
H	2.59649700	1.93869200	0.51149700
H	4.64375000	0.54944200	0.35721700
H	3.96244300	-0.36094000	-0.98397300
N	-1.67618500	-0.25609800	-0.18424100
C	-2.91536400	-0.75666500	-0.85043000
C	-2.00313500	0.70806900	0.90424900
C	-3.99320400	-0.01708300	-0.11464700
H	-2.87087600	-0.51670500	-1.91706000
C	-3.50094400	0.77426700	0.83003700
H	-1.63304200	0.31752300	1.85763200
H	-5.03920400	-0.14775700	-0.35954400
H	-4.07289400	1.40748300	1.49567500
H	-1.51128500	1.66456100	0.70014600
H	-2.97309800	-1.84289500	-0.73049200

**Int3**

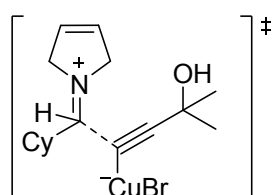


C	0.76320600	0.79410900	1.24886500
C	-0.64500200	-1.01849200	-1.52694900
C	-1.82885200	-1.23054600	-1.28460400



C	-3.19665000	-1.56544400	-0.83885100
H	1.77105200	1.21255400	1.22615000
C	-0.37141200	1.56436700	0.67212800
C	-1.02654800	2.41432600	1.78746300
C	0.10350700	2.46023300	-0.48053000
H	-1.10711200	0.85325400	0.27495900
C	-2.19446700	3.22013100	1.21308400
H	-0.27696200	3.09881600	2.20710100
H	-1.37065000	1.77208500	2.60637600
C	-1.07160600	3.25724800	-1.04399900
H	0.88258800	3.14257700	-0.11211700
H	0.55706600	1.84638600	-1.26443700
C	-1.74587900	4.09611000	0.04242500
H	-2.63996800	3.83059000	2.00479500
H	-2.97030600	2.52402900	0.86830900
H	-0.72531100	3.89468400	-1.86260800
H	-1.79651400	2.55209200	-1.47277000
H	-2.60264200	4.63842300	-0.36915100
H	-1.03693700	4.85081800	0.40890700
C	-3.89891000	-0.34443400	-0.24688100
H	-3.98195600	0.44848600	-0.99396400
H	-4.89759400	-0.62368600	0.10038300
H	-3.32799000	0.03063000	0.60885200
C	-4.02031200	-2.16692600	-1.97922800
H	-5.00730800	-2.45540900	-1.60695300
H	-4.13488500	-1.44602600	-2.79235100
H	-3.51776700	-3.05111300	-2.38133400
O	-3.11811100	-2.50435700	0.24695400
H	-2.59112600	-3.24488200	-0.07940800
Cu	1.27645900	-0.65609100	-1.47338300
Br	3.44039100	0.03781700	-0.74163700
N	0.64130700	-0.35090200	1.81841500
C	1.79810300	-1.10833800	2.36223800
C	-0.61374000	-1.13975600	1.89826800
C	1.16526200	-2.40958400	2.75836300
C	-0.14028500	-2.42146000	2.51280700
H	-1.01428100	-1.27310800	0.88545800
H	-1.35031100	-0.60697000	2.51007300
H	-0.82479200	-3.23982700	2.69408100
H	1.74653400	-3.21963400	3.17905200
H	2.55275600	-1.19144300	1.56909700
H	2.23066700	-0.55836800	3.20473800

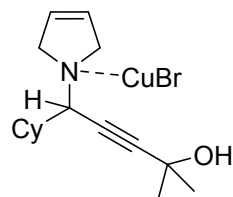
TS1



C	0.24862900	-0.64701800	0.76714000
C	-0.02152800	0.84473600	-0.77794700
C	0.95373100	1.56626600	-0.98649800
C	2.09896500	2.45889000	-1.25427400
H	-0.71041700	-1.14569700	0.62301000
C	1.45278500	-1.39080700	0.26101900
C	1.75067400	-2.52443500	1.26951000
C	1.23778300	-1.97559900	-1.13897200
H	2.30995500	-0.70593600	0.23628600
C	2.96225000	-3.34566200	0.82435400
H	0.86964400	-3.17782800	1.33422000
H	1.91154200	-2.10905000	2.27028500
C	2.44573700	-2.80435300	-1.57755900
H	0.34013200	-2.61088300	-1.12145800
H	1.04588200	-1.16662100	-1.84703500
C	2.75800500	-3.91885000	-0.57810900
H	3.14650600	-4.14648400	1.54715200
H	3.85203400	-2.70186800	0.82806400
H	2.26450800	-3.22119800	-2.57270600
H	3.31891200	-2.14264800	-1.66616500
H	3.64428200	-4.47906500	-0.89175400
H	1.92145600	-4.62991700	-0.55784900
C	3.35445100	1.64850300	-1.57243100
H	3.18926000	1.01351900	-2.44562900
H	4.18311200	2.33311700	-1.77073300
H	3.62279700	1.02057800	-0.71861900
C	1.75017500	3.40479000	-2.40865500
H	2.58938200	4.08430200	-2.57851300
H	1.54470300	2.84281800	-3.32240300
H	0.86036300	3.99101700	-2.16288600
O	2.42170700	3.21415500	-0.08500600
H	1.62064300	3.68204700	0.18387500
Cu	-1.93952900	0.30583200	-0.86840300
Br	-4.04501100	-0.58675100	-0.36235900
N	0.30896000	0.10120600	1.85323100
C	-0.91140900	0.66932700	2.44750300
C	1.50297400	0.87098100	2.21748100
C	-0.36623700	1.76838400	3.31176500

C	0.95268200	1.87702900	3.18832200
H	1.92095900	1.35756300	1.32094700
H	2.27141800	0.22090800	2.65294100
H	1.58783200	2.59376300	3.69318600
H	-1.00454900	2.38090700	3.93552600
H	-1.56830400	1.04578500	1.64714300
H	-1.46470800	-0.09676900	3.00092300

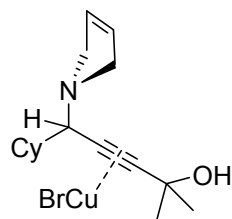
**Int4**



C	-1.42809600	0.37146300	-1.30734800
H	-1.93246000	0.57435500	-2.26783300
C	-0.37142700	-0.63730900	-1.48782900
C	0.63128400	-1.31417900	-1.47341900
N	-0.72019000	1.60339600	-0.86799400
C	0.15856000	2.17125000	-1.93263000
H	1.10591800	1.62791500	-1.98622600
H	-0.33151400	2.08768100	-2.91864300
C	-1.60183400	2.72198500	-0.45594300
H	-1.93840900	2.59278500	0.57628100
H	-2.49584100	2.77303100	-1.10205100
C	-0.72120500	3.92255600	-0.68109800
C	0.26873600	3.61197800	-1.51343400
C	1.92196800	-2.05272300	-1.41591700
H	-0.91755700	4.89158600	-0.23975100
H	1.03630600	4.27937500	-1.88414200
O	2.96683100	-1.12045200	-1.22010200
H	2.94906300	-0.82137700	-0.29434700
C	2.19303000	-2.72590300	-2.75922500
H	2.25793800	-1.97134800	-3.54569400
H	3.14742200	-3.25417000	-2.69905400
H	1.39936900	-3.43528300	-3.00493700
C	1.87547400	-3.07393500	-0.27646800
H	1.71081000	-2.56542400	0.67822600
H	1.07464200	-3.80110000	-0.43545100
H	2.83391200	-3.59814000	-0.23522700
C	-2.50463000	-0.09483700	-0.30433800
C	-3.20551900	-1.34578700	-0.85193300
C	-1.96452400	-0.35739900	1.10662200
H	-3.25675700	0.70610500	-0.24320600

C	-4.30963600	-1.83007400	0.08839400
H	-2.45599700	-2.13910300	-0.97332800
H	-3.61339900	-1.13748800	-1.84851900
C	-3.06688400	-0.85389100	2.04546800
H	-1.16299500	-1.10820400	1.04974400
H	-1.51940100	0.55256000	1.53209000
C	-3.75431500	-2.10017100	1.48733200
H	-4.77691700	-2.73104100	-0.32124100
H	-5.09580800	-1.06532500	0.15243900
H	-2.64203200	-1.05576100	3.03314000
H	-3.81395100	-0.05890500	2.17680500
H	-4.55330100	-2.42813100	2.15969100
H	-3.02482100	-2.91933900	1.43328700
Cu	0.68643600	0.94550800	0.53663100
Br	2.36257000	0.16704900	1.99637200

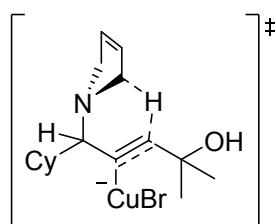
**Int5**



C	-1.56610600	-0.03942100	-0.64685700
H	-1.36065500	-0.43419700	-1.65060000
C	-0.31483800	0.60544000	-0.13348000
C	0.46382300	1.43607500	0.31895900
N	-2.57338100	1.00012500	-0.77982300
C	-2.27066400	1.99105700	-1.82829000
H	-1.21904000	1.92928500	-2.15192200
H	-2.89389600	1.82552200	-2.71650600
C	-2.91310200	1.69828600	0.47526900
H	-2.16999700	1.51446700	1.26651600
H	-3.88724400	1.36734400	0.85839800
C	-2.91416000	3.15218900	0.09439000
C	-2.55262300	3.31513600	-1.17628800
C	1.17467500	2.63632500	0.85139700
H	-2.48446300	4.25826600	-1.70657400
H	-3.18743400	3.93857800	0.78913900
Cu	1.64758500	-0.32121600	-0.21032000
Br	3.57552600	-1.58476200	-0.48823700
C	1.99189600	3.27678500	-0.27307200
H	2.46429000	4.18477900	0.10896700
H	2.76537000	2.59261700	-0.63438200

H	1.34271700	3.54061800	-1.11385000
O	0.18772700	3.52692500	1.33862100
H	-0.43274900	3.72018600	0.62026000
C	2.05285000	2.26276100	2.04101600
H	2.83416200	1.55907100	1.73918300
H	2.51807800	3.17079100	2.43136700
H	1.44313600	1.81191600	2.82637000
C	-2.03002900	-1.21925900	0.22255400
C	-3.29362000	-1.83742700	-0.38560300
C	-0.92638100	-2.27271500	0.37443800
H	-2.27330900	-0.83344400	1.22436400
C	-3.77094300	-3.04968200	0.41516100
H	-3.06227800	-2.15348600	-1.41392100
H	-4.07632300	-1.07730100	-0.46052600
C	-1.41080600	-3.49608800	1.15814600
H	-0.58849700	-2.58865400	-0.62454900
H	-0.05436200	-1.84383300	0.88617900
C	-2.66679800	-4.10085700	0.53128600
H	-4.66309100	-3.47739500	-0.05309500
H	-4.06696100	-2.72461100	1.42197400
H	-0.60795500	-4.23697000	1.21449500
H	-1.63539500	-3.19101000	2.18913100
H	-3.01042300	-4.95565000	1.12236500
H	-2.42423200	-4.48286300	-0.46955900

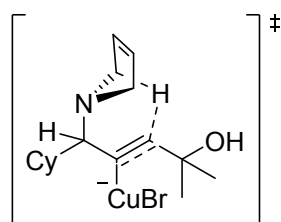
**TS2\_1**



C	-1.27307400	-0.38183400	-0.73217800
H	-0.94220400	-0.82838500	-1.67613900
C	-0.17241000	0.49863800	-0.13679200
C	-0.42476800	1.55340600	0.54466300
N	-2.39916200	0.48865400	-1.05332300
C	-2.31443800	1.22548000	-2.32181900
H	-1.26615900	1.47427200	-2.55262700
H	-2.70522500	0.61344300	-3.14271900
C	-2.86737400	1.34591900	-0.07601700
H	-1.75959200	1.79034800	0.48877400
H	-3.34150000	0.90277200	0.79957600
C	0.10145600	2.67477200	1.39522300

C	-3.44630800	2.52150400	-0.76605200
C	-3.11467400	2.46463500	-2.05744500
H	-3.99427000	3.30245200	-0.25692900
H	-3.35536900	3.19118800	-2.82265600
C	1.62825500	2.73289700	1.29035800
H	2.08804300	1.82115900	1.68178600
H	1.94252000	2.84740200	0.24779000
H	1.98441800	3.59077700	1.86674100
Cu	1.77433100	-0.04882000	-0.36283300
Br	4.00276800	-0.70008600	-0.61125800
C	-0.34637000	2.48540300	2.84131400
H	-1.43812800	2.46372400	2.89753500
H	0.05261800	1.55320500	3.24637500
H	0.01230800	3.32629100	3.43963600
O	-0.48235600	3.89889600	0.97433600
H	-0.17521600	4.07884400	0.07705200
C	-1.65776400	-1.51898500	0.22801600
C	-2.76394700	-2.38864700	-0.38288500
C	-0.43920700	-2.37546400	0.59501100
H	-2.03615200	-1.06150400	1.15650800
C	-3.14517800	-3.55002700	0.53650800
H	-2.39689500	-2.79216500	-1.33832900
H	-3.63878500	-1.77255300	-0.61475900
C	-0.82444200	-3.54606900	1.50164500
H	0.01870600	-2.75846300	-0.32970300
H	0.32001500	-1.76120600	1.09073000
C	-1.92398300	-4.40496600	0.87668100
H	-3.92357200	-4.15781900	0.06425200
H	-3.57558900	-3.14967800	1.46465400
H	0.06197800	-4.14910100	1.71921800
H	-1.18165700	-3.14939500	2.46189300
H	-2.20286300	-5.22038000	1.55158400
H	-1.54155900	-4.86816500	-0.04285100

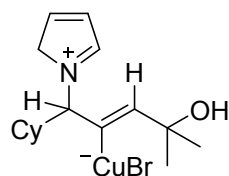
TS2\_2



C	0.13713900	-1.57372400	-0.68921400
H	0.13334100	-1.93748800	-1.72647400
C	-0.67697800	-0.26955200	-0.67510000

C	-1.95764700	-0.26582500	-0.64273900
N	-0.61861500	-2.53351500	0.10439900
C	-1.91774800	-2.78237000	-0.29271300
H	-2.38471700	-1.55976700	-0.55924900
H	-2.06203800	-3.23668600	-1.27248800
C	-0.61891500	-2.35165200	1.56405300
H	-0.59016900	-1.27478100	1.80891700
H	0.25616500	-2.82376400	2.02205100
C	-1.92423800	-2.95591700	1.98322100
C	-2.66590800	-3.22209100	0.90507200
C	-3.22667200	0.54600900	-0.62356200
H	-3.66446500	-3.63632700	0.87123600
H	-2.19488300	-3.12442300	3.01741600
Cu	0.14841900	1.51327000	-0.13144600
Br	1.13836900	3.45020100	0.72563900
C	-2.92444900	2.00938300	-0.95721700
H	-3.87067500	2.55372100	-1.01809200
H	-2.29790600	2.47516100	-0.19022200
H	-2.40209700	2.08787900	-1.91591000
O	-4.14031300	-0.00450200	-1.56033300
H	-3.79101500	0.16156700	-2.44476900
C	-3.89949900	0.41822800	0.73944700
H	-3.23987800	0.79897700	1.52317100
H	-4.82985700	0.99127700	0.73775500
H	-4.13286200	-0.62937700	0.94736800
C	1.59317300	-1.43907700	-0.23831600
C	2.28511900	-2.80360400	-0.11483900
C	2.39258500	-0.56434200	-1.21470100
H	1.60281200	-0.94024900	0.74517600
C	3.72819400	-2.64567800	0.36915000
H	2.27932800	-3.28524900	-1.10388500
H	1.72839300	-3.46942500	0.55187900
C	3.83576800	-0.38523000	-0.74210300
H	2.38563100	-1.05176600	-2.20145900
H	1.92281700	0.41712600	-1.34625800
C	4.53101500	-1.73582600	-0.56192000
H	4.20470900	-3.62775300	0.45206100
H	3.71841000	-2.21123000	1.37815300
H	4.38445400	0.23675100	-1.45560000
H	3.83016900	0.16085900	0.21028900
H	5.54488400	-1.59481200	-0.17441800
H	4.62955700	-2.22386900	-1.54130500

## Int6\_1

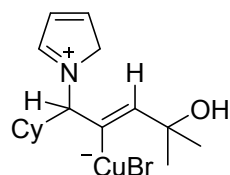


C	1.14224800	0.33157900	-0.57767400
H	0.72459200	0.75867900	-1.49752000
C	0.16078800	-0.67945700	0.02237200
C	0.63322700	-1.76559600	0.63577200
N	2.36155900	-0.38119400	-1.03190600
C	2.32364400	-1.15690200	-2.26755500
H	1.39630000	-1.74537900	-2.26385300
H	2.30618800	-0.48322200	-3.13202200
C	3.37854600	-0.75554800	-0.31364300
H	1.71124700	-2.01186900	0.67657500
H	3.56586900	-0.32255200	0.66174800
C	-0.14161500	-2.84438500	1.37250000
C	4.16405500	-1.75630000	-1.01146400
C	3.54748900	-2.00210700	-2.18192900
H	5.07106800	-2.19966600	-0.62692800
H	3.85612600	-2.69094400	-2.95665900
C	-1.65610600	-2.68797800	1.30652600
H	-1.98591600	-1.75496100	1.77298400
H	-2.00855200	-2.68336200	0.26856100
H	-2.12515000	-3.52711900	1.82710600
Cu	-1.75770500	-0.12160700	-0.29592400
Br	-3.88712900	0.72369300	-0.82562600
C	0.32753600	-2.88746400	2.82509300
H	1.40895900	-3.04790000	2.86630900
H	0.08808000	-1.94877600	3.33095100
H	-0.16131700	-3.71430100	3.34707600
O	0.23646100	-4.11418300	0.82954500
H	-0.12335100	-4.15020900	-0.06479600
C	1.50057900	1.49055700	0.36765600
C	2.47125500	2.48053100	-0.29353200
C	0.23255100	2.22378500	0.83258600
H	1.96964000	1.05869100	1.26710800
C	2.80461300	3.65742600	0.62542100
H	1.99769700	2.86207400	-1.21000200
H	3.39543200	1.97934200	-0.60505900
C	0.56752500	3.41238700	1.73653000
H	-0.32293700	2.57252900	-0.05080800
H	-0.42540800	1.52829300	1.35968900



C	1.53455900	4.38534000	1.06399000
H	3.49022500	4.34299700	0.11712700
H	3.33108400	3.28240000	1.51421400
H	-0.35758800	3.92230900	2.02049200
H	1.02106400	3.03871700	2.66503500
H	1.78142100	5.21056900	1.73930900
H	1.05023100	4.82760100	0.18313400

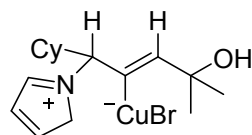
**Int6\_2**



C	1.34706400	0.13876700	-0.56933200
H	1.24208500	0.39457500	-1.63384600
C	0.17625800	-0.73302500	-0.15955700
C	0.34007300	-2.04399000	0.04876900
N	2.62502700	-0.63670000	-0.49702000
C	3.10271300	-1.40614800	-1.42396000
H	1.30579100	-2.56832600	-0.03678000
H	2.69598400	-1.37526200	-2.42926700
C	3.27711400	-0.94271800	0.77301100
H	2.50704500	-1.33071000	1.45481800
H	3.70731700	-0.03615100	1.21181700
C	4.28693300	-1.97097000	0.40015700
C	4.16988300	-2.24476800	-0.91264800
C	-0.74729900	-3.03967800	0.45268900
H	4.73815700	-2.94751500	-1.50436200
H	4.97942000	-2.41034600	1.10546800
Cu	-1.68007500	0.07918900	-0.19636300
Br	-3.83449500	1.03150300	-0.25599900
C	-1.83571600	-3.17110200	-0.61488000
H	-2.52887600	-3.96811600	-0.33065400
H	-2.40366400	-2.24316500	-0.73213100
H	-1.39233000	-3.41420200	-1.58795800
O	-0.13182900	-4.31670300	0.65255700
H	0.04043100	-4.69019500	-0.21961000
C	-1.35740500	-2.67340900	1.80195800
H	-1.84510600	-1.69586600	1.74849900
H	-2.09520900	-3.42660400	2.09126000
H	-0.57522200	-2.63494600	2.56525400
C	1.56344800	1.46054800	0.20226000
C	2.76705500	2.22640700	-0.37647200

C	0.32153300	2.36091000	0.18400600
H	1.76419100	1.21244900	1.25743200
C	3.01580600	3.55570900	0.33760500
H	2.56101400	2.42491400	-1.43897400
H	3.67953800	1.61656700	-0.35208200
C	0.57450900	3.70198000	0.87724700
H	0.01033000	2.53063100	-0.85742300
H	-0.51246200	1.86532400	0.68496300
C	1.77197500	4.44057600	0.28393300
H	3.87569500	4.06225800	-0.11248700
H	3.27571000	3.35938600	1.38717400
H	-0.33069000	4.31246200	0.81512500
H	0.75917700	3.51983500	1.94489600
H	1.94806700	5.38106900	0.81533500
H	1.55891100	4.69886000	-0.76199200

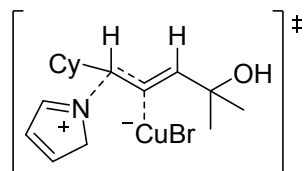
**Int7**



C	-0.99589900	0.45120800	0.98858700
H	-1.41402700	1.09826300	1.77793300
C	0.19789300	1.09225100	0.28177300
C	0.45782800	2.35306300	0.64208300
N	-0.44358200	-0.72507300	1.71683300
C	0.37171000	-0.52902600	2.90883800
H	1.09327000	0.27007100	2.68409200
H	-0.25352000	-0.20819000	3.74925100
C	-0.23561000	-1.91393600	1.23331300
H	-0.16003400	2.88344200	1.38093500
H	-0.67913800	-2.24377300	0.30106900
C	0.65743900	-2.67166200	2.08901500
C	1.01850000	-1.85824900	3.09748900
C	1.55244500	3.24669100	0.10444100
H	0.97429700	-3.68290900	1.88121600
H	1.68067400	-2.08736100	3.92160500
O	2.10503000	3.86880400	1.26817200
H	2.76618000	4.50520300	0.97010600
C	2.64811300	2.49709300	-0.64714100
H	2.26161100	2.03172600	-1.55907400
H	3.44109400	3.19574000	-0.93849000
H	3.08214700	1.71983100	-0.01208500
C	0.92262900	4.31885000	-0.79258200

H	1.68394200	5.02850000	-1.13913300
H	0.45480300	3.86270800	-1.66948000
H	0.16214900	4.87302400	-0.23565400
Cu	1.20642800	-0.26563800	-0.81660000
Br	1.86279800	-2.49961600	-1.36273000
C	-2.13379100	0.03825900	0.04873600
C	-3.28788400	-0.65865900	0.78311400
C	-2.64967200	1.27990800	-0.69087000
H	-1.72144600	-0.64085000	-0.71508500
C	-4.43055000	-1.01339700	-0.17103600
H	-3.66436700	0.02304400	1.55988700
H	-2.94188300	-1.56063100	1.30129500
C	-3.79711900	0.92957300	-1.63950700
H	-2.99607700	2.01276400	0.05373000
H	-1.82398000	1.74826700	-1.23339800
C	-4.93956200	0.22850700	-0.90313400
H	-5.24311800	-1.49587500	0.38150600
H	-4.06946900	-1.74424900	-0.90719100
H	-4.15926200	1.83609400	-2.13455700
H	-3.41745900	0.26738600	-2.42915100
H	-5.73741400	-0.04202800	-1.60202000
H	-5.37730600	0.92209800	-0.17228900

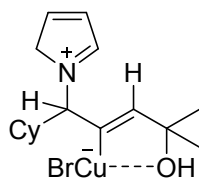
**TS3**



C	-1.10087900	0.69337900	1.17100900
H	-1.43465200	0.83855200	2.20156500
C	0.12195200	1.21099600	0.75642300
C	0.58803400	2.46322900	0.76119600
N	-0.59681400	-1.29125500	1.78183100
C	0.47408700	-1.36297700	2.76209700
H	1.14057600	-0.50068300	2.61367400
H	0.05900500	-1.29153100	3.77500700
C	-0.52924900	-2.35079300	1.05044700
H	-0.04074300	3.31302200	1.04294500
H	-1.20192600	-2.50629200	0.20941900
C	0.55009500	-3.25420000	1.45436500
C	1.16253600	-2.66430000	2.49347700
C	1.96398400	2.89941100	0.29455200
H	0.79908300	-4.18061600	0.95702800

H	2.01569000	-3.02903500	3.05054400
O	2.10770100	4.21183600	0.83227700
H	2.95279300	4.56219100	0.52788800
C	3.07516900	1.99994200	0.83809800
H	2.99966000	0.97474000	0.45957900
H	4.05171100	2.38697800	0.52666400
H	3.03606300	1.97815300	1.92992300
C	2.00987700	2.96221400	-1.23644000
H	2.97261000	3.36592200	-1.57163800
H	1.89048100	1.96611700	-1.67620700
H	1.21061200	3.60838100	-1.60917900
Cu	1.03637500	-0.20696100	-0.44280000
Br	1.61774300	-2.04608600	-1.79990000
C	-2.19411400	0.36165700	0.18471800
C	-3.40637600	-0.31859700	0.82721700
C	-2.62015400	1.67703300	-0.50281700
H	-1.77575200	-0.29103200	-0.59593900
C	-4.51032300	-0.57101500	-0.20183700
H	-3.79378900	0.33976600	1.61848600
H	-3.10322900	-1.25071800	1.31316800
C	-3.72861300	1.42298600	-1.52636300
H	-2.97972600	2.37901900	0.26357000
H	-1.74967100	2.13813700	-0.97871500
C	-4.93229000	0.72919400	-0.88819300
H	-5.36918300	-1.04778600	0.28080900
H	-4.14060100	-1.27597400	-0.95899300
H	-4.02932600	2.37009500	-1.98534500
H	-3.32976500	0.79119100	-2.33094900
H	-5.70117500	0.53164900	-1.64163400
H	-5.38092200	1.39976300	-0.14269500

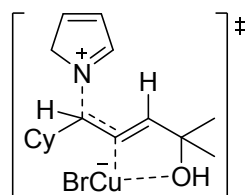
**Int8**



C	1.39707500	0.02550500	-0.55420000
H	1.20607600	0.43136100	-1.55589500
C	0.12918700	-0.57462800	0.00190500
C	0.10961700	-1.75828200	0.61399000
N	2.39003500	-1.06095800	-0.78964900
C	2.26912500	-1.90335900	-1.97527000
H	1.21170700	-2.18290000	-2.08003200

H	2.57162100	-1.33959000	-2.86536900
C	3.13635500	-1.65670100	0.09337600
H	0.98436800	-2.42673600	0.71786600
H	3.31391100	-1.21277300	1.06572200
C	-1.15467200	-2.36511900	1.20711600
C	3.65369300	-2.90871400	-0.42824700
C	3.14749900	-3.06661700	-1.66506100
H	4.31991100	-3.56709000	0.11053300
H	3.31954300	-3.88724500	-2.34823200
C	-0.81944500	-3.16925300	2.46394400
H	-0.12378700	-3.98424100	2.23760800
H	-0.36583900	-2.51284100	3.21076800
H	-1.72898400	-3.60211400	2.89077400
Cu	-1.68158700	0.33319200	-0.20780700
Br	-3.78270700	1.28511700	-0.76072200
C	-1.83323300	-3.24503500	0.15414200
H	-2.11233100	-2.62769800	-0.70531000
H	-1.16042400	-4.03868900	-0.18529400
H	-2.73351300	-3.71967500	0.56302300
O	-2.02344300	-1.29362600	1.56713800
H	-2.94313000	-1.56906200	1.46944400
C	2.00458400	1.14969500	0.30213400
C	3.28037000	1.71443200	-0.34034100
C	0.97627800	2.27011100	0.52167800
H	2.24599700	0.73347300	1.29378300
C	3.86646400	2.87575500	0.46485700
H	3.02414100	2.07080900	-1.34914200
H	4.03751700	0.93154600	-0.46808700
C	1.57165500	3.43481100	1.31487400
H	0.62735800	2.62763700	-0.45837800
H	0.09931500	1.87143500	1.03721800
C	2.83375900	3.98638400	0.65330300
H	4.76292700	3.25849700	-0.03363100
H	4.18425900	2.50733700	1.45008100
H	0.81829000	4.22002300	1.42627200
H	1.81889500	3.08879700	2.32798600
H	3.25564300	4.80233400	1.24868900
H	2.57474100	4.40756600	-0.32747900

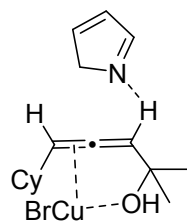
TS4



C	1.16950000	0.30208000	-0.54510900
H	1.02216800	0.53133900	-1.60465800
C	0.30003600	-0.66115700	-0.01461300
C	0.46173800	-1.86241100	0.52315900
N	2.83749900	-0.55189800	-0.82535700
C	2.85892800	-1.54600300	-1.88896900
H	1.85267600	-1.97751000	-1.97858900
H	3.10534600	-1.06701900	-2.84431800
C	3.65179900	-0.93765400	0.09832700
H	1.44531400	-2.35398500	0.56124600
H	3.77179700	-0.36680700	1.01531200
C	-0.67376800	-2.69240900	1.09101200
C	4.34363600	-2.17866100	-0.25027400
C	3.87210500	-2.55337400	-1.45178900
H	5.08302800	-2.67451600	0.36321000
H	4.14962500	-3.42730300	-2.02627600
C	-0.24428300	-3.35232800	2.40122300
H	0.61516600	-4.01159200	2.24391500
H	0.02681200	-2.58414700	3.12931500
H	-1.06321200	-3.94987000	2.81329200
Cu	-1.68504400	-0.04978500	-0.18145400
Br	-3.80826300	0.80143400	-0.80053300
C	-1.11201700	-3.73574100	0.06076200
H	-1.47364700	-3.22957600	-0.83905800
H	-0.27609200	-4.38584000	-0.21377300
H	-1.91187400	-4.36938800	0.46213200
O	-1.75236800	-1.79506300	1.35383400
H	-2.59120900	-2.27153900	1.33964300
C	1.54546000	1.52010100	0.28616000
C	2.52961800	2.43767000	-0.45092500
C	0.28614200	2.31362000	0.69286200
H	2.00696500	1.15309600	1.21705100
C	2.88244400	3.67609700	0.37432500
H	2.05976600	2.75581300	-1.39312900
H	3.43652700	1.88725200	-0.71994400
C	0.64417200	3.55950000	1.50432400
H	-0.26547400	2.60165400	-0.21339800
H	-0.38002100	1.66667100	1.27169800

C	1.62680300	4.45964500	0.75683900
H	3.57828100	4.30865200	-0.18626300
H	3.40545800	3.36334300	1.28902600
H	-0.27128300	4.10576600	1.74980500
H	1.09426200	3.24866000	2.45743100
H	1.88990700	5.33062200	1.36539700
H	1.14772900	4.83974200	-0.15530800

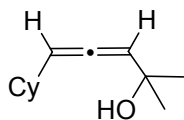
**Int9**



C	-0.32737000	0.23079900	1.44289200
H	-0.17688400	0.53130300	2.48297800
C	-0.00932100	-1.01022800	1.09663400
C	0.20327300	-2.26053900	0.77011000
N	-2.85724700	-2.32079900	-0.09358000
C	-4.28370200	-2.10274200	0.10206600
H	-4.80628400	-3.06769600	0.08786100
H	-4.45247100	-1.67288700	1.09855400
C	-2.53520000	-1.65072400	-1.14270700
H	-0.63151300	-2.95587900	0.86240800
H	-1.50823400	-1.63729100	-1.50446100
C	1.50054500	-2.78505200	0.18624100
C	-3.65596600	-0.92463200	-1.75833800
C	-4.73073900	-1.19082500	-0.99891700
H	-3.59970200	-0.30495000	-2.64382500
H	-5.74260700	-0.83076000	-1.13424900
C	1.36966700	-2.88233100	-1.33447400
H	0.52772600	-3.52389900	-1.60872100
H	1.20916100	-1.88514600	-1.75704100
H	2.27869300	-3.30897400	-1.77305000
Cu	1.77737000	0.22915600	0.49025900
Br	3.23341300	1.58617800	-0.80630600
C	1.85396000	-4.13107900	0.81234600
H	1.96771700	-4.02030000	1.89286600
H	1.07229000	-4.86865500	0.61085900
H	2.79518100	-4.50287500	0.39668100
O	2.51390200	-1.82930700	0.52325500
H	3.25653100	-1.89572500	-0.09213100
C	-1.09229500	1.20433600	0.56571300

C	-2.56789000	1.20338900	1.00358500
C	-0.51222400	2.62423800	0.63809500
H	-1.04010000	0.85084700	-0.47491600
C	-3.39432900	2.18728000	0.17426800
H	-2.61794200	1.48778700	2.06487700
H	-2.96864500	0.18728900	0.92297700
C	-1.34939300	3.61060900	-0.17842300
H	-0.50050200	2.93968200	1.69227200
H	0.52602500	2.63041000	0.28660700
C	-2.81554300	3.60024000	0.25732400
H	-4.43729200	2.17250700	0.50891500
H	-3.39491600	1.85585700	-0.87296600
H	-0.92612100	4.61535800	-0.08681900
H	-1.28427900	3.33818100	-1.24045500
H	-3.40273900	4.28886400	-0.35876600
H	-2.88761200	3.95881400	1.29326000

5

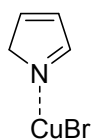


C	0.22435800	-0.77728600	-0.85929800
H	0.41540300	-1.00844100	-1.90907100
C	-0.98930500	-0.91505600	-0.39333000
C	-2.20023700	-1.02659000	0.08420000
H	-2.53728100	-1.96939800	0.51343300
C	-3.22208700	0.09355900	0.12132600
C	-2.83922100	1.25064100	-0.79583000
H	-1.87971400	1.68482800	-0.50270900
H	-2.76300100	0.89695500	-1.82618800
H	-3.60124300	2.03612100	-0.74511900
C	-3.39202900	0.56963000	1.56760000
H	-3.68190000	-0.26917300	2.20551100
H	-2.46160300	0.99830800	1.94889500
H	-4.17408200	1.33611000	1.62665300
O	-4.43392700	-0.51092600	-0.32492900
H	-5.12574000	0.16017200	-0.27810300
C	1.40748000	-0.30105000	-0.04997800
C	2.53435200	-1.34417300	-0.06632400
C	1.91799100	1.04514600	-0.58663900
H	1.08064800	-0.15738000	0.98930600
C	3.76777400	-0.85859100	0.69840700
H	2.81054700	-1.54247700	-1.11251600
H	2.16578600	-2.28868200	0.34735900



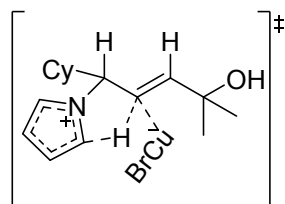
C	3.15156600	1.52912600	0.17893200
H	2.17306900	0.92374100	-1.64961500
H	1.11320400	1.78699200	-0.53761600
C	4.26498400	0.48053400	0.15079300
H	4.56148900	-1.61132300	0.64916900
H	3.50920500	-0.73936200	1.75947100
H	3.50682600	2.47719900	-0.23820900
H	2.87185400	1.72768300	1.22272100
H	5.13175500	0.82821500	0.72248100
H	4.60244100	0.34199600	-0.88558300

### Int10



N	-1.63951300	-0.08264900	-0.00003600
C	-2.45087300	1.12906500	0.00004100
H	-2.20287600	1.73287300	0.88165200
H	-2.20288600	1.73296900	-0.88151400
C	-2.44689700	-1.08908500	-0.00017300
H	-2.07243600	-2.10820600	-0.00028800
C	-3.85255600	-0.69084000	-0.00019500
C	-3.86520800	0.65272800	0.00000100
H	-4.69380500	-1.36945200	-0.00032400
H	-4.72835600	1.30524900	0.00005800
Cu	0.34754000	-0.05633100	0.00000600
Br	2.65689900	0.02592900	0.00007000

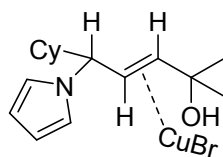
### TS5



C	-1.29062900	0.35845700	1.18146400
H	-1.81601800	1.02873400	1.87802100
C	0.04289800	0.96860400	0.71549900
C	0.18491800	2.29316800	0.59493200
N	-0.83491500	-0.80859300	1.98073500
C	0.26252300	-0.50850500	2.83957500
H	0.82627500	0.17164900	1.88265000
H	0.09820800	0.21627900	3.63232000
C	-0.61038300	-2.01653500	1.45577200

H	-0.65075100	2.98165900	0.76185200
H	-1.18616200	-2.38530000	0.61751800
C	0.46595800	-2.65216700	2.11218100
C	0.98087000	-1.73671100	3.00200000
C	1.44393800	3.00986000	0.15275600
H	0.82430300	-3.64771400	1.89748400
H	1.81161600	-1.88041700	3.67927300
O	1.29904700	4.32914600	0.67310200
H	2.04398200	4.85176500	0.35409400
C	2.72086100	2.37722300	0.70597500
H	2.88982500	1.37131200	0.30872700
H	3.58466100	2.98762100	0.42100900
H	2.67368400	2.32636000	1.79679900
C	1.48096700	3.05532200	-1.38018700
H	2.33980900	3.64601100	-1.72066000
H	1.57329100	2.04645800	-1.79550800
H	0.56713000	3.51501500	-1.76654400
Cu	1.19197400	-0.37376500	-0.33763500
Br	2.30280900	-1.97785500	-1.63950700
C	-2.25515100	-0.02789700	0.05654900
C	-3.52527400	-0.70766100	0.59306500
C	-2.63795700	1.20734100	-0.76993300
H	-1.73072200	-0.71760700	-0.62466600
C	-4.48665000	-1.07580100	-0.53929500
H	-4.02425600	-0.00794900	1.27925400
H	-3.28062700	-1.59596800	1.18570500
C	-3.60416300	0.84616100	-1.89917400
H	-3.10871800	1.94794200	-0.10561000
H	-1.73784100	1.67198600	-1.18159100
C	-4.85905000	0.15512800	-1.36624500
H	-5.38325100	-1.54929700	-0.12686200
H	-4.00700800	-1.81786700	-1.19209600
H	-3.87055100	1.74747400	-2.45977900
H	-3.09309700	0.17552000	-2.60286200
H	-5.52123500	-0.12590400	-2.19113500
H	-5.41812100	0.85739100	-0.73281900

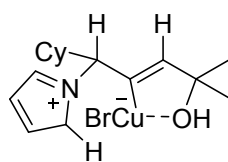
**Int11**



C	-1.53527700	0.25411600	-0.32442200
H	-1.35457000	0.09001500	-1.39535100

C	-0.28084800	0.84092100	0.29264800
C	0.57571600	1.63661400	-0.38893300
N	-2.60778800	1.23778600	-0.24916300
C	-3.24546000	1.79939500	-1.32439600
H	-2.96795900	1.52170000	-2.33104000
C	-3.14590200	1.74284700	0.90788200
H	0.38502200	1.83834500	-1.44575400
H	-2.77801900	1.43138400	1.87476600
C	-4.13746000	2.63182600	0.56511900
C	-4.20217600	2.66693400	-0.85323300
C	1.69135800	2.43779000	0.27855200
H	-4.74611900	3.19489900	1.25688300
H	-4.87249500	3.25751300	-1.45957500
O	2.13459000	1.76468200	1.44807000
C	2.84795400	2.67156800	-0.69145800
H	2.50705300	3.21172100	-1.57934500
H	3.61802900	3.26933300	-0.19710500
H	3.29383900	1.72247800	-1.00986800
C	1.08678000	3.76491400	0.74241300
H	1.86945200	4.37799400	1.19554900
H	0.64598600	4.30949000	-0.09701100
H	0.30685800	3.57686500	1.48432400
Cu	1.47547000	-0.43060400	-0.18821800
Br	3.66558900	-1.27690700	-0.21473500
H	-0.14861900	0.74837800	1.37390600
H	2.88012800	1.18618400	1.21902700
C	-1.96567600	-1.08449300	0.29850600
C	-3.22787700	-1.60775800	-0.39680100
C	-0.83956900	-2.12498900	0.24308900
H	-2.20528800	-0.90099000	1.35794300
C	-3.66456700	-2.96540100	0.15335300
H	-3.01580200	-1.70686100	-1.47256800
H	-4.03274000	-0.87243400	-0.29770900
C	-1.28574000	-3.49512000	0.76381300
H	-0.48903800	-2.22740600	-0.79788200
H	0.01810700	-1.80072700	0.85469800
C	-2.53727700	-3.99148600	0.04036800
H	-4.55657000	-3.31133600	-0.37774300
H	-3.94753000	-2.85294500	1.20865000
H	-0.46431900	-4.21009400	0.66149500
H	-1.50167000	-3.40839300	1.83686700
H	-2.85128700	-4.95598800	0.45125100
H	-2.30276900	-4.15787800	-1.01978100

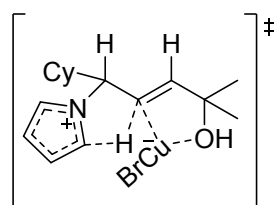
Int12



C	-1.21340800	0.20020400	0.99351800
H	-1.71254700	0.68999700	1.84799500
C	-0.05582800	0.99952300	0.41997700
C	0.11293400	2.25664100	0.83530000
N	-0.59082000	-1.02212000	1.56625400
C	0.01639200	-0.99748200	2.88929200
H	0.61038700	-0.07404100	2.95652400
H	-0.75420500	-0.97976400	3.66744200
C	-0.08997200	-2.00234700	0.87130600
H	-0.55968200	2.76093300	1.54444300
H	-0.32568400	-2.14888500	-0.17638500
C	0.80554300	-2.80539100	1.68232800
C	0.86937100	-2.22126100	2.89197800
C	1.23029200	3.14372400	0.31981300
H	1.33484100	-3.67089200	1.31180900
H	1.44765200	-2.54233100	3.74791700
O	2.19551600	2.30033400	-0.31274300
H	2.84684300	2.85560000	-0.75629500
C	0.66733500	4.12999300	-0.70740200
H	-0.12560600	4.74095400	-0.26612500
H	1.44924000	4.80643100	-1.07401700
H	0.25167500	3.57261000	-1.55082900
C	1.89892500	3.88159200	1.48110600
H	2.70106000	4.53321100	1.11682300
H	1.17513400	4.50395600	2.01613700
H	2.32714700	3.15845700	2.17970100
Cu	1.37241400	0.06712200	-0.67235400
Br	2.45009300	-1.97241300	-1.38055400
C	-2.28220800	-0.15860400	-0.04632900
C	-3.36836300	-1.08597600	0.51358000
C	-2.90767000	1.13348400	-0.58619700
H	-1.77857400	-0.65316700	-0.89160900
C	-4.45167700	-1.37750400	-0.52770000
H	-3.82843400	-0.59832500	1.38602400
H	-2.93280800	-2.02544800	0.87326300
C	-3.99593600	0.84269400	-1.62043900
H	-3.34354400	1.69005200	0.25811400
H	-2.12272800	1.76522400	-1.01090500
C	-5.07276000	-0.08278000	-1.05271000

H	-5.22005800	-2.02726000	-0.09638900
H	-4.00406600	-1.92840000	-1.36599000
H	-4.44002600	1.78114400	-1.96737900
H	-3.53709400	0.36676300	-2.49738900
H	-5.82866300	-0.30330400	-1.81320900
H	-5.58971500	0.42748800	-0.22838000

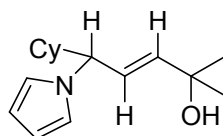
**TS6**



C	-1.38427700	0.20944300	1.18432900
H	-1.93541200	0.77036900	1.95450700
C	-0.08077700	0.90914000	0.78187300
C	0.03982800	2.23502800	0.68266800
N	-0.88482100	-1.02404800	1.84410600
C	0.18006300	-0.77423000	2.76086300
H	0.73146600	0.02491600	1.91769400
H	-0.04696800	-0.17884600	3.64120200
C	-0.55805700	-2.12296900	1.15649400
H	-0.79329700	2.92629300	0.85335400
H	-1.08225100	-2.40391900	0.25319900
C	0.53904100	-2.78039900	1.75492400
C	0.96874900	-1.97292100	2.78139500
C	1.32703500	2.91177500	0.25845200
H	0.97260200	-3.70563700	1.40624900
H	1.79373700	-2.15690600	3.45598400
O	2.34700700	1.91258400	0.24042900
H	3.07402900	2.20979400	-0.31951600
C	1.14335400	3.48436400	-1.14980200
H	0.31382700	4.19664100	-1.17704000
H	2.04904300	4.01103700	-1.47372600
H	0.93207700	2.67227700	-1.85159700
C	1.71367300	4.00487600	1.25548000
H	2.63585400	4.50174800	0.93765900
H	0.92679700	4.76110100	1.33183600
H	1.87669400	3.56388000	2.24156500
Cu	1.34464500	-0.17398300	-0.26938700
Br	2.50678900	-1.74708600	-1.61335400
C	-2.33855100	-0.08586300	0.02273900
C	-3.54863200	-0.92097800	0.47184900
C	-2.82357300	1.21741100	-0.62670700

H	-1.77670700	-0.63611200	-0.74816900
C	-4.50053300	-1.20488500	-0.69152300
H	-4.08402100	-0.35785900	1.25029300
H	-3.23207900	-1.86041100	0.93720900
C	-3.78203100	0.94145400	-1.78669500
H	-3.33433500	1.82639500	0.13514900
H	-1.96591500	1.79585000	-0.98094700
C	-4.97453400	0.09389700	-1.34392700
H	-5.35403600	-1.79337600	-0.34022300
H	-3.98009900	-1.81684300	-1.44088100
H	-4.12332700	1.88800900	-2.21771000
H	-3.23678300	0.41185500	-2.57917900
H	-5.62763800	-0.12254100	-2.19522200
H	-5.57253100	0.66261800	-0.61873900

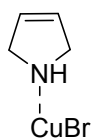
4



C	-0.26350700	0.35198800	-0.39938800
H	-0.22739600	0.22697800	-1.48934300
C	1.12113200	0.16642500	0.16073900
C	2.17563500	-0.20619800	-0.55763500
N	-0.73083300	1.71636500	-0.16536100
C	-1.22820400	2.55506300	-1.12639500
H	-1.19272400	2.27222100	-2.16848100
C	-0.90942200	2.29265000	1.06536800
H	2.06916400	-0.37693200	-1.63034000
H	-0.59188900	1.78889500	1.96659300
C	-1.51475400	3.51498200	0.88576900
C	-1.71738100	3.68281800	-0.50950200
C	3.56511900	-0.40737800	0.00977100
H	-1.77064900	4.21272000	1.66938800
H	-2.16223700	4.53262800	-1.00537600
O	3.54792600	-0.38585800	1.42918800
C	4.13853500	-1.73937300	-0.48316100
H	4.21453700	-1.75867100	-1.57417900
H	5.13384500	-1.88957700	-0.05726400
H	3.49547300	-2.57179400	-0.17619100
C	4.46435500	0.75612800	-0.40338400
H	5.47212200	0.60085200	-0.00900100
H	4.51694400	0.83797500	-1.49222300
H	4.06354900	1.68764200	0.00170200

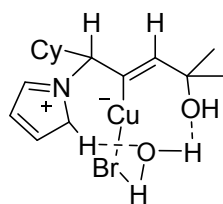
H	1.24853100	0.35396800	1.22679200
H	3.00008700	-1.12502500	1.72286000
C	-1.26983700	-0.67169800	0.16794300
C	-2.70251200	-0.35252400	-0.27432200
C	-0.88870500	-2.10008500	-0.23656200
H	-1.22899100	-0.60172700	1.26734600
C	-3.69861300	-1.38058200	0.26591600
H	-2.73778900	-0.35498600	-1.37482000
H	-2.97955800	0.65585300	0.05002600
C	-1.88761000	-3.12681300	0.30258700
H	-0.86978900	-2.15690400	-1.33589900
H	0.12503700	-2.33344900	0.10580200
C	-3.31344200	-2.80174400	-0.14558700
H	-4.70868900	-1.14046500	-0.08124800
H	-3.71817800	-1.31666100	1.36255100
H	-1.60189500	-4.13317700	-0.02075300
H	-1.84674300	-3.12293900	1.40048400
H	-4.01939000	-3.52721100	0.27165800
H	-3.37568800	-2.88987100	-1.23900700

**Int13**



N	-1.63223800	-0.00043200	0.52308300
C	-2.34762900	-1.19187700	-0.02506500
H	-1.83867700	-1.54279500	-0.93057500
H	-2.32529600	-2.00552300	0.70400600
C	-2.34673500	1.19187400	-0.02439600
H	-1.83753400	1.54290700	-0.92972300
H	-2.32375100	2.00509600	0.70512800
C	-3.72428400	0.66516100	-0.34624200
C	-3.72477700	-0.66393900	-0.34663400
H	-4.56106300	-1.30613800	-0.59347100
H	-4.56008800	1.30813600	-0.59269500
Cu	0.37166800	-0.00044100	0.23288000
Br	2.65042300	0.00021300	-0.16713700
H	-1.81052500	-0.00064700	1.52603800

Int14

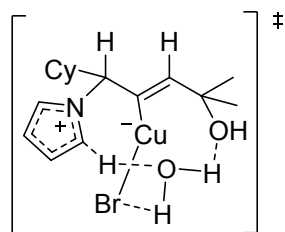


C	-1.29946500	0.28874000	0.93393400
H	-1.72019000	0.81241700	1.80972600
C	-0.17645100	1.05796500	0.26176800
C	0.14073700	2.25126500	0.77079400
N	-0.66507100	-0.93360600	1.49816500
C	0.01913200	-0.91456800	2.78452200
H	0.76609600	-0.10726700	2.73806200
H	-0.68980900	-0.74853200	3.60119900
C	-0.31271500	-1.99328900	0.83229400
H	-0.41377900	2.72091800	1.59464400
H	-0.63256100	-2.16103800	-0.18998100
C	0.53966000	-2.84826000	1.63000000
C	0.72670400	-2.22202600	2.80654600
C	1.30088700	3.07601700	0.24079200
H	0.95661500	-3.78071800	1.27930000
H	1.33093900	-2.55372200	3.64008400
O	2.33692500	2.14791100	-0.13675100
H	3.02817100	2.63122300	-0.60599100
C	0.87438000	3.86528800	-0.99708500
H	0.05058300	4.54243200	-0.75476400
H	1.70374900	4.46662900	-1.39042700
H	0.53571900	3.16638600	-1.76658600
C	1.84468900	3.99617800	1.33134700
H	2.69814900	4.57573400	0.96343100
H	1.07473600	4.69880900	1.66339400
H	2.17078800	3.40334700	2.19048700
Cu	1.07255000	0.01455700	-0.92782600
Br	2.27340500	-1.98565100	-1.53906800
O	2.65561900	-0.21213100	1.55526100
H	2.65366800	0.63371400	1.07811100
H	2.88410400	-0.86173300	0.87328400
C	-2.44910900	-0.07363500	-0.01273400
C	-3.52533200	-0.93522000	0.65923300
C	-3.06672500	1.21556200	-0.56788700
H	-2.02256300	-0.62051900	-0.86873600
C	-4.68104500	-1.23829600	-0.29723900
H	-3.91221100	-0.38985700	1.53284600
H	-3.09907000	-1.87125200	1.03849100



C	-4.22657000	0.91544900	-1.51895900
H	-3.43059400	1.82094000	0.27653300
H	-2.29077300	1.80221700	-1.06828200
C	-5.29344700	0.05107600	-0.84519100
H	-5.44105600	-1.84020900	0.21131000
H	-4.30456700	-1.84240800	-1.13386800
H	-4.66348400	1.85158700	-1.88085400
H	-3.83758900	0.38697800	-2.39974300
H	-6.10000700	-0.17897800	-1.54871500
H	-5.74500500	0.61406700	-0.01668700

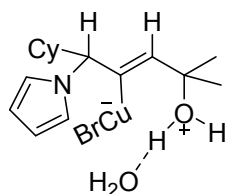
**TS7**



C	-1.39625600	0.11921700	0.90443700
H	-1.81647500	0.58956700	1.80980400
C	-0.22897000	0.90468300	0.34336700
C	0.07698900	2.05480900	0.95244600
N	-0.83562300	-1.17802300	1.37549200
C	0.05747700	-1.25342900	2.47543300
H	1.20008800	-0.77244100	2.05217900
H	-0.18543500	-0.64198500	3.34126800
C	-0.81713800	-2.33128100	0.72892700
H	-0.53138400	2.45467600	1.77479500
H	-1.32902300	-2.45576600	-0.21584900
C	-0.02906900	-3.27596500	1.42842200
C	0.45436600	-2.63362200	2.54144600
C	1.28634200	2.90652100	0.58499600
H	0.16136100	-4.28858900	1.10723300
H	1.11158500	-3.04081600	3.29807900
O	2.46817900	2.07799700	0.46145800
H	2.57619400	1.80793000	-0.46170700
C	1.06170600	3.63392100	-0.73816200
H	0.19012900	4.29003300	-0.66775900
H	1.93685900	4.23520000	-1.00441500
H	0.86323100	2.90361000	-1.53124900
C	1.60687300	3.88634200	1.70695600
H	2.48392700	4.48402700	1.44882700
H	0.75834800	4.55341400	1.88258800
H	1.81616600	3.34223900	2.63263100

Cu	0.96445800	-0.09971800	-0.91637500
Br	2.82454300	-1.42999000	-1.58864800
O	2.44114900	-0.35055600	1.69344300
H	2.41514100	0.57961400	1.34282100
H	2.75827000	-0.88724500	0.93871700
C	-2.53847300	-0.08615800	-0.09677600
C	-3.72259200	-0.86776200	0.48959400
C	-3.01873700	1.28043400	-0.60567900
H	-2.13695400	-0.62573100	-0.96978800
C	-4.84959800	-1.02594000	-0.53392000
H	-4.10124600	-0.31554800	1.36201900
H	-3.40994000	-1.85055100	0.85875800
C	-4.15080600	1.13270100	-1.62310300
H	-3.36925600	1.87122800	0.25433700
H	-2.17644800	1.82569100	-1.04101400
C	-5.32152200	0.33448800	-1.04928700
H	-5.68330300	-1.57956400	-0.09007700
H	-4.48522500	-1.62555400	-1.37959200
H	-4.48625900	2.12101700	-1.95304300
H	-3.76407300	0.61759300	-2.51306300
H	-6.10462900	0.20586400	-1.80329600
H	-5.76874300	0.89644200	-0.21788400

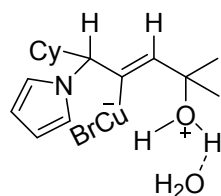
**Int15**



C	1.54283800	0.05673900	0.92715800
H	1.95551000	-0.26080800	1.89952600
C	0.24375800	-0.65457100	0.60475300
C	-0.30651700	-1.40013700	1.57189600
N	1.19797900	1.48123700	1.09449600
C	0.73430100	2.00456000	2.26922000
H	-1.45871800	1.73478900	1.59201500
H	0.86111500	1.46312900	3.19583800
C	0.89643600	2.34695500	0.07516900
H	0.19147900	-1.57395800	2.53395300
H	1.16408700	2.12094000	-0.94676900
C	0.26228900	3.44922700	0.60620000
C	0.15687400	3.23282600	2.00908700
C	-1.67016900	-2.05398000	1.45835400
H	-0.06027500	4.32007800	0.05492600

H	-0.25138900	3.91094400	2.74439400
O	-2.69803200	-1.01800800	1.08248400
H	-2.91461800	-1.03409400	0.12318800
C	-1.74122400	-3.11096900	0.36653500
H	-1.05410400	-3.92229700	0.61670400
H	-2.75218900	-3.52110100	0.27616100
H	-1.42278400	-2.69104600	-0.59295200
C	-2.15093600	-2.58511400	2.79824900
H	-3.15288400	-3.01043000	2.71139000
H	-1.46331400	-3.36124000	3.14381300
H	-2.16662700	-1.78532200	3.54379000
Cu	-0.79851700	-0.06398300	-1.00810500
Br	-2.95829100	0.48205000	-1.93706900
O	-2.32278500	1.36473700	1.31625200
H	-2.43258000	0.04915400	1.28222600
H	-2.49209100	1.67633500	0.40716900
C	2.62631700	-0.14725800	-0.13380700
C	3.90353100	0.64104900	0.17299300
C	2.93702000	-1.64155600	-0.27776100
H	2.22311300	0.19394000	-1.10108200
C	4.98101400	0.39277500	-0.88495200
H	4.28122700	0.32379800	1.15637200
H	3.68031200	1.71036800	0.25008700
C	4.01422100	-1.88920700	-1.33536100
H	3.28348200	-2.02346900	0.69466900
H	2.01958700	-2.18722600	-0.52341100
C	5.28705500	-1.09962900	-1.02547800
H	5.88968100	0.94909400	-0.63331700
H	4.63065800	0.78062300	-1.85130700
H	4.23372300	-2.95952100	-1.40557200
H	3.62851700	-1.57967900	-2.31638600
H	6.03921800	-1.26389700	-1.80392700
H	5.71688000	-1.46811900	-0.08393300

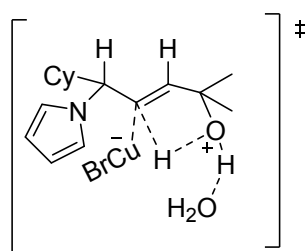
**Int16**



C	1.57894100	1.03082900	0.06813700
H	2.07135800	1.88449200	0.56112200
C	0.10386100	0.97721300	0.41725900
C	-0.37147800	1.89193700	1.27157300

N	1. 71703000	1. 27686500	-1. 36899300
C	1. 96859400	2. 49955800	-1. 92780200
H	2. 19107900	3. 34911400	-1. 29851600
C	1. 45149200	0. 37708900	-2. 37003700
H	0. 25451800	2. 64996800	1. 75340600
H	1. 23208100	-0. 65876100	-2. 15103300
C	1. 55360800	1. 03118900	-3. 57756400
C	1. 88285600	2. 38331900	-3. 29637600
C	-1. 84832100	1. 98814400	1. 60430700
H	1. 42103500	0. 58069200	-4. 55016300
H	2. 05125800	3. 17529400	-4. 01095600
O	-2. 55871200	1. 81473600	0. 28453100
C	-2. 33287300	0. 87432400	2. 52270300
H	-1. 82449200	0. 97274100	3. 48481100
H	-3. 41306400	0. 92770300	2. 68957600
H	-2. 07493000	-0. 10433400	2. 10594400
C	-2. 24300400	3. 36673300	2. 09971400
H	-3. 32309500	3. 43519500	2. 25100500
H	-1. 74524300	3. 55879100	3. 05380200
H	-1. 93151300	4. 13129300	1. 38464000
Cu	-0. 86854000	-0. 63263000	-0. 33140300
Br	-2. 40658500	-2. 38089700	-0. 87759200
H	-1. 82973300	1. 58789300	-0. 34369200
H	-3. 31983800	1. 03531200	0. 25248400
O	-4. 24173700	0. 04872800	0. 18758700
H	-3. 80253300	-0. 81375700	-0. 02834700
H	-4. 92554900	0. 17462100	-0. 48261500
C	2. 33087500	-0. 24157000	0. 49140900
C	3. 80717800	-0. 19032400	0. 08291700
C	2. 19495300	-0. 47210200	2. 00090500
H	1. 86036500	-1. 10063600	-0. 01674600
C	4. 55759000	-1. 44603600	0. 53096400
H	4. 26728900	0. 69333700	0. 55009800
H	3. 89164300	-0. 05684200	-1. 00010000
C	2. 95199900	-1. 72353500	2. 45023600
H	2. 59572400	0. 40828900	2. 52681000
H	1. 13673900	-0. 54689900	2. 27381500
C	4. 42409600	-1. 66297900	2. 03913000
H	5. 61195200	-1. 37499000	0. 24503400
H	4. 14502300	-2. 31713400	0. 00401400
H	2. 86041000	-1. 84787800	3. 53419100
H	2. 48595100	-2. 60548300	1. 99023100
H	4. 94300300	-2. 57806500	2. 34258700
H	4. 91086300	-0. 83079900	2. 56614600

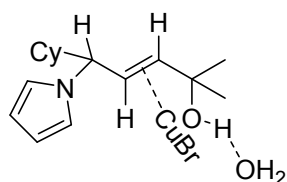
TS8



C	1.51486700	0.95838600	0.54841300
H	1.94913700	1.41931700	1.44842700
C	0.00932900	1.13713700	0.54760200
C	-0.60447800	1.78228700	1.54256300
N	2.08995800	1.68340500	-0.58258500
C	3.07235100	2.63252500	-0.49461100
H	3.42605300	2.96358800	0.47093200
C	1.83263300	1.42772000	-1.90458800
H	-0.11836400	2.18400400	2.43467600
H	1.08752500	0.70068400	-2.19587600
C	2.65337100	2.22782000	-2.66602100
C	3.44220800	2.99575400	-1.76903000
C	-2.08472100	2.10422000	1.36719300
H	2.67652400	2.26086100	-3.74524400
H	4.18989200	3.73174700	-2.02488800
O	-2.26357600	1.98030500	-0.08336700
C	-2.99232600	1.10425800	2.07460900
H	-2.82009200	1.16078600	3.15247900
H	-4.04706700	1.31723500	1.87744600
H	-2.76617300	0.08289700	1.74920300
C	-2.39328800	3.54347500	1.74324900
H	-3.44241800	3.77687100	1.54391500
H	-2.19761900	3.69540700	2.80845100
H	-1.76156100	4.22473000	1.16917400
Cu	-0.85748800	-0.51692200	-0.39389800
Br	-2.16547500	-2.36118900	-1.09803100
H	-1.23762400	1.53566600	-0.31294200
H	-3.01867400	1.33631000	-0.36537200
O	-4.05001300	0.35629600	-0.81874000
H	-3.70225900	-0.56085900	-0.81721000
H	-4.36586500	0.50695900	-1.71792400
C	1.95500500	-0.51882500	0.51894400
C	3.47725600	-0.65716000	0.41821000
C	1.42531500	-1.29128400	1.73228100
H	1.52858900	-0.97692200	-0.39371700
C	3.89733500	-2.12776100	0.36788300

H	3.93214200	-0.17496000	1.29704400
H	3.84151100	-0.12222700	-0.46504400
C	1.84111700	-2.76261700	1.68017800
H	1.82595100	-0.82350900	2.64471900
H	0.33226500	-1.21377000	1.80021200
C	3.36011400	-2.90467500	1.57092900
H	4.98823100	-2.20373100	0.31735500
H	3.50619300	-2.57671600	-0.55514100
H	1.46833800	-3.28793300	2.56521900
H	1.36382300	-3.23273900	0.80939800
H	3.63885700	-3.96094000	1.49927200
H	3.82391100	-2.51464900	2.48769300

**Int17**



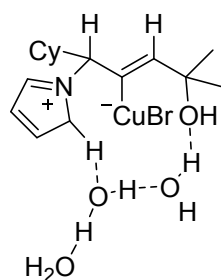
C	-1.51510600	0.18141500	-0.28100300
H	-1.17310700	-0.09643400	-1.28747200
C	-0.41427100	0.96438000	0.41312600
C	0.41096100	1.81534000	-0.23604000
N	-2.66829500	1.05082800	-0.48008300
C	-3.25147500	1.33137100	-1.68787400
H	-2.84295800	0.92187100	-2.60048400
C	-3.37645500	1.67195300	0.51728400
H	0.32842700	1.91984400	-1.32094000
H	-3.07485000	1.58286100	1.55091600
C	-4.41882900	2.35719300	-0.06152200
C	-4.34062200	2.13992100	-1.46288400
C	1.33188600	2.79543000	0.47795500
H	-5.15212700	2.95043400	0.46423000
H	-5.00514100	2.52993600	-2.21922600
O	1.47267900	2.44694900	1.83900400
C	2.69478100	2.85634100	-0.21537800
H	2.59045100	3.13741200	-1.26717500
H	3.32306900	3.59626200	0.28684100
H	3.20336500	1.88510600	-0.17936600
C	0.64623600	4.16335500	0.45360800
H	1.29084300	4.89469500	0.94716300
H	0.45365400	4.49066100	-0.57144800
H	-0.30399100	4.10753100	0.99027900
Cu	1.46356100	-0.18237500	-0.05872000

Br	3.17133400	-1.48839800	-1.12284000
H	-0.39254900	0.97001800	1.50436900
H	2.11639800	1.72421300	1.91144500
O	2.86889400	-0.08359800	1.84498500
H	3.50830700	-0.52264800	1.25507700
H	2.70194900	-0.70434500	2.56372700
C	-1.91458500	-1.10392300	0.46389400
C	-3.03543200	-1.83070900	-0.28825700
C	-0.71134000	-2.03163500	0.67586000
H	-2.29882600	-0.80884600	1.45368200
C	-3.42728800	-3.14053300	0.39589100
H	-2.68595700	-2.04714500	-1.30938600
H	-3.90315900	-1.16986200	-0.38175200
C	-1.10963000	-3.35069000	1.34477200
H	-0.23940500	-2.24704200	-0.29634000
H	0.04718100	-1.53799300	1.30378200
C	-2.21675900	-4.05856600	0.56400900
H	-4.21300600	-3.63993100	-0.17923300
H	-3.85221700	-2.91793100	1.38421800
H	-0.22958500	-3.99438300	1.43809900
H	-1.46535200	-3.14082700	2.36262700
H	-2.50317800	-4.98452400	1.07246800
H	-1.83513100	-4.34258900	-0.42578500

**water cluster**

O	0.10716500	1.57578400	0.11811500
H	0.03511000	2.09531900	-0.68849300
H	-0.66199000	0.97161500	0.10127200
O	1.32035700	-0.87778500	-0.10178800
O	-1.42526500	-0.68767000	-0.09332500
H	-0.52785900	-1.07277300	-0.13766300
H	-1.83286800	-1.06421700	0.69212700
H	1.17936300	0.08913000	-0.05824200
H	1.79018400	-1.10170700	0.70698200

**Int18**



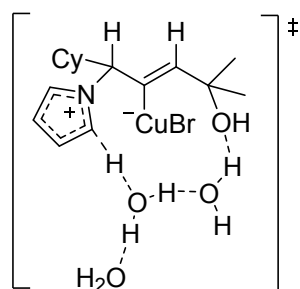
C	1.48333600	0.04202500	-0.90656800
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H	1.97361600	0.38501900	-1.83356000
C	0.25947900	0.85796300	-0.56108100
C	0.08357400	1.97616800	-1.27073700
N	1.08821400	-1.36029400	-1.20423600
C	1.31283000	-1.98061800	-2.49908900
H	0.68883300	-1.43182100	-3.22003900
H	2.37315300	-1.93486700	-2.76832600
C	0.44553700	-2.17182500	-0.42566600
H	0.75930300	2.27114500	-2.08658500
H	0.13549200	-1.87879500	0.57413300
C	0.22640200	-3.44455500	-1.08352600
C	0.76175700	-3.34881100	-2.31436300
C	-1.01323700	2.99406000	-1.03918700
H	-0.30587700	-4.27043300	-0.63636800
H	0.76318900	-4.10080900	-3.09213000
O	-1.91653300	2.46394200	-0.05378300
H	-2.50941000	3.16863800	0.23448800
C	-0.40297000	4.28734000	-0.49580800
H	0.33830600	4.68523400	-1.19430200
H	-1.17313000	5.05487500	-0.35095100
H	0.08831900	4.08796200	0.46008900
C	-1.78769400	3.24847000	-2.33392300
H	-2.56588000	4.00401500	-2.17754200
H	-1.11639000	3.61166600	-3.11755500
H	-2.25872500	2.32248300	-2.67381500
Cu	-1.02534300	0.36159000	0.89485000
Br	-2.26532200	-0.90487100	2.52791000
O	-1.44136600	-1.28756500	-2.77637500
H	-1.89283000	-0.46079700	-2.53414000
H	-1.81424000	-1.89746200	-2.12430800
O	-3.23340700	0.31678100	-1.37719800
O	-2.62767500	-2.45682700	-0.36679100
H	-3.47346300	-2.91766800	-0.39598700
H	-2.54080400	-2.14369500	0.55611200
H	-2.87107000	1.02764000	-0.82407800
H	-3.18960000	-0.48738100	-0.83902500
C	2.53869000	0.02534900	0.21765600
C	3.73734100	-0.86623800	-0.13169700
C	3.00244500	1.45186500	0.52756600
H	2.04503800	-0.37304200	1.11932600
C	4.80334500	-0.84397000	0.96602100
H	4.18129300	-0.50276400	-1.07151700
H	3.41161600	-1.89906300	-0.31008500
C	4.07318200	1.47129000	1.62018100



H	3.40850900	1.89577600	-0.39466400
H	2.14024000	2.05839400	0.81616800
C	5.26418000	0.58471500	1.25403300
H	5.65159300	-1.47327700	0.67793400
H	4.38164000	-1.27813100	1.88235300
H	4.40153000	2.49992200	1.80036900
H	3.63178500	1.11139800	2.55922900
H	6.00801500	0.59047700	2.05721600
H	5.75633400	0.99176600	0.36001800

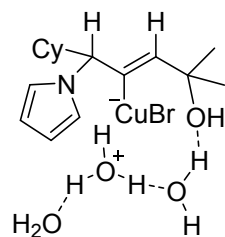
**TS9**



C	-1.58521000	0.17634500	0.97185500
H	-2.11647100	0.67324400	1.80364800
C	-0.24762400	0.82679100	0.70158100
C	0.00411600	1.92568400	1.42109900
N	-1.36193500	-1.20883900	1.46728100
C	-0.66856900	-1.45499800	2.68928500
H	0.52317300	-1.46911400	2.31011500
H	-0.80376800	-0.71507500	3.47309000
C	-1.62852900	-2.35706200	0.88708200
H	-0.70294200	2.29784000	2.17782300
H	-2.02655600	-2.40853500	-0.11650100
C	-1.28857000	-3.43747300	1.74849400
C	-0.77668000	-2.88502500	2.88793700
C	1.20121300	2.84098600	1.28226500
H	-1.39507600	-4.48254200	1.50042200
H	-0.36934400	-3.40730700	3.74312100
O	2.11507700	2.26998600	0.33270600
H	2.67867200	2.97124300	-0.01551500
C	0.73346900	4.19842100	0.75422400
H	-0.00425500	4.63918000	1.42985400
H	1.57366800	4.89933600	0.67294700
H	0.27257600	4.07007700	-0.22873100
C	1.92060300	2.98847900	2.62461300
H	2.77431900	3.66880700	2.53547500
H	1.24292500	3.38802600	3.38466200
H	2.28246400	2.01264300	2.96016200

Cu	1.01124800	0.14072100	-0.69607700
Br	2.50941000	-0.79460200	-2.35650400
O	1.76404700	-1.87602300	1.70067400
H	2.42006800	-1.17157800	1.44891900
H	1.49908700	-2.32787800	0.86981800
O	3.53305000	-0.07562600	0.86426000
O	0.86750700	-3.13307100	-0.61975800
H	1.33703700	-3.96817300	-0.72602300
H	1.22908900	-2.55751800	-1.32034700
H	3.09907600	0.79420800	0.77841600
H	3.69904100	-0.34459400	-0.05373000
C	-2.52403300	0.18184800	-0.24502600
C	-3.94506400	-0.28945300	0.10594300
C	-2.59430500	1.58543800	-0.86386200
H	-2.09023700	-0.47801500	-1.01355600
C	-4.86156000	-0.28313400	-1.11901300
H	-4.35289500	0.39789700	0.86108000
H	-3.94344800	-1.28300700	0.56702100
C	-3.51782600	1.61140300	-2.08321500
H	-2.95872100	2.29094400	-0.10150700
H	-1.58904800	1.91263500	-1.14092500
C	-4.92226300	1.10966200	-1.74605100
H	-5.86372600	-0.62403000	-0.83926200
H	-4.47819500	-0.99801000	-1.86018200
H	-3.56235300	2.62556500	-2.49302200
H	-3.08569400	0.97418400	-2.86681600
H	-5.55229500	1.10052100	-2.64128200
H	-5.39067200	1.80147500	-1.03258100

**Int19**

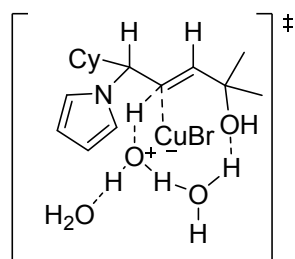


C	-1.55510900	-0.09644400	0.78799400
H	-1.99876900	0.24502300	1.73707000
C	-0.39793100	0.80023400	0.37449200
C	-0.37989400	2.01814200	0.94489200
N	-1.09065800	-1.46888200	1.06074400
C	-0.95618200	-2.01724000	2.30440800
H	1.22140400	0.46649900	1.81632100
H	-1.18903400	-1.43765500	3.18606900

C	-0.75285800	-2.40429000	0.12062800
H	-1.14644900	2.30889400	1.67757900
H	-0.80481300	-2.18319600	-0.93597800
C	-0.40996700	-3.57360600	0.77237000
C	-0.53613100	-3.32553500	2.16778200
C	0.55022600	3.17247000	0.61562200
H	-0.11985300	-4.49874500	0.29562900
H	-0.35905700	-4.02271300	2.97329700
O	1.49563300	2.82344200	-0.40439400
H	1.00368500	2.36036300	-1.10053100
C	-0.28381100	4.35124700	0.10500200
H	-1.01706900	4.66373700	0.85378400
H	0.36877100	5.19674800	-0.12774100
H	-0.82550400	4.06403300	-0.80163200
C	1.37269700	3.59417900	1.83125300
H	2.03563200	4.42241500	1.56652500
H	0.70905900	3.92103900	2.63570800
H	1.98027000	2.76724500	2.20964200
Cu	1.00473100	-0.08361500	-0.77979000
Br	2.93025600	-1.12947400	-1.77058300
O	2.11867000	0.15518600	2.07397900
H	2.80194600	0.67595400	1.41599600
H	2.18143900	-0.88621600	1.83208800
O	3.55618500	1.34640100	0.47805100
O	2.32376400	-2.19407300	1.38325600
H	1.48827100	-2.69756200	1.41842500
H	2.61133500	-2.20008700	0.45030100
H	2.92197600	1.98404300	0.06658700
H	3.80502600	0.72848400	-0.23338900
C	-2.69456700	-0.12725000	-0.25281200
C	-3.81468600	-1.08512300	0.17723200
C	-3.26519200	1.27550500	-0.49276000
H	-2.27388900	-0.48116600	-1.20743600
C	-4.96436200	-1.10521600	-0.83185600
H	-4.19690700	-0.75267600	1.15421800
H	-3.41922700	-2.09598100	0.31909400
C	-4.41843200	1.25383000	-1.49850700
H	-3.62520600	1.67760700	0.46713500
H	-2.47553600	1.94834600	-0.83848200
C	-5.52713100	0.29754300	-1.06024500
H	-5.75036400	-1.78494300	-0.48736900
H	-4.59619500	-1.50531900	-1.78637200
H	-4.81372300	2.26593900	-1.63279600
H	-4.03282300	0.93218500	-2.47556600

H	-6.32957000	0.27327000	-1.80471400
H	-5.97041300	0.66471900	-0.12444900

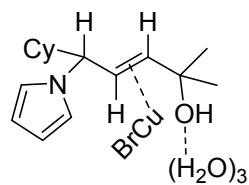
**TS10**



C	-1.56111900	0.04246100	1.08431700
H	-2.10284000	0.46535600	1.94447000
C	-0.21615000	0.73131300	0.92407700
C	-0.12276400	2.03964700	1.20944900
N	-1.35076800	-1.38041500	1.40506900
C	-0.97357700	-1.82327100	2.64465300
H	0.95664500	0.02843800	1.36176500
H	-0.85144500	-1.12179600	3.45741700
C	-1.39284300	-2.44896400	0.54779700
H	-0.97810700	2.59136400	1.61851600
H	-1.68085000	-2.33694100	-0.48634500
C	-1.07523800	-3.59010300	1.25979300
C	-0.79717400	-3.18675300	2.59427800
C	1.12616800	2.88960100	1.04629100
H	-1.07396800	-4.59698600	0.86695200
H	-0.51079500	-3.81970400	3.42055600
O	1.98469800	2.36177900	0.02325800
H	1.58364000	2.53272300	-0.84024900
C	0.73924000	4.31953400	0.67104300
H	0.13838500	4.77853500	1.46046300
H	1.63944600	4.92029400	0.51889100
H	0.14605900	4.33051100	-0.25073300
C	1.95389800	2.86781800	2.33041300
H	2.84822000	3.48521800	2.20902100
H	1.36437400	3.25921800	3.16327800
H	2.25136700	1.84559600	2.57626400
Cu	0.91929600	-0.03779100	-0.66988400
Br	2.25217700	-1.01974500	-2.37632600
O	1.90949700	-0.53936300	1.90512000
H	2.73827800	-0.18794900	1.45238100
H	1.85730500	-1.48804000	1.56802900
O	3.86553600	0.36381900	0.42314600
O	1.84613900	-2.78391000	0.61792800

H	0.94609600	-3.14961800	0.62726500
H	2.05764800	-2.59434800	-0.31094500
H	3.47822800	1.22201000	0.17963000
H	3.84413300	-0.15329400	-0.39820500
C	-2.49082000	0.18558300	-0.14335200
C	-3.85766000	-0.47189900	0.11528100
C	-2.71270800	1.64588800	-0.55909000
H	-2.00508200	-0.31530200	-0.99725500
C	-4.76622500	-0.38898100	-1.11192300
H	-4.33418000	0.05818000	0.95321000
H	-3.74209300	-1.51204600	0.42996100
C	-3.62724900	1.74554900	-1.78340400
H	-3.16447100	2.19303100	0.28276400
H	-1.75793200	2.13162100	-0.77722400
C	-4.97294800	1.06119400	-1.54590000
H	-5.72709300	-0.86747100	-0.89749800
H	-4.30881800	-0.95325600	-1.93648300
H	-3.77260000	2.79740700	-2.05015200
H	-3.12661900	1.26903400	-2.63728500
H	-5.59131700	1.11009100	-2.44780300
H	-5.51595900	1.59777600	-0.75604600

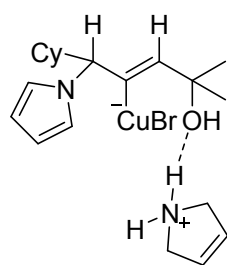
**Int20**



C	1.45322600	0.37126100	-0.58119300
H	1.24285000	0.68891300	-1.61234900
C	0.32633100	-0.53485100	-0.12049800
C	-0.51129900	-1.16230000	-0.98217500
N	2.70784700	-0.37909200	-0.64906000
C	3.33926700	-0.73526800	-1.81698700
H	0.31961000	-0.81024600	0.93894500
H	2.89250500	-0.50613100	-2.77378500
C	3.49133700	-0.74034200	0.41795500
H	-0.38794200	-1.00698300	-2.05779200
H	3.13858600	-0.62080100	1.43242100
C	4.63334000	-1.33221100	-0.07578000
C	4.53558800	-1.33196400	-1.49557000
C	-1.54762300	-2.20918400	-0.55624600
H	5.44491000	-1.72292900	0.52074300
H	5.26098400	-1.71151900	-2.19980200

O	-2.17016000	-1.80029300	0.66808900
H	-2.96501400	-1.27208300	0.47676700
C	-2.60322800	-2.38872300	-1.64295500
H	-2.14204700	-2.73475700	-2.57219600
H	-3.33181300	-3.13646800	-1.31985700
H	-3.12805800	-1.44716200	-1.83871200
C	-0.83200500	-3.52045500	-0.24294800
H	-1.56823700	-4.27762200	0.03911100
H	-0.26436900	-3.87844900	-1.10609000
H	-0.13661200	-3.37508300	0.58632800
O	1.44345000	-2.06124000	2.26722800
H	0.65855700	-2.47833600	2.66522600
H	1.76499300	-2.69023500	1.60041600
O	-1.09040200	-3.02253600	2.97441200
O	2.25806300	-3.47347200	-0.14403800
H	1.91106400	-2.76313600	-0.69962000
H	3.20698700	-3.28538700	-0.14008200
H	-1.60334200	-2.59942700	2.26579800
H	-1.48688600	-2.73073900	3.80044400
C	1.64924300	1.63816200	0.27541000
C	2.73211400	2.52496300	-0.35309900
C	0.34510900	2.42079100	0.46483300
H	1.98845500	1.32013700	1.27187200
C	2.93494500	3.82668200	0.42273100
H	2.42817400	2.76611600	-1.38326100
H	3.67077700	1.96537900	-0.42013200
C	0.55401700	3.74340500	1.21136400
H	-0.10624300	2.63453500	-0.52057400
H	-0.36826000	1.82592600	1.06271300
C	1.62372400	4.60266500	0.54008400
H	3.70125700	4.43426600	-0.06809500
H	3.31047800	3.59382300	1.42811200
H	-0.39797000	4.27821900	1.27612600
H	0.86615800	3.51789700	2.23939000
H	1.77129200	5.52797700	1.10530600
H	1.28159700	4.89228000	-0.46274800
Cu	-1.57753200	0.68464700	-0.24908500
Br	-3.89860200	1.14929900	-0.30522400

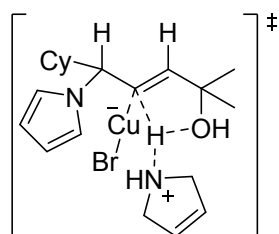
Int21



C	1.68248600	-0.84151800	-0.58499200
H	1.97088100	-1.40338800	-1.48932500
C	0.49560100	0.06079500	-0.84149800
C	-0.07943400	0.00810900	-2.05192800
N	1.26573400	-1.87673500	0.38514200
C	0.91804200	-3.15515800	0.05436300
H	-1.26394500	-1.94051600	0.96735900
H	1.07494000	-3.51935400	-0.95102400
C	0.97281000	-1.66036000	1.70343200
H	0.33933300	-0.60276900	-2.86500200
H	1.16345700	-0.70386300	2.16817800
C	0.43068400	-2.82135900	2.22641300
C	0.39789300	-3.77655800	1.17281200
H	0.13440000	-2.97133200	3.25443600
H	0.06940800	-4.80409200	1.23377200
Cu	-0.26972400	1.24013000	0.59911400
Br	-1.91797600	2.37704800	1.88786400
C	-3.23203500	-1.12335600	0.93417700
C	-4.26445000	-1.58919700	-0.05102900
C	-3.74057000	-2.36613000	-0.99149700
C	-2.26448700	-2.55932900	-0.79238000
N	-1.94703400	-1.56996100	0.29009900
H	-1.51838400	-0.74279900	-0.17104400
H	-3.33106800	-1.60604300	1.91114100
H	-5.30530700	-1.30618000	0.03842300
H	-4.27578900	-2.83528200	-1.80709300
H	-1.64318600	-2.31168800	-1.65903300
H	-3.18778300	-0.03971300	1.08146800
H	-1.99746000	-3.56225600	-0.44748900
C	2.91992800	-0.08825600	-0.08413700
C	4.09081300	-1.02942000	0.21516000
C	3.33132300	0.97828900	-1.10469400
H	2.64087600	0.43576800	0.84490000
C	5.32929200	-0.25848500	0.67742600
H	4.33414800	-1.58645100	-0.70223500
H	3.79762100	-1.76994500	0.96744000

C	4.57043500	1.74684300	-0.64274200
H	3.54289200	0.48188700	-2.06445900
H	2.49538300	1.66299600	-1.28175100
C	5.73562500	0.80132800	-0.34793700
H	6.15600000	-0.95234700	0.86195400
H	5.10906000	0.23294800	1.63497400
H	4.85754900	2.48553000	-1.39821000
H	4.32217500	2.30690200	0.26910800
H	6.60513000	1.36423600	0.00719600
H	6.03839100	0.30219800	-1.27898800
C	-1.33874300	0.79241500	-2.42352900
C	-2.00605200	0.17716200	-3.64992100
H	-2.90122400	0.74413400	-3.91616900
H	-1.32016300	0.17074400	-4.50170100
H	-2.30621400	-0.85477000	-3.43949800
C	-1.00408600	2.26249700	-2.67014900
H	-0.27149000	2.35788200	-3.47603900
H	-1.90383300	2.82382200	-2.94321600
H	-0.56515300	2.70098600	-1.76654200
O	-2.31031000	0.69311400	-1.36191700
H	-2.32839100	1.51441300	-0.84653600

**TS11**

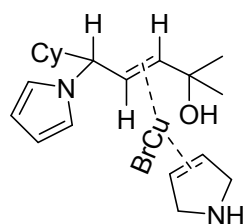


C	1.29911500	1.26207100	0.76926100
H	1.59042400	1.72203500	1.72702500
C	0.02278800	0.45979800	0.90505500
C	-0.37950600	0.04855900	2.11758400
N	1.02995500	2.39051200	-0.14406500
C	0.45515800	3.56445400	0.25716100
H	-1.37724500	2.32448100	-1.12821900
H	0.34743300	3.78528100	1.30963900
C	1.03076000	2.33904100	-1.51189000
H	0.18989900	0.27035500	3.02967300
H	1.42833900	1.48469700	-2.03985900
C	0.47086300	3.50683900	-1.99198600
C	0.10106800	4.28862300	-0.86235000
H	0.37109900	3.77644500	-3.03321300
H	-0.33769600	5.27567100	-0.86792700



Cu	-0.32530600	-1.15613400	-0.38477000
Br	-0.57431300	-3.01165500	-1.81369900
C	-2.67692500	0.75090500	-1.58125700
C	-4.08928200	0.87090200	-1.08502400
C	-4.16929800	1.66042100	-0.02039900
C	-2.82377000	2.20445000	0.36439500
N	-1.90023700	1.59942300	-0.63171400
H	-1.03626100	0.92258100	-0.02979800
H	-2.54823700	1.11476100	-2.60549500
H	-4.91106100	0.34829500	-1.55915800
H	-5.06976400	1.89904000	0.53228100
H	-2.50815400	1.88747600	1.36580000
H	-2.30808000	-0.28361600	-1.54829400
H	-2.76452300	3.29643200	0.31428100
C	2.49345000	0.42483900	0.27688300
C	3.74434400	1.28745500	0.05971400
C	2.80804300	-0.71607900	1.25466600
H	2.21185900	-0.04260900	-0.68190000
C	4.92800800	0.44958200	-0.42577200
H	4.00464400	1.76429800	1.01674300
H	3.53749400	2.09567700	-0.64789700
C	3.99626500	-1.55265400	0.77643400
H	3.03351800	-0.28218800	2.24159100
H	1.93119000	-1.35907300	1.38360700
C	5.23631800	-0.68858000	0.54699700
H	5.80657600	1.08866200	-0.56200800
H	4.68769400	0.02666700	-1.41078000
H	4.20716500	-2.34405000	1.50280400
H	3.72056900	-2.05148300	-0.16238300
H	6.06398000	-1.29994600	0.17309500
H	5.56245600	-0.26254400	1.50601700
C	-1.61553200	-0.79575100	2.35767400
C	-2.43780400	-0.22999900	3.51769100
H	-2.74955300	0.79570300	3.30434800
H	-3.33403600	-0.83738000	3.67876100
H	-1.85494100	-0.22977900	4.44328000
C	-1.20328600	-2.24220900	2.65036900
H	-0.69458500	-2.67582300	1.78251300
H	-0.52799600	-2.28793600	3.50949100
H	-2.08417800	-2.85272900	2.88180500
O	-2.38790800	-0.74170300	1.15594300
H	-3.00260200	-1.48550200	1.14364500

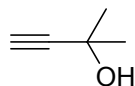
Int22



C	-1.67150400	0.58175300	-1.03224500
H	-1.67776200	0.65270300	-2.12730200
C	-0.45730000	1.31565300	-0.49864900
C	0.63201300	1.61154300	-1.22650500
N	-2.86951400	1.27087700	-0.57108400
C	-3.89476700	1.70186400	-1.37022800
H	-1.46612900	0.27946600	3.57082800
H	-3.80771600	1.65329100	-2.44601100
C	-3.22692400	1.42435500	0.74485200
H	0.67807900	1.27164100	-2.26260300
H	-2.55463300	1.10230000	1.52935800
C	-4.48735000	1.97519700	0.78168500
C	-4.91178600	2.15316900	-0.56244700
H	-5.04034800	2.22797700	1.67449400
H	-5.84884800	2.57010200	-0.90030300
Cu	1.25635300	-0.22504300	0.32174700
Br	3.27756900	-1.13727800	-0.78319700
C	-0.43818700	-1.38061000	2.87993400
C	1.00051000	-1.39025500	2.42551800
C	1.54261000	-0.17385200	2.62375000
C	0.50801600	0.77422400	3.17183000
N	-0.74637800	0.05697200	2.89188100
H	-0.55026400	1.67995700	0.52728000
H	-0.49780700	-1.85265800	3.87574600
H	1.53917700	-2.27889900	2.11234600
H	2.58868500	0.08541400	2.50059600
H	0.53442600	1.75309900	2.67934100
H	-1.11652800	-1.92974500	2.21852900
H	0.69277800	0.93594200	4.24720300
C	-1.68895500	-0.91368600	-0.64549100
C	-3.07685100	-1.55134400	-0.77803200
C	-0.68934600	-1.71344200	-1.49163700
H	-1.39378800	-0.96559100	0.41597000
C	-3.04200900	-3.01866900	-0.33859700
H	-3.39599200	-1.48738700	-1.82905200
H	-3.81256600	-0.99634300	-0.18769700
C	-0.61651600	-3.16670800	-1.02395900

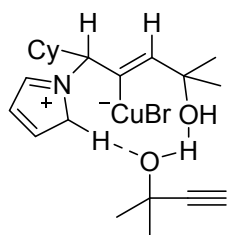
H	-1.03194200	-1.68608000	-2.53714100
H	0.31637500	-1.27502700	-1.49790100
C	-1.99396100	-3.82592700	-1.10793000
H	-4.03336200	-3.46729800	-0.45788900
H	-2.80904700	-3.05969700	0.73539000
H	0.12063900	-3.71601300	-1.61673400
H	-0.25696200	-3.18637600	0.01631500
H	-1.95333700	-4.85340900	-0.73211900
H	-2.29235900	-3.88570100	-2.16343300
C	1.79242100	2.48968600	-0.74142500
C	1.26425200	3.85115500	-0.29787700
H	0.72775100	4.34215000	-1.11345900
H	0.57872000	3.73820700	0.54632400
H	2.10057900	4.48116800	0.01468300
C	2.82527300	2.63647600	-1.85427900
H	3.65985200	3.25019800	-1.50542600
H	3.20408100	1.65254500	-2.15113600
H	2.38008900	3.11960600	-2.72876700
O	2.40653900	1.91097700	0.42041800
H	3.11009300	1.30918800	0.11530800

1



O	0.74285900	-0.03773500	1.38918000
H	0.32009500	-0.79684200	1.80857900
C	0.31606400	0.00265500	0.03395500
C	0.83570600	-1.22475600	-0.72071200
H	0.55037100	-1.18614600	-1.77482800
H	1.92530000	-1.25502400	-0.64067400
H	0.42293200	-2.14135100	-0.28924000
C	0.90091800	1.29039200	-0.54052900
H	0.62131200	1.40539200	-1.58973000
H	0.53293000	2.14734800	0.02607400
H	1.98996400	1.25099000	-0.45680100
C	-1.16363200	0.03632600	-0.03500800
C	-2.36780300	0.03431200	-0.08313200
H	-3.43329700	0.04394000	-0.12426300

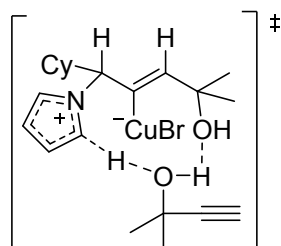
Int23



C	1.56554200	0.69097400	-1.09235500
H	1.72815600	1.41365500	-1.91019300
C	0.45566400	1.11041600	-0.13757200
C	-0.09932500	2.30645000	-0.35111400
N	1.05380500	-0.53595900	-1.76431100
C	0.07034500	-0.45065200	-2.83717900
H	-0.73654900	0.22133900	-2.50794900
H	0.53232800	-0.06088800	-3.75046400
C	1.05753500	-1.73713200	-1.26492200
H	0.25700900	2.99306800	-1.13188400
H	1.64530700	-2.00383300	-0.39365900
C	0.15558600	-2.60290200	-1.99605200
C	-0.42982700	-1.84749600	-2.94408700
C	-1.26731500	2.85582700	0.44620400
H	-0.00700500	-3.64319200	-1.75557100
H	-1.16845000	-2.15896600	-3.67082700
O	-1.90511200	1.74856100	1.10235000
H	-2.82338900	1.98867800	1.29069100
C	-0.77256100	3.83968600	1.50643800
H	-0.22134700	4.66364100	1.04298900
H	-1.61394900	4.26017600	2.06816300
H	-0.10775300	3.31686200	2.19831000
C	-2.26406500	3.51760100	-0.50727200
H	-3.11442000	3.93312800	0.04625600
H	-1.78435000	4.33601200	-1.05179300
H	-2.64286000	2.78268300	-1.22362800
Br	-0.00499500	-2.63779700	1.89282900
O	-2.41481000	0.06421700	-1.12033300
H	-1.98022200	0.56852300	-0.40608100
C	-3.64094100	-0.42869400	-0.60089700
C	-3.38094200	-1.32447000	0.61215100
H	-4.31575000	-1.73317500	1.00496100
H	-2.71450800	-2.14267200	0.32611300
H	-2.88920000	-0.75546600	1.40733100
Cu	-0.08876800	-0.34641400	1.15481600
C	-4.30196900	-1.20796300	-1.73559600
H	-5.26631000	-1.61033400	-1.41908900

H	-4.45143300	-0.55568600	-2.59881400
H	-3.64468700	-2.03527400	-2.01823800
C	-4.51836000	0.70148500	-0.19935900
C	-5.23310400	1.60936800	0.14992700
H	-5.88207000	2.40536600	0.43757700
C	2.90655800	0.42406000	-0.40036500
C	3.98660700	-0.07897300	-1.36694600
C	3.37531400	1.70419900	0.30289400
H	2.74051100	-0.32940500	0.38636600
C	5.32208900	-0.29610900	-0.65212100
H	4.11923900	0.67044000	-2.16132300
H	3.67244400	-1.00611400	-1.86042200
C	4.71338400	1.49132900	1.01243400
H	3.47930900	2.50150700	-0.44909700
H	2.60792500	2.03208200	1.00999700
C	5.78488500	0.98260600	0.04684400
H	6.07718300	-0.64076000	-1.36600600
H	5.20333200	-1.09281900	0.09446000
H	5.03610300	2.42389800	1.48613200
H	4.57611000	0.75747900	1.81776000
H	6.72636800	0.80702000	0.57708200
H	5.98417500	1.75374700	-0.71012400

**TS12**

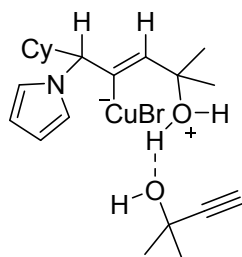


C	-1.33293000	-0.83570500	-0.98666300
H	-1.39354600	-1.69358600	-1.67751200
C	-0.37809400	-1.09821200	0.16943800
C	0.23612200	-2.28569700	0.12902700
N	-0.73400800	0.25152100	-1.80049900
C	0.26374700	0.01515100	-2.77281000
H	1.41542600	-0.24595200	-2.09224100
H	0.15385500	-0.88266700	-3.37650600
C	-0.86160700	1.55648700	-1.60989800
H	0.02526300	-3.01136100	-0.67008800
H	-1.47586600	1.96065800	-0.81383900
C	-0.05496500	2.25782500	-2.53720000
C	0.58577200	1.30799300	-3.29999000

C	1.36069200	-2.73445000	1.03658500
H	0.02823900	3.33253000	-2.59866900
H	1.27594500	1.47858700	-4.11565200
O	2.55999500	-2.42120500	0.26700300
H	3.34150400	-2.37489200	0.83407500
C	1.42279700	-2.01935400	2.37938000
H	0.49318600	-2.17157500	2.93277000
H	2.25025300	-2.41602900	2.97976500
H	1.56798900	-0.94305700	2.25826900
C	1.32359900	-4.24661200	1.23531200
H	2.18893700	-4.58556700	1.81394600
H	0.41465100	-4.53408800	1.77104700
H	1.33454200	-4.75229000	0.26638700
Br	-0.16608400	2.76375500	2.14592000
O	2.53818800	-0.62429200	-1.56484100
H	2.42250500	-1.34498500	-0.85683500
C	3.44124400	0.37991300	-1.03890700
C	2.73103900	1.21809500	0.01970100
H	3.39564300	1.99193100	0.41025400
H	1.84774200	1.70071300	-0.41244400
H	2.40917200	0.58720200	0.85121300
Cu	-0.21161500	0.53817000	1.33252900
C	3.91754700	1.23014600	-2.21408000
H	4.69686900	1.91597300	-1.87674000
H	4.32001200	0.59056200	-3.00199100
H	3.08363700	1.81851600	-2.60282600
C	4.59339800	-0.32970400	-0.44610100
C	5.54717800	-0.87382900	0.05080000
H	6.40541700	-1.34393500	0.47588000
C	-2.75927000	-0.48349100	-0.54710200
C	-3.69420600	-0.19900900	-1.72959500
C	-3.31654800	-1.62810500	0.30837300
H	-2.71355400	0.40806700	0.09918000
C	-5.11907700	0.09869200	-1.25738100
H	-3.70706700	-1.08370300	-2.38341600
H	-3.31817500	0.63351400	-2.33474100
C	-4.74331000	-1.33682600	0.77506700
H	-3.30491800	-2.55136200	-0.29112400
H	-2.65643900	-1.79846500	1.16411600
C	-5.66925600	-1.04680300	-0.40712200
H	-5.76776300	0.28489600	-2.11952100
H	-5.11311800	1.02021500	-0.65988800
H	-5.12251000	-2.17954600	1.36206700
H	-4.72838900	-0.46593000	1.44390600

H	-6.67830500	-0.80990200	-0.05466100
H	-5.75202200	-1.94853400	-1.02956400

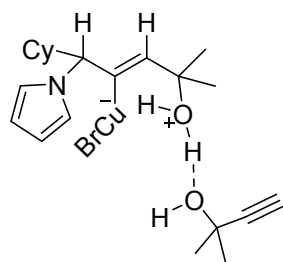
**Int24**



C	1.67763000	1.03225800	0.76073800
H	1.97383000	1.64388000	1.62914400
C	0.61719700	0.00851000	1.12515800
C	0.03855600	0.15112600	2.32361500
N	1.05281900	1.98284900	-0.17778500
C	0.61594800	3.23407900	0.15213000
H	-1.30244800	1.44068800	-0.37809000
H	0.81608700	3.63901200	1.13324800
C	0.65191800	1.69007800	-1.45696900
H	0.34923300	0.90469500	3.05737400
H	0.90113700	0.74688500	-1.92330800
C	-0.04212100	2.78164300	-1.94932800
C	-0.06337500	3.76462900	-0.92350300
C	-1.15742700	-0.67345200	2.74885000
H	-0.44678300	2.86884700	-2.94821500
H	-0.50813700	4.74774600	-0.97153000
O	-2.04513600	-0.72407700	1.54377000
H	-2.96442100	-0.95969700	1.75061100
C	-0.81770200	-2.12098600	3.06142000
H	-0.13813200	-2.15257100	3.91666600
H	-1.71388300	-2.70170100	3.30591700
H	-0.31672500	-2.56949400	2.19991100
C	-1.94669300	0.00770100	3.85592300
H	-2.84354100	-0.56375700	4.11901900
H	-1.32380500	0.08284800	4.75061800
H	-2.23730000	1.01774000	3.55267500
Br	-0.77394400	-2.70055600	-2.02231000
O	-2.09166600	1.25760700	0.17830700
H	-1.99294300	0.21876000	0.89553200
C	-3.29670000	1.25390700	-0.64411500
C	-3.06582900	0.39243700	-1.88180400
H	-3.97142300	0.37037000	-2.49183000
H	-2.25256700	0.82594800	-2.47230200

H	-2.78642600	-0.63065200	-1.61553400
Cu	0.05036500	-1.31034800	-0.29426700
C	-3.62930400	2.70279000	-0.98686700
H	-4.55723200	2.74334800	-1.56096900
H	-3.74230300	3.28976400	-0.07368500
H	-2.81562000	3.12248000	-1.58338500
C	-4.34810100	0.67455200	0.21577900
C	-5.21872700	0.19849300	0.90044200
H	-6.01550200	-0.20445400	1.48555800
C	2.94315100	0.41332700	0.16050500
C	3.95489400	1.47484800	-0.28119800
C	3.57503400	-0.55550900	1.16560800
H	2.64289300	-0.17612400	-0.72163900
C	5.22524600	0.83499500	-0.84427400
H	4.21657100	2.09511300	0.58968300
H	3.50131700	2.14357900	-1.02093900
C	4.84811300	-1.19160300	0.60522700
H	3.81655300	0.00063000	2.08468600
H	2.84670900	-1.32613500	1.44204300
C	5.85423600	-0.12594800	0.16631900
H	5.94148700	1.61107600	-1.13365800
H	4.97191400	0.28070700	-1.75807600
H	5.29510800	-1.85761100	1.35057100
H	4.58324000	-1.81602200	-0.25860900
H	6.74773100	-0.59552700	-0.25815900
H	6.18184300	0.44375800	1.04717800

**Int25**



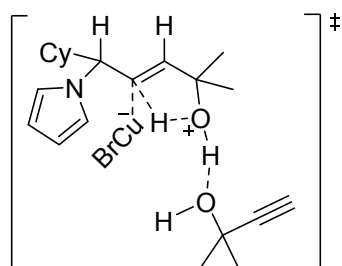
C	-2.38543500	1.07237700	0.03267100
H	-2.81446100	2.01454400	-0.34489500
C	-0.88233600	1.04449300	-0.17022600
C	-0.31813500	2.10764600	-0.75744400
N	-2.68672000	1.05646500	1.46517200
C	-3.21144300	2.10549600	2.16824900
H	-3.45735400	3.02889900	1.66436100
C	-2.46584400	0.01082700	2.32435100
H	-0.89032800	2.96920200	-1.11742000



H	-2.06466500	-0.92992700	1.97264900
C	-2.85828400	0.39842100	3.58634800
C	-3.33304800	1.73206300	3.48763000
C	1.18338300	2.23364500	-0.92430800
H	-2.81491900	-0.21424500	4.47479400
H	-3.72361000	2.34601100	4.28554800
O	1.76924100	1.80729500	0.39477900
H	2.49719600	0.99447800	0.37650700
C	1.74973500	1.30561700	-1.98937600
H	1.31976300	1.58239100	-2.95515900
H	2.83933100	1.39646100	-2.05279700
H	1.46931800	0.26750700	-1.78204500
C	1.63304200	3.66998400	-1.11575100
H	2.72432700	3.72991800	-1.13655800
H	1.24057400	4.04711800	-2.06389100
H	1.25457700	4.29846600	-0.30637200
Br	1.36454200	-2.64752200	0.67256400
H	0.99001000	1.50946900	0.91953000
Cu	0.00806400	-0.70995400	0.29154100
O	3.29684000	-0.07085200	0.53799000
H	2.83566500	-0.94195100	0.63419800
C	4.59894900	-0.24526100	-0.06545000
C	4.48023700	-1.17311900	-1.27502600
H	5.46043400	-1.30469100	-1.73793700
H	4.10259000	-2.14754300	-0.95123800
H	3.79198300	-0.75900800	-2.01412000
C	5.53150200	-0.82321800	0.99770000
H	6.53857000	-0.94214000	0.59241300
H	5.56781700	-0.16051700	1.86366200
H	5.15516700	-1.80178500	1.30979600
C	5.04362000	1.09914500	-0.47267300
C	5.42172800	2.19149200	-0.81176400
H	5.76957200	3.15610400	-1.10689500
C	-3.09911000	-0.08343600	-0.68856800
C	-4.60811300	-0.06641700	-0.42363200
C	-2.81257800	-0.04560800	-2.19324000
H	-2.69091400	-1.02965400	-0.29335600
C	-5.32025700	-1.20154200	-1.16176100
H	-5.01189600	0.89865900	-0.76611600
H	-4.79931600	-0.12736500	0.65284000
C	-3.53028100	-1.17739900	-2.93155700
H	-3.15192300	0.92423200	-2.58946200
H	-1.73236500	-0.09711100	-2.37011100
C	-5.03592500	-1.15012000	-2.66351500

H	-6.39769400	-1.15446500	-0.97290600
H	-4.97063600	-2.16312900	-0.76177500
H	-3.32977600	-1.11114800	-4.00609900
H	-3.12169000	-2.13888400	-2.59165600
H	-5.53033800	-1.98149400	-3.17667900
H	-5.45786700	-0.22380000	-3.07752800

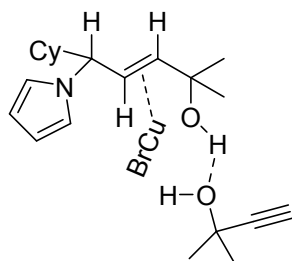
TS13



C	-2.10372300	1.19897700	-0.42135100
H	-2.67489600	1.75573500	-1.17932000
C	-0.66476700	1.04341700	-0.86613100
C	-0.26719200	1.42440900	-2.08290900
N	-2.15375100	2.01535700	0.78996000
C	-2.84992900	3.18551100	0.92686000
H	-3.37088000	3.61202200	0.08197600
C	-1.59634100	1.68410200	1.99804500
H	-0.91258000	1.83073300	-2.86517800
H	-1.00831600	0.78359800	2.11406400
C	-1.93655200	2.65584200	2.91129600
C	-2.73387900	3.61245300	2.22961800
C	1.23359900	1.41654000	-2.36141600
H	-1.64041700	2.67595300	3.94983100
H	-3.16818400	4.51095400	2.64191800
O	1.80171300	1.41807800	-1.01222200
H	2.44688100	0.63429200	-0.81068100
C	1.69266400	0.16196400	-3.09641400
H	1.22642500	0.12657900	-4.08441200
H	2.77944600	0.15553700	-3.22312500
H	1.39033900	-0.73709900	-2.54782200
C	1.68473900	2.69476900	-3.04679100
H	2.77179200	2.70364200	-3.16084500
H	1.22643800	2.76513700	-4.03737100
H	1.38291200	3.56284800	-2.45680200
Br	1.03190000	-2.77854900	0.64458900
H	0.81917700	1.24392800	-0.45099900
Cu	0.09906400	-0.67815800	0.04288800
O	3.28781800	-0.47710600	-0.30008600

H	2.79271800	-1.30512000	-0.12106700
C	3.95232200	-0.07802900	0.92412800
C	4.78438400	-1.25724000	1.42380000
H	5.33512700	-0.97407900	2.32306300
H	4.11899900	-2.09291000	1.66346800
H	5.49303800	-1.56645800	0.65351200
C	2.91362700	0.35666200	1.96313500
H	3.41535500	0.69782900	2.87153300
H	2.30586400	1.18300800	1.58093700
H	2.26741000	-0.49120400	2.21006300
C	4.81444300	1.05819600	0.55821600
C	5.51384600	1.99872800	0.28388500
H	6.13459300	2.83092100	0.03972000
C	-2.82259200	-0.14706900	-0.19302500
C	-4.25724600	0.06260400	0.30344800
C	-2.80548600	-1.01333600	-1.45749100
H	-2.27918400	-0.69117700	0.60205100
C	-4.97287400	-1.27218200	0.52149800
H	-4.80421200	0.65123900	-0.44898100
H	-4.25098500	0.65074900	1.22713500
C	-3.52482400	-2.34512000	-1.23624300
H	-3.29808400	-0.45568700	-2.26905300
H	-1.77466300	-1.19596000	-1.78655500
C	-4.95691800	-2.12624100	-0.74679900
H	-6.00097700	-1.09452600	0.85316300
H	-4.46925500	-1.81870900	1.33021300
H	-3.51833800	-2.93106900	-2.16075600
H	-2.96829900	-2.92659200	-0.48859400
H	-5.44860200	-3.08766600	-0.56697100
H	-5.53181700	-1.61568200	-1.53189400

**Int26**

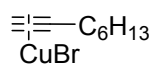


C	-2.15298600	0.14999100	-0.18883300
H	-2.07558800	-0.16711400	-1.23762000
C	-0.93431100	0.98913200	0.15878800
C	-0.35943900	1.83868300	-0.72144200
N	-3.34025400	0.99305000	-0.11452500

C	-4.23873500	1.18569900	-1.13042800
H	-4.07649400	0.73151200	-2.09738600
C	-3.77827900	1.65241300	1.00560200
H	-0.74274300	1.88278000	-1.74423100
H	-3.20596500	1.63031700	1.92176100
C	-4.96557500	2.27544700	0.69835800
C	-5.25934900	1.97783600	-0.65901100
C	0.64637900	2.90829600	-0.32126300
H	-5.55315300	2.88133900	1.37208500
H	-6.11817500	2.30450700	-1.22612200
O	1.23815500	2.58271300	0.92034500
H	2.04620700	2.07230800	0.75736100
C	1.70294500	3.09198000	-1.41196400
H	1.23885400	3.37861900	-2.35976100
H	2.40038700	3.87821400	-1.11126700
H	2.27122800	2.16962500	-1.57387300
C	-0.13913300	4.20489600	-0.10460200
H	0.55744500	5.00574700	0.15526500
H	-0.69172500	4.48889200	-1.00420700
H	-0.84966300	4.07076200	0.71471200
Br	1.97268300	-1.68432900	-2.12103000
H	-0.62032600	1.04560200	1.20342100
Cu	0.86147400	-0.07530700	-0.70163400
O	3.08517000	0.44066700	0.11885500
H	3.29794200	-0.13292000	-0.64150000
C	3.55726700	-0.20528000	1.31732800
C	4.86183500	-0.94012800	1.01197900
H	5.25835300	-1.40381200	1.91744500
H	4.67010600	-1.72226700	0.26950600
H	5.60229000	-0.24045400	0.61916400
C	2.48064100	-1.16254300	1.83396600
H	2.79988400	-1.63966300	2.76377200
H	1.56356300	-0.59798300	2.03531300
H	2.28373800	-1.93254900	1.07987000
C	3.77685600	0.87256500	2.29827300
C	3.92452300	1.75598300	3.10309300
H	4.05746500	2.53980000	3.81403800
C	-2.31035800	-1.10715000	0.68286100
C	-3.59784500	-1.85630300	0.32367000
C	-1.09289200	-2.02668100	0.54987000
H	-2.38427900	-0.77945200	1.73278800
C	-3.75108000	-3.14252300	1.13768800
H	-3.56669600	-2.10790700	-0.74744000
H	-4.46221000	-1.20098700	0.47235700

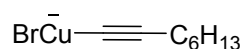
C	-1.25239300	-3.31873700	1.35501800
H	-0.93263400	-2.27383200	-0.51061500
H	-0.18717300	-1.50941400	0.89547100
C	-2.53551800	-4.05413300	0.96846700
H	-4.66694700	-3.66307400	0.84109100
H	-3.86388700	-2.88435800	2.19962000
H	-0.37687500	-3.95713500	1.20004600
H	-1.28628200	-3.07184800	2.42498100
H	-2.64850700	-4.96123600	1.57074800
H	-2.46493500	-4.37366400	-0.07981200

**CuBr-6**



C	3.11586200	0.27685700	0.87621300
C	2.59534600	1.19238100	0.26199900
C	2.04097500	2.34317500	-0.46874700
H	2.08439900	3.21113000	0.19902400
H	2.70672600	2.54781100	-1.31337900
C	0.59911500	2.12497500	-0.95984200
H	0.33412500	2.96535100	-1.60964900
H	0.56674400	1.22475600	-1.58900600
C	-0.42391100	2.00493200	0.16807700
H	-0.08465200	1.26945500	0.91426600
H	-0.49180300	2.96081400	0.70459900
C	-1.79932200	1.57590100	-0.33605400
H	-2.21159900	2.35543900	-0.99145800
H	-1.68481200	0.66917700	-0.94336900
C	-2.77468700	1.27542000	0.79843400
H	-2.33283200	0.50035800	1.43729900
H	-2.90517200	2.16929700	1.42238300
C	-4.12558600	0.79165200	0.28059900
H	-4.81838300	0.58345000	1.09977300
H	-4.58871900	1.54016900	-0.37061700
H	-4.00078700	-0.12872100	-0.29775100
H	3.69450800	-0.41744000	1.44982700
Cu	1.28275200	-0.66436600	0.17914100
Br	-0.53812300	-2.04846300	-0.25803100

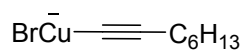
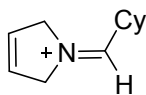
**Int27**



C	0.76888900	1.95551300	-0.11562000
C	-0.28372600	1.32843200	-0.08001300

Cu	-1.97507700	0.34021400	-0.02372900
Br	-4.04261100	-0.84907700	0.04129200
C	2.06196100	2.64911400	-0.14410900
H	2.32918900	2.91605600	-1.17763300
H	2.00215000	3.59731200	0.40691100
C	3.19878200	1.80007900	0.44886700
H	4.13252600	2.38067400	0.44278900
H	2.96115400	1.58038500	1.49707200
C	3.40157500	0.48851500	-0.30184600
H	2.44556500	-0.04821100	-0.31506400
H	3.65073000	0.70696100	-1.35066400
C	4.49198400	-0.38996700	0.30477300
H	4.23975000	-0.60988600	1.35164400
H	5.44382700	0.16157500	0.32996000
C	4.69301800	-1.70373000	-0.44688800
H	3.74342800	-2.25186500	-0.46746700
H	4.94215300	-1.48495400	-1.49313300
C	5.78171800	-2.57774700	0.17020300
H	5.91222000	-3.51519900	-0.37818100
H	6.74421900	-2.05488700	0.17687700
H	5.53650300	-2.82774000	1.20760300

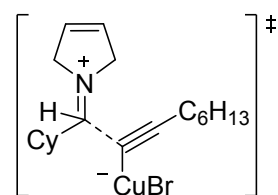
**Int28**



C	-1.13452600	-0.83368300	1.22431400
C	-0.36762100	1.62283800	-1.40321000
C	0.59763800	2.37947300	-1.38278200
H	-1.88783900	-1.62085100	1.17324900
C	0.23355100	-1.09619900	0.70315100
C	1.08360300	-1.66682700	1.86499100
C	0.18737100	-2.09136300	-0.46685200
H	0.67217000	-0.15144600	0.35185000
C	2.49311100	-1.99665900	1.37140300
H	0.60417400	-2.57845300	2.24707800
H	1.12448800	-0.95175600	2.69468600
C	1.59857800	-2.43575100	-0.94152900
H	-0.33170700	-3.00333800	-0.13877600
H	-0.39896300	-1.66867800	-1.28843100
C	2.46013000	-2.97787400	0.19956800
H	3.08568600	-2.39989000	2.19921300
H	2.97940800	-1.06649500	1.04891000

H	1.54073200	-3.16116700	-1.75814300
H	2.06051200	-1.52950000	-1.35589600
H	3.47939300	-3.17698800	-0.14894600
H	2.04907400	-3.93706900	0.54234300
Cu	-1.95284800	0.47751100	-1.40330900
Br	-3.69418700	-1.09100400	-0.92187400
N	-1.49727500	0.25641000	1.79999600
C	-2.87882900	0.47850500	2.29712400
C	-0.66822100	1.48122600	1.91814300
C	-2.83281700	1.91460500	2.72482100
C	-1.63466800	2.45299500	2.52749900
H	-0.33452900	1.77734600	0.91077700
H	0.20434700	1.27378900	2.54816400
H	-1.35158400	3.47575100	2.73950700
H	-3.70234900	2.41667500	3.12814800
H	-3.57118500	0.27170800	1.46998400
H	-3.08761900	-0.21615200	3.11749600
C	1.75129200	3.28913800	-1.35836200
H	2.13543600	3.42484400	-2.37776800
H	1.43013600	4.28097000	-1.01826200
C	2.89172400	2.78447600	-0.46067800
H	3.67363200	3.55188300	-0.40275700
H	2.50816700	2.64583800	0.55981100
C	3.49227100	1.47435100	-0.95719300
H	2.68303400	0.73884700	-1.06557400
H	3.90406600	1.62255300	-1.96490900
C	4.57544300	0.91258900	-0.04164600
H	5.37994300	1.64932200	0.08673200
H	4.15405900	0.75413400	0.96219600
C	5.16326000	-0.39861700	-0.56141100
H	4.34224000	-1.07147100	-0.84407100
H	5.71889100	-0.20104100	-1.48596700
C	6.06515000	-1.09299400	0.45389600
H	6.48975700	-2.01678000	0.05191100
H	6.89463900	-0.44400500	0.75197000
H	5.50320900	-1.34747800	1.35957000

**TS14**



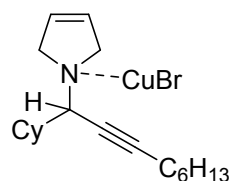
C	-0.66386700	0.28876700	0.93968900
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C	-0.61548100	0.65130900	-1.29077400
C	0.24611800	1.42257300	-1.71010700
H	-1.48493300	-0.43072800	0.94180300
C	0.71189800	-0.28381000	1.12111600
C	0.91996000	-0.50840400	2.63708600
C	0.87060600	-1.60988400	0.36714100
H	1.46064200	0.43344700	0.75727000
C	2.28601600	-1.13932200	2.91146700
H	0.12926900	-1.17604000	3.00611000
H	0.81508300	0.43677400	3.18083000
C	2.22686700	-2.25114900	0.65972200
H	0.06448600	-2.28938300	0.68134700
H	0.74149300	-1.43489100	-0.70426700
C	2.44411500	-2.46009600	2.15819000
H	2.41157700	-1.28898300	3.98835400
H	3.07381100	-0.44274000	2.59140100
H	2.31164900	-3.19952600	0.12028100
H	3.01913500	-1.59521200	0.27467200
H	3.43462100	-2.88758000	2.34410800
H	1.70799900	-3.18146800	2.53671200
Cu	-2.25469800	-0.47271800	-1.28582800
Br	-4.11251300	-1.64425900	-0.44271700
N	-1.00038400	1.48551600	1.36473900
C	-2.40146900	1.93681100	1.31852700
C	-0.06865800	2.61435700	1.39557600
C	-2.26553700	3.41711300	1.52315900
C	-0.99070700	3.78871600	1.56783900
H	0.47152300	2.64040800	0.43512500
H	0.66274900	2.50192200	2.20382000
H	-0.62029300	4.79821500	1.69120300
H	-3.12574400	4.06934300	1.60145000
H	-2.82962100	1.68234400	0.33634800
H	-2.99280300	1.43040700	2.08799500
C	1.29132400	2.31228400	-2.23297300
H	1.39963200	2.13684600	-3.31081000
H	0.98062800	3.35757300	-2.11824600
C	2.65149300	2.09200800	-1.55002800
H	3.35410000	2.85528000	-1.90432700
H	2.54330700	2.25013200	-0.46748300
C	3.22939900	0.70334700	-1.80540800
H	2.45926900	-0.05290200	-1.59808800
H	3.47394400	0.60557200	-2.87178300
C	4.46639700	0.40841000	-0.96224000
H	5.18835900	1.23166300	-1.05130800



H	4.17503500	0.37893900	0.09934500
C	5.14925500	-0.90509200	-1.34178700
H	4.39170500	-1.69196300	-1.44761800
H	5.60901700	-0.79450900	-2.33108900
C	6.19692200	-1.33651300	-0.32067800
H	6.70205800	-2.25704800	-0.62318500
H	6.95872300	-0.56177900	-0.18823500
H	5.73254200	-1.51337700	0.65609600

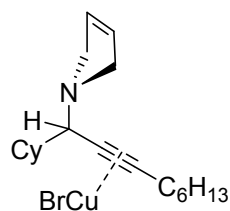
**Int29**



C	1.73660600	-0.65814100	1.38708300
H	2.10549000	-1.02920800	2.35944600
C	1.03183100	-1.73845700	0.68102600
C	0.37192200	-2.52640000	0.04508800
N	0.73478100	0.40951400	1.64705200
C	-0.31651500	-0.01887600	2.61345800
H	-1.07600300	-0.63125700	2.12092500
H	0.13080900	-0.62585700	3.42050600
C	1.29425400	1.65632800	2.22992100
H	1.71960100	2.29449300	1.45067200
H	2.09261900	1.42307000	2.95636800
C	0.09871100	2.24402800	2.93333500
C	-0.81050900	1.29782600	3.14987300
H	0.03922000	3.28339000	3.23063000
H	-1.75843000	1.41321500	3.66016200
C	2.96546700	-0.15880400	0.59430300
C	3.96971400	-1.30713500	0.42329900
C	2.61513800	0.45709300	-0.76442600
H	3.45220100	0.61266300	1.20975000
C	5.22308600	-0.85170700	-0.32644700
H	3.48386000	-2.11526800	-0.13870600
H	4.23649500	-1.71724000	1.40513500
C	3.86896200	0.89134700	-1.52819100
H	2.05484000	-0.27889300	-1.35807500
H	1.96129700	1.33094100	-0.64647200
C	4.85794400	-0.26260800	-1.68916800
H	5.91321600	-1.69346100	-0.44131900
H	5.74724200	-0.09040700	0.26758600
H	3.57899200	1.29346400	-2.50327900

H	4.35843800	1.70846800	-0.98024200
H	5.75743300	0.07635000	-2.21284800
H	4.40244100	-1.04547400	-2.31025900
Cu	-0.32082300	0.84073200	-0.10333800
Br	-1.38680200	1.58039700	-2.05712200
C	-0.51052900	-3.42346200	-0.70753600
H	-0.41008300	-3.19512700	-1.77500600
H	-0.18730700	-4.46005900	-0.56740300
C	-1.98006700	-3.25433200	-0.28073400
H	-2.08738400	-3.57560600	0.76259500
H	-2.59660200	-3.92720200	-0.88747200
C	-2.46771900	-1.81698500	-0.42753800
H	-1.80936700	-1.16631700	0.16525500
H	-2.34966200	-1.47415600	-1.46333600
C	-3.90256100	-1.59069300	0.03486900
H	-4.59638700	-2.12765300	-0.62619500
H	-4.03884100	-2.02269900	1.03743900
C	-4.26481300	-0.10690100	0.06654600
H	-4.08477800	0.33286600	-0.92068900
H	-3.57072300	0.41211500	0.74413800
C	-5.70392900	0.14018900	0.50689700
H	-5.93486300	1.20792800	0.53723400
H	-6.40872000	-0.33406700	-0.18352100
H	-5.88851400	-0.27458400	1.50370600

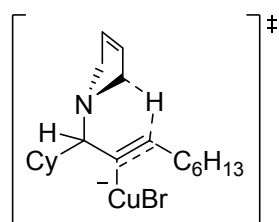
**Int30**



C	-2.18072000	-0.06941400	0.35109000
H	-1.96146400	0.22699800	1.38703800
C	-1.08202400	-0.98864000	-0.10333000
C	-0.33792500	-1.84244100	-0.56517600
N	-3.45345200	-0.75481700	0.36177200
C	-3.58568500	-1.82074600	1.36130400
H	-2.62528200	-2.33114700	1.55921800
H	-3.94287300	-1.41325400	2.31536000
C	-3.94499600	-1.23575900	-0.93379400
H	-3.12524000	-1.51966100	-1.61960000
H	-4.53682200	-0.46110100	-1.43950700
C	-4.75896400	-2.44230100	-0.55554700

C	-4.56006700	-2.76660700	0.71746600
H	-5.39607700	-2.96442900	-1.25920800
H	-5.00564100	-3.60214300	1.24366700
Cu	0.83538100	-0.39756600	0.75654400
Br	2.55532500	0.65966500	1.93272100
C	-2.21732700	1.21945200	-0.49417600
C	-3.31270700	2.15325000	0.03405500
C	-0.85951300	1.93270200	-0.50912300
H	-2.46217400	0.93783700	-1.53015100
C	-3.36773300	3.46260900	-0.75360300
H	-3.09609900	2.37585600	1.08950500
H	-4.27770800	1.63907100	0.01455000
C	-0.91897900	3.25280500	-1.28140000
H	-0.54018500	2.12950700	0.52669800
H	-0.09537600	1.28831600	-0.96329600
C	-2.01315100	4.17145700	-0.73771800
H	-4.14734300	4.11166600	-0.34238200
H	-3.65040500	3.24766700	-1.79345900
H	0.05706500	3.74539800	-1.23946300
H	-1.12349200	3.03676200	-2.33887200
H	-2.05579100	5.09685000	-1.32085500
H	-1.76584400	4.45508300	0.29400500
C	0.48911400	-2.89959300	-1.17521400
H	0.18620400	-3.85871100	-0.74301300
H	0.25213500	-2.93709600	-2.24489500
C	1.99822700	-2.67741100	-0.97834100
H	2.21103100	-2.62078300	0.09834800
H	2.52786200	-3.56000500	-1.35237300
C	2.52716300	-1.42279300	-1.67167900
H	2.47682200	-1.55317600	-2.76092700
H	1.87089100	-0.56619400	-1.44936500
C	3.94588400	-1.06057300	-1.23977200
H	3.99585500	-1.07088900	-0.14353100
H	4.65011500	-1.82153200	-1.60264500
C	4.37031400	0.32275600	-1.72446000
H	4.32287100	0.36412300	-2.82064500
H	3.64692700	1.05523900	-1.34385300
C	5.76729500	0.69791000	-1.24081800
H	6.06127300	1.68995000	-1.59278200
H	5.79802200	0.70510800	-0.14715800
H	6.51322300	-0.02044700	-1.59641600

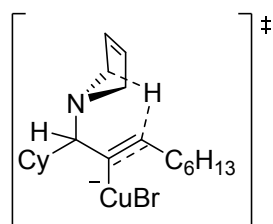
TS15\_1



C	-2.03643600	0.04892200	0.47680300
H	-1.97098100	0.41443300	1.50772000
C	-0.83123800	-0.82471900	0.13828300
C	-0.89281900	-1.85011800	-0.63320700
N	-3.22382300	-0.79909800	0.41423700
C	-3.53060100	-1.60409100	1.60311600
H	-2.60035800	-1.93064600	2.09467500
H	-4.10699900	-1.01156900	2.32274700
C	-3.42986000	-1.57066700	-0.70406100
H	-2.18164300	-2.04950100	-0.94360200
H	-3.58578000	-1.06162800	-1.65438800
C	-4.23649600	-2.73896900	-0.29032700
C	-4.28133100	-2.77394400	1.04373500
H	-4.66326900	-3.44970800	-0.98491800
H	-4.76332200	-3.52221300	1.65920700
Cu	0.96119100	-0.21693600	0.91694600
Br	2.92431100	0.68560700	1.83393000
C	-2.14227800	1.27127800	-0.45232000
C	-3.38003300	2.10242500	-0.09179100
C	-0.87470600	2.13353600	-0.39186500
H	-2.24775100	0.90258200	-1.48534200
C	-3.50078300	3.35548000	-0.96012000
H	-3.29742600	2.40377800	0.96332900
H	-4.28023000	1.48476600	-0.17403900
C	-1.00548600	3.39899200	-1.24389000
H	-0.68148000	2.41260000	0.65527900
H	-0.00564100	1.55658300	-0.72739900
C	-2.24013600	4.21401200	-0.86051800
H	-4.38488700	3.92950300	-0.66481200
H	-3.65224200	3.05653800	-2.00659700
H	-0.09710800	4.00049600	-1.14443700
H	-1.08038600	3.11018900	-2.30130200
H	-2.32628400	5.09859100	-1.49960900
H	-2.12982300	4.57526200	0.17076800
C	-0.09546600	-2.90084300	-1.32882300
H	-0.41499200	-3.88473600	-0.96691500
H	-0.32987400	-2.87165600	-2.40085400

C	1.41769500	-2.72591300	-1.12919500
H	1.62837500	-2.67634000	-0.05237600
H	1.91858700	-3.62591800	-1.50488200
C	1.99296300	-1.49402300	-1.82338500
H	1.88682700	-1.60254100	-2.91164200
H	1.39877500	-0.61022100	-1.55058600
C	3.45323000	-1.23624800	-1.45743400
H	3.56344900	-1.27990100	-0.36608500
H	4.08721400	-2.03066400	-1.87502600
C	3.94520400	0.12917200	-1.92880400
H	3.85275200	0.20092400	-3.02092000
H	3.28884900	0.89702900	-1.49871300
C	5.38136600	0.40455000	-1.49584300
H	5.72719600	1.37946000	-1.84928200
H	5.44883100	0.39729200	-0.40380800
H	6.06423300	-0.35720400	-1.88693200

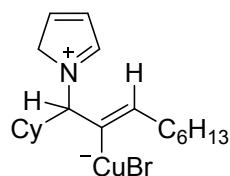
**TS15\_2**



C	-2.09947300	0.83114300	-0.63103800
H	-2.70175400	0.99250800	-1.53622100
C	-0.62235500	1.04029300	-1.02017500
C	-0.12603400	2.21425100	-1.18783900
N	-2.41508900	1.91376800	0.29217000
C	-2.26369400	3.19692500	-0.17934000
H	-1.08089100	3.09733700	-0.86061400
H	-2.89999400	3.51041200	-1.00575900
C	-1.82560700	1.84263700	1.63802800
H	-0.84429400	1.33925000	1.59045200
H	-2.46407800	1.26726900	2.31665600
C	-1.67707600	3.28142400	2.02352500
C	-1.95376600	4.06248100	0.97512300
H	-1.92249100	5.14252000	0.92896000
H	-1.38395000	3.60285800	3.01432400
Cu	0.65567300	-0.52088200	-0.65430300
Br	1.77878700	-2.41822600	0.16625500
C	-2.43852800	-0.55078000	-0.06881300
C	-3.86268100	-0.61934400	0.49738600
C	-2.28104700	-1.63273000	-1.14698700

H	-1.72309700	-0.77673000	0.74012000
C	-4.14729900	-2.00305600	1.08738500
H	-4.57263000	-0.41246500	-0.31699600
H	-4.02595100	0.15762300	1.25102900
C	-2.54559600	-3.02480500	-0.57285700
H	-2.99838100	-1.42156500	-1.95471900
H	-1.28263500	-1.60202000	-1.59787200
C	-3.94121200	-3.10656900	0.04797000
H	-5.16638700	-2.03721200	1.48611500
H	-3.46862100	-2.17395100	1.93392600
H	-2.43109800	-3.77731000	-1.35879700
H	-1.78043000	-3.24278500	0.18370800
H	-4.10080500	-4.08969200	0.50180500
H	-4.69494200	-2.99493400	-0.74360500
C	1.09444800	2.97662800	-1.57981200
H	1.20631700	3.84671800	-0.92103800
H	0.95197300	3.36564400	-2.59463100
C	2.36782100	2.11831300	-1.51323200
H	3.17870700	2.66236400	-2.01116400
H	2.20495000	1.19915100	-2.09169000
C	2.79035900	1.76977100	-0.08737500
H	3.07916400	2.68884500	0.44117100
H	1.93043500	1.36221000	0.46492900
C	3.92828200	0.75393000	-0.03424100
H	3.65228600	-0.12608900	-0.63043000
H	4.83001800	1.18159100	-0.49443900
C	4.23578400	0.28823800	1.38617300
H	4.54939000	1.14614300	1.99596700
H	3.31036200	-0.10321900	1.82683800
C	5.29843500	-0.80484700	1.41536800
H	6.23029000	-0.46290900	0.95225600
H	5.52532400	-1.11607300	2.43842900
H	4.94221900	-1.68182700	0.86647300

**Int31\_1**

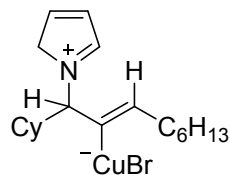


C	-1.88633400	0.00767100	0.40936400
H	-1.73886200	0.33220800	1.44683600
C	-0.77956200	-0.97165700	0.00541200
C	-1.05633100	-1.96921300	-0.83778900

N	-3.18405500	-0.71206600	0.43854800
C	-3.47111600	-1.62503400	1.54097200
H	-2.56844200	-2.22512900	1.71957400
H	-3.69677500	-1.05418600	2.44932200
C	-3.96789400	-0.97952000	-0.56441300
H	-2.08763300	-2.14119300	-1.20424800
H	-3.89489500	-0.43185600	-1.49618800
C	-4.90011800	-2.03813900	-0.22272100
C	-4.61678600	-2.43021600	1.03298700
H	-5.66678700	-2.41540500	-0.88388100
H	-5.11443200	-3.19732100	1.61069500
Cu	0.97741400	-0.40952900	0.86009100
Br	2.82852800	0.60601700	1.92517600
C	-1.97195300	1.26405500	-0.47409100
C	-3.06940400	2.22259900	0.01437200
C	-0.61741800	1.98884400	-0.52108200
H	-2.19590000	0.94010900	-1.50377400
C	-3.13584100	3.49968400	-0.82519500
H	-2.84675100	2.49052000	1.05755500
H	-4.04899800	1.72933800	0.02104300
C	-0.69164900	3.27394800	-1.34745800
H	-0.29814500	2.22359500	0.50526100
H	0.14398400	1.32423100	-0.93815700
C	-1.78464500	4.21335900	-0.84027200
H	-3.91943200	4.15850600	-0.43731900
H	-3.41931600	3.24126900	-1.85499500
H	0.28307200	3.77013200	-1.33034100
H	-0.89779500	3.01493700	-2.39524000
H	-1.83485200	5.11450600	-1.45949000
H	-1.53758800	4.53885000	0.17898700
C	-0.10619900	-2.99405700	-1.42110900
H	-0.41408800	-3.98480800	-1.05785800
H	-0.27036300	-3.02534600	-2.50840100
C	1.38182800	-2.78740800	-1.14958700
H	1.92829500	-3.69047800	-1.44811100
H	1.54255000	-2.68090400	-0.06760500
C	1.97329100	-1.57922600	-1.87526700
H	1.93647900	-1.75057000	-2.96017400
H	1.33637700	-0.70439400	-1.68845800
C	3.40251700	-1.25636500	-1.44155700
H	3.46951800	-1.30364800	-0.34647900
H	4.09292900	-2.01653000	-1.83265600
C	3.85188900	0.13467100	-1.87918500
H	3.79144200	0.21879400	-2.97291500

H	3.14771800	0.86648900	-1.46103100
C	5.25850300	0.46839600	-1.39375400
H	5.57237900	1.46302100	-1.72215000
H	5.28704600	0.44793900	-0.30008400
H	5.98750200	-0.25682200	-1.77112300

**Int31\_2**

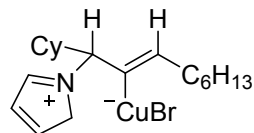


C	-1.92656900	-0.08028400	0.47873100
H	-1.93270600	0.27263300	1.51973700
C	-0.74204100	-1.00914200	0.29110500
C	-0.92188800	-2.30003300	-0.01601900
N	-3.23058000	-0.81671800	0.34322500
C	-3.84194900	-1.12545000	-0.94563600
H	-4.23515900	-0.21486800	-1.41052300
H	-3.05946800	-1.53733800	-1.59791800
C	-3.77088100	-1.55237900	1.26331900
H	-1.92807400	-2.73607000	-0.14087800
H	-3.40299400	-1.51591600	2.28328900
C	-4.83959000	-2.37052500	0.72320600
C	-4.89370100	-2.12079100	-0.59833900
H	-5.45325000	-3.04299000	1.30481700
H	-5.56960200	-2.55359100	-1.32356200
Cu	1.00998500	-0.11535800	0.83498800
Br	2.86919200	1.21170800	1.47208500
C	-2.00906900	1.16443400	-0.43465900
C	-3.16283000	2.07625700	0.01573300
C	-0.70081100	1.96350500	-0.48402300
H	-2.20168700	0.81852500	-1.46354300
C	-3.29702000	3.32526400	-0.85612100
H	-2.96223800	2.38449600	1.05235200
H	-4.11570700	1.53069600	0.03891100
C	-0.83880700	3.22779900	-1.33681800
H	-0.39422700	2.23544300	0.53642800
H	0.09940200	1.34196600	-0.89427800
C	-1.98947900	4.11563700	-0.86817200
H	-4.12477100	3.94440100	-0.49537200
H	-3.54853900	3.02566200	-1.88351800
H	0.10759200	3.77544900	-1.31552300
H	-1.01456700	2.93729800	-2.38220700



H	-2.08064000	4.99774500	-1.50981300
H	-1.77882100	4.47840600	0.14659500
C	0.12593200	-3.37936900	-0.19751300
H	-0.07576900	-4.16311800	0.54673200
H	-0.05020100	-3.86127500	-1.17125200
C	1.59391600	-2.97233000	-0.10948200
H	2.20792500	-3.88036500	-0.05881900
H	1.77148900	-2.44233900	0.83736100
C	2.08084100	-2.11418500	-1.27737100
H	1.99634200	-2.68799300	-2.21120600
H	1.41490100	-1.24923300	-1.39522100
C	3.51521100	-1.62246100	-1.08799800
H	3.63601700	-1.25058500	-0.06220800
H	4.21499000	-2.46176900	-1.20525200
C	3.88866300	-0.49254000	-2.04294800
H	3.77439900	-0.82889000	-3.08258700
H	3.17666800	0.32977100	-1.89186700
C	5.30336900	0.02359100	-1.80182600
H	5.56302600	0.82851300	-2.49502300
H	5.38809500	0.41314000	-0.78283400
H	6.04054300	-0.77719200	-1.92402900

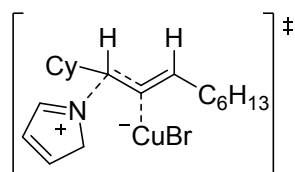
**Int32**



C	-1.75239200	0.54644400	1.03842700
H	-2.32936900	1.08102400	1.81232600
C	-0.52022300	1.32317200	0.57648600
C	-0.38469600	2.55240500	1.09427500
N	-1.22994500	-0.66855800	1.72670500
C	-0.60536900	-0.55325100	3.03817700
H	0.07575400	0.30855700	3.00071500
H	-1.36494700	-0.36655100	3.80535400
C	-0.87269000	-1.78637200	1.16698900
H	-1.13492500	2.93581300	1.80250600
H	-1.15604700	-2.04182600	0.15293000
C	-0.05218800	-2.57640200	2.06634800
C	0.10820100	-1.85327800	3.18884600
H	0.36283200	-3.54037000	1.81156800
H	0.66706500	-2.12787000	4.07340700
Cu	0.68132900	0.13217900	-0.53975700
Br	1.51369500	-2.02614600	-1.20018700

C	-2.69953900	0.16667200	-0.10531500
C	-3.89911400	-0.67842500	0.34601100
C	-3.18808800	1.44556500	-0.79792200
H	-2.11834800	-0.39695300	-0.85372600
C	-4.82429900	-1.00498500	-0.82918900
H	-4.45995000	-0.11144100	1.10361900
H	-3.57331300	-1.60662100	0.83055800
C	-4.11672300	1.12490200	-1.96908400
H	-3.72349000	2.06199500	-0.05956300
H	-2.32685700	2.02883500	-1.13340400
C	-5.30371100	0.26920500	-1.52565000
H	-5.67623200	-1.59790400	-0.48110900
H	-4.27803300	-1.62736500	-1.55102900
H	-4.46631900	2.05344700	-2.43136000
H	-3.54803800	0.58386700	-2.73734600
H	-5.93767500	0.01796500	-2.38192400
H	-5.92428300	0.84780500	-0.82771800
C	0.69645700	3.56370000	0.78289100
H	0.20734300	4.45347900	0.36293100
H	1.14474400	3.90456800	1.72841300
C	1.80115100	3.09671200	-0.16257800
H	1.33596400	2.62704400	-1.04012100
H	2.35283300	3.96688300	-0.53802400
C	2.78844800	2.11856600	0.47948200
H	2.23368700	1.38360800	1.07908700
H	3.43225300	2.66031700	1.18576500
C	3.64991000	1.37838400	-0.54188000
H	3.00242200	0.94291000	-1.31938100
H	4.30467200	2.09164200	-1.06184100
C	4.48121300	0.25365700	0.06834200
H	3.80208500	-0.43540900	0.58776400
H	5.16074200	0.66836300	0.82487200
C	5.26493500	-0.52488600	-0.98313300
H	5.87211700	-1.31243700	-0.52891300
H	4.57375400	-0.99783100	-1.68747200
H	5.93360200	0.13558200	-1.54545900

**TS16**

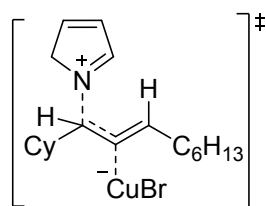


C	-1.72332200	0.79255900	1.13920400
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H	-2.03964800	0.89983600	2.18048700
C	-0.66595400	1.55064400	0.63951900
C	-0.49151800	2.87855000	0.74512000
N	-0.73655300	-1.01551100	1.84798600
C	0.34612300	-0.77633100	2.78940400
H	0.79022100	0.20640100	2.57377600
H	-0.04964800	-0.73968600	3.81204300
C	-0.44098400	-2.07469900	1.17567500
H	-1.29384100	3.48709800	1.17898700
H	-1.07783100	-2.43627400	0.37126200
C	0.82914700	-2.67740600	1.58836500
C	1.31244200	-1.89821500	2.56958500
H	1.27440900	-3.55249700	1.13676600
H	2.24179400	-2.01922600	3.11103100
Cu	0.44313500	0.28592600	-0.57586300
Br	1.27138900	-1.57288500	-1.80092000
C	-2.73419800	0.15048300	0.22470800
C	-3.74010000	-0.74844400	0.94890300
C	-3.47118600	1.28450700	-0.52251600
H	-2.19450600	-0.43899400	-0.53153200
C	-4.77408100	-1.31725800	-0.02507100
H	-4.25543800	-0.15024100	1.71486400
H	-3.21541600	-1.55113400	1.47563500
C	-4.50758100	0.71319400	-1.49115800
H	-3.97087300	1.93002700	0.21481400
H	-2.74350700	1.90466200	-1.05385200
C	-5.50236100	-0.19934500	-0.77370400
H	-5.48827300	-1.94729400	0.51449100
H	-4.26423700	-1.96559500	-0.75096900
H	-5.03102600	1.53185400	-1.99508700
H	-3.98587400	0.14150100	-2.27013400
H	-6.21668200	-0.62068100	-1.48793200
H	-6.08326500	0.39503700	-0.05495900
C	0.66381300	3.71587200	0.25682800
H	0.25482300	4.48305600	-0.41435900
H	1.05124800	4.27554400	1.12201400
C	1.81222600	2.99131900	-0.43731700
H	1.40728400	2.39143400	-1.26751100
H	2.47139900	3.73095400	-0.90696400
C	2.64062400	2.09767500	0.48752200
H	3.17043200	2.72113100	1.22017200
H	1.96209100	1.46423700	1.07524000
C	3.62869900	1.20320700	-0.26317000
H	4.49376200	1.79426900	-0.59213600

H	3.15327800	0.81467000	-1.17430800
C	4.09241500	0.00886200	0.56681000
H	3.20212600	-0.56579400	0.86102700
H	4.56785500	0.36083500	1.49275500
C	5.03556600	-0.90545100	-0.20726500
H	5.93043700	-0.36431900	-0.53172800
H	5.35850700	-1.75633600	0.39887200
H	4.52811900	-1.29511600	-1.09510000

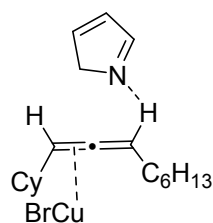
**TS17**



C	1.66344900	0.13250600	-0.45746700
H	1.70846900	0.33778800	-1.53103100
C	0.88896300	-0.97489900	-0.06777300
C	1.17930100	-2.08826400	0.60016400
N	3.52548800	-0.43051600	-0.40987800
C	3.88637500	-1.43061700	-1.40336100
H	2.99386100	-2.02968300	-1.62975900
H	4.20427100	-0.93966900	-2.33120300
C	4.23188300	-0.64816200	0.64663500
H	2.23421300	-2.28265800	0.84578700
H	4.10799100	-0.04236100	1.54081100
C	5.16853000	-1.75982800	0.47674700
C	4.96704300	-2.23910600	-0.76248500
H	5.86871300	-2.10745800	1.22362900
H	5.47583700	-3.06527800	-1.24152700
Cu	-0.93989500	-0.39448500	-0.86524700
Br	-2.85427500	0.52566500	-1.88950600
C	1.70647000	1.38506200	0.40842900
C	2.60249400	2.47138300	-0.19957000
C	0.29408500	1.95062100	0.66295700
H	2.10531400	1.07950500	1.38917500
C	2.64522900	3.72727300	0.67310700
H	2.19821800	2.73384500	-1.18802000
H	3.61249300	2.08290800	-0.36230200
C	0.34117000	3.21103600	1.52812900
H	-0.18591200	2.17979100	-0.29953500
H	-0.32195300	1.18658500	1.14876200
C	1.24079800	4.28155300	0.91223200

H	3.28495100	4.48234100	0.20516200
H	3.10505000	3.47898500	1.64015200
H	-0.67510000	3.59211200	1.66544000
H	0.72146000	2.94873300	2.52511700
H	1.28207600	5.16489200	1.55726800
H	0.81285800	4.60508500	-0.04586200
C	0.25117700	-3.18274500	1.06862700
H	0.54520300	-4.11365100	0.56469000
H	0.45258900	-3.35809100	2.13535400
C	-1.24340000	-2.94370400	0.87303600
H	-1.44119000	-2.72173900	-0.18676900
H	-1.78476500	-3.87373400	1.08393100
C	-1.81210100	-1.82452300	1.74618800
H	-1.71902000	-2.10416300	2.80454000
H	-1.19533700	-0.92325800	1.62479800
C	-3.26500400	-1.48575200	1.41253700
H	-3.92820600	-2.27730500	1.78725900
H	-3.39122700	-1.46098100	0.32213500
C	-3.70170000	-0.13149300	1.96491000
H	-3.01937700	0.63449600	1.57078500
H	-3.59561600	-0.12189400	3.05808700
C	-5.12872700	0.22259300	1.56061900
H	-5.83732700	-0.53284100	1.91652300
H	-5.43486100	1.18969400	1.96851200
H	-5.20172300	0.27581200	0.47012700

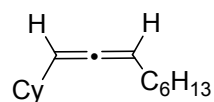
### Int33



C	0.75210100	0.39906200	-1.53366600
H	0.59041800	0.93825000	-2.47236500
C	0.60743100	-0.92527300	-1.52035400
C	0.72747800	-2.22992800	-1.49757100
N	3.71039200	-1.94227800	-0.42839100
C	5.07356600	-1.43834200	-0.33550500
H	5.77792700	-2.26189900	-0.50923900
H	5.24994400	-0.70680500	-1.13526900
C	3.16052100	-1.69461200	0.70747300
H	1.73368500	-2.57311800	-1.75059600
H	2.12442200	-1.96971000	0.90074700

C	4.04364100	-1.01161700	1.66446400
C	5.21599300	-0.84360200	1.03208100
H	3.77690600	-0.71449600	2.67039600
H	6.11522500	-0.37840200	1.41544200
Cu	-1.39711800	0.13555600	-1.11142000
Br	-3.51742500	1.05330800	-0.70025500
C	1.31837800	1.20608900	-0.37847900
C	2.78056700	1.56707500	-0.69319200
C	0.49648500	2.47453000	-0.10416000
H	1.30810000	0.57304000	0.52143700
C	3.39822400	2.41515100	0.42014700
H	2.80719500	2.12940000	-1.63790800
H	3.34944500	0.64450300	-0.84928500
C	1.12718400	3.32644500	0.99906100
H	0.43802800	3.06039200	-1.03330800
H	-0.53555300	2.21712400	0.16613200
C	2.57826500	3.68069000	0.67035700
H	4.43365500	2.66550700	0.16511400
H	3.43660900	1.81937900	1.34177400
H	0.53235100	4.23208800	1.15078600
H	1.09706100	2.76617400	1.94361900
H	3.02091200	4.26727500	1.48171300
H	2.60119300	4.31154000	-0.22849400
C	-0.27586000	-3.29620500	-1.13539500
H	-0.54030500	-3.83623300	-2.05295700
H	0.25078700	-4.02591900	-0.50670300
C	-1.53944300	-2.83265700	-0.41578800
H	-2.18567600	-3.70366500	-0.25591500
H	-2.12526700	-2.16210600	-1.06463700
C	-1.28237400	-2.15953600	0.93374200
H	-0.67782200	-2.82696500	1.56399400
H	-0.66369600	-1.25810400	0.79693400
C	-2.57354900	-1.77128100	1.65500500
H	-3.03383800	-2.66757700	2.09152300
H	-3.28853900	-1.37082200	0.92580500
C	-2.35389100	-0.71543000	2.73506500
H	-1.89146600	0.16434600	2.26573100
H	-1.64080600	-1.08882400	3.48221600
C	-3.65842500	-0.29637500	3.40401400
H	-4.15126400	-1.15329000	3.87466100
H	-3.49167000	0.46085800	4.17441000
H	-4.34218500	0.12200400	2.65928100

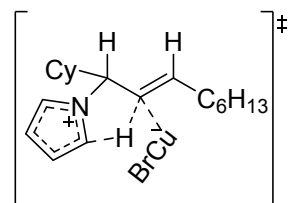
8



C	-0.40091600	-1.91376700	0.74530100
H	-0.66673400	-2.19851600	1.76511500
C	0.69478900	-2.38879900	0.21114300
C	1.79869300	-2.80427700	-0.35459400
H	1.77416300	-3.73180900	-0.92559700
C	-1.33844300	-0.95786000	0.04488800
C	-2.74779300	-1.55321800	-0.08783300
C	-1.39924700	0.38323600	0.79179700
H	-0.94684100	-0.77237000	-0.96580600
C	-3.71019000	-0.57316500	-0.76301400
H	-3.12110000	-1.79726100	0.91772000
H	-2.69840800	-2.49485500	-0.64462400
C	-2.35865000	1.36400000	0.11485700
H	-1.73593500	0.19557300	1.82215400
H	-0.39168100	0.80937300	0.86211100
C	-3.75931100	0.76168600	-0.01672600
H	-4.71112500	-1.01230700	-0.82914700
H	-3.37419000	-0.39504000	-1.79381400
H	-2.39336200	2.30527500	0.67401400
H	-1.97719400	1.60565000	-0.88736400
H	-4.42943600	1.46052200	-0.52825800
H	-4.17583500	0.59831900	0.98669000
C	3.13231500	-2.09171800	-0.26423400
H	3.55041800	-2.00952500	-1.27638500
H	3.82700200	-2.73150400	0.29489000
C	3.06680500	-0.70704700	0.37901800
H	2.55987300	-0.78706100	1.34939400
H	4.08601100	-0.35829300	0.58473500
C	2.34434400	0.33048000	-0.47910600
H	2.88106500	0.45774300	-1.42949000
H	1.34531000	-0.04233400	-0.73772200
C	2.20157500	1.68267600	0.21338100
H	3.19456000	2.10259700	0.42540500
H	1.72113600	1.53642500	1.19158800
C	1.38616000	2.68394100	-0.60187800
H	1.90830200	2.89498400	-1.54342100
H	0.42995600	2.22058800	-0.88108300
C	1.12061800	3.98323800	0.15224800
H	0.54973400	4.69222400	-0.45294400
H	0.55139800	3.78796000	1.06726700

H 2.05841600 4.46720300 0.44308300

**TS18**

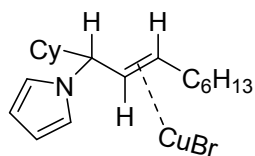


C	-2.06261400	0.44754500	0.99319400
H	-2.68155200	0.89983800	1.78258600
C	-0.75178900	-0.12691700	1.55889800
C	-0.11694700	0.44780000	2.58895900
N	-2.77391100	-0.77887000	0.55061600
C	-2.71146100	-1.83991200	1.50198600
H	-1.45598800	-1.59335700	1.70142300
H	-3.19215200	-1.68029900	2.46342000
C	-2.61254200	-1.32168500	-0.65940300
H	-0.49267100	1.38253300	3.02385100
H	-2.40613700	-0.71538300	-1.53116900
C	-2.70284600	-2.72969100	-0.58972100
C	-2.81206000	-3.05194100	0.74289500
H	-2.63908000	-3.39782000	-1.43528000
H	-2.90483200	-4.04110100	1.17013600
Cu	0.27729300	-1.24522500	0.16360700
Br	1.25240900	-2.29042500	-1.71139700
C	-1.88640500	1.46952900	-0.13410100
C	-3.23318100	1.91585100	-0.72523000
C	-1.11062800	2.69902600	0.35792400
H	-1.27615800	1.00449700	-0.92550400
C	-3.04111400	2.92925500	-1.85571900
H	-3.82446400	2.37601500	0.07995300
H	-3.81526200	1.05908200	-1.08138800
C	-0.91349200	3.71665900	-0.76716300
H	-1.66919200	3.16656200	1.18326000
H	-0.14096400	2.39368300	0.76079500
C	-2.24782300	4.14556400	-1.37713100
H	-4.01464900	3.23595800	-2.25111000
H	-2.50087000	2.44682300	-2.68162400
H	-0.36807100	4.58642800	-0.38772000
H	-0.28517600	3.26522600	-1.54683600
H	-2.08431800	4.84425300	-2.20353800
H	-2.83489400	4.68076000	-0.61825000
C	1.17149300	-0.06200100	3.17002900
H	1.12829300	-0.01850700	4.26448300



H	1.30453100	-1.11404500	2.88459400
C	2.38832200	0.74500600	2.67693300
H	2.24152300	1.80832900	2.91071600
H	3.27310200	0.42276700	3.23918800
C	2.65424100	0.57847500	1.18342500
H	2.73699900	-0.49292900	0.94333400
H	1.79497000	0.95045500	0.60760500
C	3.91274900	1.28980600	0.69563900
H	4.79021300	0.88213900	1.21624800
H	3.86257800	2.35444700	0.96540600
C	4.10555900	1.15352000	-0.81342900
H	4.10530300	0.09053300	-1.08232000
H	3.23817700	1.59101000	-1.32427700
C	5.38641500	1.82070500	-1.30523800
H	5.50224900	1.71702400	-2.38704500
H	5.38885500	2.88960500	-1.06727000
H	6.26595100	1.37442200	-0.83018900

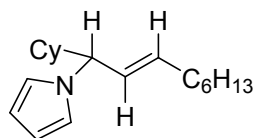
**Int34**



C	2.01695100	0.40898200	0.10457500
H	1.70773600	0.15502900	1.12836900
C	0.88764900	1.16907100	-0.58009400
C	0.10832100	2.07233900	0.05992900
N	3.16350900	1.29634400	0.25036200
C	3.70392400	1.70090800	1.44315500
H	3.28048700	1.36321500	2.37823800
C	3.88646600	1.84290100	-0.77996300
H	0.24100400	2.18883400	1.14039500
H	3.62184900	1.64922800	-1.80934700
C	4.89647800	2.60208100	-0.23766200
C	4.78164400	2.51119700	1.17514900
H	5.63511100	3.15894600	-0.79481400
H	5.41835300	2.97894800	1.91100100
Cu	-0.90494500	0.04381300	0.24413100
Br	-2.32525900	-1.49472700	1.29901600
H	0.83826800	1.10608000	-1.66961400
C	2.40693500	-0.89280900	-0.61390200
C	3.56651900	-1.57873900	0.11769900
C	1.21196800	-1.84465900	-0.74478900
H	2.74835500	-0.62689000	-1.62763700

C	3.95444400	-2.90033100	-0.54675000
H	3.25586500	-1.77311700	1.15557000
H	4.42684500	-0.90328200	0.16310100
C	1.60517600	-3.17114000	-1.40083600
H	0.79605200	-2.04730500	0.25466800
H	0.40762100	-1.38267800	-1.33680700
C	2.75418200	-3.84179700	-0.64841400
H	4.76844600	-3.37183100	0.01246500
H	4.34059100	-2.69607000	-1.55483200
H	0.73206300	-3.82878900	-1.44210100
H	1.91428900	-2.98059500	-2.43759500
H	3.03847500	-4.77430400	-1.14598400
H	2.41579100	-4.10907700	0.36150500
C	-0.82873100	3.05000900	-0.59606300
H	-0.49429900	4.05129500	-0.30118400
H	-0.72788900	2.98635200	-1.68584900
C	-2.30026200	2.84431200	-0.19038600
H	-2.34489300	2.53831600	0.86445000
H	-2.83763100	3.79561000	-0.25547500
C	-3.01432500	1.80425800	-1.05611100
H	-3.22354200	2.23673200	-2.04348600
H	-2.34579500	0.94907300	-1.26261600
C	-4.29474500	1.26850600	-0.42405700
H	-4.06328900	0.89989300	0.58350400
H	-5.01755800	2.08800700	-0.30895100
C	-4.91945100	0.12725400	-1.22125800
H	-5.18344000	0.47853800	-2.22743600
H	-4.16648900	-0.66188900	-1.34161900
C	-6.14510400	-0.45396900	-0.52417500
H	-6.91118500	0.31273700	-0.36844600
H	-6.59241000	-1.26316400	-1.10687900
H	-5.86410900	-0.85763000	0.45324800

7

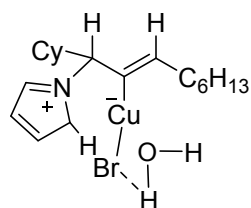


C	-1.44085800	-0.46985500	0.31148900
H	-1.28300700	-0.45610600	1.39779900
C	-0.40574400	-1.36752200	-0.31207300
C	0.49781300	-2.05840000	0.37787700
N	-2.78661100	-1.00492300	0.10930600
C	-3.68363500	-1.28254000	1.10466400

H	-3.39396700	-1.18968700	2.14125300
C	-3.39619000	-1.18589100	-1.10432200
H	0.49950800	-1.98037900	1.46787900
H	-2.86101200	-1.01289800	-2.02653100
C	-4.69186200	-1.59174000	-0.88025200
C	-4.87542000	-1.65318300	0.52606900
H	-5.42096300	-1.82310800	-1.64275400
H	-5.77246100	-1.93958600	1.05458300
H	-0.41418400	-1.43041200	-1.40185500
C	-1.35385700	0.97882200	-0.20554300
C	-2.46258300	1.84987200	0.39472900
C	0.02695100	1.58301200	0.07500300
H	-1.49651000	0.95025800	-1.29827300
C	-2.36558600	3.29767400	-0.08814900
H	-2.37013400	1.82633600	1.49168300
H	-3.44293700	1.42805200	0.14957900
C	0.11767200	3.03425700	-0.40093800
H	0.21419200	1.54194200	1.15941200
H	0.80613300	0.97772100	-0.40042400
C	-0.98926700	3.89368500	0.21140300
H	-3.15427900	3.89998100	0.37420000
H	-2.54124200	3.32585500	-1.17227500
H	1.10362100	3.44550500	-0.16002700
H	0.02494800	3.05683900	-1.49543400
H	-0.92581100	4.92062300	-0.16325800
H	-0.84682400	3.94225800	1.29975700
C	1.55496000	-2.93607700	-0.22516300
H	1.38093300	-3.97655700	0.07669700
H	1.47267000	-2.90253200	-1.31817600
C	2.96979300	-2.52114600	0.19955100
H	3.07957100	-2.65616600	1.28400500
H	3.69577500	-3.19605900	-0.27001400
C	3.30423200	-1.07557500	-0.16221900
H	3.08449100	-0.90552200	-1.22641600
H	2.64182100	-0.39983000	0.39488300
C	4.75664000	-0.70661400	0.12377400
H	4.98332700	-0.91201500	1.17934800
H	5.42138600	-1.35563800	-0.46284900
C	5.07561000	0.75474300	-0.18488000
H	4.83825000	0.96084600	-1.23622200
H	4.41607900	1.39946900	0.40996900
C	6.53356200	1.10855100	0.09353300
H	7.20534500	0.49550800	-0.51543600
H	6.74422900	2.15797700	-0.12752900

H 6.78393800 0.92933700 1.14395100

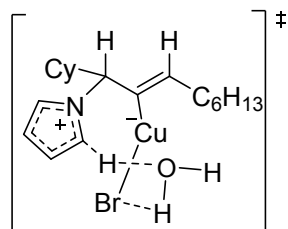
**Int35**



C	1.88295300	-0.18759900	0.94442200
H	2.44734000	-0.43448700	1.85929800
C	0.60466300	-1.00868500	0.81462100
C	0.48652000	-2.02059300	1.68922600
N	1.52983500	1.25009000	1.10964300
C	1.45617500	1.90184900	2.41019900
H	0.75121900	1.34951400	3.04282000
H	2.44976700	1.91459300	2.87298900
C	1.08572100	2.05067300	0.18888400
H	1.26053400	-2.16764100	2.45761900
H	1.03348000	1.75698500	-0.85338700
C	0.69615600	3.32540600	0.75407700
C	0.92256500	3.25094300	2.07804100
H	0.27413500	4.13653800	0.17924700
H	0.73393900	4.01285100	2.82231600
Cu	-0.72420600	-0.26258000	-0.51645200
Br	-1.90981700	1.62682200	-1.43765500
O	-1.35718900	1.16637800	2.15142700
H	-1.05767900	0.26527500	1.96346600
H	-1.80669700	1.44182900	1.33765900
C	2.83091400	-0.35167200	-0.25694800
C	4.08378700	0.52714600	-0.14489500
C	3.23087200	-1.82383800	-0.40996400
H	2.27295500	-0.06982500	-1.16492900
C	5.02275500	0.32586100	-1.33656900
H	4.61450400	0.26107500	0.78172000
H	3.81550500	1.58692600	-0.06090300
C	4.17626300	-2.02810200	-1.59527100
H	3.72721000	-2.14898300	0.51749000
H	2.33327100	-2.43759500	-0.51977600
C	5.41788800	-1.14346800	-1.48446100
H	5.91133200	0.95533400	-1.22330800
H	4.51373200	0.65679900	-2.25212100
H	4.46167100	-3.08255500	-1.66372600
H	3.64171400	-1.78487400	-2.52352900

H	6.06489200	-1.27791000	-2.35722100
H	6.00173200	-1.44819500	-0.60513500
C	-0.57302100	-3.10062500	1.73105500
H	-0.04598300	-4.06211000	1.66231700
H	-1.03921000	-3.10468600	2.72786000
C	-1.66281400	-3.04441500	0.66087600
H	-1.19718600	-2.81935300	-0.30888800
H	-2.11791600	-4.03626400	0.55546300
C	-2.77018200	-2.03028600	0.95338200
H	-3.38520400	-2.39442500	1.78740400
H	-2.33825000	-1.08485500	1.30591600
C	-3.65753200	-1.73587000	-0.25311200
H	-3.02857600	-1.41637900	-1.09885900
H	-4.15958700	-2.65766700	-0.57920600
C	-4.69038400	-0.64526800	0.01575300
H	-5.37025200	-0.97597300	0.81168300
H	-4.16924600	0.24500700	0.39093500
C	-5.47489200	-0.27133200	-1.23738500
H	-6.23450400	0.48566300	-1.02557900
H	-4.79594600	0.13532900	-1.99329200
H	-5.97890000	-1.14627700	-1.66180600

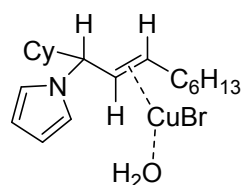
**TS19**



C	1.94462600	-0.07222900	0.86446100
H	2.44337500	-0.26214900	1.82949100
C	0.67141000	-0.89752800	0.71344900
C	0.53718600	-1.90553700	1.59413400
N	1.62224900	1.37958400	0.89554100
C	1.28197800	2.07646700	2.07427500
H	-0.00811500	1.68478300	2.18468000
H	1.78315900	1.79428600	2.99440200
C	1.35510300	2.15408800	-0.15058900
H	1.30091600	-2.04327500	2.37470600
H	1.42526700	1.77690500	-1.16235500
C	0.94429500	3.43072100	0.28056000
C	0.95888300	3.40518700	1.65890800
H	0.64129800	4.23897000	-0.36698400
H	0.68498200	4.20647100	2.33167600

Cu	-0.67093000	-0.17430000	-0.61647800
Br	-2.24059500	1.59456400	-1.11710600
O	-1.16634900	1.11743600	2.10707400
H	-0.90107500	0.19301300	1.90261300
H	-1.63827000	1.43225200	1.29914700
C	2.97363000	-0.35572300	-0.24702300
C	4.23774900	0.50342000	-0.10485300
C	3.34934400	-1.84312400	-0.25632800
H	2.49575200	-0.13805400	-1.21578100
C	5.26221500	0.19122700	-1.19800600
H	4.68568600	0.29881600	0.87915700
H	3.99038300	1.56992700	-0.12023200
C	4.37922300	-2.15669400	-1.34363700
H	3.76399300	-2.10601600	0.72915600
H	2.45107600	-2.45030600	-0.39339100
C	5.63127700	-1.29209900	-1.20221200
H	6.15444300	0.81086500	-1.06117300
H	4.83659500	0.45968900	-2.17477200
H	4.64044300	-3.21926700	-1.31077600
H	3.92494400	-1.97448200	-2.32722600
H	6.34018100	-1.50765000	-2.00812700
H	6.13694700	-1.53919900	-0.25860400
C	-0.49556900	-3.01201300	1.61443200
H	0.06177500	-3.95350500	1.51260400
H	-0.94936300	-3.06307900	2.61542100
C	-1.60047500	-2.96618100	0.55986000
H	-1.16437700	-2.68400100	-0.40860800
H	-2.00995700	-3.97422000	0.42504400
C	-2.75640200	-2.02732100	0.90464000
H	-3.28600100	-2.41584500	1.78528900
H	-2.37618000	-1.03990900	1.20192500
C	-3.73696000	-1.82932400	-0.24683800
H	-3.19758400	-1.41177500	-1.10964000
H	-4.13160300	-2.80406200	-0.56675200
C	-4.88901000	-0.89245900	0.10464300
H	-5.48742100	-1.33746100	0.91032400
H	-4.47210400	0.04419500	0.49477300
C	-5.76860900	-0.58248300	-1.10202700
H	-6.60689100	0.06571600	-0.83367100
H	-5.18066700	-0.07296500	-1.87160500
H	-6.17812900	-1.50064800	-1.53663300

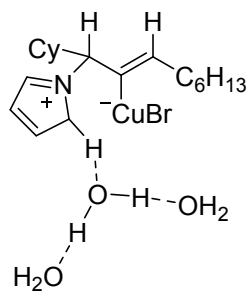
## Int36



C	2.00228500	-0.42790300	0.07844800
H	1.66803200	-0.24065300	-0.95247300
C	0.86352200	-1.08975500	0.84368300
C	0.04526500	-2.00190800	0.27221400
N	3.12023500	-1.35621400	-0.03408100
C	3.63224300	-1.83419700	-1.21178900
H	-1.53806100	2.59605400	0.74633200
H	3.18762200	-1.55124300	-2.15523200
C	3.85927800	-1.84847100	1.01151400
H	0.16102000	-2.19479400	-0.79809900
H	3.61448000	-1.59536200	2.03299000
C	4.85070200	-2.64925400	0.49449600
C	4.70723300	-2.63976600	-0.91856700
H	5.59293900	-3.18410600	1.06833200
H	5.31987400	-3.16157800	-1.63828700
Cu	-0.90288200	0.05071100	-0.11333900
Br	-1.75074100	0.46607000	-2.36512500
O	-2.04724200	1.78327600	0.64058200
H	0.82723100	-0.94022300	1.92484200
H	-2.47555100	1.85898500	-0.23129200
C	2.46115300	0.90925000	0.68252800
C	3.61712700	1.49979200	-0.13236300
C	1.30074000	1.90697700	0.77598500
H	2.82373500	0.71174700	1.70436900
C	4.06417900	2.85575800	0.41495500
H	3.28108000	1.62087800	-1.17331200
H	4.45523800	0.79580100	-0.14814300
C	1.75391100	3.26872500	1.31147200
H	0.86719900	2.03623100	-0.23085200
H	0.51151500	1.50497700	1.42639300
C	2.89745700	3.84217600	0.47507000
H	4.87344700	3.25707600	-0.20262900
H	4.47480300	2.71958900	1.42466000
H	0.90761000	3.96482700	1.33405800
H	2.08990700	3.14810400	2.34998500
H	3.22492400	4.80142200	0.88805200
H	2.53620400	4.03842500	-0.54344500
C	-0.94603000	-2.87428200	0.99254200

H	-0.68680500	-3.91252100	0.75616400
H	-0.83317500	-2.75348200	2.07660800
C	-2.40295700	-2.59027700	0.57895100
H	-2.43431200	-2.34582400	-0.49193600
H	-3.00623700	-3.49470800	0.70794200
C	-3.03434700	-1.45330600	1.38834700
H	-3.29218700	-1.82556400	2.38903300
H	-2.30591200	-0.64426400	1.56996700
C	-4.26697600	-0.85761100	0.71496800
H	-3.97053200	-0.44690000	-0.26130100
H	-4.98798800	-1.65946500	0.50306200
C	-4.94148200	0.23046700	1.54681100
H	-5.25674600	-0.19063200	2.51017200
H	-4.20372500	1.01062400	1.76960900
C	-6.14260400	0.84206500	0.83107400
H	-6.61508900	1.62446300	1.43063000
H	-5.83992200	1.28455100	-0.12359800
H	-6.89900700	0.08091100	0.61547500

### Int37



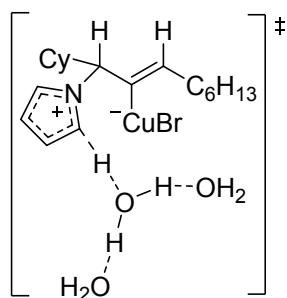
C	-1.88875100	0.55847500	0.84285900
H	-2.29546800	1.18644400	1.65194500
C	-0.62432800	1.15242600	0.22446300
C	-0.53678300	2.49162500	0.29919300
N	-1.54982500	-0.73072000	1.49993000
C	-1.08448200	-0.81563100	2.87196000
H	-0.12455600	-0.24500600	2.97437800
H	-1.82630700	-0.42397500	3.57358200
C	-1.37479000	-1.87575200	0.90516000
H	-1.29474800	3.06473100	0.85408500
H	-1.57670400	-2.01406200	-0.15151000
C	-0.86445500	-2.86118600	1.82720600
C	-0.72492500	-2.24336400	3.01962200
H	-0.62910000	-3.88039200	1.55808400
H	-0.34066600	-2.66182800	3.94020100
Cu	0.52768000	-0.23035900	-0.69611400



Br	1.03367900	-2.38499700	-1.69483600
O	1.69042500	-0.04591200	3.26425500
H	1.82010900	0.91559000	3.20117600
H	2.12755100	-0.43248000	2.48686800
O	1.41257000	2.65615200	2.69073200
O	2.71882300	-1.26889400	0.92680100
H	3.46599700	-1.02832200	0.36739300
H	2.23248000	-1.92389200	0.39965800
H	0.76715500	2.35183400	2.03024400
H	2.11891900	3.04863500	2.16697000
C	-3.01365400	0.32801800	-0.19152600
C	-4.25004800	-0.33697700	0.43438000
C	-3.41955200	1.64859300	-0.85877800
H	-2.61464100	-0.32210500	-0.98641100
C	-5.36613300	-0.54491900	-0.59233700
H	-4.61828300	0.31239500	1.24251300
H	-3.99483700	-1.29677900	0.89679400
C	-4.53838100	1.44259200	-1.88190900
H	-3.75882900	2.34853900	-0.07973900
H	-2.54980100	2.10377300	-1.33697200
C	-5.76066600	0.77461300	-1.25394400
H	-6.23182500	-1.01073900	-0.11061200
H	-5.01690900	-1.24552000	-1.36288700
H	-4.81190500	2.40460400	-2.32683900
H	-4.16217600	0.81215000	-2.69882500
H	-6.53777000	0.60841700	-2.00665800
H	-6.18822200	1.44408900	-0.49513400
C	0.46371500	3.38747900	-0.40232300
H	-0.10767300	4.02906400	-1.08715500
H	0.90221700	4.08346100	0.32970700
C	1.57998800	2.69615900	-1.18238900
H	1.14544100	1.90799700	-1.81314600
H	2.03444800	3.41750500	-1.87196800
C	2.68684800	2.10822600	-0.30673600
H	2.25850400	1.49489000	0.49826400
H	3.23289700	2.93538200	0.17507000
C	3.67477300	1.25080900	-1.09346400
H	3.16306100	0.33405200	-1.42851200
H	3.97505500	1.77371600	-2.01131400
C	4.92537800	0.89186300	-0.29063600
H	5.51092900	1.80278500	-0.11766000
H	4.63426600	0.54261300	0.71051000
C	5.79134700	-0.15578300	-0.98642500
H	6.11396200	0.20195200	-1.96867100

H	6.68355100	-0.39708900	-0.40378800
H	5.23600900	-1.08644700	-1.15317100

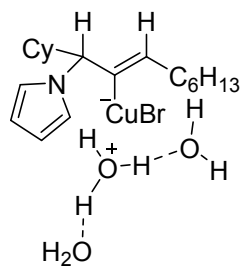
**TS20**



C	-1.90286700	0.48567300	0.81242600
H	-2.31415500	1.08226500	1.64284000
C	-0.64268800	1.11289700	0.22766900
C	-0.56020600	2.44900300	0.36047800
N	-1.59094400	-0.83464000	1.41861400
C	-1.30397400	-1.03029000	2.80086200
H	-0.12653300	-0.63669900	2.94838800
H	-1.93162200	-0.47536600	3.49534500
C	-1.36568900	-1.95559900	0.76498000
H	-1.33835700	2.99441400	0.91670600
H	-1.40992200	-2.00563000	-0.31684600
C	-1.03386500	-2.99899300	1.67270600
C	-1.06595500	-2.45326900	2.92573800
H	-0.78882700	-4.01098500	1.38716600
H	-0.84076200	-2.94637000	3.86184000
Cu	0.52171100	-0.18225900	-0.78030500
Br	1.37327200	-2.10793900	-1.94607200
O	1.25839300	-0.33767800	3.09923700
H	1.36894500	0.64017800	3.11341000
H	1.77223300	-0.69513400	2.33892400
O	1.11653200	2.32963600	2.88932000
O	2.66106000	-1.39670300	1.02566300
H	3.24799400	-0.85178800	0.48739100
H	2.23588100	-1.97768400	0.37163200
H	0.53076600	2.21929300	2.11673600
H	1.88474700	2.80047900	2.54838900
C	-3.02938800	0.30057000	-0.23140200
C	-4.26690600	-0.37554200	0.37966100
C	-3.42813700	1.64067800	-0.86131000
H	-2.63668600	-0.33380100	-1.04210700
C	-5.38767000	-0.54815900	-0.64788500
H	-4.62890400	0.25253900	1.20750300

H	-4.01056200	-1.34868400	0.81222700
C	-4.55212700	1.46934400	-1.88559400
H	-3.76134400	2.32157800	-0.06285000
H	-2.55780800	2.10477200	-1.33045500
C	-5.77634900	0.79133400	-1.27172900
H	-6.25486200	-1.02146200	-0.17615100
H	-5.04598200	-1.22975200	-1.43861500
H	-4.82166300	2.44472300	-2.30325100
H	-4.18280300	0.85931100	-2.72101100
H	-6.55691000	0.65096100	-2.02622500
H	-6.19727300	1.44241900	-0.49330900
C	0.46387000	3.38116900	-0.25611500
H	-0.07176900	4.02960600	-0.96287200
H	0.83818000	4.06732500	0.52039700
C	1.65092200	2.73925000	-0.97171700
H	1.28807900	1.97830200	-1.67639800
H	2.15003200	3.50005600	-1.58377900
C	2.69161300	2.12551100	-0.03470500
H	2.20607800	1.45330700	0.68683000
H	3.16288300	2.93281500	0.54882800
C	3.77567900	1.34673600	-0.77667100
H	3.32115200	0.45859000	-1.24567000
H	4.16002500	1.94791500	-1.61098800
C	4.94503500	0.93521100	0.12065500
H	5.50186300	1.83344500	0.41320300
H	4.56669000	0.51237100	1.06327400
C	5.87973000	-0.06328200	-0.55727000
H	6.27726100	0.35100800	-1.48858400
H	6.72379700	-0.32734100	0.08413100
H	5.34856800	-0.98663300	-0.81338500

**Int38**

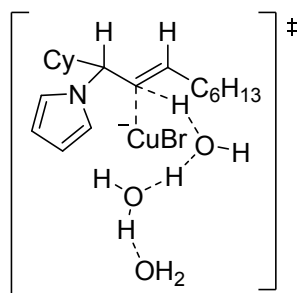


C	-2.03124800	-0.02904000	0.88981900
H	-2.55880100	0.00852200	1.85747500
C	-0.72145600	0.73932200	0.94778100
C	-0.61255300	1.58817100	1.99015300
N	-1.80964000	-1.47126000	0.64498900

C	-2.06490100	-2.46340800	1.54446400
H	0.12683900	-3.22287400	1.51686500
H	-2.40349900	-2.22328800	2.54224500
C	-1.43024700	-2.03346900	-0.54364400
H	-1.42881700	1.63830400	2.72733800
H	-1.21129500	-1.41696400	-1.40555800
C	-1.43648900	-3.40781900	-0.40147300
C	-1.83605200	-3.68667400	0.93618700
H	-1.22013300	-4.12969000	-1.17715000
H	-1.98592000	-4.65784900	1.38528800
Cu	0.56552600	0.47530000	-0.57697200
Br	2.09700500	0.01672700	-2.36868900
O	1.04356500	-2.87672700	1.59327000
H	1.00854400	-1.99479300	2.17397100
H	1.42859200	-2.76112800	0.60776200
O	0.84612400	-0.86178000	2.99205100
O	1.80546500	-2.76763400	-0.73561300
H	2.21841000	-1.96331700	-1.11787500
H	0.97958500	-2.85650200	-1.23335100
H	0.31689500	-0.18613700	2.49278200
H	1.67308500	-0.42119200	3.22558000
C	-2.99969200	0.52740400	-0.17476000
C	-4.29230600	-0.29738900	-0.24764000
C	-3.32366200	2.00096700	0.09841400
H	-2.49153400	0.47546900	-1.15133300
C	-5.26829300	0.26874500	-1.28106700
H	-4.76865500	-0.28390500	0.74463900
H	-4.06688500	-1.34466000	-0.47658700
C	-4.30325000	2.56346900	-0.93361000
H	-3.76536500	2.08288600	1.10387400
H	-2.40239800	2.58948200	0.11052900
C	-5.58742200	1.73628800	-0.99520300
H	-6.18483200	-0.32990900	-1.29604900
H	-4.81942900	0.18537400	-2.28025600
H	-4.52993300	3.60878300	-0.70014600
H	-3.82290100	2.55704100	-1.92154500
H	-6.26647600	2.13645000	-1.75509200
H	-6.10905800	1.80944300	-0.03088200
C	0.47695600	2.59545700	2.29553600
H	-0.00493000	3.58262800	2.31044400
H	0.82071500	2.44089800	3.33075200
C	1.69113100	2.65330000	1.36911200
H	1.35545000	2.70712900	0.32409100
H	2.23298600	3.58737400	1.56079800

C	2.67171200	1.49221500	1.52604300
H	2.15711400	0.54351400	1.31753800
H	3.01502500	1.44531800	2.57296600
C	3.87553200	1.58966700	0.59288400
H	3.51683400	1.77050600	-0.42836000
H	4.49226700	2.45391300	0.87336900
C	4.72501500	0.32234700	0.58823100
H	5.12264400	0.13659300	1.59515300
H	4.07531600	-0.52968800	0.34307400
C	5.86167900	0.39084000	-0.42641100
H	6.52123300	1.23905600	-0.21709900
H	6.46828100	-0.51831400	-0.41613400
H	5.45513800	0.51796900	-1.43428900

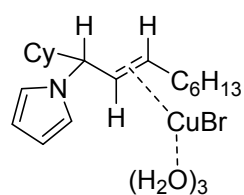
**TS21**



C	-2.03774400	0.15874000	-1.04974700
H	-2.68899700	0.18417800	-1.93625800
C	-0.66785300	-0.40147800	-1.40827700
C	-0.60626300	-1.37791800	-2.33280200
N	-1.91562400	1.56670000	-0.62044700
C	-2.18563000	2.64997800	-1.40401000
H	0.19631800	3.74750600	-0.90873500
H	-2.48618400	2.51724600	-2.43320600
C	-1.56149200	1.99917300	0.63137800
H	-1.52968500	-1.70865900	-2.82517500
H	-1.34635400	1.29676700	1.42628500
C	-1.62321000	3.37836600	0.64992200
C	-2.01803400	3.79647900	-0.65135100
H	-1.43375100	4.01071900	1.50632200
H	-2.19179400	4.80790700	-0.98895600
Cu	0.58242600	-0.30622100	0.24104300
Br	1.72029200	-0.44194200	2.32725200
O	1.09985800	3.40685900	-1.02493100
H	0.99903100	2.33222400	-1.80936900
H	1.41230200	3.16725300	-0.10697700
O	0.84924000	1.45370200	-2.43701200

O	1.67456200	2.74003500	1.43467800
H	2.14157700	1.91706300	1.65830500
H	0.79900300	2.60199500	1.81858600
H	0.29661800	0.59486000	-1.83905700
H	1.69119200	1.13377900	-2.78518800
C	-2.78676200	-0.64618800	0.03953000
C	-4.13757000	0.00383900	0.37682000
C	-3.00096700	-2.10894700	-0.36693500
H	-2.16193500	-0.65423700	0.94843800
C	-4.88966300	-0.77512900	1.45719900
H	-4.74497200	0.02841100	-0.54063400
H	-3.99779500	1.04275400	0.69114500
C	-3.75637300	-2.88787700	0.71290800
H	-3.57456500	-2.13705800	-1.30659500
H	-2.04009200	-2.59195800	-0.56359700
C	-5.09553400	-2.23271600	1.04751800
H	-5.85078400	-0.29242700	1.66177100
H	-4.31264900	-0.74029900	2.39146500
H	-3.90397000	-3.92234600	0.38628700
H	-3.13714300	-2.92744700	1.61927000
H	-5.60560300	-2.78665000	1.84211300
H	-5.74669400	-2.26968600	0.16329800
C	0.62599700	-2.09459600	-2.84223000
H	0.29238700	-3.05900600	-3.23936300
H	1.01372700	-1.55071900	-3.71891300
C	1.76821500	-2.34418900	-1.84476000
H	1.33861700	-2.57491100	-0.85942500
H	2.31220400	-3.24399900	-2.15592400
C	2.79140200	-1.21826300	-1.69484200
H	2.29471100	-0.28961500	-1.38252300
H	3.25127200	-1.00673300	-2.67258200
C	3.87038200	-1.52924000	-0.66029200
H	3.38659500	-1.88395100	0.25880700
H	4.50817400	-2.34650900	-1.02263100
C	4.72359000	-0.31225100	-0.31362200
H	5.23619000	0.05229300	-1.21386800
H	4.05498900	0.49438700	0.01888000
C	5.73440100	-0.60817700	0.78930800
H	6.40949100	-1.41804400	0.49485400
H	6.34245100	0.26907900	1.02417900
H	5.21428600	-0.91509600	1.70187800

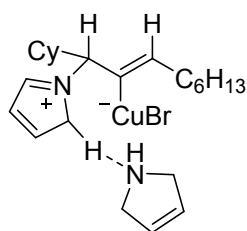
## Int39



C	2.32356100	-0.65018900	-0.17530400
H	2.03267000	-0.62996100	-1.23423600
C	1.17073700	-1.24331200	0.61671900
C	0.28597500	-2.09209200	0.04800000
N	3.45467700	-1.56972300	-0.08783800
C	4.03948400	-2.20953000	-1.14786100
H	-0.06871400	3.73159100	1.54584900
H	3.64349500	-2.08691300	-2.14562000
C	4.14342500	-1.87515500	1.05791900
H	0.35083700	-2.24106400	-1.03315900
H	3.83950100	-1.47180900	2.01302700
C	5.17606500	-2.72067400	0.72447700
C	5.11047800	-2.93329400	-0.67808100
H	5.89349400	-3.14138600	1.41344500
H	5.76941000	-3.54548200	-1.27551800
Cu	-0.72221500	-0.01342900	0.15715400
Br	-2.00988400	0.79769100	-1.75502600
O	-0.71132200	3.26478000	2.08854500
H	-0.78017000	1.46789700	2.32537900
H	-1.54681000	3.25268100	1.58873500
O	-1.22953100	0.61708800	2.13871700
O	-3.09076900	2.32328600	0.96811900
H	-2.92998000	1.98030600	0.06489500
H	-4.00453800	2.62643100	0.98014600
H	1.18508400	-1.12207900	1.70204100
H	-2.14951500	0.91077700	2.01927700
C	2.75461100	0.77477600	0.22147800
C	4.01479700	1.17675200	-0.55858200
C	1.62556000	1.78483200	-0.01868800
H	2.99989300	0.77505000	1.29576200
C	4.44181600	2.61358200	-0.26195300
H	3.80357900	1.07833100	-1.63445800
H	4.82836400	0.48109300	-0.33116200
C	2.06118900	3.23312000	0.22448500
H	1.25732100	1.68318700	-1.05028000
H	0.77747700	1.57961200	0.64898500
C	3.31392800	3.59604100	-0.57136600
H	5.33669800	2.86207300	-0.84070500

H	4.71715300	2.69868900	0.79826500
H	1.24144700	3.90849800	-0.05211500
H	2.26234700	3.37457200	1.29616700
H	3.61996300	4.62295300	-0.34813900
H	3.08187900	3.55559500	-1.64378100
C	-0.67737100	-2.99940000	0.76753000
H	-0.22564500	-3.99938900	0.73481800
H	-0.74087000	-2.71696300	1.82563500
C	-2.07875700	-3.04582000	0.12887600
H	-1.99034300	-2.82821700	-0.94377000
H	-2.48969200	-4.05776900	0.20740100
C	-3.06402200	-2.05958500	0.75592100
H	-2.57165300	-1.09035900	0.91132400
H	-3.34388500	-2.40752100	1.75947400
C	-4.30646500	-1.81751700	-0.09331800
H	-3.98745900	-1.52410200	-1.10150700
H	-4.88171800	-2.74814100	-0.19398600
C	-5.19403900	-0.71507700	0.47770500
H	-5.55097300	-1.00584400	1.47430000
H	-4.57535800	0.18228500	0.61636600
C	-6.37590700	-0.38716600	-0.42955300
H	-6.99879700	-1.27173700	-0.59587300
H	-7.01247400	0.39253200	-0.00197000
H	-6.02200800	-0.04010000	-1.40515700

**Int40**



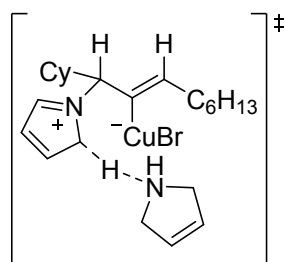
C	1.88509700	0.88871000	0.83808700
H	2.37323400	1.46988800	1.63795500
C	0.56620300	0.26987200	1.29195600
C	0.35538400	0.28834100	2.61704800
N	1.58645300	1.89324500	-0.22154400
C	1.23553400	3.27403000	0.08093400
H	0.33384600	3.26992300	0.73157000
H	2.06183000	3.78429300	0.58506300
C	1.34759800	1.64192800	-1.47563900
H	1.10332500	0.74376100	3.28308700
H	1.46197100	0.65084800	-1.90149400
C	0.89716400	2.83328200	-2.16212400



C	0.85819700	3.82203600	-1.24679300
H	0.63097800	2.86391500	-3.20862000
H	0.55513700	4.84930100	-1.40059700
Cu	-0.47834600	-0.48269600	-0.27656400
Br	-1.02361900	-0.79408100	-2.59221300
C	-2.31043700	2.45497000	-0.43898900
C	-3.70015300	1.93242700	-0.15692500
C	-3.98289200	2.06608900	1.13613100
C	-2.81022200	2.68722900	1.86310300
N	-1.69623100	2.62513600	0.89543200
H	-1.19249100	1.76052100	1.09650700
H	-2.36261300	3.41926400	-0.96767300
H	-4.36082200	1.55297100	-0.92758000
H	-4.92252000	1.81981300	1.61726100
H	-2.53704500	2.15876200	2.78339100
H	-1.71437500	1.77764000	-1.06276400
H	-3.03162200	3.72821600	2.13821300
C	2.89558300	-0.14706000	0.31270200
C	4.20910600	0.49346600	-0.15627200
C	3.17692800	-1.19461200	1.39665000
H	2.43022800	-0.68048100	-0.53185200
C	5.20761800	-0.55890300	-0.64607000
H	4.64874600	1.04110400	0.69070600
H	4.02853200	1.23124400	-0.94691000
C	4.17828500	-2.24433200	0.91100100
H	3.57696300	-0.68329800	2.28578300
H	2.23941200	-1.66724700	1.70001500
C	5.48207200	-1.60247800	0.43689200
H	6.13766200	-0.07379700	-0.95968200
H	4.79484800	-1.05803400	-1.53317300
H	4.37378300	-2.96731500	1.70915700
H	3.72921200	-2.80492400	0.07997200
H	6.17233700	-2.36554700	0.06346200
H	5.97633200	-1.11525900	1.28848900
C	-0.82789500	-0.27462500	3.37500600
H	-0.46266400	-1.05985600	4.05464300
H	-1.20568200	0.51527600	4.03970500
C	-1.97271500	-0.83154200	2.52976000
H	-2.88073200	-0.90021300	3.14170200
H	-2.21025000	-0.11898300	1.72667200
C	-1.67561600	-2.20174200	1.91503100
H	-1.72111200	-2.97266000	2.69588600
H	-0.64188500	-2.21308700	1.54368400
C	-2.62715100	-2.56050800	0.77340300

H	-2.72230000	-1.70100300	0.09091300
H	-3.63591800	-2.73698500	1.17197400
C	-2.16861300	-3.76675400	-0.04092100
H	-2.08383000	-4.64319600	0.61508200
H	-1.16130200	-3.56264600	-0.42943500
C	-3.10168800	-4.06218900	-1.21063900
H	-3.12692100	-3.20583600	-1.89161400
H	-2.77013100	-4.93510600	-1.77898100
H	-4.12134900	-4.25473000	-0.85993600

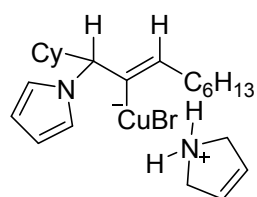
**TS22**



C	1.88732700	0.84565600	0.76147300
H	2.38739900	1.43309300	1.54925100
C	0.57263400	0.24129600	1.24531400
C	0.37063000	0.29724300	2.57124500
N	1.60944900	1.83456300	-0.31744300
C	1.26658400	3.20229700	-0.05920800
H	0.12587600	3.11501700	0.38309100
H	1.89943800	3.70566100	0.66949900
C	1.37741900	1.56235000	-1.58320400
H	1.12960300	0.76405700	3.21697100
H	1.43912300	0.55425800	-1.97659000
C	1.01262400	2.74773200	-2.28859900
C	1.01674700	3.76355200	-1.37877500
H	0.76765600	2.78477800	-3.33956000
H	0.77749600	4.80367400	-1.55745200
Cu	-0.48663600	-0.55200000	-0.29360000
Br	-1.28516900	-0.92045200	-2.51314800
C	-2.22942300	2.58691100	-0.51909400
C	-3.62171100	2.61429600	0.06201700
C	-3.58140800	2.86737900	1.36708100
C	-2.15404800	3.04368200	1.82881000
N	-1.35028700	2.58842200	0.67353900
H	-1.06037600	1.62506300	0.86349900
H	-2.03957400	3.48025500	-1.13227400
H	-4.51338700	2.47834500	-0.53807100
H	-4.43431300	2.98024300	2.02562500

H	-1.89325900	2.45000700	2.71118100
H	-2.02054800	1.70938400	-1.14391400
H	-1.94014000	4.09561700	2.06215300
C	2.88359600	-0.21719500	0.26009700
C	4.20085700	0.38970600	-0.24274200
C	3.16260300	-1.23228000	1.37505200
H	2.40484600	-0.77050200	-0.56396600
C	5.17922600	-0.69357600	-0.70569900
H	4.65652900	0.95983900	0.58054500
H	4.02028100	1.10208900	-1.05552700
C	4.14508500	-2.31161700	0.91757500
H	3.57842300	-0.69643100	2.24237000
H	2.22332700	-1.68325300	1.70470000
C	5.45198500	-1.70345500	0.40887700
H	6.11234500	-0.23319700	-1.04643700
H	4.74970000	-1.21716000	-1.57059100
H	4.33972800	-3.00879900	1.73872400
H	3.68085100	-2.89506100	0.11092700
H	6.12899700	-2.48772400	0.05527100
H	5.96043300	-1.19376900	1.23867300
C	-0.80638000	-0.23748000	3.36057600
H	-0.43956200	-1.02134300	4.04088300
H	-1.15801400	0.56345500	4.02677200
C	-1.98017300	-0.78902200	2.55169800
H	-2.87460900	-0.82847700	3.18514800
H	-2.22535800	-0.09014100	1.73679000
C	-1.72029600	-2.17987600	1.96794000
H	-1.73585900	-2.92094600	2.77856300
H	-0.70335600	-2.21363300	1.55406400
C	-2.72192500	-2.57365300	0.88342800
H	-2.82882700	-1.74664700	0.16498100
H	-3.71546100	-2.71907200	1.32991200
C	-2.30971400	-3.82232000	0.10893300
H	-2.20345600	-4.66759600	0.80182000
H	-1.31904300	-3.64631300	-0.33192300
C	-3.29529000	-4.16310300	-1.00382200
H	-3.34601300	-3.33789500	-1.72082200
H	-2.99393600	-5.06318700	-1.54603200
H	-4.29942500	-4.33191200	-0.60018900

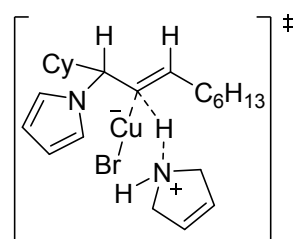
## Int41



C	2.06329000	-0.38321100	-0.81486200
H	2.66743600	-0.67965400	-1.68842200
C	0.57865200	-0.34730100	-1.15479600
C	0.25349000	-0.68531600	-2.41488000
N	2.29832800	-1.44832000	0.18550400
C	2.65377200	-2.72950000	-0.13248400
H	0.31221300	-2.93430300	0.87315100
H	2.92416900	-2.98295200	-1.14788100
C	2.01119000	-1.38146700	1.52161700
H	1.05492300	-0.92809600	-3.12929900
H	1.69054500	-0.45831400	1.98457600
C	2.19184600	-2.63962000	2.06882000
C	2.60243200	-3.50045100	1.01257500
H	2.07596300	-2.89306100	3.11246900
H	2.86791600	-4.54501800	1.08737700
Cu	-0.54128500	0.45212000	0.35215600
Br	-1.68829800	0.93489000	2.37472500
C	-1.80536500	-2.73513800	0.87436800
C	-2.67900600	-3.36584500	-0.17350200
C	-1.96127100	-3.91148300	-1.15068700
C	-0.48617200	-3.73458500	-0.91601400
N	-0.45787700	-2.75206400	0.21166000
H	-0.25013400	-1.79152400	-0.20616900
H	-1.76256800	-3.32475800	1.79543300
H	-3.75867500	-3.36459600	-0.09494400
H	-2.34927600	-4.43952400	-2.01246300
H	0.06130700	-3.29534700	-1.75603900
H	-2.06444900	-1.70417600	1.14248200
H	0.01904200	-4.65589800	-0.60900800
C	2.60654800	0.96221400	-0.31262300
C	4.09045900	0.88615300	0.06417900
C	2.37801500	2.05222800	-1.36660100
H	2.03127100	1.24994000	0.58365300
C	4.61733300	2.24187600	0.54001700
H	4.65901000	0.56690100	-0.82226000
H	4.25041900	0.12483200	0.83475000
C	2.90900300	3.40737200	-0.89446300
H	2.89265000	1.75670200	-2.29395400

H	1.31185200	2.12006500	-1.60649300
C	4.38806100	3.32571200	-0.51420300
H	5.68114200	2.16511900	0.78762400
H	4.09581400	2.52311000	1.46497200
H	2.75327300	4.16168600	-1.67243600
H	2.32905900	3.73009800	-0.01915600
H	4.74364800	4.29500400	-0.14993000
H	4.97770500	3.08581400	-1.40980600
C	-1.12454600	-0.79666200	-3.03331600
H	-1.11602200	-0.25314200	-3.98875400
H	-1.28962700	-1.84950700	-3.31411900
C	-2.30220000	-0.30567400	-2.19416500
H	-3.23839600	-0.66711100	-2.63804600
H	-2.25657000	-0.76011900	-1.19359400
C	-2.36782100	1.21411400	-2.04915600
H	-2.55069600	1.66574100	-3.03347700
H	-1.38652400	1.58949100	-1.72827100
C	-3.43348700	1.67019100	-1.05377500
H	-3.37508700	1.04940100	-0.14911800
H	-4.43380400	1.51068300	-1.47992300
C	-3.27069300	3.12743000	-0.63154700
H	-3.32220200	3.77786100	-1.51478400
H	-2.26667600	3.24981800	-0.20370000
C	-4.30721000	3.54895200	0.40426900
H	-4.20055300	2.93948500	1.30701200
H	-4.18742600	4.59761400	0.68876000
H	-5.32408500	3.41787900	0.01909400

**TS23**

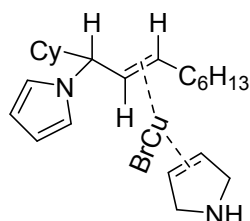


C	2.08824300	0.12222900	0.85433000
H	2.71848000	0.27767800	1.74434700
C	0.66530700	0.59941500	1.11824000
C	0.29784600	0.80237600	2.39618300
N	2.67689900	0.96938100	-0.19955800
C	3.31000900	2.15678600	0.04617700
H	1.04700200	2.76118200	-1.05524300
H	3.56696500	2.43653600	1.05815800
C	2.45399600	0.85129000	-1.54618000

H	1.03042100	0.61368600	3.19200600
H	1.94617200	-0.00741600	-1.96339400
C	2.96833600	1.97175800	-2.16960800
C	3.51364900	2.80519200	-1.15437800
H	2.97556000	2.15045700	-3.23480600
H	4.02289700	3.74835200	-1.28824100
Cu	-0.58224600	-0.26796800	-0.32474200
Br	-1.55597300	-1.29892000	-2.20660400
C	-1.04604000	2.95037900	-1.12852100
C	-1.80398200	3.88759500	-0.22935800
C	-1.01922000	4.38736700	0.72075800
C	0.38546900	3.86279500	0.59922800
N	0.24828600	2.78959900	-0.41531000
H	0.27756200	1.66074200	0.20766200
H	-0.89335800	3.36750100	-2.13025900
H	-2.85375800	4.10900800	-0.37714900
H	-1.31349900	5.09540600	1.48578800
H	0.77556400	3.41984200	1.52481200
H	-1.52643500	1.96935800	-1.25513200
H	1.09538300	4.62802000	0.26467200
C	2.19590700	-1.36761500	0.47604800
C	3.65420100	-1.78381900	0.24335000
C	1.55301300	-2.25953800	1.54495200
H	1.63747100	-1.53445800	-0.46079100
C	3.76414300	-3.26436900	-0.12614400
H	4.21865400	-1.59769900	1.16957700
H	4.10665600	-1.16141700	-0.53523100
C	1.66289900	-3.73923200	1.17314900
H	2.05573900	-2.07907700	2.50803300
H	0.50154700	-1.98759100	1.68506300
C	3.11677300	-4.14989400	0.93890600
H	4.81537800	-3.53638900	-0.26643500
H	3.26217100	-3.43193700	-1.08848700
H	1.21087900	-4.35424300	1.95793600
H	1.08274500	-3.91605800	0.25720400
H	3.17368700	-5.20344200	0.64678300
H	3.67550200	-4.04866800	1.87977000
C	-1.02904100	1.31766600	2.90717700
H	-0.91122400	2.39046800	3.12602800
H	-1.22733200	0.84981900	3.88022100
C	-2.24051700	1.11102300	1.99870600
H	-2.01607300	1.48784200	0.99236800
H	-3.07052500	1.72960000	2.36154100
C	-2.70140300	-0.34344200	1.90936000

H	-1.84417300	-0.99237800	1.67285300
H	-3.05617100	-0.67439700	2.89471500
C	-3.79121700	-0.55629600	0.86158500
H	-4.69880300	-0.01209500	1.15878100
H	-3.46306700	-0.12249500	-0.09370100
C	-4.11758800	-2.02789100	0.62592700
H	-3.19167400	-2.54797900	0.34956400
H	-4.47560800	-2.47955800	1.56059000
C	-5.14416000	-2.21723600	-0.48597500
H	-4.74809700	-1.82347100	-1.42701100
H	-5.38193500	-3.27335000	-0.63672200
H	-6.07654600	-1.69021400	-0.25659500

**Int42**



C	2.17606900	-0.59750800	-0.75138200
H	2.00488100	-0.47503200	-1.82901200
C	0.93588600	-1.22564300	-0.13660000
C	-0.05149400	-1.76451200	-0.89017800
N	3.23755700	-1.59253500	-0.61392900
C	3.92564200	-2.18168500	-1.64004900
H	1.60122800	-0.37864400	3.82011700
H	3.66928500	-1.96458600	-2.66691800
C	3.76009800	-2.01502000	0.58244600
H	-0.03226800	-1.57680700	-1.96659000
H	3.35035900	-1.65607300	1.51679400
C	4.79117000	-2.88525300	0.31412100
C	4.89675200	-2.99145400	-1.09866300
H	5.39695700	-3.39227300	1.05051600
H	5.60080100	-3.59150700	-1.65550400
Cu	-0.83117400	0.22143600	0.00086400
Br	-2.39577300	1.68476800	-1.11909300
C	0.65212700	1.22332400	2.90775400
C	-0.75293900	1.19711100	2.36133000
C	-1.28609400	-0.02231900	2.52767900
C	-0.29397000	-0.94005500	3.19544500
N	0.97026000	-0.20545800	3.04684900
H	1.00014400	-1.43828300	0.93177400
H	0.65460200	1.77260900	3.86439000

H	-1.27113700	2.06889800	1.97337800
H	-2.31469600	-0.29954000	2.32194000
H	-0.23349500	-1.92970800	2.72378100
H	1.36534600	1.72314600	2.24412700
H	-0.59352700	-1.10181500	4.24438600
C	2.64902800	0.76024700	-0.19208000
C	4.02018500	1.11709800	-0.79040200
C	1.63711800	1.87347800	-0.48640100
H	2.75993200	0.65628400	0.89927900
C	4.50321200	2.50063700	-0.35610000
H	3.93503600	1.09602600	-1.88798500
H	4.75503500	0.35377900	-0.51654800
C	2.13581400	3.26543800	-0.08883300
H	1.38841600	1.86984400	-1.55732400
H	0.69149900	1.70061300	0.04418200
C	3.48809800	3.58080500	-0.72392800
H	5.47611200	2.71039300	-0.81159500
H	4.65635700	2.50451400	0.73206000
H	1.38398200	4.00944500	-0.36928200
H	2.24356100	3.31806200	1.00403700
H	3.83782400	4.56715100	-0.40302100
H	3.37704800	3.61968300	-1.81577100
C	-1.06284300	-2.78736000	-0.43822800
H	-0.67236800	-3.75074800	-0.79189600
H	-1.07636600	-2.84909200	0.65794000
C	-2.48504300	-2.57650500	-0.98890500
H	-2.42571300	-2.03835900	-1.94398300
H	-2.94315400	-3.54724200	-1.20645000
C	-3.39339100	-1.80046400	-0.03859700
H	-3.59426700	-2.40868300	0.85589000
H	-2.87716800	-0.89529500	0.30412600
C	-4.69955200	-1.34300600	-0.67591700
H	-4.45797600	-0.75443500	-1.56996200
H	-5.28454800	-2.21334200	-1.00485400
C	-5.53038500	-0.47699600	0.26744300
H	-5.77299100	-1.04796000	1.17397500
H	-4.91432200	0.37702700	0.57729600
C	-6.81072100	0.03366500	-0.38577700
H	-7.44498600	-0.79732300	-0.71154100
H	-7.39414900	0.65264600	0.30072200
H	-6.57246700	0.63992600	-1.26480400