

# Theoretical Study of Copper Hydride Complexes Catalyzing Terminal Alkyne Hydroalkylation for C(sp<sup>2</sup>)-C(sp<sup>3</sup>) Bond Formation

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**Table S1. Energy statistics for all stationary points.**

Energies calculated at B3LYP(D3)/BSI (6-31g(d), SDD) level in gas phase, and correction solvation energies calculated at  $\omega$ B97X-D/BSII (6-311g(d, p), SDD) in Benzene/THF(7:3) of reaction pathways. (unit: Hartree)

	<i>ZPE</i>	<i>U</i>	<i>H</i>	<i>G</i>	<i>sol E</i>
<b>Cata1</b>	0.571016	0.602351	0.603295	0.515712	-1357.99279
<b>R1</b>	0.191814	0.202393	0.203337	0.155716	-426.299348
<b>INT1M</b>	0.766468	0.80951	0.810455	0.699557	-1784.29895
<b>INT1aM</b>	0.765138	0.808663	0.809608	0.697309	-1784.30026
<b>TS1M</b>	0.765199	0.80795	0.808894	0.698529	-1784.27909
<b>TS1aM</b>	0.764049	0.80717	0.808114	0.696258	-1784.28181
<b>INT2M</b>	0.770268	0.813794	0.814738	0.701673	-1784.36732
<b>INT2aM</b>	0.770472	0.813913	0.814857	0.700138	-1784.35693
<b>R2</b>	0.18965	0.200761	0.201705	0.152508	-492.545195
<b>IM1</b>	0.961373	1.017922	1.018866	0.877776	-2276.91471
<b>TS2</b>	0.959195	1.015343	1.016287	0.878293	-2276.88106
<b>INT3a</b>	0.772591	0.817722	0.818666	0.701279	-1797.7753
<b>INT3b</b>	0.185085	0.195218	0.196162	0.149334	-479.101591
<b>TS3</b>	0.96158	1.016522	1.017466	0.883061	-2276.86055
<b>TS4</b>	0.960361	1.015696	1.01664	0.881637	-2276.8585
<b>TS5(MECP)</b>	—	—	—	—	-2276.89462
<b>TS6</b>	0.960916	1.016232	1.017176	0.880795	-2276.88828
<b>INT4</b>	0.964133	1.019012	1.019957	0.886083	-2276.93179
<b>TS7</b>	0.963833	1.018261	1.019205	0.886155	-2276.93235
<b>Cata2</b>	0.565908	0.598877	0.599821	0.507027	-1370.878
<b>P</b>	0.39618	0.416874	0.417818	0.347922	-906.122683

For all stable points, thermodynamic corrections were performed on the transition states at a pressure of one megapascal and room temperature. Single-point energy corrections were carried out using SMD (a 7:3 mixture of benzene and tetrahydrofuran) as the solvent.

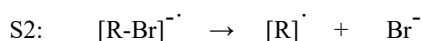
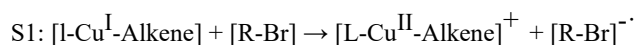
**Table S2. Calculation of the OSET energy barrier using Marcus theory.**

Marcus theory calculations for the free energy of activation of single electron transfer at  $\omega$ B97X-D/BSII (6-311g\*\*, SDD) rate determining step. (unit: Hartree)

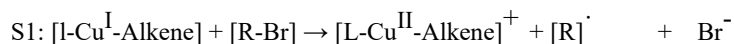
	<i>ZPE</i>	<i>E</i>	<i>H</i>	<i>G</i>
<b>INT2aM</b>	-1783.573207	-1783.530465	-1783.529521	-1783.651571
<b>R2</b>	-492.351725	-492.340899	-492.339955	-492.389625
<b>INT2aM<sup>+</sup></b>	-1783.384304	-1783.342109	-1783.341165	-1783.459803
<b>R2<sup>·</sup></b>	-492.462256	-492.450093	-492.449148	-492.503952
<b>INT3-b</b>	-478.912265	-478.902421	-478.901477	-478.948195
<b>Br<sup>·</sup></b>	-13.349628	-13.348212	-13.347268	-13.366458
<b>Br<sup>-</sup></b>	-13.540639	-13.539223	-13.538279	-13.556815

We used the modified Marcus theory to estimate the barriers for the stepwise outer-sphere single electron transfer (OSET-SW) and the concerted dissociative electron transfer (OSET-C) processes in the reduction of  $\alpha$ -Bromine by copper(I) compound. The DFT calculations were performed at the  $\omega$ -B97XD/6-311g\*\*// $\omega$ B97X-D/SDD/6-31G(d) level of theory in benzene/THF from 7:3 at 25°C (see Computational Methods in the manuscript for details).

OSET-SW:



OSET-C:



The following equation was used to calculate the activation free energy of activation ( $\Delta G_{OSET-SW}^\ddagger$ ) in the OSET-SW pathway:

$$\Delta G_{OSET-SW}^{\ddagger} = \Delta G_0^{\ddagger} \left( 1 + \frac{\Delta_r G^{\ominus}}{4\Delta G_0^{\ddagger}} \right)^2$$

Here,  $\Delta_r G^{\ominus} = 48.59$  kcal/mol is the reaction energy of eq. s1 obtained from DFT calculations. The intrinsic barrier is determined using  $\Delta G_0^{\ddagger} = \lambda_0 / 4$ , where  $\lambda_0$  is the solvent reorganization energy that can be calculated as follows:

$$\lambda_0 = A \times [(2r_D)^{-1} + (2r_A)^{-1} - (r_D + r_A)^{-1}]$$

Where  $r_D$  and  $r_A$  are the hard sphere radii of electron donor and acceptor, respectively. A is an empirical constant. Here we use  $A = 99$  kcal mol<sup>-1</sup> Å as suggested in the Coote and Matyjaszewski's study.<sup>[1]</sup>

Thus,

$$\begin{aligned} \lambda_0 &= 99 \times [(2r_{[A3-aM]})^{-1} + (2r_{[A4]})^{-1} - (r_{[A3-aM]} + r_{[A4]})^{-1}] \\ &= 99 \times [1/(2 \times 9.817) + 1/(2 \times 5.112) - 1/(9.817 + 5.112)] \\ &= 8.09 \text{ kcal/mol} \end{aligned}$$

Leading to

$$\Delta G_0^{\ddagger} = \lambda_0 / 4 = 2.02 \text{ kcal/mol}$$

Thus,

$$\Delta G_{OSET-SW}^{\ddagger} = 2.02 \times \left( 1 + \frac{48.59}{8.09} \right)^2 = 99.26 \text{ kcal/mol}$$

The dissociation of the radical anion SW1 is highly exothermic (Figure 3) and is expected to be very fast. Therefore, the rate-determining step in the OSET-SW pathway is the outer-sphere single electron transfer (eq. s1).

In the OSET-C pathway (eq. s3), the electron transfer occurs with simultaneous alkyl halide bond dissociation to form the INT3b radical and the Br<sup>-</sup> anion in a polar solvent (benzene/THF from 7:3) cage. Thus, the "sticky" model<sup>5</sup> is used to estimate the free energy of activation of the OSET-C pathway:

$$\begin{aligned} \Delta G_{OSET-C}^{\ddagger} &= \Delta G_0^{\ddagger} \left( 1 + \frac{\Delta_r G^{\ominus} - D_p}{4\Delta G_0^{\ddagger}} \right)^2 \\ \Delta G_0^{\ddagger} &= \frac{R2(BDE) + \lambda_0}{4} \end{aligned}$$

where  $\Delta G_0^{\ddagger}$  is the intrinsic barrier;  $\Delta_r G^{\ominus} = 47.93$  kcal/mol is the DFT-calculated reaction energy for eq. s3;  $D_p$  is the interaction energy between MMA• and Br<sup>-</sup> in the solvent cage, and the experimental data of  $D_p = 1.13$  kcal/mol is used in our calculation;  $D_{MMA-Br}$  is the MMA-Br bond dissociation enthalpy calculated using DFT ( $D_{R2} = 57.24$  kcal/mol);  $\lambda_0$  is the solvent reorganization energy that is the same as that in the OSET-SW pathway ( $\lambda_0 = 8.09$  kcal/mol).

$$\begin{aligned} \Delta G_0^{\ddagger} &= \frac{(\sqrt{D_{R2}} - \sqrt{D_p})^2 + \lambda_0}{4} = \frac{(\sqrt{57.24} - \sqrt{1.13})^2 + 8.09}{4} = 12.60 \text{ kcal/mol} \\ \Delta G_{OSET-C}^{\ddagger} &= \Delta G_0^{\ddagger} \left( 1 + \frac{\Delta_r G^{\ominus} - D_p}{4\Delta G_0^{\ddagger}} \right)^2 = 8.88 \times \left( 1 + \frac{47.93 - 1.13}{4 \times 12.60} \right)^2 = 46.87 \text{ kcal/mol} \end{aligned}$$

**Table S3. Calculated electronic ( $E_{\text{HOMO}}$ ), steric ( $V_{\text{bur}\%}$ ), and backbone flexibility ( $\Delta E_{\text{dist}}$ ) parameters for alkenyl copper(I). (unit: Hartree)**

To further understand the influence of ligands on electron transfer, we used the SambVca web server software to calculate the buried volume percentage  $V_{\text{bur}\%}$  of the catalyst, combined with the energy  $E_{\text{HOMO}}$  of the highest occupied orbital and the distortion energy  $\Delta E_{\text{dist}}$  of the catalyst, to describe the electronic effect, steric effect, and skeleton flexibility effect in the ISET process. After calculation,  $E_{\text{HOMO}} = -4.9$  eV,  $V_{\text{bur}\%} = 46.1$ ,  $\Delta E_{\text{dist}} = 14.64$  kcal·mol<sup>-1</sup>. Details of the calculations can be found in Table S3 & Figure S1. Compared with the guiding data in the literature, it is known that the distinct electronic effect of NHC ligands promotes the occurrence of the reaction with a lower energy barrier in the process of catalytic activation of C-Br bonds by alkenyl copper(I) complexes.

	$E+ZPE$	$E$	$H$	$G$	$EE$
TS2	-2275.92186	-2275.865712	-2275.864768	-2276.002762	-2276.88106
F-TS2	-2275.917527	-2275.861405	-2275.860461	-2275.999271	-2276.876623

$\Delta E$  The bond angle of TS2 (Cu---Br---C) was fixed at 179°, referred to as F-TS2, for constrained optimization, and the difference between F-TS2 and TS2 was calculated.

$$\Delta E = E_{\text{F-TS2}} - E_{\text{TS2}} = 2.78 \text{ kcal}\cdot\text{mol}^{-1}$$

Figure S1. The buried volume values and steric maps of NHC-Cu.

%V Free	%V Buried	% V Tot/V Ex
53.9	46.1	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	27.1	17.7	44.9	<b>60.5</b>	39.5
NW	24.3	20.6	44.9	<b>54.1</b>	45.9
NE	23.0	21.9	44.9	<b>51.3</b>	48.7
SE	22.2	22.6	44.9	<b>49.6</b>	50.4

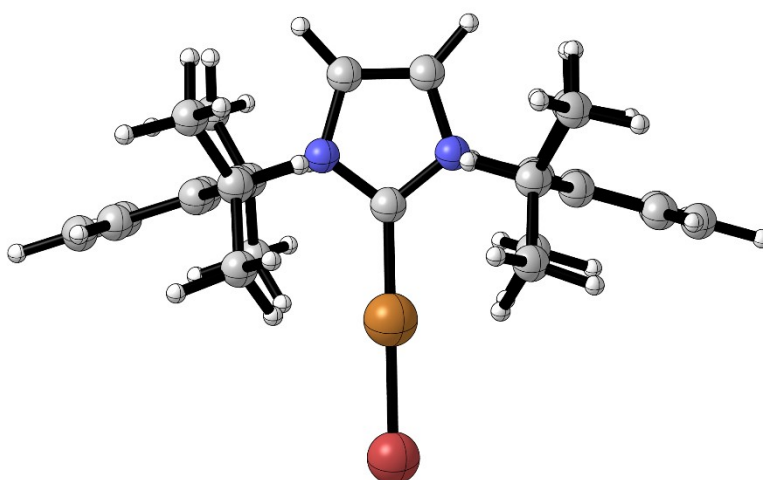
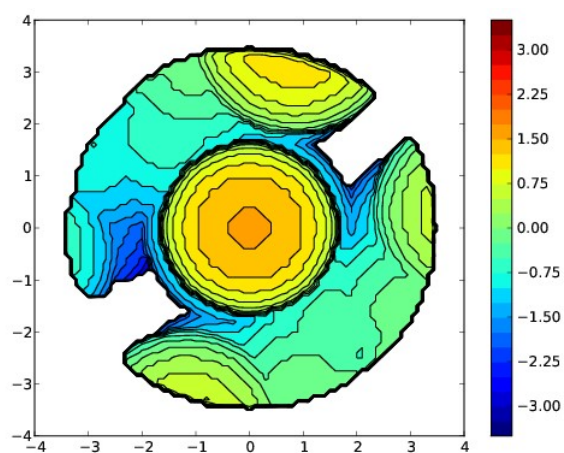


Figure S2. Performing a flexible scan on the dihedral angle ( $\angle C1-C2-Cu-H$ ) of INT2aM, with a step size of  $20^\circ$

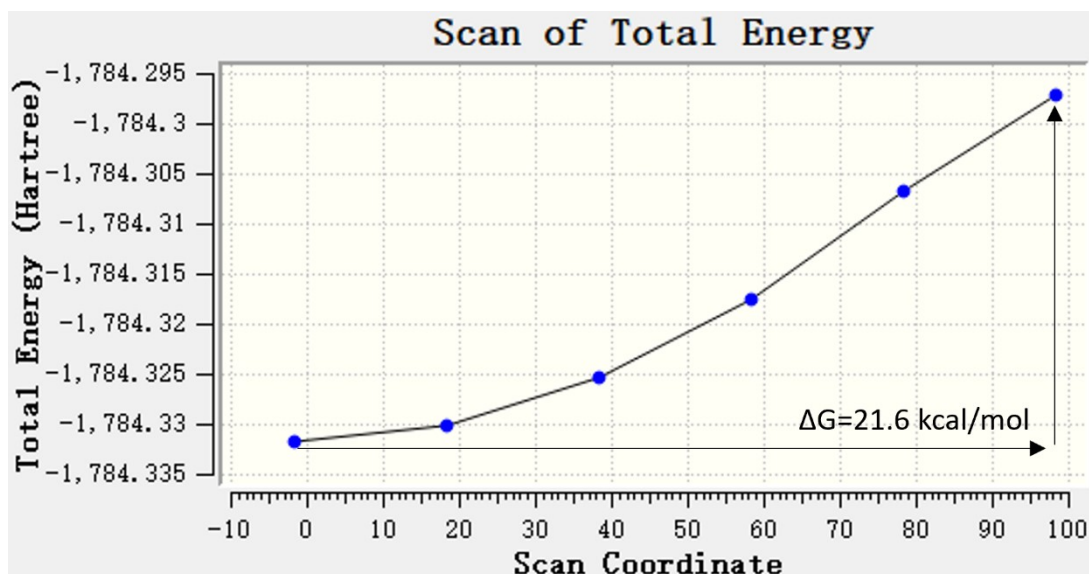
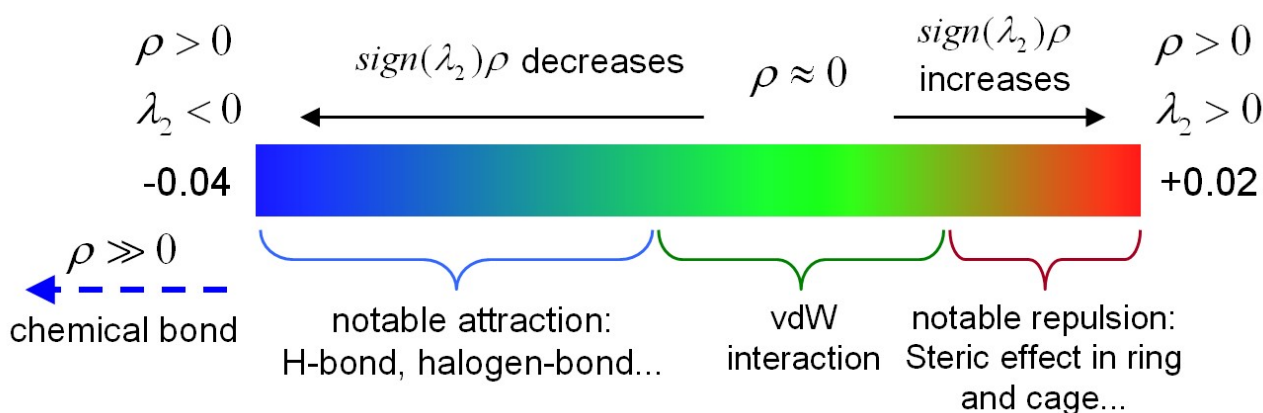
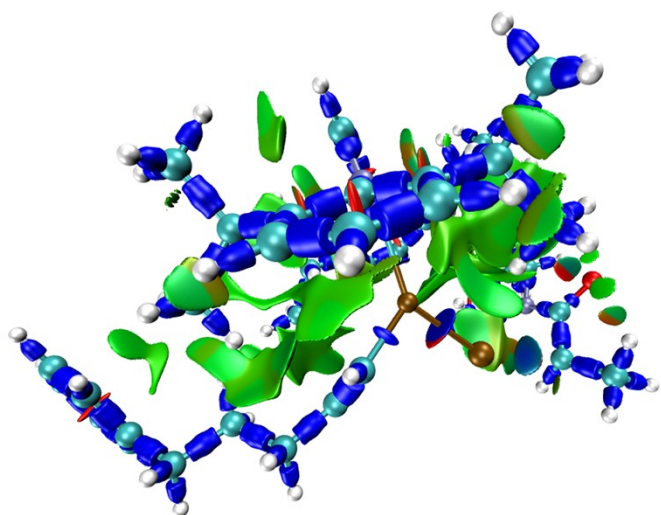


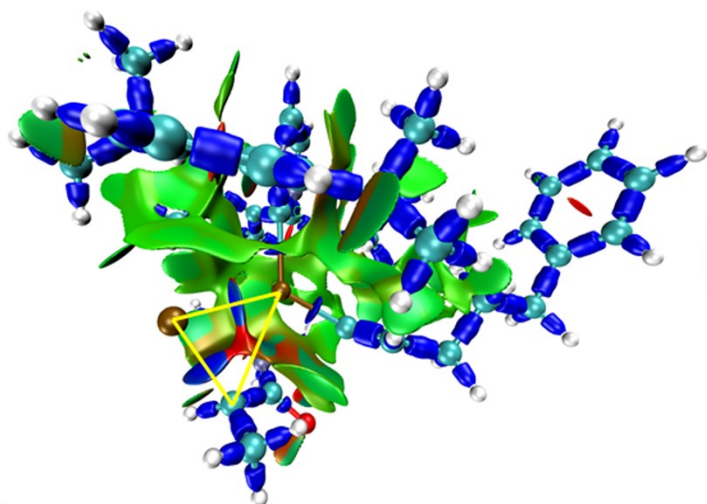
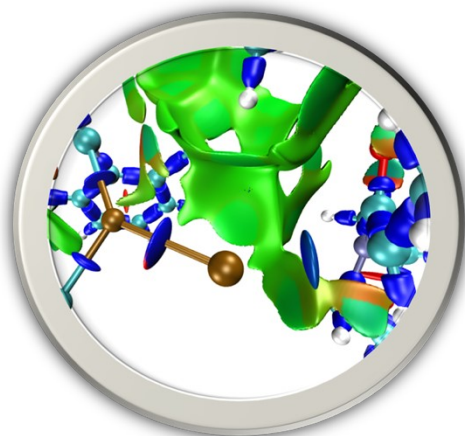
Figure S3. The visualization of different interaction forms between INT2aM and R2. (Observation perspective as the primary reaction coordinate Cu-Br-C.)



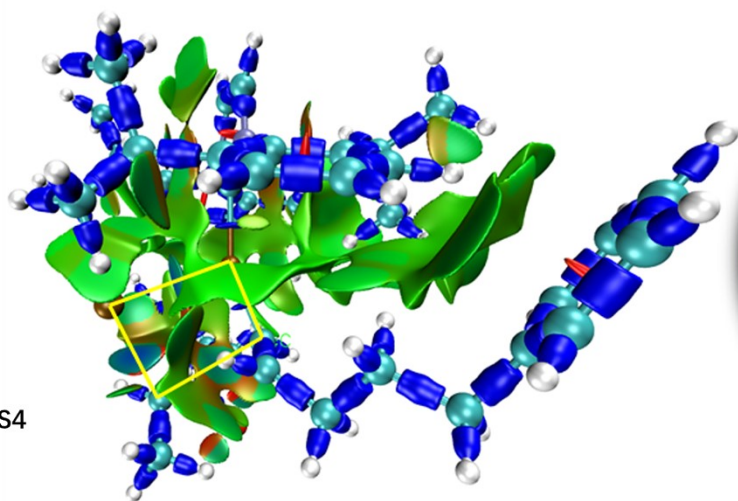
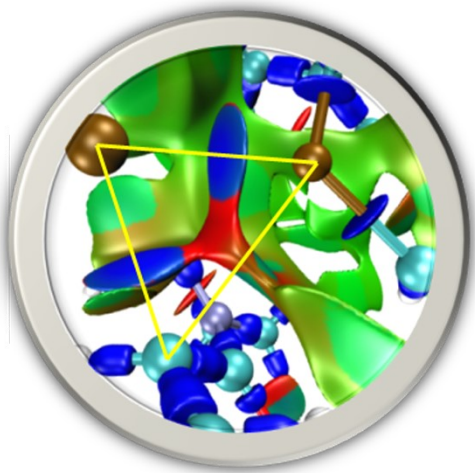
The above color scheme indicates that if an IRI contour is predominantly green, it implies the presence of a van der Waals interaction region (or it could be a very weak hydrogen bond, where dispersion forces dominate). If the contour color is noticeably reddish, it suggests the presence of steric hindrance. If it is bright red, it indicates strong steric hindrance. If the contour color is noticeably bluish, it suggests a significant attractive interaction. If the contour is entirely blue, it means that the region either exhibits relatively strong weak interactions, with the electron density of the interacting region reaching a level of  $\geq 0.04$  a.u., or it involves chemical bonding, where the electron density in the bonding region is typically significantly greater than 0.04 a.u. The equivalent surface is 0.08.



TS2



TS3



TS4

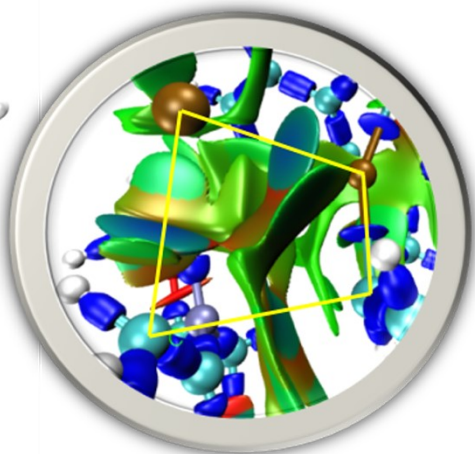
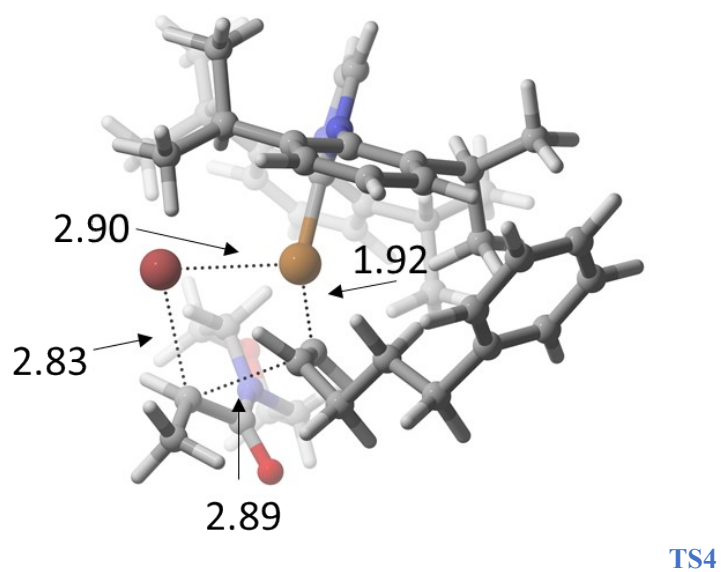
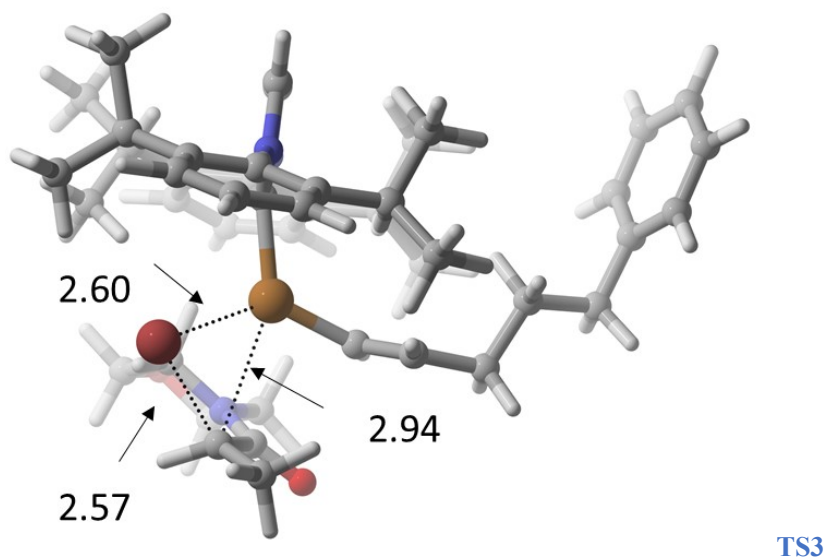
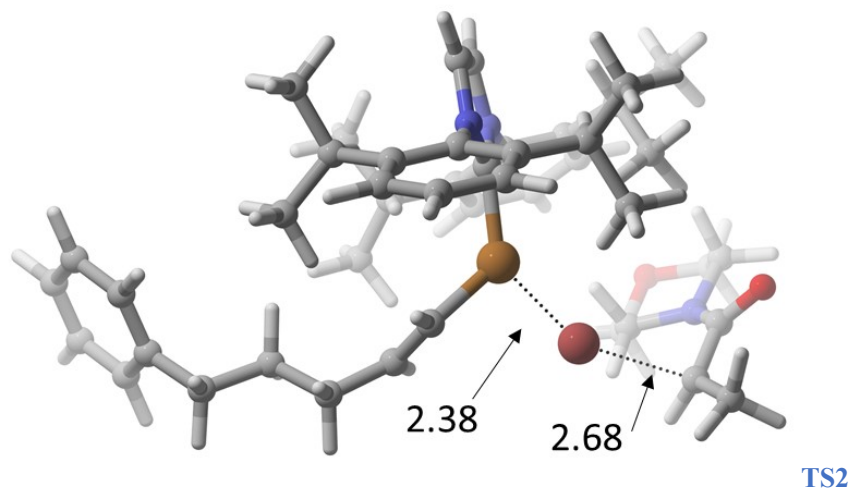




Figure S4. INT2aM and R2 are involved in different reaction forms to form C-C bonds. (Observation perspective as the primary reaction coordinate Cu-Br-C.)



### Figure S5. Das Activation-Strain-Modell am Beispiel einer metallvermittelten C-Br-Bindungsaktivierung

Distortion/interaction model and energy decomposition analysis (EDA) calculations in Figure 5 were performed to dissect the computed gas-phase activation energy ( $\Delta E^\ddagger$ ). The activation energy was first decomposed into the distortion energy of the two reactive fragments, i.e. the alkene copper(I) and the  $\alpha$ -bromo amide, to reach their transition state geometries ( $\Delta E_{\text{strain}} = \Delta E_{\text{dist}}(\text{INT2aM}) + \Delta E_{\text{dist}}(\text{R2})$ ) and the interaction energy ( $\Delta E_{\text{int}}$ ) between these two fragments (eq. 1)

Here, the distortion energies were calculated from the energy difference between the distorted fragment in the transition state geometry and the same fragment in the fully optimized ground state geometry. Then,  $\Delta E_{\text{int}}$  is calculated from  $\Delta E_{\text{int}} = \Delta E_{\text{strain}} - \Delta E^\ddagger$ .

$$\Delta E^\ddagger = \Delta E_{\text{strain}} + \Delta E_{\text{int}}$$

$$\Delta E^\ddagger = \underbrace{\Delta E_{\text{strain}} + \Delta E_{\text{exrep}}}_{\text{steric effects } (\Delta E_{\text{steric}})} + \underbrace{\Delta E_{\text{ele}} + \Delta E_{\text{pol}}}_{\text{electronic effects } (\Delta E_{\text{electronic}})} + \underbrace{\Delta E_{\text{corr/disp}} + \Delta E_{\text{desol}}}_{\text{dispersion desolvation}} + \underbrace{\Delta E_{\text{orbital}}}_{\text{orbital Interaction } (\Delta E_{\text{orbital}})}$$

(1)

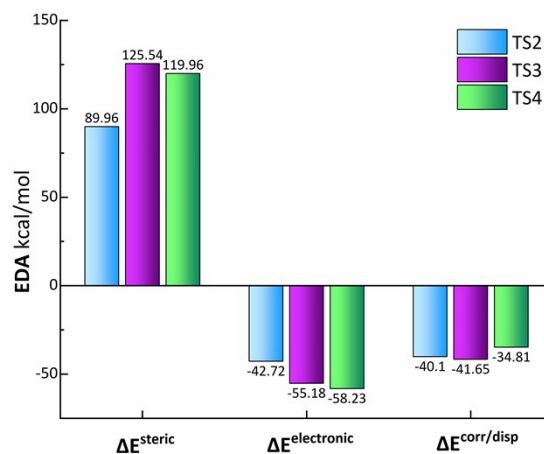
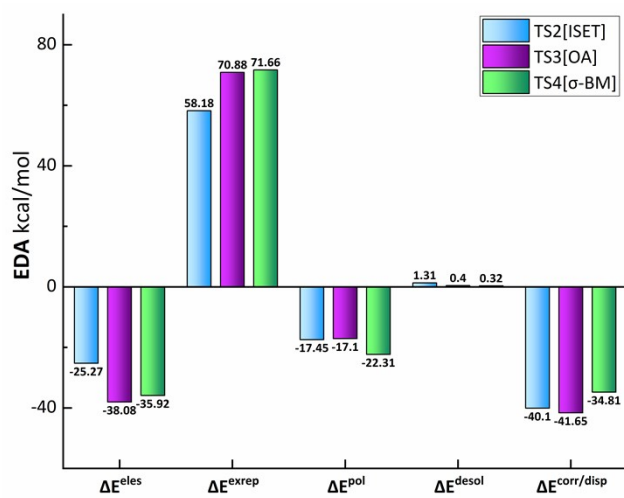
	$\Delta E_{\text{strain}}$	$\Delta E_{\text{exrep}}$	$\Delta E_{\text{eles}}$	$\Delta E_{\text{pol}}$	$\Delta E_{\text{corr/disp}}$	$\Delta E_{\text{desol}}$
<b>ISSET[2.06]</b>	6.35	17.44	-6.65	-2.28	-17.07	0.31
<b>ISSET[2.30]</b>	22.76	45.46	-19.77	-11.25	-26.11	0.62
<b>ISSET[TS2]</b>	31.78	58.18	-25.27	-17.45	-40.1	1.31
<b>OA[2.06]</b>	15.84	35.50	-16.25	-5.33	-28.54	0.01
<b>OA[2.30]</b>	30.08	63.71	-31.95	-11.87	-34.25	0.28
<b>OA[TS3]</b>	51.51	74.03	-38.08	-17.1	-41.65	0.4
<b><math>\sigma</math>-BM [2.06]</b>	16.7	32.80	-12.84	-4.4	-28.2	0.07
<b><math>\sigma</math>-BM [2.30]</b>	20.2	54.25	-25.26	-9.87	-32.17	0.21
<b><math>\sigma</math>-BM [2.60]</b>	34.59	60.04	-29.32	-12.95	-32.52	0.46
<b><math>\sigma</math>-BM [TS4]</b>	48.3	71.66	-35.92	-22.31	-34.81	0.32

In this system, the activation energy of the transition state is decomposed into reaction strain ( $\Delta E_{\text{strain}}$ ) (In other literature, it is also referred to as distortion energy ( $\Delta E_{\text{dist}}$ )) and interaction ( $\Delta E_{\text{int}}$ ) between the alkenyl copper and  $\alpha$ -

bromo amide fragments. Using the GKS-EDA method,  $\Delta E_{\text{int}}$  is further broken down into electrostatic interaction  $\Delta E_{\text{eles}}$ , Pauli repulsion  $\Delta E_{\text{exrep}}$ , polarization effects and charge transfer effects, along with several other components collectively termed polarization interaction  $\Delta E_{\text{pol}}$ , desolvation  $\Delta E_{\text{desol}}$ , dispersion, and correlation energy  $\Delta E_{\text{corr/disp}}$ .

Due to variations in energy decomposition models, our quantification model for steric-electronic effects, as per formula (1), allows for the quantitative assessment of steric hindrance, electronic effects, and dispersion effects. Steric hindrance,  $\Delta E_{\text{steric}}$ , is calculated as the sum of  $\Delta E_{\text{strain}}$  and  $\Delta E_{\text{exrep}}$ , with impacts on the three reaction types being  $\Delta E_{\text{steric}}(\text{TS2}) = 89.96 \text{ kcal} \cdot \text{mol}^{-1}$ ,  $\Delta E_{\text{steric}}(\text{TS3}) = 125.54 \text{ kcal} \cdot \text{mol}^{-1}$ , and  $\Delta E_{\text{steric}}(\text{TS4}) = 119.96 \text{ kcal} \cdot \text{mol}^{-1}$ . Electronic effects,  $\Delta E_{\text{electronic}}$ , are represented by  $\Delta E_{\text{ele}}$  and  $\Delta E_{\text{pol}}$ , and their effects are  $\Delta E_{\text{electronic}}(\text{TS2}) = -42.72 \text{ kcal} \cdot \text{mol}^{-1}$ ,  $\Delta E_{\text{electronic}} = -55.18 \text{ kcal} \cdot \text{mol}^{-1}$ , and  $\Delta E_{\text{electronic}}(\text{TS4}) = -58.23 \text{ kcal} \cdot \text{mol}^{-1}$ . From the points and transition states selected along the IRC, spatial steric hindrance  $\Delta E_{\text{steric}}$  and dispersion-related energy promote the ISET pathway, while electronic effects enhance the non-radical pathway.

Figure S6. The SMD solvation model was used to perform EDA of TS2, TS3, TS4 in Benzene/THF (7:3) mixture solvent at  $\omega$ B97X-D/BSII (6-311g(d, p), SDD) levels, respectively.(c) Steric-electronic effects were applied to TS2, TS3, TS4.



## EPS and EPS (INF) of mixed solvents

EPS and EPSINF of mixed solvent Benzene/THF (7:3)

Calculation of static permittivity (eps):

Benzene( $\epsilon/\epsilon_0$ )=2.2706

THF( $\epsilon/\epsilon_0$ )=7.4257

According to the original literature, the volume ratio of mixed solvents:

Benzene/THF=7: 3

So the static permittivity (eps) of Benzene/THF is  $(7/10) * 2.2706 + (3/10) * 7.4257 = 3.81713$

The calculation of dynamic permittivity (epsinf):

The refractive index of Benzene is 1.5011

The refractive index of THF is 1.4050

According to the original literature, the volume ratio of mixed solvents:

Benzene/THF=7: 3

So the dynamic permittivity (EPSINF) of Benzene/THF mixed solvent is  $(7/10) * (1.5011)^2 + (3/10) * (1.4050)^2 \approx 2.169518347$

## Cartesian Coordinates

### Catal

Cu -0.31167107 0.38461538 0.00000000  
C 0.36725193 0.38442038 4.11273400  
C -0.99086207 0.38437638 4.11269200  
H 1.08459393 0.38439838 4.91815100  
H -1.70825207 0.38431338 4.91806600  
N 0.75936093 0.38447938 2.77917300  
N -1.38289407 0.38442138 2.77910800  
C -0.31174007 0.38450838 1.93502700  
C 2.01448693 2.94299038 2.26392500  
C 1.63813993 3.52331838 0.88644600  
C 2.81321993 3.95637238 3.10169700  
H 1.08035893 2.74544638 2.79987300  
H 1.03966593 2.80946638 0.30942400  
H 1.05774593 4.44623038 1.00456900  
H 2.53736493 3.75653738 0.30397400  
H 3.08265793 3.54226738 4.08005000  
H 3.73846393 4.25945538 2.59867300  
H 2.21775593 4.86212538 3.26446800  
C -2.63799207 -2.17408062 2.26370600  
C -2.26164907 -2.75440562 0.88622300  
C -3.43672807 -3.18746862 3.10146600  
H -1.70386507 -1.97654662 2.79966000  
H -1.66316507 -2.04056262 0.30920200  
H -1.68127007 -3.67732762 1.00434200  
H -3.16087807 -2.98760762 0.30374900  
H -3.70618007 -2.77336862 4.07981700  
H -4.36196407 -3.49055862 2.59843100

H -2.84126007 -4.09321862 3.26424100  
C -4.69300207 -0.82456962 1.61815600  
C -3.37512007 -0.85222062 2.08871100  
C -2.74864507 0.38440238 2.32199900  
C -3.37524807 1.62101638 2.08899800  
C -4.69312607 1.59333838 1.61843500  
C -5.34650807 0.38437738 1.38878400  
H -5.20704407 -1.75901462 1.41395100  
H -5.20726407 2.52777638 1.41443900  
H -6.36800407 0.38436738 1.01794000  
C 4.06959893 -0.82440962 1.61850200  
C 2.75171793 -0.85209762 2.08905500  
C 2.12513393 0.38451038 2.32213500  
C 2.75162193 1.62113738 2.08891800  
C 4.06950693 1.59349838 1.61837000  
C 4.72300193 0.38455738 1.38893600  
H 4.58372193 -1.75884262 1.41444200  
H 4.58355493 2.52795038 1.41420700  
H 5.74449793 0.38457538 1.01809300  
C 2.81359093 -3.18739462 3.10171700  
C 2.01465593 -2.17397562 2.26418600  
H 1.08065093 -1.97647262 2.80036500  
H 3.08332293 -2.77331662 4.08000000  
H 2.21813693 -4.09312762 3.26464200  
H 3.73867793 -3.49051462 2.59842600  
C 1.63799693 -2.75424362 0.88676400  
H 1.03935893 -2.04038562 0.30992100  
H 2.53709693 -2.98738762 0.30406900  
H 1.05766993 -3.67718662 1.00497300  
C -2.63823207 2.94290438 2.26426300

H -1.70416207 2.74536438 2.80031500  
C -2.26175307 3.52341938 0.88689700  
H -1.68144907 4.44636638 1.00519700  
H -1.66315407 2.80968538 0.30986200  
H -3.16092807 3.75662838 0.30434300  
C -3.43713307 3.95614538 3.10204200  
H -2.84171107 4.86188338 3.26505100  
H -4.36228907 4.25929638 2.59889800  
H -3.70673907 3.54189338 4.08028600  
H -0.31156207 0.38473638 -1.52317400

**R1**

C -0.96153840 -0.05305040 0.00000000  
C -1.82027040 -0.09536840 0.84793900  
H -0.19958840 -0.01535740 -0.74494100  
C -2.88276440 -0.14725140 1.85184600  
H -2.77359940 -1.06046840 2.45432800  
H -2.76848440 0.69312560 2.55150300  
C -4.29540740 -0.10925540 1.23332300  
H -4.41140340 -0.94834640 0.53681900  
H -4.40967040 0.80553560 0.63951300  
C -5.39898740 -0.17086040 2.30495300  
H -5.27357140 0.67126160 2.99905700  
C -6.78455840 -0.13712140 1.69947000  
C -7.44013440 -1.32275840 1.34304900  
C -7.42134940 1.08249160 1.43434600  
C -8.69790340 -1.29308140 0.73914600  
H -6.95966040 -2.27816340 1.54423600  
C -8.67876040 1.11822560 0.83033000

H -6.92634040 2.01233760 1.70739300  
C -9.32170440 -0.07097340 0.48058900  
H -9.19209540 -2.22421340 0.47393300  
H -9.15807040 2.07439260 0.63640300  
H -10.30248740 -0.04545140 0.01328400  
H -5.27283640 -1.08649440 2.89827300

**INTIM**

Cu 0.35145886 0.06631300 0.00000000  
C 0.56289686 -0.55683800 -4.12912100  
C 0.93236786 0.74436700 -4.07675600  
H 0.36694686 -1.21095800 -4.96286300  
H 1.12753886 1.46299900 -4.85589600  
N 0.43342486 -0.98716400 -2.80826100  
N 1.01912986 1.08129700 -2.72799400  
C 0.70934586 0.01969200 -1.92070400  
C -2.35271114 -1.22982600 -2.02559400  
C -3.46307614 -1.36446900 -0.97459200  
C -2.94620214 -0.94533900 -3.41986800  
H -1.76609314 -0.36249500 -1.71786100  
H -3.04223114 -1.59612000 0.00886900  
H -3.99926714 -0.41293700 -0.89205900  
H -4.19812214 -2.13569000 -1.23653400  
H -2.16305614 -0.75985600 -4.16238500  
H -3.55283714 -1.79066900 -3.76811200  
H -3.58872514 -0.05719800 -3.38271200  
C 3.71189986 2.11046000 -2.27793500  
C 4.85352586 2.41356200 -1.29448400  
C 4.20167286 2.30314700 -3.72787400

H 3.44386286 1.05659200 -2.15331800	H 2.21743786 -4.67071600 -4.59815800
H 4.50653886 2.38005100 -0.25606900	C 3.22378986 -4.05587800 -2.06030100
H 5.65328186 1.67801100 -1.41704400	H 3.05392686 -3.84025900 -1.00146300
H 5.28926786 3.40408400 -1.47143300	H 3.09251586 -5.13309700 -2.21011800
H 3.43924986 2.00285700 -4.45434100	H 4.26648286 -3.82139500 -2.29933200
H 4.44643686 3.35620200 -3.91283000	C -1.37902714 2.66202200 -2.42209000
H 5.09961986 1.70274800 -3.90705200	H -1.31933314 1.57279400 -2.39995900
C 2.56481086 4.27866900 -1.60711400	C -2.44593414 3.05818600 -1.39044000
C 2.46336886 2.94596900 -2.02634700	H -3.39080214 2.55538400 -1.63011900
C 1.17280286 2.43925300 -2.26151400	H -2.13768914 2.74402500 -0.38978300
C 0.00459686 3.21061900 -2.09511100	H -2.64218914 4.13726600 -1.38991000
C 0.16416786 4.53602100 -1.67625900	C -1.79926114 3.08814900 -3.84304000
C 1.42893086 5.06467400 -1.43198600	H -2.77554714 2.65810200 -4.09703400
H 3.54308786 4.70691800 -1.41614700	H -1.87794014 4.17977100 -3.91595400
H -0.71253314 5.16094100 -1.53921700	H -1.07625314 2.75219400 -4.59458100
H 1.53046686 6.09616200 -1.10442900	H -1.01075514 0.81055900 0.15531000
C 0.29678986 -4.66479000 -2.26047300	C 0.72395086 -0.33560000 1.86234500
C 0.81622586 -3.39464400 -2.54172900	C 1.69371686 -0.82282100 1.22831900
C -0.05800914 -2.29600300 -2.45260100	H 0.14871086 -0.09589500 2.73695300
C -1.41226314 -2.42933800 -2.07546300	C 2.98541786 -1.53210400 1.08339500
C -1.87404414 -3.71951500 -1.79178300	H 3.52469786 -1.51384500 2.04286400
C -1.03380014 -4.82669100 -1.88875000	H 2.78264786 -2.58985600 0.86305800
H 0.94210086 -5.53494900 -2.32939500	C 3.87499286 -0.94589500 -0.02129200
H -2.90703014 -3.86174800 -1.49367200	H 4.02932986 0.12117000 0.17081700
H -1.41851614 -5.81932800 -1.66972900	H 3.32961786 -1.00784500 -0.96892700
C 2.48135386 -3.61955600 -4.43210700	C 5.23689486 -1.65119300 -0.13160800
C 2.27492186 -3.23794700 -2.95312400	H 5.07108986 -2.72558000 -0.28607800
H 2.53919286 -2.18113600 -2.83961100	C 6.10253486 -1.10528400 -1.24795000
H 1.86220786 -3.01041500 -5.09807700	C 7.34007086 -0.50751600 -0.97666800
H 3.52996386 -3.48192100 -4.72281200	C 5.67864586 -1.16842700 -2.58456700



C 8.13192286 0.01257200 -2.00366200	H -6.14620571 3.37586959 1.35454300
H 7.68444086 -0.44379900 0.05306000	H -4.69009571 2.59663659 -0.48877000
C 6.46795186 -0.65742400 -3.61511100	H -6.40217371 -1.32821541 -0.19871200
H 4.71769886 -1.61469700 -2.82207400	H -7.85390671 -0.56292041 1.65773000
C 7.69888486 -0.06088300 -3.32845100	C -4.49878171 0.09711259 -1.55356800
H 9.08641286 0.47545000 -1.76689900	H -4.95860571 -0.71609041 -2.13096300
H 6.11895186 -0.72105600 -4.64267700	H -4.29008571 0.91096959 -2.26074600
H 8.31257686 0.34177300 -4.12961200	C 1.08765929 0.47574159 3.98646700
H 5.77059686 -1.55847700 0.82295000	C 2.34047829 0.68872259 3.51075000
	H 0.69692129 0.46029559 4.99129500
<b>INT1aM</b>	H 3.27163429 0.90173359 4.01146000
	N 0.27752929 0.25811159 2.87686700
Cu 0.07294429 0.14588859 0.00000000	N 2.25567529 0.59848259 2.12015100
H -0.62993071 1.48544059 -0.39853000	C 0.98457229 0.33395959 1.71117400
C 0.07355829 -1.74431141 -0.71151800	C -1.55333771 2.49351159 2.74022300
C -0.83143871 -1.07676241 -1.26535100	C -1.61156171 3.15483759 4.13089100
H 0.63342529 -2.63664541 -0.50787000	C -2.32006971 3.31675959 1.69339300
C -2.09491471 -0.75240241 -1.96310500	H -0.50901871 2.47741759 2.41556200
H -1.92854471 0.09507359 -2.63778800	H -1.00686171 2.60376759 4.86103900
H -2.42137071 -1.60960341 -2.57103800	H -1.23548671 4.18396159 4.08502700
C -3.17558171 -0.37691141 -0.92896100	H -2.64225071 3.18570959 4.50488300
H -2.76586871 0.41798559 -0.29714700	H -2.23958871 2.83914459 0.71257800
H -3.36351471 -1.23100041 -0.26602300	H -3.37961371 3.43047659 1.94987700
C -7.09179071 1.45579059 1.63674000	H -1.88564471 4.32114459 1.62311600
C -6.20530971 2.34296459 1.02016800	C 3.05648129 3.28415459 1.44614800
C -5.39101871 1.90611359 -0.02582500	C 1.91530629 3.67679259 0.48369700
C -5.44878371 0.58149359 -0.48045500	C 3.98216529 4.48011859 1.72138200
C -6.34619971 -0.29615941 0.14131900	H 2.59526229 3.01109459 2.40152200
C -7.16136571 0.13334559 1.19100900	H 1.21490229 2.85090759 0.31924500
H -7.72735771 1.79335859 2.45112000	H 1.35491929 4.52904859 0.88843200

H 2.32394829 3.97082859 -0.49116300  
H 4.82676329 4.20053359 2.36176700  
H 4.38546429 4.90616659 0.79548200  
H 3.41959029 5.27566359 2.22269000  
C 4.87300729 2.18937859 0.02715900  
C 3.79160029 2.06121159 0.90778000  
C 3.36075829 0.75733159 1.21276200  
C 3.94220829 -0.39732741 0.65374000  
C 5.01998229 -0.21244141 -0.21934600  
C 5.48338929 1.06606559 -0.52497200  
H 5.23536729 3.17697159 -0.23823400  
H 5.50011529 -1.07357141 -0.67173300  
H 6.32108629 1.18717759 -1.20687000  
C -2.92465971 -1.61982341 2.95118700  
C -1.54739571 -1.36927441 2.94370200  
C -1.13524071 -0.02457041 2.90096300  
C -2.03732871 1.05151259 2.82036100  
C -3.40342671 0.74665959 2.83351500  
C -3.84313271 -0.57311241 2.90009300  
H -3.28302371 -2.64383741 2.98559300  
H -4.13585871 1.54233159 2.76269600  
H -4.90888571 -0.78038441 2.88309300  
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C -0.53613071 -2.50791941 2.99683700  
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H -1.19016371 -3.39859441 1.11651900  
H -0.12574071 -4.43725241 2.09096800  
H -1.81735971 -4.23658441 2.55163900  
C -0.27373171 -2.93421541 4.45443600  
H 0.09646229 -2.09480841 5.05321700

H -1.19469771 -3.30213141 4.92267800  
H 0.47376529 -3.73579141 4.49482900  
C 3.42559229 -1.78828841 1.00788500  
H 2.34661029 -1.69987041 1.16439000  
C 3.62104129 -2.81724341 -0.11549400  
H 3.10335229 -3.74844041 0.14382200  
H 3.21461029 -2.45105841 -1.06416300  
H 4.67725829 -3.06906741 -0.26784500  
C 4.05691429 -2.28951041 2.32213900  
H 3.65471129 -3.27425041 2.58972700  
H 5.14499229 -2.38210741 2.21911400  
H 3.85082029 -1.60551541 3.15166500

#### **TS1M**

Cu -1.45225454 0.57029177 0.00000000  
C -2.28776754 0.44400177 -4.02480800  
C -1.85291854 1.72432877 -3.94007500  
H -2.65510054 -0.13479623 -4.85722900  
H -1.76380254 2.50063177 -4.68284400  
N -2.19919254 -0.09065123 -2.74112100  
N -1.50269054 1.94070277 -2.60863600  
C -1.73135954 0.83037177 -1.84239100  
C -5.02038354 -0.38837823 -2.15941700  
C -5.36606254 0.05001977 -0.72266400  
C -6.28719354 -0.69459423 -2.97668600  
H -4.52452554 0.45774577 -2.64435000  
H -4.46094054 0.32961877 -0.17255300  
H -6.04258954 0.91324077 -0.73976200  
H -5.86372954 -0.76196423 -0.17830200

H -6.03876554 -1.01679523 -3.99452400	H -3.96677754 -4.89390123 -1.40621800
H -6.89155854 -1.48236223 -2.51285000	C 0.09460746 -2.23283323 -3.97733200
H -6.91517254 0.20130777 -3.04430300	C -0.25340454 -2.20733623 -2.47557800
C 1.32336946 2.61091977 -2.40097400	H -0.03257654 -1.20581923 -2.09110700
C 2.65313346 2.87805277 -1.67906500	H -0.47158654 -1.48148423 -4.53587100
C 1.56020246 2.60645677 -3.92519800	H 1.16159846 -2.02618723 -4.12635100
H 0.98895246 1.60800377 -2.11022000	H -0.12451854 -3.21698223 -4.40912500
H 2.51355146 2.95762377 -0.59589800	C 0.63885446 -3.19001123 -1.70378200
H 3.35290446 2.06294777 -1.87646300	H 0.36166146 -3.22843523 -0.64582700
H 3.12426446 3.80386277 -2.03126000	H 0.58251846 -4.20574123 -2.11305200
H 0.66358546 2.31557177 -4.47997100	H 1.68502846 -2.87434023 -1.76901000
H 1.86741346 3.60171177 -4.26938400	C -3.64510354 3.65349577 -1.68284300
H 2.35856446 1.89774677 -4.17457500	H -3.69868154 2.62262177 -2.04226300
C 0.51464646 4.87085577 -1.53082000	C -4.24400154 3.65816677 -0.26455700
C 0.21937846 3.58568377 -2.00010500	H -5.28508154 3.31535377 -0.29430700
C -1.14171354 3.22882077 -2.07678600	H -3.67951154 2.98455477 0.38863600
C -2.18175854 4.07877777 -1.66050100	H -4.23409954 4.66327077 0.17357200
C -1.82940454 5.35264377 -1.19719600	C -4.46703854 4.52314877 -2.65128900
C -0.49718854 5.74839377 -1.14254400	H -5.50760854 4.17901577 -2.68331000
H 1.54810446 5.18992177 -1.45523400	H -4.47189454 5.57418477 -2.33930500
H -2.60885454 6.03544377 -0.87127400	H -4.06026454 4.47807077 -3.66840100
H -0.24088454 6.74120777 -0.78187100	H -2.40593954 0.92327577 1.22884300
C -2.24065954 -3.70963323 -1.90455600	C -1.01760054 0.19999077 1.89397300
C -1.74156054 -2.44875523 -2.24757700	C -0.04738854 -0.21819723 1.16193100
C -2.67220054 -1.39841123 -2.37076200	H -1.38041754 0.30661577 2.90462100
C -4.04714254 -1.56092423 -2.12576900	C 1.29994146 -0.84884623 1.21898400
C -4.49315554 -2.84242723 -1.77720200	H 1.78246646 -0.71579623 2.20144900
C -3.60242854 -3.90633623 -1.67692600	H 1.17745146 -1.93307723 1.08031400
H -1.56031154 -4.54764723 -1.80025800	C 2.21123046 -0.30705323 0.10887300
H -5.54668454 -3.00333923 -1.56941000	H 2.38496746 0.76166677 0.27973700

H 1.66520646 -0.37215023 -0.83878800	C -7.19118307 -1.01059822 -1.71106400
C 3.56329846 -1.02728023 -0.03317200	C -6.31491307 -1.21523822 -0.64358900
H 3.38302346 -2.09856923 -0.19998500	C -6.13484207 -0.23441922 0.34115000
C 4.36198846 -0.44846523 -1.18099900	C -6.86113707 0.95899778 0.22963100
C 5.45376046 0.39927477 -0.95724500	C -7.74024407 1.16999178 -0.83413200
C 3.96550446 -0.68203723 -2.50696900	H -8.59210707 0.34541778 -2.63990200
C 6.12598746 1.00438977 -2.02243400	H -7.31881107 -1.78649122 -2.46205400
H 5.77331346 0.59614877 0.06372900	H -5.75578307 -2.14598622 -0.57405300
C 4.63183346 -0.08098223 -3.57487500	H -6.73321107 1.73087378 0.98566300
H 3.11772646 -1.33456723 -2.70219000	H -8.29714707 2.10144078 -0.89876900
C 5.71509546 0.76977877 -3.33556400	C -5.12832907 -0.42851922 1.45296300
H 6.96812146 1.66253877 -1.82448100	H -5.48782707 0.04870878 2.37457300
H 4.30630546 -0.27638723 -4.59368000	H -5.01937607 -1.49875522 1.67417800
H 6.23385646 1.24235277 -4.16521100	C 0.56087593 0.73666378 -3.99967100
H 4.13225646 -0.94721823 0.90188900	C 1.82314493 0.44281178 -3.59531400
<b>TS1aM</b>	H 0.14904993 0.93475478 -4.97654000
	H 2.74487893 0.33114178 -4.14392300
	N -0.22677907 0.75054078 -2.85419800
Cu -0.24535807 0.37135278 0.00000000	N 1.76897993 0.28887978 -2.21187000
H -1.22560307 -0.80853722 0.41123900	C 0.50595093 0.47498078 -1.73332500
C -0.46360907 1.35353278 1.71626100	C -2.00786707 -1.51720822 -3.21737600
C -1.34697607 0.41936278 1.65221400	C -2.36447907 -1.98118222 -4.64175100
H -0.32396307 2.21377478 2.35915000	C -2.52854207 -2.50207822 -2.15501900
C -2.66776907 -0.07864322 2.13725200	H -0.91690807 -1.50945522 -3.13247900
H -2.60972607 -1.14831322 2.37911700	H -1.94909507 -1.30320922 -5.39677000
H -2.92573807 0.45729278 3.06278600	H -1.96974107 -2.98675022 -4.82993700
C -3.75386407 0.14966078 1.07129100	H -3.45122607 -2.01316922 -4.78434400
H -3.41959907 -0.29961022 0.12913900	H -2.22362607 -2.17373922 -1.15628100
H -3.84641707 1.22545178 0.87402500	H -3.62214207 -2.58096622 -2.17821000
C -7.90653607 0.18542678 -1.81200300	H -2.11719807 -3.50301222 -2.33418000

C 2.33824093 -2.48788222 -1.62037300	H -0.11867707 3.09067478 -2.45416500
C 1.42986393 -3.06078122 -0.51441400	H -1.01485407 3.19120178 -0.15254300
C 3.19288493 -3.58929622 -2.27125600	H -0.50515207 4.79753178 -0.71685800
H 1.68257293 -2.08403822 -2.39861100	H -2.23005507 4.38716378 -0.65633800
H 0.76663093 -2.28749922 -0.11186800	C -1.37578707 4.57539178 -3.34385300
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H 2.02854593 -3.46720822 0.30992200	H -2.37495007 5.01375078 -3.23779000
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H 2.54548593 -4.34958222 -2.72348100	H 2.46510893 2.53338478 -1.87854300
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C -2.51494307 -0.10299722 -2.96535500	C -1.69967117 1.47199936 4.01573800
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<b>IM1</b>	H 5.95761822 4.72587941 -3.07866794
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H 11.65556232 3.21694343 -3.16817159	C 5.35455332 2.16655143 1.42143241
H 11.38817932 1.59988343 -3.81363259	C 4.57613732 3.31749043 1.65033141
C 6.15656532 6.50181643 2.21282941	C 3.19364132 3.28095843 1.92016941
C 5.58566832 5.36794643 2.69634541	C 2.60007132 2.01806743 2.01392241
H 6.57330632 7.36257043 2.71048641	C 3.34241932 0.85639343 1.81106041
H 5.40020332 5.03265943 3.70448041	H 5.25458932 0.01595243 1.33367441
N 6.12870832 6.39432543 0.82767041	H 1.54219832 1.93005043 2.22763141
N 5.22105432 4.60642943 1.59059741	H 2.83956332 -0.10419257 1.85316941
C 5.54673732 5.23143543 0.42761641	C 6.38001132 9.14160743 -1.65404459
C 8.97775132 6.28958543 0.34210841	C 5.81342232 8.24603943 -0.73790559
C 9.72832632 6.95160843 1.51397041	C 6.68381132 7.34785143 -0.09741559
C 9.96298832 5.61501943 -0.62726559	C 8.06773932 7.29806343 -0.35150459
H 8.34742032 5.49463143 0.75428141	C 8.58359532 8.22612243 -1.26242859
H 9.03452732 7.38004143 2.24583041	C 7.74908232 9.13785643 -1.90780359
H 10.35858532 6.21859543 2.03098741	H 5.73820832 9.84394243 -2.17737259
H 10.37361432 7.76108843 1.15208641	H 9.64706832 8.22825543 -1.47999559
H 9.43100332 5.16396043 -1.46851959	H 8.16892932 9.84334543 -2.61981559
H 10.70150132 6.32279743 -1.02170359	C 3.54743432 7.76845143 -1.74132159
H 10.51436932 4.82338043 -0.10651659	C 4.30992632 8.24439643 -0.48993159
C 6.84812132 2.25863443 1.11380441	H 4.09417432 7.53154643 0.31147541
C 7.38055732 1.06805543 0.30372541	H 3.87649532 6.77400243 -2.05975259
C 7.66632132 2.43451443 2.40951941	H 2.47247832 7.71465743 -1.53483159
H 7.00757232 3.14787143 0.49453441	H 3.69966532 8.45772643 -2.58051859
H 6.78411532 0.90416443 -0.59963759	C 3.80775332 9.62203743 -0.02055659
H 8.41131432 1.26717143 -0.00511159	H 4.33817932 9.95525143 0.87891941
H 7.38662232 0.14118243 0.88960841	H 3.94466132 10.38670143 -0.79382059

H 2.73735932 9.57322943 0.20977941	O -5.57103300 -0.86105000 -1.98572000
C 2.38008332 4.56889443 2.02770341	O -4.09444800 -4.47859200 1.02854600
H 3.00850332 5.32041443 2.52054141	C -4.01117600 -0.59725300 -4.32029000
C 2.03317932 5.11643643 0.62391441	H -4.78656900 -1.03697900 -4.97106100
H 1.58387132 6.11339043 0.71041541	H -4.41855600 0.33290400 -3.91877500
H 2.91804632 5.19517543 -0.01356559	H -3.13148400 -0.39031400 -4.93616500
H 1.31282132 4.47763443 0.10415041	H -3.06540800 -2.40422300 -3.46789900
C 1.10914132 4.42642243 2.87885741	Cu 0.12229500 0.66319500 -0.73287000
H 0.65084532 5.41064443 3.02492641	H 1.42754400 -1.99320200 -1.43856900
H 0.36000432 3.79502343 2.38822941	C 1.43933000 0.04535300 -1.96214000
H 1.32526732 3.99743043 3.86400441	C 1.93945000 -1.20021200 -1.98969000
Br 3.78974032 3.75953643 -2.95467759	H 1.94898700 0.80618600 -2.57209000
	C 3.23786900 -1.61653800 -2.63866100
<b>F-TS2</b>	H 3.09646000 -2.53053900 -3.23702900
	H 3.58068100 -0.83160100 -3.32712100
C -5.37467300 -3.93836000 0.72297200	C 4.32588000 -1.87658000 -1.57983300
H -5.92949900 -4.63363300 0.07153900	H 3.97776600 -2.64165800 -0.87158800
H -5.90672500 -3.85232200 1.67597500	H 4.47345500 -0.96174900 -0.99079500
C -3.30346400 -4.59449100 -0.14690000	C 8.59455200 -2.87089100 0.97629600
H -2.33258900 -4.98790400 0.16993800	C 7.92566200 -3.97274900 0.43871500
H -3.76813600 -5.31155100 -0.84452100	C 6.99855700 -3.79605300 -0.59092400
C -5.27689300 -2.57086400 0.05482600	C 6.72373200 -2.52105900 -1.10310300
H -4.86246300 -1.84401200 0.76451200	C 7.40213400 -1.42306400 -0.55321600
H -6.26158800 -2.21615200 -0.25125200	C 8.32903600 -1.59298900 0.47593600
C -3.11159200 -3.24469500 -0.83493300	H 9.31875300 -3.00634700 1.77548600
H -2.53535100 -3.38370000 -1.75031200	H 8.12721500 -4.97165300 0.81855600
H -2.53042400 -2.58309300 -0.17883300	H 6.48086100 -4.65879700 -1.00598500
N -4.41424600 -2.63786400 -1.12654200	H 7.19904000 -0.42574200 -0.93977400
C -4.61183500 -1.63781700 -2.07656300	H 8.84764900 -0.72896400 0.88502700
C -3.68701500 -1.54956000 -3.22414700	C 5.67638700 -2.31715900 -2.17486000

H 6.01554900 -1.55516200 -2.89024700	C -0.42363700 -1.24080200 2.41841000
H 5.53656000 -3.24390200 -2.74708400	C -1.35495400 -0.18658600 2.33975800
C -0.22069400 3.21863500 2.52375900	C -2.74449300 -0.36348900 2.49994800
C -0.77805600 2.12482900 3.10346900	C -3.18616400 -1.65672900 2.79738700
H 0.02997000 4.19021300 2.91743400	C -2.29437200 -2.72453000 2.88090900
H -1.12090100 1.94306300 4.10966500	H -0.25497200 -3.36439100 2.74221800
N 0.02158100 2.87522700 1.19993500	H -4.24181200 -1.84406500 2.95344300
N -0.86239100 1.14927900 2.11334400	H -2.67613400 -3.72270000 3.06457300
C -0.36906200 1.59887200 0.92677800	C 0.73896100 5.20870600 -1.59523400
C 2.91378400 2.69772600 1.20606000	C 0.00931500 4.47031900 -0.65560000
C 3.79556800 3.53352200 2.15206200	C 0.74072600 3.68169700 0.24824300
C 3.73654900 1.63063500 0.46089600	C 2.14531200 3.59129000 0.23711800
H 2.19073200 2.16032300 1.82685300	C 2.82618100 4.35407900 -0.71888400
H 3.19764000 4.25955400 2.71562600	C 2.13139400 5.15443400 -1.62461800
H 4.30887600 2.88208700 2.86937900	H 0.20983900 5.82222900 -2.31840000
H 4.56043700 4.08953800 1.59680100	H 3.91089500 4.31098200 -0.76139200
H 3.09188200 1.01690000 -0.17556500	H 2.67855700 5.73358100 -2.36401400
H 4.50843600 2.08714200 -0.17065300	C -2.04790000 3.68532100 -1.87154700
H 4.24073500 0.97191300 1.17928700	C -1.51378400 4.48000800 -0.66335300
C 1.07930600 -1.00595300 2.27392100	H -1.86056500 3.96818300 0.24049300
C 1.84148400 -2.22411300 1.73232400	H -1.66757200 2.65879500 -1.87353300
C 1.68778700 -0.53261300 3.60896000	H -3.14313400 3.63962700 -1.84488000
H 1.22893300 -0.20571000 1.54342800	H -1.74800400 4.16040700 -2.81347900
H 1.37418900 -2.60859700 0.82076800	C -2.08954200 5.90710900 -0.62951200
H 2.86848300 -1.93445800 1.48491600	H -1.70129700 6.47446400 0.22437900
H 1.89537300 -3.03786000 2.46558700	H -1.84812200 6.46503800 -1.54195300
H 1.21478700 0.38903600 3.96370600	H -3.18190500 5.86959800 -0.54837500
H 1.56447900 -1.29885200 4.38414000	C -3.71761000 0.80002500 2.30531800
H 2.76063000 -0.33769400 3.48869700	H -3.27347600 1.68848900 2.77332700
C -0.93251600 -2.51960400 2.68281400	C -3.90590600 1.12815700 0.80619100

H -4.50954300 2.03798300 0.69941900  
H -2.95267400 1.28477200 0.29650500  
H -4.42688400 0.32341000 0.27800400  
C -5.08247000 0.58296900 2.97873400  
H -5.67611600 1.50084200 2.90978000  
H -5.65842700 -0.20792500 2.48506100  
H -4.97896600 0.32072000 4.03794700  
Br -1.65886500 -0.38766100 -1.92184100

### INT3a

Br -0.74933682 0.57029177 0.00000000  
Cu -2.76390082 0.35182777 -1.17993400  
H -5.32720082 -1.12571523 -1.44257000  
C -4.49676382 0.38716477 -0.27180500  
C -5.49522582 -0.42448623 -0.62502600  
H -4.61611582 1.11909777 0.53400200  
C -6.89919182 -0.43701423 -0.06592500  
H -7.11158182 -1.39590923 0.43200600  
H -7.00521682 0.34659777 0.69604300  
C -7.92521882 -0.22087223 -1.19130200  
H -7.85031082 -1.03813623 -1.91999000  
H -7.67206882 0.69123977 -1.74191900  
C -11.89957782 0.72882877 -4.13043900  
C -11.75478582 -0.58260723 -3.67345700  
C -10.96490382 -0.85209323 -2.55346800  
C -10.30956882 0.17971777 -1.86994600  
C -10.46488382 1.49288177 -2.33831200  
C -11.25128982 1.76808377 -3.45782700  
H -12.51550482 0.94046977 -5.00036700

H -12.25921682 -1.39710523 -4.18724200  
H -10.85518982 -1.87630523 -2.20254300  
H -9.96391682 2.30588677 -1.81615500  
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C -9.38342682 -0.11269723 -0.71103400  
H -9.45529582 0.68609877 0.03939100  
H -9.67684082 -1.04423223 -0.20985600  
C -4.04813482 -0.58619323 -5.07233000  
C -4.17251282 0.76438277 -5.09090200  
H -4.24823182 -1.33156323 -5.82380700  
H -4.49522782 1.44339977 -5.86353300  
N -3.56090782 -0.92670923 -3.81126300  
N -3.75599282 1.21792877 -3.84398900  
C -3.37229582 0.18548977 -3.04830100  
C -0.71589882 -1.49366223 -3.52499800  
C -0.48428382 -1.39063423 -5.04706500  
C 0.60861918 -1.74415023 -2.79158200  
H -1.07017082 -0.52136423 -3.17469900  
H -1.40230982 -1.12905323 -5.58376300  
H 0.26390318 -0.61939723 -5.26471500  
H -0.11748182 -2.34370523 -5.44676400  
H 0.45103918 -1.84203923 -1.71363500  
H 1.12508918 -2.63683423 -3.16501500  
H 1.27374218 -0.88902223 -2.95010200  
C -1.15204182 2.31066377 -4.48618600  
C 0.11365318 2.25870777 -3.61146500  
C -0.83828582 2.83070377 -5.90164000  
H -1.50642382 1.28308477 -4.59670200  
H -0.10638182 1.86612477 -2.61378100  
H 0.86491418 1.61063877 -4.07901000

H 0.56073418 3.25265777 -3.49399700  
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H -0.45073182 3.85569677 -5.87249000  
H -0.08053882 2.19850077 -6.37908700  
C -2.03227682 4.48659177 -3.53422100  
C -2.25453582 3.13719277 -3.83447600  
C -3.51960782 2.60642077 -3.52115800  
C -4.54336682 3.35887077 -2.91634900  
C -4.26818982 4.70388977 -2.64414500  
C -3.02817382 5.26244077 -2.94904500  
H -1.06609682 4.92852577 -3.75823400  
H -5.02914282 5.32233877 -2.18040200  
H -2.83678282 6.30776577 -2.72206300  
C -3.75986082 -4.52451723 -2.86340100  
C -4.17457382 -3.23950223 -3.23881200  
C -3.17553482 -2.26165523 -3.41160400  
C -1.79835682 -2.53160123 -3.22892700  
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C -2.41749882 -4.81345923 -2.65052100  
H -4.50124882 -5.30541223 -2.72875600  
H -0.40841682 -4.07093823 -2.66428000  
H -2.11944682 -5.81281723 -2.34530100  
C -6.55591382 -3.54301523 -2.37156800  
C -5.65771082 -2.97538623 -3.48730300  
H -5.81862182 -1.89234823 -3.51682600  
H -6.25255482 -3.18083023 -1.38514600  
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H -6.53194282 -4.63801823 -2.35139600  
C -6.09096482 -3.55674523 -4.84926400  
H -5.49658182 -3.15546023 -5.67700000

H -5.96909382 -4.64619423 -4.85761200  
H -7.14522482 -3.33019323 -5.04630700  
C -5.90161782 2.74728977 -2.59760000  
H -5.75289882 1.67224777 -2.46450900  
C -6.49465782 3.27743577 -1.28260200  
H -7.40960382 2.72846877 -1.03608900  
H -5.79007682 3.14867477 -0.45533400  
H -6.76335282 4.33787977 -1.34871300  
C -6.88537582 2.95493777 -3.76646700  
H -7.84985882 2.48035177 -3.54920900  
H -7.06116682 4.02332277 -3.94205300  
H -6.49966182 2.52142377 -4.69607000

**INT3b**

C -0.61671083 0.29177718 0.00000000  
H -0.08611783 0.42000518 -0.95759000  
H -1.43614483 1.01517218 0.05016600  
C -0.24315083 -2.02961382 0.01333000  
H -0.78633283 -2.97817882 0.07733000  
H 0.30305217 -1.99754382 -0.94567400  
C 0.36685817 0.49315418 1.15439900  
H -0.17813483 0.44688018 2.10638300  
H 0.87893517 1.45199018 1.07282400  
C 0.76285217 -1.90155082 1.16607800  
H 1.51959617 -2.68266582 1.08318800  
H 0.23629917 -2.03465482 2.12048700  
N 1.37155317 -0.57207382 1.14764100  
C 2.63540217 -0.27803882 0.64167900  
C 3.64551617 -1.33294982 0.65620500



O 2.91705317 0.86369618 0.25128100	H -11.20001800 1.36551193 0.46280700
O -1.21814183 -1.00026082 0.06382700	H -9.60276300 -1.78067007 2.90873000
C 4.98433917 -1.10291982 0.05235700	H -10.88000000 -0.92880607 4.84996500
H 5.23859817 -1.89735782 -0.66469400	C -9.45320600 -0.73833707 0.39269500
H 5.01485517 -0.13452482 -0.45138500	H -9.28766200 -1.82153907 0.46899700
H 5.77263717 -1.12085982 0.82076500	H -9.96600500 -0.56511207 -0.56254000
H 3.47128717 -2.26341882 1.18729500	C -2.47881300 -1.93850107 -0.99867200
	C -1.79289500 -0.67061107 -1.44946500
<b>TS3</b>	H -0.72146400 -0.78879107 -1.58574100
	C -2.50356300 0.10659793 -2.50950900
Br -0.90848800 1.25994693 0.00000000	H -3.53482600 0.30259893 -2.20834200
Cu -3.16838500 0.37539093 0.93444800	H -1.97683300 1.03457993 -2.73456100
H -5.66900800 1.13159293 -0.72433200	H -2.53451600 -0.51857107 -3.41332700
C -4.69724300 -0.51329607 0.17313200	O -3.34503600 -2.37514207 -1.75914500
C -5.73386800 0.07961893 -0.44273000	C -3.82959500 2.61693893 4.43936500
H -4.85374300 -1.57145007 0.42329000	C -3.86967900 1.36985593 4.96687700
C -7.09027600 -0.55110007 -0.66483700	H -4.01966300 3.58426593 4.87536400
H -7.47954600 -0.34601907 -1.67377400	H -4.08401100 1.02048893 5.96424600
H -7.00806900 -1.64249807 -0.56808500	N -3.46799300 2.47128293 3.10213600
C -8.08851500 -0.02316007 0.38487100	N -3.53653300 0.49503193 3.93549800
H -8.25043400 1.05398793 0.23936700	C -3.27335400 1.16074893 2.76950800
H -7.63253800 -0.12193107 1.37791900	C -0.83609600 3.64968993 3.30175300
C -11.76562500 0.70690093 3.75546800	C -0.81252300 4.48640793 4.59688900
C -11.85322600 1.34567793 2.51641300	C 0.56832000 3.59616093 2.67657600
C -11.12904400 0.86217093 1.42493400	H -1.10288100 2.62308493 3.56809400
C -10.30724800 -0.26617707 1.54738200	H -1.78582300 4.48542093 5.09805700
C -10.23147600 -0.89986007 2.79641800	H -0.06957700 4.08798093 5.29835100
C -10.95159500 -0.42003007 3.89184000	H -0.54859600 5.52805993 4.37805700
H -12.32967500 1.08132593 4.60562300	H 0.56349300 3.02248493 1.74571800
H -12.48777000 2.22056493 2.39860800	H 0.96136200 4.59718093 2.46508600

H 1.26453300 3.11564693 3.37388600	C -5.53105700 3.37958493 1.25843600
C -0.91472700 -0.19025107 4.89996700	H -5.36820900 2.29675593 1.31671100
C 0.04774600 -0.04884007 3.70544200	H -5.60777900 3.44668893 -0.93243000
C -0.14193500 -0.46112207 6.20227700	H -7.14055100 3.03261993 -0.14635700
H -1.41407400 0.77500493 5.02677300	H -6.57800500 4.70530693 -0.14041400
H -0.48523900 0.22694193 2.79119300	C -6.45130400 3.78385293 2.42944500
H 0.79642600 0.72634293 3.90575400	H -6.02322400 3.52000193 3.39998500
H 0.57962700 -0.99086407 3.52548300	H -6.63477800 4.86542093 2.41961500
H -0.82134000 -0.59421207 7.05158500	H -7.41730400 3.27259693 2.34228700
H 0.48503300 -1.35689007 6.12871900	C -5.63704700 -1.45398607 3.34788600
H 0.52220000 0.38249793 6.42237200	H -5.49130900 -0.65099507 2.61646200
C -1.68995600 -2.60708207 4.77575300	C -6.38119200 -2.59146907 2.63100900
C -1.97951800 -1.24674407 4.61592500	H -7.28453300 -2.19750207 2.15727300
C -3.26055800 -0.90551807 4.13740100	H -5.77104700 -3.04992407 1.84704400
C -4.25343500 -1.86271707 3.84794000	H -6.69314700 -3.37678307 3.33071100
C -3.91082200 -3.20759107 4.04122600	C -6.51851700 -0.91003107 4.49226500
C -2.64289300 -3.57752307 4.48522400	H -7.50100800 -0.61605507 4.10417700
H -0.70431500 -2.91158607 5.11240800	H -6.67196700 -1.67760007 5.26126500
H -4.63856900 -3.98156107 3.82563000	H -6.07533700 -0.03278407 4.97083700
H -2.39044000 -4.62800307 4.58879700	C -0.17951700 -3.34159907 1.51328600
C -3.84600300 5.17347793 0.57344500	C -1.09051300 -2.18597707 1.09475200
C -4.16550600 4.05633293 1.35479100	C -2.76921100 -3.84616207 0.48176600
C -3.17302600 3.59009093 2.23876000	C -1.79152300 -4.93624107 0.91411800
C -1.89663600 4.17541693 2.34018900	H -1.65580800 -1.82647007 1.96423500
C -1.63549300 5.29450693 1.54074700	H -0.49307500 -1.35663807 0.72029100
C -2.59979300 5.78961593 0.66902300	H 0.47895600 -3.61344407 0.67020900
H -4.57574200 5.56870993 -0.12385100	H 0.44162000 -3.04035607 2.36108900
H -0.66493500 5.77693293 1.59557400	H -3.42029600 -3.58415207 1.32675700
H -2.37831800 6.65682193 0.05247800	H -3.38554400 -4.17395207 -0.35556300
C -6.24832300 3.66144193 -0.07063800	H -2.33340900 -5.79155207 1.32904700

H -1.20652800 -5.27705507 0.04311400  
O -0.91914500 -4.47634907 1.93981000  
N -2.02381700 -2.65379807 0.07414700

**TS4**

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C 0.30111907 0.88199238 1.00608700  
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C 1.52585107 1.68047738 1.37413000  
H 1.81306107 2.36127038 0.55714100  
H 1.32055407 2.29314138 2.26215500  
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H 2.88924107 0.09569538 0.78298500  
H 2.34332607 0.00482738 2.43637100  
C 6.65407907 -1.83297062 3.33399800  
C 6.70575307 -1.32181262 2.03455200  
C 5.87602607 -0.26127362 1.66400700  
C 4.97949407 0.30763438 2.57840900  
C 4.94634907 -0.20755162 3.88214300  
C 5.77356107 -1.26711762 4.26022000  
H 7.29770807 -2.65910862 3.62356000  
H 7.39283607 -1.74953162 1.30880300  
H 5.91540107 0.12636538 0.64826500  
H 4.25781307 0.22416738 4.60548500  
H 5.73094807 -1.65008962 5.27669200  
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H 3.76977407 2.03948738 2.98894500  
H 4.41279707 1.98869538 1.34745100

Cu -1.32547193 -1.23840862 1.58975500  
C -0.54856993 -5.30381562 1.87089600  
C -1.80552593 -5.30847062 2.38130400  
H 0.16883107 -6.09576562 1.72621800  
H -2.42281293 -6.10568362 2.76378300  
N -0.26199893 -3.98531762 1.53260300  
N -2.25224693 -3.99157762 2.33423000  
C -1.30952893 -3.15539662 1.81321900  
C 0.17690207 -3.60208562 -1.30877900  
C 0.12185607 -5.10547762 -1.65065300  
C 0.32629507 -2.76987362 -2.59045600  
H -0.78121693 -3.31658362 -0.86241700  
H -0.07276593 -5.71928262 -0.76521100  
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H 0.41500807 -1.70439762 -2.36084100  
H 1.19405307 -3.08282362 -3.18502300  
H -0.56578293 -2.89591262 -3.21205000  
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C -5.36218493 -5.71886362 0.66551400  
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H -4.61590893 -2.46159562 -0.37204100  
H -5.12717493 -3.84040262 -1.35273500  
H -6.24544093 -3.15433862 -0.16333500  
H -4.93500393 -6.42222262 1.39016900  
H -6.42624793 -5.60210962 0.90289300  
H -5.28857793 -6.16801162 -0.33158000  
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C -4.67361793 -3.75227362 2.09408200

C -3.51415393 -3.54951462 2.86191400	H -1.96604793 -0.65622462 4.25323500
C -3.53319093 -2.93389862 4.12901100	H -2.86050193 -0.75937762 5.78813900
C -4.77622693 -2.52635562 4.62612900	C -2.30572893 -3.49367362 6.26782900
C -5.94687193 -2.73845862 3.90224700	H -1.37186293 -3.34866462 6.82379700
H -6.81011793 -3.49871762 2.08829800	H -3.13238293 -3.16912762 6.91055000
H -4.82766193 -2.03131062 5.59129600	H -2.42899093 -4.56632362 6.07952100
H -6.89680393 -2.39602662 4.29973400	Br -2.27768593 -0.71824362 -1.09457400
C 3.26784407 -2.84115562 1.65655600	N -3.96553993 1.31726038 2.19488000
C 2.01072007 -3.28333762 2.08540100	C -4.33704193 1.63356238 3.57115000
C 1.03637907 -3.52528362 1.09794000	C -5.86042993 1.58127738 3.70417700
C 1.26422007 -3.32572762 -0.27677200	O -6.38264493 0.33141838 3.27036800
C 2.54008407 -2.88645862 -0.65076800	C -4.51604793 0.05071238 1.72563600
C 3.52898507 -2.65142662 0.30253300	C -6.03182793 0.06869838 1.91677600
H 4.04365507 -2.62028162 2.38131800	C -2.98202693 2.04947238 1.58028000
H 2.76035107 -2.71640762 -1.69891900	C -2.70930793 1.79906138 0.13577900
H 4.50960507 -2.29923662 -0.00387000	O -2.45066893 3.02775838 2.11962500
C 1.41814407 -2.05095762 4.19863200	C -1.74200393 2.67963238 -0.56578300
C 1.70663807 -3.42914762 3.57287500	H -3.95163593 2.62381638 3.81690700
H 0.79857907 -4.03061662 3.68263000	H -3.88399193 0.89920638 4.25155900
H 0.62768307 -1.52617362 3.65141000	H -6.30676193 2.40261438 3.11827500
H 1.10450307 -2.16363262 5.24399300	H -6.15808393 1.69600038 4.75115800
H 2.31936307 -1.42881062 4.17968500	H -4.25833493 -0.12959462 0.68415300
C 2.82545807 -4.15598162 4.33870700	H -4.07178293 -0.77072862 2.30842100
H 3.04780307 -5.13139762 3.89125400	H -6.45600893 -0.90510962 1.66707800
H 3.75177407 -3.57109462 4.35164000	H -6.47478493 0.83393538 1.25619300
H 2.52292407 -4.31698062 5.38016200	H -3.55407093 1.46928538 -0.45470700
C -2.27074793 -2.69807762 4.95046100	H -0.98293293 3.06092838 0.11475700
H -1.41134293 -3.05260662 4.37615100	H -2.31461793 3.53362838 -0.96934700
C -2.04309393 -1.19714062 5.20242900	H -1.28579393 2.16559738 -1.41323500
H -1.11134193 -1.04163162 5.75734500	

**TS6 (MECP)**

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N -1.30917061 2.27663797 4.08099800	N -1.30917061 2.27663797 4.08099800
H -0.85543761 0.46419097 0.00000000	N -1.80408961 0.34864797 4.90782200
C -1.76729661 -0.58577303 1.58397500	C -2.04312261 1.15845597 3.84073900
C -0.84974261 -0.43322503 0.62001700	C 0.47310639 2.66128197 1.81102400
H -1.70283861 -1.48627503 2.20267700	C 1.76432839 2.78942997 2.64593800
C 0.31393439 -1.38005303 0.39526400	C 0.80315939 2.71716697 0.31121100
H 0.01744539 -2.40819603 0.64155600	H 0.04255439 1.67491297 2.01147200
H 0.62491339 -1.37941003 -0.65891300	H 1.56423839 2.68548297 3.71677900
C 1.50370839 -0.98337803 1.28863400	H 2.48376639 2.00986397 2.36898200
H 1.16569739 -0.97601303 2.33090500	H 2.23526839 3.76657797 2.48272300
H 1.80620239 0.04703297 1.07007800	H -0.10573161 2.70841997 -0.29978300
C 5.55092639 -0.72689103 4.24380700	H 1.37838139 3.61371797 0.05239900
C 4.78650339 -1.88485403 4.39816300	H 1.41099939 1.85237597 0.02797000
C 3.90340639 -2.28116603 3.39090200	C -0.37505461 -2.17887803 4.57385900
C 3.76631439 -1.53104203 2.21574100	C -0.09723961 -3.34980703 3.61445800
C 4.54319039 -0.37207203 2.07217200	C 0.57683539 -2.27188403 5.78369500
C 5.42720339 0.02837097 3.07482800	H -0.14758661 -1.25229303 4.03683100
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H 4.87909739 -2.48350503 5.30082500	H 0.90962339 -3.25413503 3.19692100
H 3.31463939 -3.18740903 3.51682000	H -0.14604861 -4.31569203 4.12965100
H 4.44943339 0.22099497 1.16466700	H 0.44538739 -1.43354903 6.47383000
H 6.02070339 0.92948297 2.94283800	H 0.39646439 -3.19660503 6.34482900
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H 3.16195339 -1.80911103 0.16058800	C -2.55015161 -3.27902603 5.29667800
H 2.43162939 -2.94451203 1.29142400	C -1.83330661 -2.10835603 5.01320700
Cu -3.09201761 0.68135797 2.20384600	C -2.51159461 -0.88486003 5.16741300
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H 0.02434639 2.95440197 5.64428800	C -3.88354061 -3.22800703 5.69124300

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C -1.40323861 3.51086297 3.33008900  
C -0.55233561 3.71008197 2.22796500  
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H -3.78235761 -2.46642503 1.41650700  
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O -6.14766961 -3.88999103 3.33740800  
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**INT4**  
  
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C -3.87293658 -1.51822443 -1.14343600	C -3.16430258 1.48566857 3.03073400
H -2.79312458 -2.67222343 0.27141500	C -2.98794658 0.29204357 3.64188200
C -5.15883558 -2.31166543 -1.17428400	H -3.62442258 2.39926357 3.36784100
H -5.51149058 -2.40402243 -2.21096000	H -3.23680258 -0.04647843 4.63364400
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C -10.06812658 -0.46852343 2.71140100	C -0.91491058 4.03728457 3.58857200
C -9.95369358 0.08581457 1.43392000	C 1.03419042 3.59972557 2.06284100
C -9.18170658 -0.55018743 0.46045200	H -0.43447858 2.16246657 2.64252400
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C -8.63677358 -2.29558343 2.02607900	H -0.24861358 3.87851957 4.44482200
C -9.40851158 -1.66392843 3.00402300	H -0.91714258 5.10857057 3.35453900
H -10.67031258 0.02445657 3.46977100	H 1.38486842 3.11158357 1.15185300
H -10.46869458 1.01259057 1.19426400	H 1.15809442 4.68412057 1.95579300
H -9.09678158 -0.11338943 -0.53265800	H 1.67630542 3.28164757 2.89255200
H -8.12842558 -3.22882643 2.25988400	C 0.44039842 -0.70903043 3.51218500
H -9.49693258 -2.10811943 3.99227200	C 1.89427242 -1.02238743 3.12910500
C -7.59180458 -2.37553943 -0.28224300	C 0.37170442 -0.03473543 4.89734800
H -7.42667358 -3.43385143 -0.04166000	H 0.08537042 0.00730957 2.76947700
H -8.04739658 -2.34864643 -1.28089900	H 1.94429642 -1.53314943 2.16307600
C -1.06017558 -3.10510243 -1.88422000	H 2.45266442 -0.08634543 3.02942700
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H -2.16473058 -0.85461043 -3.13743800	H 0.99491142 0.86747157 4.91012600
H -0.75796358 0.21360957 -2.85270400	C 0.00019642 -3.18998343 3.84960700

C -0.47288958 -1.92874143 3.46698800	H -5.70666758 -3.83985443 1.57058500
C -1.82706958 -1.83696043 3.08035700	H -4.06511058 -4.34774843 1.13630600
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C -2.16251558 -4.18375043 3.45531000	C -5.04721858 -2.55063643 3.95189600
C -0.82837758 -4.30841043 3.83158700	H -6.09377658 -2.41737643 3.65360200
H 1.03611942 -3.30055343 4.15117300	H -4.99111258 -3.39390843 4.65065800
H -2.79419758 -5.06501743 3.44536600	H -4.73791258 -1.65004243 4.48858400
H -0.43032158 -5.28314843 4.09652400	C 1.07616542 -4.61073143 0.78141000
C -3.15623858 3.88134757 -0.93968000	C 0.12161242 -3.51621443 0.30443100
C -3.34481658 2.74487657 -0.14376700	C -1.20341558 -5.26970543 -0.75975600
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C -1.36581458 3.41319757 1.18583700	H -0.60118958 -3.29597043 1.10070100
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C -2.10929258 4.76528157 -0.69323300	H 1.88912842 -4.73515143 0.04605900
H -3.83803758 4.08141057 -1.75834400	H 1.50965342 -4.33117543 1.74487700
H -0.42457458 5.23698257 0.54728400	H -2.04046358 -5.20126043 -0.04413900
H -1.98035158 5.64020557 -1.32481000	H -1.60295358 -5.56367943 -1.73112200
C -5.00922958 1.78501157 -1.82178700	H -0.68587158 -7.23797143 -0.01661500
C -4.54276858 1.82675457 -0.35772700	H 0.58573742 -6.45973843 -0.99942000
H -4.24406258 0.81256957 -0.07732900	O 0.40317442 -5.84650443 0.97878900
H -4.17779158 1.57602357 -2.50382800	N -0.57625758 -3.95738743 -0.90058300
H -5.76444058 1.00399457 -1.95494200	
H -5.46943158 2.73102357 -2.12951400	<b>TS8</b>
C -5.71187258 2.23812457 0.56215400	
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H -6.04470358 3.25715557 0.33064400	Cu -2.24660327 -1.32138141 0.10447200
H -6.56403358 1.56023857 0.43343300	H -4.65096727 -1.73750241 -1.77902300
C -4.17107158 -2.81720143 2.71040700	C -3.48385427 -2.72223341 -0.34348500
H -4.26556258 -1.95774843 2.03927600	C -4.58618327 -2.56992341 -1.08292400
C -4.71055758 -4.05304343 1.96949600	H -3.36366827 -3.57948241 0.31803200



C -5.80142227 -3.46181041 -1.00102900	H -4.89954527 1.53048759 3.52916700
H -6.18842327 -3.64383941 -2.01405200	H -4.22034427 -0.82023841 4.85321600
H -5.52037127 -4.43938141 -0.59273900	N -3.77216627 0.59060759 1.94054200
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C -9.27818327 -3.66948941 2.24088900	H -1.77151327 3.44387759 4.58532900
C -10.10158127 -3.08201641 3.20456900	H -2.46827527 4.57012059 3.40434900
H -11.46012927 -1.46436841 3.64754100	H 0.02601773 2.57358259 1.40099000
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C -6.88034527 1.01162459 0.62474300	
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## **Cata2**

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H 3.89706752 4.76493655 -2.49770800  
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H -5.03632448 -1.25989245 -1.32701100	H -3.52410248 -2.22513845 -4.05289800
H -6.19965948 0.87614355 -0.90009600	Br -0.16573748 0.84199955 2.27928500
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C 2.27020252 0.89955255 -2.25754000	
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H 4.70458052 -1.26004245 -1.32693300	H -0.67436265 2.18545509 3.05849100
H 4.72019852 3.02651155 -1.29307600	C 1.25812435 2.73020509 1.19776700
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