Electronic Supplementary Information for:

Synergetic argentophilic and through space electronic interactions in single-crystal-to-single-crystal photocycloaddition reaction: a mechanistic study

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S1. Computational Details

S1.1 Model Setup

The X-ray crystal structure of $[Ag_2\text{-}(4\text{-pyr-ph-cb})_2][CF_3SO_3]_2$ (CCDC 945408) was used to construct the initial QM/MM model.[1] There were 31 crystal units of $[Ag_2\text{-}(4\text{-pyr-ph-cb})_2]$ $[CF_3SO_3]_2$ included in the model, accounting for a total number of 3658 atoms. The AMBER-parm99 force field[2] was employed for the chosen system. The charge distribution of $[Ag_2\text{-}(4\text{-pyr-ph-cb})_2][CF_3SO_3]_2$ were recalculated with restrained electrostatic potential (RESP) using the tleap module of AMBER10.[3] Because the parameters for Ag(I) is not available in the general Amber force field (GAFF), we used the same force constants as Cu(I) for instead in the MM minimization,[4] which has turned to be reasonable in our investigations.

S1.2 QM/MM Computational Protocol

The QM/MM partitioning chosen are shown in Figure S1. To describe the [2+2] photodimerization accurately, $[Ag_2\text{-}(4\text{-pyr-ph-cb})_2]^{2+}$ with 102 atoms is only adopted in the QM subsystem. The MM subsystem includes the other 30 molecules of $[Ag_2\text{-}(4\text{-pyr-ph-cb})_2]^{2+}$ and their counterpart anions.
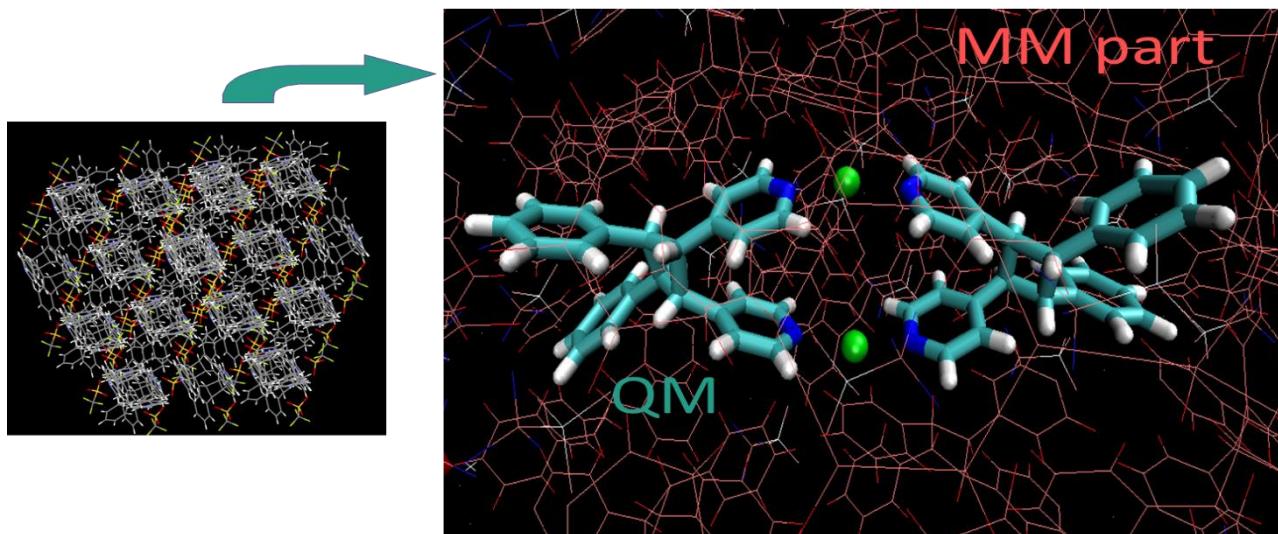

Fig. S1 *Illustration of the QM/MM computational model.*

S1.3 QM Method:

The pedal-like conformational change of the QM part have been studied using the density functional theory (DFT) with the B3LYP functional. The stationary structures and

scanned transition states are obtained. The minimum energy profile (MEP) is mapped via intrinsic reaction coordinate (IRC) [5] computations to connect the above critical points.

The [2+2] photodimerization calculations of the QM parts after the pedal motion are conducted with the complete active space self-consistent field (CASSCF) method. [6] To consider dynamic electron correlation effects, the single-point energies of the optimized geometries are recalculated at the multi-configuration second-order perturbation (CASPT2) level of theory. [7] The active space of 10 electrons in 10 orbitals (10e/10o) is applied. These orbitals are schematically shown in Figure S2 and Figure S3, which includes d_z^2 orbital of Ag(I), σ orbital of Ag⋯Ag and the rest high-lying occupied π and low-lying π* orbitals that are mainly distributed in the 4-stilbz moiety. For Ag(I) ions, we chose the energy-consistent scalar-relativistic WB-adjusted 28-electron core pseudopotential[8-9] associated with the optimized (8s7p6d)/[6s5p3d]) valence basis set to account for the relativistic effects involved. The pseudopotentials and basis set of the Ag atoms can be found in the homepage of the Dolg group (http://www.tc.uni-koeln.de/PP/index.en.html) and the basis set library of the Molcas program package.[10] The 6-31G* basis set is applied for the carbon atoms of C=C double bonds in the reaction center, while the STO-3G basis set is adopted for the rest C, H, N atoms. Due to the limitation of computer memory for CASPT2 computations with 102 atoms, the 6-31G basis set for C=C is used in the single point energy calculations. The critical points including minima, conical intersections, and singlet-triplet state crossings, are explicitly optimized by using the state-averaged CASSCF method. A two-roots equally weighted (0.5:0.5) or three-roots differently weighted (0.0:0.5:0.5) state-averaged approach is used for critical points in the excited states, whereas single root optimization is adopted in the ground and the lowest-lying triplet state. Single-point energy corrections at all optimized structures are determined from the 5-root state-averaged CASPT2//CASSCF calculations to include dynamical electron correlation. The calculations are performed without an ionization potential-electron affinity (IPEA) shift but included an energy level shift of 0.2 a.u. to avoid intruder state problems.
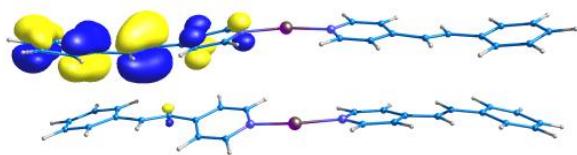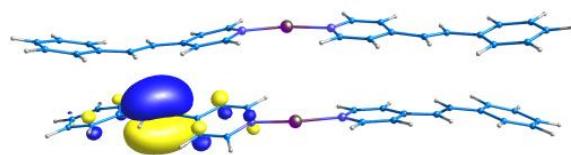
π orbital   **π orbital**
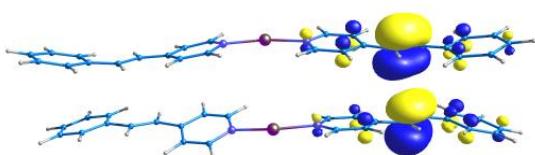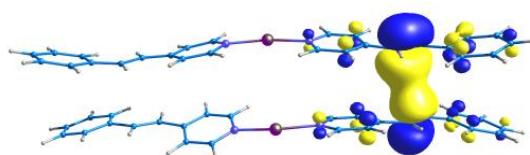
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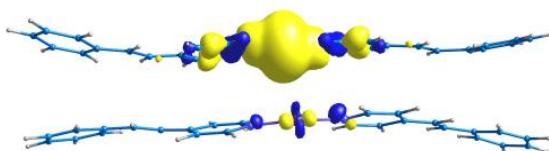
d_{z^2} orbital   **σ orbital**
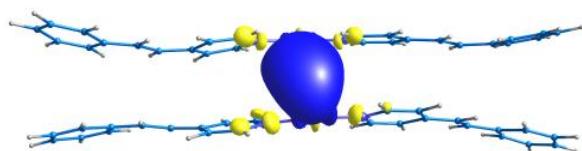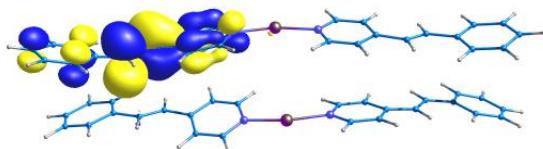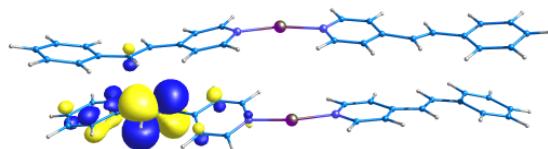
π* orbital   **π* orbital**
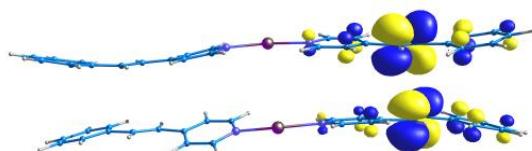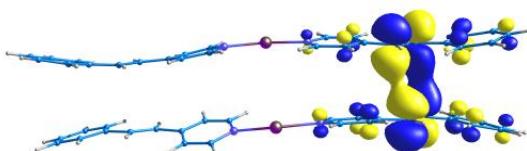
π* orbital   **π* orbital**

Fig. S2 *Molecular orbitals of **1** used in defining the active space for the CASPT2//CASSCF (10e/10o) calculations of the first [2+2] PCA reaction.*

π orbital

π orbital

π orbital

π orbital

d_{z^2} orbital

σ orbital

π* orbital

π* orbital
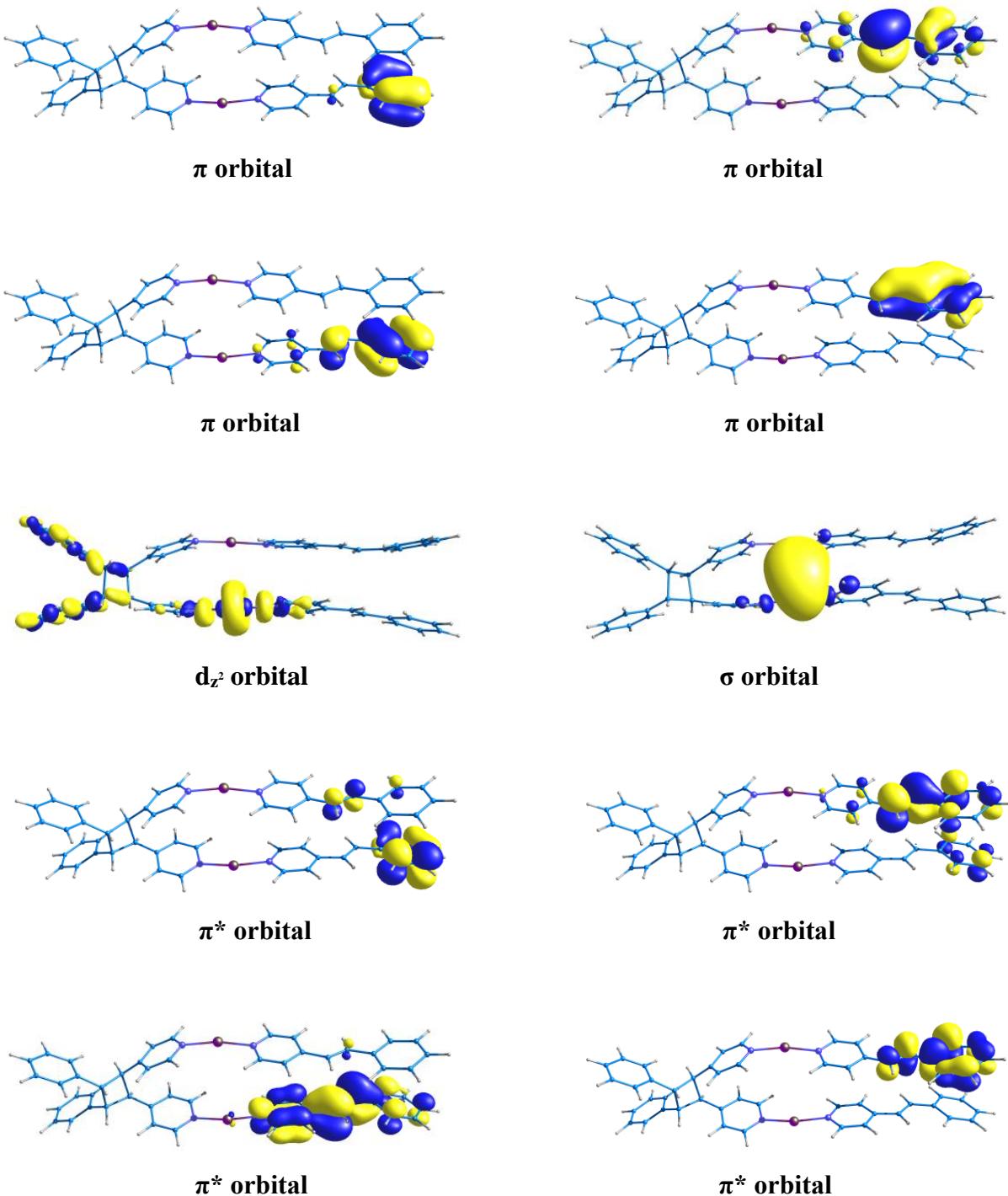
π* orbital

π* orbital

Fig. S3 *Molecular orbitals of **Reactant 2** used in defining the active space for the CASPT2//CASSCF (10e/10o) calculations of the second [2+2] PCA reaction.*

S1.4 Packages and Tool

The DFT and CASSCF computations are performed using GAUSSIAN03.[11] The CASPT2 calculations for QM part are conducted with Molcas program package.[12] The MM energy minimizations are treated with the AMBER99[2] force field using TINKER4.2 package.[13]

The theoretical investigations of intermolecular interactions in the crystal structures of $[Ag_2(4\text{-stilbz})_4][CO_2CF_3]_2$ are investigated via Hirshfeld surface analysis (Isovalue: 0.5) using Crystal Explorer 17.5. [14]

S1.5 ISC rate constant calculation

The ISC rates[15] between singlet and triplet state for [2+2] PCA reaction are estimated by eq. 1

$$k_{ISC}^{IF} = \frac{2\pi}{h} \cdot < {}^1\Psi_0^I|H_{SO}| {}^3\Psi_0^F >^2 \cdot | < X_0|X_n > |^2 \cdot \rho \qquad (eq.1)$$

Where k_{ISC}^{IF} : the rate constant for ISC, $< {}^1\Psi_0^I|H_{SO}| {}^3\Psi_0^F >$: the electronic coupling between the initial and final states, $| < X_0|X_n > |$:Franck−Condon factor, the value is 1, $\rho = \frac{1}{\Delta E^{IF}}$: the reciprocal of the energy difference between the initial state and the final state.

S1.6 Rate constant calculations with the transition state theory

The rates via an energy barrier in an adiabatic potential energy surface can be estimated using the transition state theory as follows (eq.2)

$$k_{TS} = \frac{k_B T}{h} \exp\left[-\frac{\Delta G^{\neq}}{k_B T}\right] \qquad (eq.2)$$

In which k_{TS} is the rate constant for chemical reaction, $\Delta G^{\neq}$ is the Gibbs free energy barrier, k_B is the Boltzmann constant (8.62×10^{-5} eV/K) and T is the absolute temperature (298 K). Although the value of $\Delta G^{\neq}$ can be obtained by frequency analyses as the sum of potential energy barrier ($\Delta E^{\neq}$) and the Gibbs correction, we should not overlook the anharmonic effect in the **1** complex under low-frequency vibrational mode. The TST rate obtained using $\Delta E^{\neq}$ can be considered as the lower bound of an accurate value since $\Delta G^{\neq}$ is usually smaller than $\Delta E^{\neq}$. On one hand, we can reoptimize the minima and transition states at the TD-B3LYP/PCM level, then the frequency analyses to correct the Gibbs free energy. On the other hand, if the geometries optimized at the DFT level are similar to the CASSCF results, add the correction terms to the potential energy barriers at the CASPT2//CASSCF level. The realistic process may take place at the rates ranging from k_{TS} ($\Delta E^{\neq}$) as a lower bound to $k_{TS}{}'$ ($\Delta G^{\neq}$) as an upper bound.

S1.7 Irradiative rates calculation

The irradiative rates[16] (fluorescence and phosphorescence) are calculated as follows (eq.3)

$$k_r^{F/P} = \frac{2\pi v^2 e^2}{\varepsilon_0 m c^3} f_{S_{ALPP} \to S_0} \qquad \textbf{(eq.3)}$$

in which v is the emission energy, e is the elementary electric charge, ε_0 is the vacuum permittivity, m is the mass of an electron, c is the speed of light, and $f_{S_{ALPP} \to S_0}$ is the oscillator strength of the $S_{ALPP} \to S_0$ radiative transition.

S1.8 References:

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S2 Orbital analysis of Ag-σ in $S_{ALP\Sigma}$ ($^1\pi\sigma$) state

$$\Phi_\sigma = 39.8\%Ag_{B-5s} + 20.4\%Ag_{B-5p} + 6.5\%Ag_{B-4d} + 27.9\%Ag_{A-5s} + 6.4\%Ag_{A-4d} \qquad \textbf{(eq.4)}$$

S3. Supplementary Figures

S3.1 Pedal-like Conformational Change
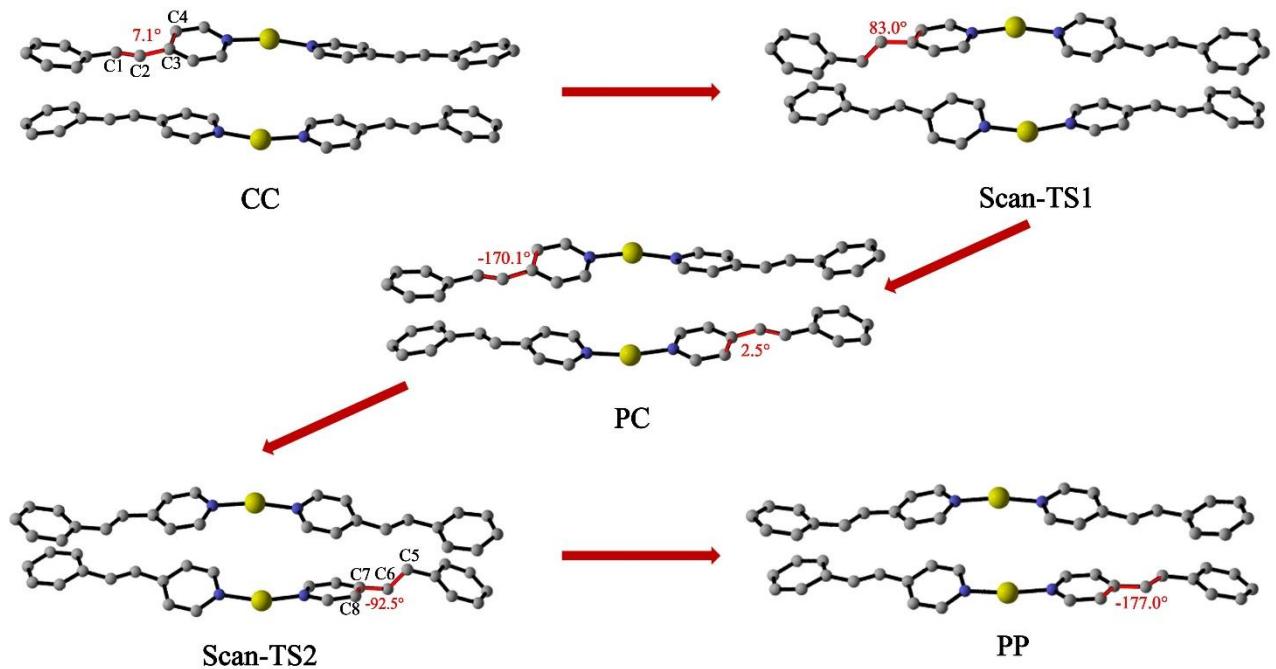
Fig. S4 The molecule structure of the important point during the pedal motion. The red lines indicate the mode of torsional deformation, which are defined as the reaction coordinate of C1C2C3C4, C5C6C7C8 dihedral angles, respectively.
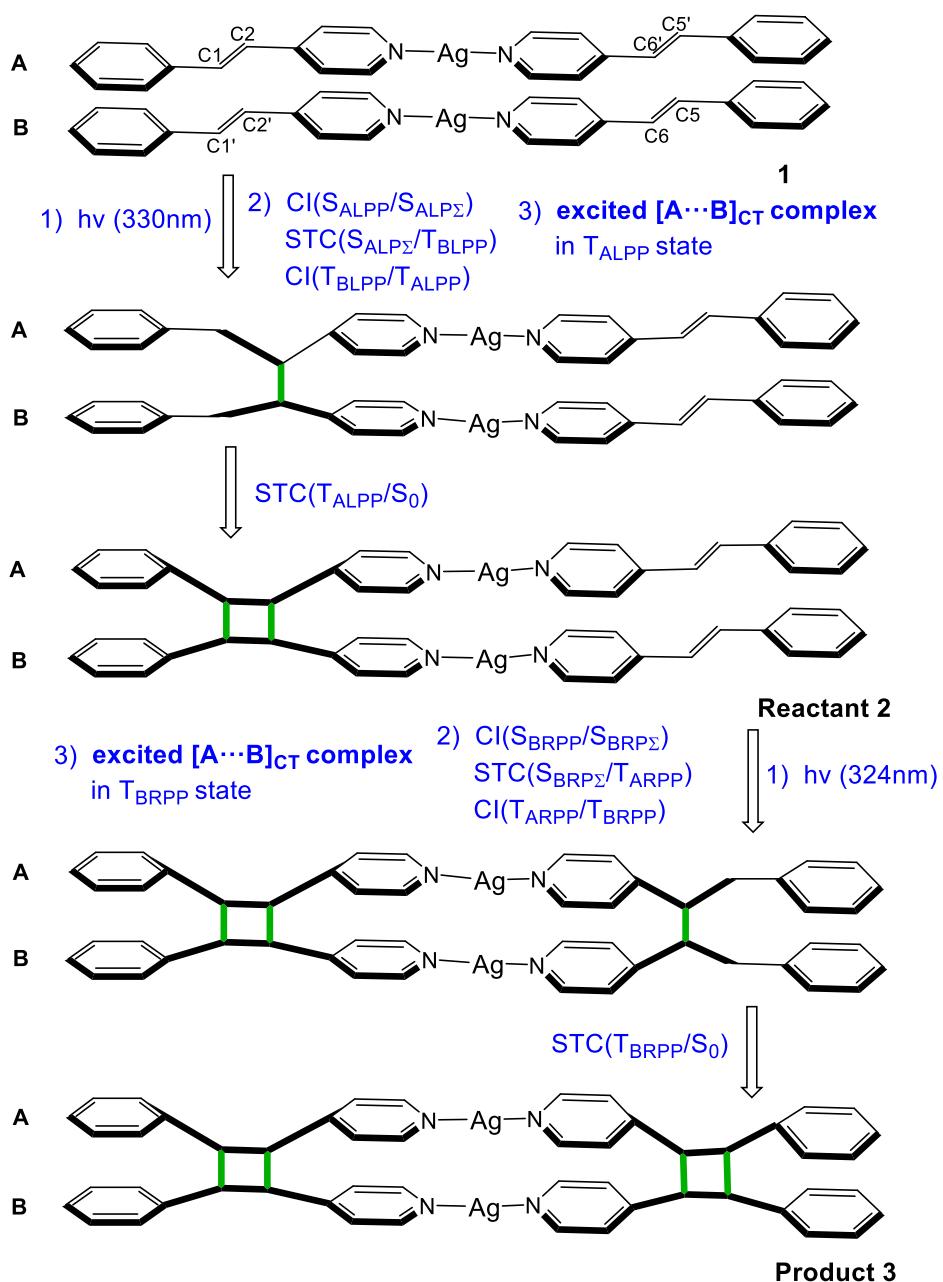
Fig. S5 *Schematic illustration of the photophysical and photochemical processes involved for the twice [2+2] PCA.*

S4. Supplementary Tables

Table S1 *Absolute energies (A.E., Hartree) and relative energies (R.E., kcal/mol) for the pedal motion from CC to PC by using the SCAN method. The corresponding energy profiles are plotted in Figure 1 (left pannel) of the main article.*

C1C2C3C4	DFT（B3LYP）	
	A.E	**R.E**
CC(-175.3º)	-2489.914686	0.0
-172.3º	-2489.914474	0.1
-169.3º	-2489.914177	0.3
-166.3º	-2489.913804	0.6
-163.3º	-2489.913363	0.8
-160.3º	-2489.912837	1.2
-157.3º	-2489.912217	1.5
-154.3º	-2489.911511	2.0
-151.3º	-2489.910699	2.5
-148.3º	-2489.909775	3.1
-145.3º	-2489.908735	3.7
-142.3º	-2489.907576	4.5
-139.3º	-2489.906285	5.3
-136.3º	-2489.904867	6.2
-133.3º	-2489.903315	7.1
-130.3º	-2489.901635	8.2
-127.3º	-2489.899829	9.3
-124.3º	-2489.897889	10.5
-121.3º	-2489.895833	11.8

-118.3º	-2489.893656	13.2
-115.3º	-2489.891376	14.6
-112.3º	-2489.888987	16.1
-109.3º	-2489.887196	17.3
-106.3º(Scan-TS1)	-2489.878753	22.5
-103.3º	-2489.879374	22.2
-100.3º	-2489.880123	21.7
-97.3º	-2489.880975	21.2
-94.3º	-2489.881923	20.6
-91.3º	-2489.882937	19.9
-88.3º	-2489.884004	19.3
-85.3º	-2489.885119	18.6
-82.3º	-2489.886276	17.8
-79.3º	-2489.887456	17.1
-76.3º	-2489.888659	16.3
-73.3º	-2489.889865	15.6
-70.3º	-2489.891063	14.8
-67.3º	-2489.89225	14.1
-64.3º	-2489.893412	13.3
-61.3º	-2489.894555	12.6
-58.3º	-2489.89566	11.9
-55.3º	-2489.896736	11.3
-52.3º	-2489.897774	10.6
-49.3º	-2489.898763	10.0

-46.3º	-2489.899701	9.4
-43.3º	-2489.900584	8.8
-40.3º	-2489.901412	8.3
-37.3º	-2489.902175	7.9
-34.3º	-2489.902876	7.4
-31.3º	-2489.903521	7.0
-28.3º	-2489.904101	6.6
-25.3º	-2489.904625	6.3
-22.3º	-2489.905091	6.0
-19.3º	-2489.905508	5.8
-16.3º	-2489.905866	5.5
-13.3º	-2489.90617	5.3
-10.3º	-2489.906431	5.2
-7.3º	-2489.906639	5.0
-4.3º	-2489.906794	5.0
-1.3º	-2489.906904	4.9
1.7º	-2489.906966	4.8
4.7(PC)	-2489.906997	4.8

Table S2 *Absolute energies (A.E., Hartree) and relative energies (R.E., kcal/mol) for the pedal motion from PC to PP by using the SCAN method. The corresponding energy profiles are plotted in Figure 1 (right pannel) of the main article.*

C5C6C7C8	DFT（B3LYP）	
	A.E	R.E
PC(-175.4º)	-2489.906923	4.9
-178.4º	-2489.906999	4.8
178.6º	-2489.907011	4.8
175.6º	-2489.906961	4.8
172.6º	-2489.906845	4.9
169.6º	-2489.906665	5.0
166.6º	-2489.906423	5.2
163.6º	-2489.906111	5.4
160.6º	-2489.905729	5.6
157.6º	-2489.905272	5.9
154.6º	-2489.904743	6.2
151.6º	-2489.904144	6.6
148.6º	-2489.903465	7.0
145.6º	-2489.902709	7.5
142.6º	-2489.901878	8.0
139.6º	-2489.900968	8.6
136.6º	-2489.899968	9.2
133.6º	-2489.898877	9.9
130.6º	-2489.897697	10.7

127.6º	-2489.896433	11.5
124.6º	-2489.895088	12.3
121.6º	-2489.893672	13.2
118.6º	-2489.89218	14.1
115.6º	-2489.890623	15.1
112.6º	-2489.889016	16.1
109.6º	-2489.88736	17.1
106.6º	-2489.885692	18.2
103.6º	-2489.883841	19.4
100.6º(Scan-TS2)	-2489.878861	22.4
97.6º	-2489.879791	21.9
94.6º	-2489.880843	21.2
91.6º	-2489.881985	20.5
88.6º	-2489.883188	19.8
85.6º	-2489.88443	19.0
82.6º	-2489.885694	18.2
79.6º	-2489.886964	17.4
76.6º	-2489.888229	16.6
73.6º	-2489.889478	15.8
70.6º	-2489.890707	15.0
67.6º	-2489.891904	14.3
64.6º	-2489.893062	13.6
61.6º	-2489.894183	12.9
58.6º	-2489.895249	12.2

55.6º	-2489.89626	11.6
52.6º	-2489.897214	11.0
49.6º	-2489.898107	10.4
46.6º	-2489.898945	9.9
43.6º	-2489.899721	9.4
40.6º	-2489.900434	8.9
37.6º	-2489.90109	8.5
34.6º	-2489.901672	8.2
31.6º	-2489.902192	7.8
28.6º	-2489.902657	7.5
25.6º	-2489.90306	7.3
22.6º	-2489.903698	6.9
19.6º	-2489.903698	6.9
16.6º	-2489.903936	6.7
13.6º	-2489.904124	6.6
10.6º	-2489.904256	6.5
7.6º	-2489.904328	6.5
4.6º（PP）	-2489.90436	6.5

Table S3 *Absolute energies (A.E., Hartree), relative energies (R.E., kcal/mol) and MM energies (hartree) for the first [2+2] PCA reaction pathway. The corresponding energy profiles are plotted in Figure 3 (left pannel) of the main article.*

Reactant 1	MM part	CASPT2	
	A.E.	A.E.	R.E.
S_0-min			
Root1		-2485.124397	0
Root2($^1\pi\sigma$)		-2484.977507	92.2
Root3($^1\pi\pi^*$)	7.699245	-2484.986228	86.6
Root4		-2484.911998	133.3
Root5		-2484.910573	134.2
$S_{ALPP}(^1\pi\pi^*)$-1			
Root1		-2485.124369	0.1
Root2($^1\pi\sigma$)		-2484.978294	91.7
Root3($^1\pi\pi^*$)	7.699244	-2484.986948	86.3
Root4		-2484.908674	135.4
Root5		-2484.903176	138.9
CI[$S_{ALPP}(^1\pi\pi^*)$ /$S_{ALP\Sigma}(^1\pi\sigma)$]			
Root1		-2485.125733	-0.9
Root2($^1\pi\pi^*$)		-2484.993383	82.1
Root3($^1\pi\sigma$)	7.699078	-2484.98633	86.5
Root4		-2484.91692	130.1
Root5		-2484.912436	132.9
$S_{ALP\Sigma}(^1\pi\sigma)$-1			
Root1		-2485.125716	-1.3
Root2($^1\pi\sigma$)	7.698385	-2484.991187	83.1
$S_{ALP\Sigma}(^1\pi\sigma)$-2			
Root1		-2485.125422	-1.5
Root2($^1\pi\sigma$)	7.697886	-2484.990403	83.3

STC[$S_{ALP\Sigma}$($^1\pi\sigma$)/T_{BLPP}($^3\pi\pi^*$)]			
Root1		-2485.125745	-1.9
Root2 ($^1\pi\sigma$)	7.697493	-2484.994182	80.6
Root3 ($^3\pi\pi^*$)		-2484.998971	77.6
T_{BLPP}($^3\pi\pi^*$)-1			
Root1 (S_0)		-2485.125744	-1.9
Root2 [T_{ALPP}($^3\pi\pi^*$)]	7.697492	-2485.030449	57.9
Root3 [T_{BLPP}($^3\pi\pi^*$)]		-2485.019606	64.7
T_{BLPP}($^3\pi\pi^*$)-2			
Root1 (S_0)		-2485.126111	-1.8
Root2 [T_{ALPP}($^3\pi\pi^*$)]	7.697481	-2485.030909	57.6
Root3 [T_{BLPP}($^3\pi\pi^*$)]		-2485.020972	63.8
T_{BLPP}($^3\pi\pi^*$)-3			
Root1 (S_0)		-2485.126020	-1.7
Root2 [T_{ALPP}($^3\pi\pi^*$)]	7.698147	-2485.030997	57.9
Root3 [T_{BLPP}($^3\pi\pi^*$)]		-2485.025263	61.5
CI[T_{BLPP}($^3\pi\pi^*$)/T_{ALPP}($^3\pi\pi^*$)]			
Root1 (S_0)		-2485.122396	0.2
Root2 [T_{ALPP}($^3\pi\pi^*$)]	7.697518	-2485.035113	55.0
Root3 [T_{BLPP}($^3\pi\pi^*$)]		-2485.029988	58.2
T_{ALPP}($^3\pi\pi^*$)-1			
Root1 (S_0)	7.705796	-2485.120513	6.6
Root2 ($^3\pi\pi^*$)		-2485.043657	54.8
T_{ALPP}($^3\pi\pi^*$)-2			
Root1 (S_0)	7.699863	-2485.109848	9.5
Root2 ($^3\pi\pi^*$)		-2485.044277	50.7
T_{ALPP}($^3\pi\pi^*$)-3	[A⋯B]$_{CT}$ complex		
Root1 (S_0)	7.69833	-2485.109944	8.5

Root2 ($^3\pi\pi^*$)		-2485.047785	47.5
$T_{ALPP}(^3\pi\pi^*)$-4			
Root1 (S_0)	7.697883	-2485.101324	13.7
Root2 ($^3\pi\pi^*$)		-2485.042485	50.6
$T_{ALPP}(^3\pi\pi^*)$-5			
Root1 (S_0)	7.695048	-2485.095953	15.3
Root2 ($^3\pi\pi^*$)		-2485.035978	52.9
$T_{ALPP}(^3\pi\pi^*)$-6			
Root1 (S_0)	7.697115	-2485.062326	37.6
Root2 ($^3\pi\pi^*$)		-2485.034724	54.9
$T_{ALPP}(^3\pi\pi^*)$-7			
Root1 (S_0)	7.695651	-2485.054926	41.4
Root2 ($^3\pi\pi^*$)		-2485.038133	51.9
$T_{ALPP}(^3\pi\pi^*)$-8			
Root1 (S_0)	7.695783	-2485.048239	45.7
Root2 ($^3\pi\pi^*$)		-2485.039504	51.1
$T_{ALPP}(^3\pi\pi^*)$-9			
Root1 (S_0)	7.695832	-2485.046593	46.7
Root2 ($^3\pi\pi^*$)		-2485.040639	50.5
$STC[T_{ALPP}(^3\pi\pi^*)/S_0]$			
Root1 (S_0)	7.695056	-2485.045236	47.1
Root2 ($^3\pi\pi^*$)		-2485.040083	50.3
S_0-1			
Root1	7.694177	-2485.065774	33.6
S_0-2			
Root1	7.693539	-2485.076066	26.8

S$_0$-3			
Root1	7.693222	-2485.077749	25.5
S$_0$-4			
Root1	7.691937	-2485.079478	23.6
S$_0$-5			
Root1	7.691499	-2485.090956	16.2
S$_0$-6			
Root1	7.69107	-2485.098003	11.5
S$_0$-7			
Root1	7.690817	-2485.10395	7.6
S$_0$-8			
Root1	7.690419	-2485.108252	4.6
S$_0$-9			
Root1	7.688541	-2485.111988	1.1
S$_0$-10	**Reactant 2**		
Root1	7.689816	-2485.121724	-4.2

Table S4 *Absolute energies (A.E., Hartree), relative energies (R.E., kcal/mol) and MM energies (hartree) for the second [2+2] PCA reaction pathway. The corresponding energy profiles are plotted in Figure 3 (right pannel) of the main article.*

Reactant 2	MM part	CASPT2	
	A.E.	A.E.	R.E.
S_0-min			
Root1		-2485.102217	0
Root2		-2484.955996	91.8
Root3 ($^1\pi\sigma$)	7.687563	-2484.941363	100.9
Root4 ($^1\pi\pi^*$)		-2484.961517	88.2
Root5		-2484.913976	118.1
$S_{BRPP}(^1\pi\pi^*)$-1			
Root1		-2485.103127	0.2
Root2 ($^1\pi\pi^*$)		-2484.966572	85.5
Root3 ($^1\pi\sigma$)	7.688202	-2484.953525	93.7
Root4		-2484.942131	100.9
Root5		-2484.948946	96.6
CI[$S_{BRPP}(^1\pi\pi^*)$/$S_{BRP\Sigma}(^1\pi\sigma)$]			
Root1		-2485.099533	2.1
Root2 ($^1\pi\sigma$)		-2484.962099	88.3
Root3 ($^1\pi\pi^*$)	7.688280	-2484.966528	85.6
Root4		-2484.951375	95.1
Root5		-2484.933404	106.4
$S_{BRP\Sigma}(^1\pi\sigma)$-1			
Root1	7.687729	-2485.098664	2.3
Root2 ($^1\pi\sigma$)		-2484.963994	86.6
$S_{BRP\Sigma}(^1\pi\sigma)$-2			
Root1	7.687919	-2485.099516	1.9
Root2 ($^1\pi\sigma$)		-2484.964877	86.4

$S_{BRP\Sigma}(^1\pi\sigma)$-3			
Root1	7.688091	-2485.099710	1.9
Root2 ($^1\pi\sigma$)		-2484.967087	85.1
STC[$S_{BRP\Sigma}(^1\pi\sigma)/T_{ARPP}(^3\pi\pi*)$]			
Root1		-2485.101185	1.8
Root2 ($^1\pi\sigma$)	7.689394	-2484.971889	82.9
Root3 ($^3\pi\pi*$)		-2484.975961	80.3
$T_{ARPP}(^3\pi\pi*)$-1			
Root1 (S_0)		-2485.101437	1.3
Root2 [$T_{BRPP}(^3\pi\pi*)$]	7.688844	-2485.014964	55.6
Root3 [$T_{ARPP}(^3\pi\pi*)$]		-2484.991673	70.2
$T_{ARPP}(^3\pi\pi*)$-2			
Root1 (S_0)		-2485.099539	2.1
Root2 [$T_{BRPP}(^3\pi\pi*)$]	7.688280	-2485.014525	55.5
Root3 [$T_{ARPP}(^3\pi\pi*)$]		-2485.005542	61.1
$T_{ARPP}(^3\pi\pi*)$-3			
Root1 (S_0)		-2485.099993	1.8
Root2 [$T_{BRPP}(^3\pi\pi*)$]	7.688232	-2485.007298	59.9
Root3 [$T_{ARPP}(^3\pi\pi*)$]		-2485.010386	58.0
CI[$T_{ARPP}(^3\pi\pi*)/T_{BRPP}(^3\pi\pi*)$]			
Root1 (S_0)		-2485.099840	1.9
Root2 [$T_{ARPP}(^3\pi\pi*)$]	7.688218	-2485.010839	57.8
Root3 [$T_{BRPP}(^3\pi\pi*)$]		-2485.012939	56.5
$T_{BRPP}(^3\pi\pi*)$-1			
Root1 (S_0)	7.689531	-2485.089798	9.0
Root2 ($^3\pi\pi*$)		-2485.021710	51.8
$T_{BRPP}(^3\pi\pi*)$-2			

Root1 (S_0)	7.688179	-2485.086523	10.2
Root2 ($^3\pi\pi^*$)		-2485.022694	50.3
$T_{BRPP}(^3\pi\pi^*)$-3			
Root1 (S_0)	7.690321	-2485.079032	16.3
Root2 ($^3\pi\pi^*$)		-2485.025537	49.9
$T_{BRPP}(^3\pi\pi^*)$-4			
Root1 (S_0)	7.690300	-2485.077187	17.5
Root2 ($^3\pi\pi^*$)		-2485.025980	49.6
$T_{BRPP}(^3\pi\pi^*)$-5	**[A···B]$_{CT}$ complex**		
Root1 (S_0)	7.687866	-2485.074005	17.9
Root2 ($^3\pi\pi^*$)		-2485.024648	48.9
$T_{BRPP}(^3\pi\pi^*)$-6			
Root1 (S_0)	7.686438	-2485.071251	18.8
Root2 ($^3\pi\pi^*$)		-2485.019099	51.5
$T_{BRPP}(^3\pi\pi^*)$-7			
Root1 (S_0)	7.686470	-2485.064752	22.8
Root2 ($^3\pi\pi^*$)		-2485.014697	54.3
$T_{BRPP}(^3\pi\pi^*)$-8			
Root1 (S_0)	7.686266	-2485.058765	26.5
Root2 ($^3\pi\pi^*$)		-2485.010329	56.9
$T_{BRPP}(^3\pi\pi^*)$-9			
Root1 (S_0)	7.687739	-2485.058059	26.9
Root2 ($^3\pi\pi^*$)		-2485.012017	56.7
$T_{BRPP}(^3\pi\pi^*)$-10			
Root1 (S_0)	7.685790	-2485.050186	32.0
Root2 ($^3\pi\pi^*$)		-2485.009062	57.5

$T_{BRPP}(^3\pi\pi^*)$-11			
Root1(S_0)	7.686178	-2485.049854	32.5
Root2($^3\pi\pi^*$)		-2485.018249	51.9
$T_{BRPP}(^3\pi\pi^*)$-12			
Root1(S_0)	7.686482	-2485.047008	34.6
Root2($^3\pi\pi^*$)		-2485.019864	51.0
$T_{BRPP}(^3\pi\pi^*)$-13			
Root1(S_0)	7.686867	-2485.046904	34.7
Root2($^3\pi\pi^*$)		-2485.028464	45.9
$T_{BRPP}(^3\pi\pi^*)$-14			
Root1(S_0)	7.687504	-2485.046840	34.7
Root2($^3\pi\pi^*$)		-2485.037477	40.6
$T_{BRPP}(^3\pi\pi^*)$-15			
Root1(S_0)	7.687546	-2485.044193	36.4
Root2($^3\pi\pi^*$)		-2485.039023	39.7
$STC[T_{BRPP}(^3\pi\pi^*)/S_0]$			
Root1 (S_0)	7.688415	-2485.044746	36.6
Root2 ($^3\pi\pi^*$)		-2485.042261	38.2
S_0-1			
Root1	7.687462	-2485.051809	31.6
S_0-2			
Root1	7.687643	-2485.059597	26.8
S_0-3			
Root1	7.687235	-2485.066961	21.9
S_0-4			
Root1	7.687535	-2485.069258	20.7

S$_0$-5			
Root1	7.687564	-2485.080187	13.9
S$_0$-6	**Product 3**		
Root1	7.685196	-2485.092091	4.9

S5. Cartesian Coordinates

Coordinates for Fig. 2

CC

Ag	10.554080000	1.062758000	3.891748000
Ag	9.946517000	5.766095000	5.125157000
C	6.463159000	2.435894000	4.154293000
H	5.975974000	3.341597000	3.764156000
C	7.819602000	2.227600000	3.879825000
H	8.406237000	2.966803000	3.310322000
N	8.516943000	1.095769000	4.326208000
C	7.777089000	0.133980000	5.018366000
H	8.335423000	-0.776661000	5.292253000
C	6.428120000	0.311822000	5.346673000
H	5.904400000	-0.480700000	5.897463000
C	5.740288000	1.500029000	4.955741000
C	4.358266000	1.796390000	5.320805000
H	3.897693000	2.600011000	4.752390000
C	3.647540000	1.198492000	6.307937000
H	4.147306000	0.424376000	6.893328000
C	2.236182000	1.380029000	6.634854000
C	1.646267000	0.427805000	7.516898000
H	2.293011000	-0.301377000	8.026634000
C	0.252694000	0.363014000	7.672257000
H	-0.170576000	-0.414629000	8.318265000
C	-0.581651000	1.269284000	6.983525000
H	-1.676149000	1.210432000	7.078959000
C	-0.006908000	2.259336000	6.150800000
H	-0.657091000	2.964315000	5.614576000
C	1.383144000	2.320228000	5.979533000
H	1.813764000	3.085548000	5.322153000
C	12.800141000	3.290017000	0.956999000
H	12.482010000	3.993150000	0.175758000
C	11.845388000	2.737962000	1.814832000
H	10.775326000	2.987523000	1.734605000
N	12.178193000	1.829758000	2.827859000
C	13.530675000	1.516490000	2.978513000
H	13.753482000	0.825465000	3.808589000
C	14.525988000	2.044311000	2.142794000
H	15.570456000	1.747107000	2.314523000
C	14.178031000	2.939792000	1.084375000
C	15.117266000	3.486942000	0.107889000
H	14.662917000	4.110987000	-0.663426000
C	16.455731000	3.282068000	0.073828000
H	16.897587000	2.659133000	0.855256000
C	17.393326000	3.741652000	-0.943216000
C	17.073024000	4.688317000	-1.958763000
H	16.102526000	5.198702000	-1.942707000
C	17.997719000	4.962100000	-2.975566000
H	17.748406000	5.684079000	-3.764720000
C	19.262930000	4.327263000	-2.991818000
H	19.974993000	4.552301000	-3.797662000

C	19.614681000	3.434424000	-1.959655000
H	20.604729000	2.960020000	-1.942599000
C	18.685920000	3.153301000	-0.946509000
H	18.929717000	2.466310000	-0.133262000
C	6.064995000	4.833920000	6.937622000
H	5.046403000	5.234686000	6.845533000
C	7.083615000	5.420622000	6.189069000
H	6.899928000	6.267183000	5.516350000
N	8.405035000	4.977757000	6.240362000
C	8.689828000	3.900147000	7.087683000
H	9.737345000	3.558269000	7.086582000
C	7.711991000	3.303592000	7.888152000
H	7.983355000	2.489184000	8.573146000
C	6.365140000	3.770153000	7.838360000
C	5.373321000	3.191670000	8.726380000
H	5.737663000	2.471038000	9.457435000
C	4.059111000	3.504108000	8.686697000
H	3.716280000	4.212494000	7.930469000
C	3.032195000	3.091407000	9.616563000
C	3.197234000	2.057949000	10.580722000
H	4.111660000	1.447059000	10.588554000
C	2.191100000	1.843175000	11.526872000
H	2.333277000	1.072838000	12.292150000
C	1.015820000	2.633189000	11.518595000
H	0.228761000	2.466357000	12.262426000
C	0.835904000	3.636620000	10.550184000
H	-0.076634000	4.239971000	10.547707000
C	1.839907000	3.858497000	9.600040000
H	1.759168000	4.640202000	8.837369000
C	13.811223000	6.625619000	3.164514000
H	14.209475000	7.371988000	2.464778000
C	12.472968000	6.712600000	3.561339000
H	11.798193000	7.509471000	3.206806000
N	11.893771000	5.795372000	4.439064000
C	12.721699000	4.801404000	4.974198000
H	12.244242000	4.098571000	5.676417000
C	14.071398000	4.687731000	4.625524000
H	14.680140000	3.896100000	5.087893000
C	14.641880000	5.580112000	3.668468000
C	16.025189000	5.362996000	3.268108000
H	16.532119000	4.577332000	3.827743000
C	16.708921000	6.018914000	2.300469000
H	16.197351000	6.809348000	1.747291000
C	18.121522000	5.846083000	1.974591000
C	18.753435000	6.829880000	1.160080000
H	18.140793000	7.623792000	0.707768000
C	20.149040000	6.824569000	0.992157000
H	20.626293000	7.606347000	0.387522000
C	20.932998000	5.830091000	1.615525000
H	22.026530000	5.833982000	1.506703000
C	20.314814000	4.820992000	2.389782000
H	20.926570000	4.049008000	2.876205000

C	18.924308000	4.822005000	2.562275000
H	18.451245000	4.039068000	3.168430000

Scan-TS1

Ag	10.651812000	1.091969000	3.871035000
Ag	9.906227000	5.732658000	5.200999000
C	6.557427000	2.479811000	4.139393000
H	6.074947000	3.400867000	3.779552000
C	7.923860000	2.294837000	3.896856000
H	8.520975000	3.065838000	3.382489000
N	8.615549000	1.145506000	4.305893000
C	7.862721000	0.144287000	4.924176000
H	8.420931000	-0.773955000	5.171924000
C	6.501374000	0.293806000	5.213743000
H	5.971021000	-0.529708000	5.710116000
C	5.815714000	1.496069000	4.863254000
C	4.429930000	1.782577000	5.221157000
H	4.012263000	2.670495000	4.753959000
C	3.683804000	1.104988000	6.129567000
H	4.147799000	0.244441000	6.617404000
C	2.296376000	1.335322000	6.530397000
C	1.721487000	0.421498000	7.464656000
H	2.368243000	-0.323277000	7.951933000
C	0.336749000	0.414046000	7.699368000
H	-0.080743000	-0.327427000	8.390847000
C	-0.501030000	1.333173000	7.031631000
H	-1.590688000	1.313532000	7.183289000
C	0.062165000	2.287064000	6.150020000
H	-0.589718000	3.003962000	5.632111000
C	1.442549000	2.298439000	5.909848000
H	1.862829000	3.034165000	5.215540000
C	12.923509000	3.293768000	0.947618000
H	12.615133000	4.005289000	0.169893000
C	11.960272000	2.735151000	1.789667000
H	10.890945000	2.985007000	1.700970000
N	12.283597000	1.818895000	2.798750000
C	13.633947000	1.502601000	2.960168000
H	13.846184000	0.808094000	3.790120000
C	14.638161000	2.033175000	2.136589000
H	15.681392000	1.735224000	2.313909000
C	14.299046000	2.937816000	1.083816000
C	15.238546000	3.490544000	0.114057000
H	14.782097000	4.144678000	-0.630143000
C	16.570145000	3.256080000	0.030296000
H	17.031121000	2.594608000	0.767643000
C	17.455932000	3.739506000	-1.021890000
C	17.081120000	4.755578000	-1.948914000
H	16.134996000	5.296178000	-1.818801000
C	17.918158000	5.059888000	-3.029126000
H	17.624501000	5.836139000	-3.748302000
C	19.151836000	4.386951000	-3.195105000
H	19.794640000	4.631210000	-4.050147000

C	19.563699000	3.426919000	-2.250154000
H	20.534425000	2.924735000	-2.355248000
C	18.721854000	3.111124000	-1.172618000
H	19.020816000	2.360159000	-0.436014000
C	5.923437000	5.015519000	6.883057000
H	4.899640000	5.370013000	6.694180000
C	6.995422000	5.515115000	6.136542000
H	6.857525000	6.291996000	5.379502000
N	8.302816000	5.085019000	6.331933000
C	8.532977000	4.127317000	7.326771000
H	9.576428000	3.784230000	7.415867000
C	7.509601000	3.671031000	8.168819000
H	7.721600000	2.958126000	8.979359000
C	6.181440000	4.115999000	7.941976000
C	5.081455000	3.842145000	8.886428000
H	4.982564000	4.541319000	9.716603000
C	4.116720000	2.956789000	8.670180000
H	4.214801000	2.283522000	7.826108000
C	2.985533000	2.812094000	9.598357000
C	3.065727000	1.811297000	10.588171000
H	3.923801000	1.124166000	10.603575000
C	2.079577000	1.759227000	11.577031000
H	2.205902000	1.027616000	12.377398000
C	0.991584000	2.657595000	11.552571000
H	0.209527000	2.602253000	12.318315000
C	0.900148000	3.632078000	10.542291000
H	0.051656000	4.324940000	10.523140000
C	1.911551000	3.726006000	9.571619000
H	1.894815000	4.494079000	8.789303000
C	13.792610000	6.562175000	3.299356000
H	14.203197000	7.336929000	2.638451000
C	12.451967000	6.645709000	3.688985000
H	11.790602000	7.466765000	3.366423000
N	11.854113000	5.696457000	4.520139000
C	12.669232000	4.674116000	5.021859000
H	12.181529000	3.946130000	5.691037000
C	14.021993000	4.562446000	4.678369000
H	14.619358000	3.748582000	5.116942000
C	14.609898000	5.485728000	3.759796000
C	15.990901000	5.267926000	3.345816000
H	16.491268000	4.454502000	3.870552000
C	16.673730000	5.952186000	2.395333000
H	16.161729000	6.765880000	1.877561000
C	18.080074000	5.784003000	2.039790000
C	18.697688000	6.777022000	1.224136000
H	18.077422000	7.577047000	0.793630000
C	20.090249000	6.774909000	1.030532000
H	20.556845000	7.564211000	0.426936000
C	20.886806000	5.774171000	1.627883000
H	21.978661000	5.782200000	1.500565000
C	20.282653000	4.754872000	2.400157000
H	20.902356000	3.976012000	2.865339000

| C | 18.895440000 | 4.753952000 | 2.598522000 |
| H | 18.433799000 | 3.965156000 | 3.204316000 |

PC

Ag	10.537972000	1.096543000	3.942367000
Ag	10.167164000	5.624303000	5.420865000
C	6.449552000	2.477678000	4.190091000
H	5.972509000	3.397267000	3.821601000
C	7.810637000	2.276938000	3.936450000
H	8.407329000	3.032378000	3.399238000
N	8.499279000	1.132009000	4.364577000
C	7.746569000	0.153553000	5.019265000
H	8.300442000	-0.762974000	5.282380000
C	6.391012000	0.322474000	5.324364000
H	5.857618000	-0.483260000	5.846087000
C	5.710106000	1.519441000	4.948738000
C	4.324200000	1.810803000	5.298331000
H	3.877741000	2.634152000	4.749424000
C	3.602369000	1.207896000	6.273242000
H	4.090921000	0.419318000	6.848777000
C	2.195891000	1.405428000	6.606692000
C	1.603272000	0.458158000	7.491013000
H	2.245602000	-0.280831000	7.991701000
C	0.211668000	0.411421000	7.662852000
H	-0.209897000	-0.364315000	8.311209000
C	-0.619254000	1.331519000	6.988579000
H	-1.713050000	1.288812000	7.099705000
C	-0.040297000	2.316276000	6.152306000
H	-0.686123000	3.034670000	5.628725000
C	1.348403000	2.359726000	5.965398000
H	1.781235000	3.125760000	5.310708000
C	12.817675000	3.356765000	1.064651000
H	12.514422000	4.101614000	0.316549000
C	11.858403000	2.821466000	1.927767000
H	10.800266000	3.125566000	1.885645000
N	12.173495000	1.863580000	2.899689000
C	13.512467000	1.483022000	3.006814000
H	13.720185000	0.754325000	3.807801000
C	14.512421000	1.993787000	2.165897000
H	15.547189000	1.648695000	2.302786000
C	14.180245000	2.937546000	1.146263000
C	15.116802000	3.476841000	0.164832000
H	14.662733000	4.146472000	-0.566902000
C	16.445510000	3.228807000	0.069758000
H	16.904068000	2.557440000	0.800048000
C	17.337402000	3.726147000	-0.972391000
C	16.967394000	4.759652000	-1.881382000
H	16.019772000	5.294656000	-1.743937000
C	17.811483000	5.092190000	-2.948096000
H	17.513558000	5.878640000	-3.654287000
C	19.050237000	4.429680000	-3.118402000
H	19.700723000	4.697364000	-3.962036000

C	19.458742000	3.453158000	-2.188094000
H	20.435372000	2.962135000	-2.292365000
C	18.608985000	3.108678000	-1.124910000
H	18.908888000	2.348798000	-0.397245000
C	6.061263000	5.262264000	6.568553000
H	5.132750000	5.766913000	6.275168000
C	7.297855000	5.741749000	6.144591000
H	7.412721000	6.668250000	5.571770000
N	8.485930000	5.074833000	6.428268000
C	8.414142000	3.905285000	7.197883000
H	9.373397000	3.388298000	7.362735000
C	7.212559000	3.446709000	7.733929000
H	7.213133000	2.563430000	8.385983000
C	5.998596000	4.142108000	7.433855000
C	4.719310000	3.853691000	8.035728000
H	3.892705000	4.471665000	7.687638000
C	4.514023000	2.958037000	9.020568000
H	5.344444000	2.330705000	9.350383000
C	3.288542000	2.775733000	9.758624000
C	3.321540000	1.819938000	10.802807000
H	4.226713000	1.211439000	10.948207000
C	2.228064000	1.693683000	11.660271000
H	2.311240000	0.977094000	12.479765000
C	1.082083000	2.495018000	11.474428000
H	0.228150000	2.409667000	12.157004000
C	1.020402000	3.414304000	10.402226000
H	0.114941000	4.014530000	10.247588000
C	2.117664000	3.561851000	9.548055000
H	2.086875000	4.287609000	8.724469000
C	13.888273000	6.535974000	3.286952000
H	14.243911000	7.296008000	2.578648000
C	12.569881000	6.602169000	3.748868000
H	11.865437000	7.392348000	3.440175000
N	12.050047000	5.666678000	4.643907000
C	12.909086000	4.673365000	5.126647000
H	12.471211000	3.957534000	5.841501000
C	14.238144000	4.579199000	4.706737000
H	14.876291000	3.788338000	5.125890000
C	14.752057000	5.491793000	3.736634000
C	16.117542000	5.288724000	3.277714000
H	16.635660000	4.476073000	3.784930000
C	16.784171000	5.985303000	2.327023000
H	16.268723000	6.804280000	1.820530000
C	18.191691000	5.819095000	1.977508000
C	18.814682000	6.819275000	1.176561000
H	18.196916000	7.620726000	0.744965000
C	20.208741000	6.820245000	0.998011000
H	20.678933000	7.614982000	0.405036000
C	20.999976000	5.816267000	1.596786000
H	22.092718000	5.824659000	1.481537000
C	20.390307000	4.791312000	2.356368000
H	21.007240000	4.011975000	2.824049000

| C | 19.001793000 | 4.786581000 | 2.540271000 |
| H | 18.537231000 | 3.993010000 | 3.138823000 |

Scan-TS2

Ag	10.589791000	1.208008000	3.904713000
Ag	10.168813000	5.533558000	5.557115000
C	6.492722000	2.588955000	4.241279000
H	6.012165000	3.521836000	3.912792000
C	7.858227000	2.412691000	3.987439000
H	8.450532000	3.200124000	3.492463000
N	8.554267000	1.253424000	4.364158000
C	7.801481000	0.237492000	4.961187000
H	8.358250000	-0.688533000	5.180619000
C	6.441465000	0.380555000	5.264729000
H	5.912045000	-0.455149000	5.742252000
C	5.752134000	1.590329000	4.947196000
C	4.363257000	1.863722000	5.306985000
H	3.928233000	2.728612000	4.814199000
C	3.628375000	1.210252000	6.240649000
H	4.105982000	0.383335000	6.770479000
C	2.224574000	1.410052000	6.591459000
C	1.631001000	0.458571000	7.472437000
H	2.270895000	-0.293837000	7.955784000
C	0.241506000	0.427913000	7.666457000
H	-0.182130000	-0.345695000	8.316480000
C	-0.588422000	1.362271000	7.011525000
H	-1.680791000	1.331577000	7.138555000
C	-0.009860000	2.347940000	6.176662000
H	-0.654124000	3.078934000	5.668638000
C	1.377300000	2.381575000	5.974631000
H	1.808031000	3.153126000	5.324916000
C	12.870732000	3.087355000	0.739440000
H	12.563686000	3.637643000	-0.160229000
C	11.899011000	2.614613000	1.632946000
H	10.821818000	2.774488000	1.463462000
N	12.225250000	1.879512000	2.778197000
C	13.578108000	1.671444000	3.037330000
H	13.793586000	1.090772000	3.950018000
C	14.591936000	2.157538000	2.186350000
H	15.645353000	1.944131000	2.423225000
C	14.251128000	2.881208000	1.008981000
C	15.277091000	3.155440000	-0.041530000
H	15.508137000	2.302306000	-0.681464000
C	16.074745000	4.220555000	-0.186403000
H	15.876016000	5.125844000	0.386499000
C	17.181242000	4.224115000	-1.172179000
C	17.185972000	5.139944000	-2.253481000
H	16.391163000	5.892522000	-2.327234000
C	18.179746000	5.043515000	-3.242402000
H	18.165490000	5.720421000	-4.108212000
C	19.236978000	4.119881000	-3.103339000
H	20.049166000	4.118583000	-3.843101000

C	19.261558000	3.237566000	-2.004562000
H	20.096419000	2.535625000	-1.878009000
C	18.219258000	3.266264000	-1.059562000
H	18.216406000	2.583745000	-0.199956000
C	6.037819000	5.243567000	6.618923000
H	5.116146000	5.753113000	6.312463000
C	7.283054000	5.701642000	6.195373000
H	7.416221000	6.614501000	5.602478000
N	8.458008000	5.024047000	6.508615000
C	8.366705000	3.863422000	7.289384000
H	9.318441000	3.338855000	7.470280000
C	7.155827000	3.421550000	7.812426000
H	7.138893000	2.544257000	8.471895000
C	5.955396000	4.131768000	7.494131000
C	4.672972000	3.854595000	8.089508000
H	3.859684000	4.509555000	7.779713000
C	4.453321000	2.908129000	9.021764000
H	5.270098000	2.244590000	9.310949000
C	3.236253000	2.723387000	9.765932000
C	3.285131000	1.768582000	10.809122000
H	4.188624000	1.153924000	10.937613000
C	2.211125000	1.657056000	11.690350000
H	2.313641000	0.943873000	12.510292000
C	1.066893000	2.465543000	11.522028000
H	0.222286000	2.394431000	12.216250000
C	0.987678000	3.379821000	10.447764000
H	0.081617000	3.982929000	10.309921000
C	2.068488000	3.517482000	9.573235000
H	2.028060000	4.238838000	8.746524000
C	13.874086000	6.468266000	3.439292000
H	14.223370000	7.238553000	2.738628000
C	12.560156000	6.530942000	3.913889000
H	11.854844000	7.328074000	3.626285000
N	12.048204000	5.581552000	4.797514000
C	12.906192000	4.578907000	5.257833000
H	12.474053000	3.858342000	5.970029000
C	14.228293000	4.483677000	4.819277000
H	14.867021000	3.685480000	5.219380000
C	14.736579000	5.410156000	3.859493000
C	16.088499000	5.197729000	3.365859000
H	16.580045000	4.319413000	3.780804000
C	16.770738000	5.964573000	2.480851000
H	16.278974000	6.854742000	2.080901000
C	18.158013000	5.782930000	2.064783000
C	18.764337000	6.786884000	1.254157000
H	18.142462000	7.605293000	0.861507000
C	20.150375000	6.770789000	1.021699000
H	20.610302000	7.567700000	0.423422000
C	20.949098000	5.746795000	1.575633000
H	22.037632000	5.744751000	1.423187000
C	20.353020000	4.714847000	2.337748000
H	20.973683000	3.916418000	2.766753000

C	18.973169000	4.727365000	2.574546000
H	18.519710000	3.932529000	3.178665000

PP

Ag	10.378336000	1.558740000	3.638258000
Ag	10.182006000	5.511816000	5.538647000
C	6.308235000	2.712560000	4.267423000
H	5.781705000	3.639286000	4.014802000
C	7.654042000	2.596093000	3.914430000
H	8.183753000	3.411383000	3.396497000
N	8.410089000	1.455621000	4.217476000
C	7.744890000	0.399945000	4.848484000
H	8.357017000	-0.501469000	5.018678000
C	6.398444000	0.479406000	5.230954000
H	5.931467000	-0.386677000	5.719589000
C	5.645405000	1.666442000	4.977115000
C	4.263464000	1.889378000	5.385864000
H	3.799449000	2.763401000	4.937624000
C	3.551720000	1.191365000	6.302282000
H	4.040072000	0.349881000	6.798377000
C	2.146141000	1.369334000	6.654510000
C	1.556139000	0.380180000	7.493709000
H	2.199765000	-0.382074000	7.956446000
C	0.164982000	0.320793000	7.662866000
H	-0.252651000	-0.490435000	8.268891000
C	-0.669039000	1.270557000	7.034884000
H	-1.762985000	1.220574000	7.140908000
C	-0.093046000	2.296398000	6.248279000
H	-0.742222000	3.036939000	5.761076000
C	1.295345000	2.352974000	6.061378000
H	1.722856000	3.150034000	5.439024000
C	13.272482000	3.423659000	0.998034000
H	13.198281000	4.212754000	0.238528000
C	12.129569000	3.068102000	1.717897000
H	11.157218000	3.561403000	1.555264000
N	12.131015000	2.059129000	2.693775000
C	13.344951000	1.425566000	2.959245000
H	13.312017000	0.650461000	3.741268000
C	14.518604000	1.761266000	2.271556000
H	15.458259000	1.249875000	2.522651000
C	14.511573000	2.754000000	1.249400000
C	15.745303000	2.977470000	0.503891000
H	16.559514000	2.314188000	0.795777000
C	15.968559000	3.889873000	-0.473537000
H	15.164275000	4.579395000	-0.740319000
C	17.176597000	4.026255000	-1.280389000
C	17.175679000	4.975522000	-2.340370000
H	16.334743000	5.671747000	-2.432951000
C	18.225529000	5.008931000	-3.270642000
H	18.192581000	5.709620000	-4.116537000
C	19.349838000	4.176877000	-3.097482000
H	20.187367000	4.245424000	-3.805953000

C	19.405741000	3.288305000	-1.997958000
H	20.296442000	2.665230000	-1.842082000
C	18.324341000	3.196168000	-1.111613000
H	18.357623000	2.489457000	-0.273513000
C	6.066460000	5.243642000	6.661982000
H	5.143130000	5.760818000	6.376645000
C	7.306295000	5.693833000	6.216828000
H	7.435136000	6.609257000	5.626586000
N	8.479779000	5.001472000	6.502537000
C	8.393010000	3.834529000	7.274864000
H	9.343022000	3.298363000	7.431565000
C	7.187720000	3.399339000	7.817674000
H	7.173620000	2.515482000	8.468611000
C	5.989331000	4.124979000	7.528513000
C	4.712359000	3.851994000	8.136390000
H	3.903719000	4.522744000	7.848335000
C	4.487057000	2.884894000	9.045676000
H	5.297621000	2.206656000	9.318032000
C	3.266937000	2.695989000	9.783892000
C	3.312128000	1.739522000	10.825917000
H	4.215545000	1.125469000	10.957966000
C	2.234564000	1.627859000	11.703155000
H	2.334842000	0.917057000	12.526167000
C	1.089165000	2.433345000	11.527423000
H	0.239626000	2.361722000	12.215080000
C	1.013159000	3.347597000	10.453203000
H	0.105424000	3.947463000	10.310985000
C	2.098946000	3.488810000	9.585813000
H	2.060273000	4.210094000	8.759186000
C	13.873793000	6.501353000	3.427945000
H	14.231245000	7.303530000	2.768972000
C	12.564952000	6.556848000	3.916085000
H	11.866138000	7.375348000	3.676694000
N	12.050551000	5.573161000	4.759906000
C	12.898432000	4.536430000	5.162018000
H	12.462370000	3.788897000	5.843285000
C	14.214949000	4.444931000	4.704747000
H	14.845015000	3.616160000	5.055025000
C	14.726149000	5.413695000	3.788992000
C	16.078170000	5.221543000	3.290404000
H	16.590042000	4.362742000	3.721982000
C	16.736199000	5.977994000	2.380010000
H	16.221501000	6.838539000	1.946883000
C	18.132043000	5.819037000	1.987928000
C	18.742877000	6.843314000	1.208667000
H	18.120480000	7.664568000	0.823122000
C	20.133043000	6.842668000	0.999480000
H	20.596897000	7.655751000	0.426584000
C	20.929659000	5.812394000	1.543696000
H	22.020018000	5.819576000	1.408587000
C	20.329343000	4.761396000	2.274979000
H	20.949503000	3.958073000	2.695199000

| C | 18.946317000 | 4.760090000 | 2.491662000 |
| H | 18.488913000 | 3.948740000 | 3.071359000 |

Coordinates for Fig. 3

S₀-Min (Reactant 1)

Ag	10.465708954	1.433454086	3.800538831
Ag	10.177832086	5.581771359	5.519742261
C	6.341319415	2.662291819	4.289629829
H	5.829279994	3.570754258	4.010721071
C	7.675439449	2.522378736	3.973546237
H	8.206458552	3.315511470	3.457359120
N	8.394523119	1.406427882	4.307814487
C	7.724270496	0.390089825	4.923781901
H	8.309721565	-0.502000314	5.129655902
C	6.388403860	0.478364898	5.268495883
H	5.912238582	-0.362678682	5.752696722
C	5.675849867	1.645600356	4.981944688
C	4.270668086	1.881565376	5.365102804
H	3.826340456	2.738800234	4.892634861
C	3.552064691	1.197025100	6.270161744
H	4.020873855	0.360696135	6.768914106
C	2.128213643	1.384465624	6.607263738
C	1.540643362	0.429242819	7.433418276
H	2.162122961	-0.331414038	7.889049042
C	0.170159500	0.404804715	7.620433273
H	-0.254121626	-0.376888308	8.231811434
C	-0.634593283	1.349589885	7.003730001
H	-1.711852342	1.324711469	7.123987330
C	-0.053510049	2.335348001	6.210273749
H	-0.679700728	3.073377678	5.725075628
C	1.313104569	2.358551577	6.017221581
H	1.745714082	3.124986075	5.389412783
C	13.283282313	3.362468002	1.054174881
H	13.181547246	4.129605063	0.299931680
C	12.180060622	2.991649194	1.787704429
H	11.211606830	3.458292271	1.630478518
N	12.222457774	2.017322391	2.752994244
C	13.422386713	1.427321726	2.999293191
H	13.428402929	0.671599379	3.779136485
C	14.566153858	1.766140091	2.295850142
H	15.501922171	1.277453967	2.529589818
C	14.514724392	2.728819983	1.290967566
C	15.745895585	2.972076610	0.511246888
H	16.558885039	2.317112368	0.781636284
C	15.938690626	3.890881061	-0.452391566
H	15.133338946	4.570381205	-0.694160930
C	17.141101300	4.052691521	-1.293725765
C	17.103258406	5.007378910	-2.305576214
H	16.264524902	5.684247327	-2.361362625
C	18.121064539	5.086122405	-3.239899148
H	18.061031285	5.803988814	-4.048344774
C	19.233148467	4.270183269	-3.122593903

H	20.040775609	4.358305511	-3.839281554
C	19.316839330	3.363121552	-2.070212525
H	20.198621986	2.745954107	-1.959092409
C	18.274750048	3.242566228	-1.173413518
H	18.336242878	2.523279538	-0.369364360
C	6.060361962	5.220758898	6.671567294
H	5.153182408	5.732104901	6.388744015
C	7.287026417	5.662007754	6.222385293
H	7.395038320	6.557868270	5.625667618
N	8.436772419	5.004886199	6.518727040
C	8.364319428	3.877417956	7.295141297
H	9.305983305	3.370930023	7.484974534
C	7.179393617	3.428865936	7.824173975
H	7.179710647	2.565069026	8.472535276
C	5.994300639	4.124618758	7.521789236
C	4.699482890	3.839498781	8.129965134
H	3.903489059	4.506191427	7.840561325
C	4.462695217	2.876088170	9.040806764
H	5.268136995	2.209400979	9.311666351
C	3.236235548	2.685353729	9.780302018
C	3.271209835	1.749035516	10.809297868
H	4.163943184	1.149100676	10.942366631
C	2.203781212	1.629505954	11.669180629
H	2.283080704	0.934234471	12.488200005
C	1.074016102	2.411596087	11.485883420
H	0.230860317	2.330080894	12.157576833
C	1.007436761	3.312957713	10.430765634
H	0.111310746	3.901381150	10.287720081
C	2.083449724	3.458380453	9.586367182
H	2.046754896	4.175504797	8.777254269
C	13.919901964	6.480506049	3.431429842
H	14.271624809	7.258366654	2.769301339
C	12.629680464	6.541653909	3.914235590
H	11.949825814	7.348447491	3.654231747
N	12.121883722	5.593256199	4.750196152
C	12.943906973	4.582089484	5.158819225
H	12.519495600	3.854319544	5.844107911
C	14.246452799	4.478075817	4.715948404
H	14.866362938	3.668775331	5.076034969
C	14.747277366	5.417586656	3.808709937
C	16.117916399	5.217020250	3.308926129
H	16.615919287	4.366910605	3.745435096
C	16.768459074	5.961208169	2.397767897
H	16.263820091	6.814984700	1.968314043
C	18.175851159	5.795634376	1.988028721
C	18.766341742	6.804423434	1.229302838
H	18.155780048	7.624945144	0.871651578
C	20.131434414	6.791269516	0.987442450
H	20.583845560	7.595575489	0.423279430
C	20.913491606	5.762586886	1.488536882
H	21.984636530	5.758753526	1.329321396
C	20.326176352	4.727773685	2.209340463

H	20.936507377	3.923051884	2.598460528
C	18.969540619	4.742610603	2.456216186
H	18.525128252	3.944432841	3.033043512

CI(S$_{ALPP}$/S$_{ALP\Sigma}$)

Ag	10.412527964	1.468352453	3.728830043
Ag	10.122904863	5.627447664	5.449873560
C	6.284737190	2.694783091	4.236816030
H	5.769042954	3.604038094	3.967767875
C	7.617215981	2.558501179	3.908076618
H	8.144848456	3.355669625	3.393269013
N	8.339760418	1.440881798	4.230509406
C	7.674585886	0.420125317	4.844459475
H	8.262820745	-0.472059815	5.041414283
C	6.342372001	0.504616159	5.201789958
H	5.872067626	-0.339362576	5.686492150
C	5.626016398	1.672974632	4.930518285
C	4.225573924	1.900238538	5.338468466
H	3.767551160	2.758643307	4.881087478
C	3.530777594	1.202276099	6.255662552
H	4.017831620	0.364546026	6.733644336
C	2.114762502	1.376615496	6.633275605
C	1.557186575	0.412940064	7.471785849
H	2.196073534	-0.347724857	7.902909464
C	0.192914434	0.378654416	7.699957077
H	-0.208474912	-0.409547646	8.318667518
C	-0.635833844	1.322167830	7.113892057
H	-1.708799191	1.289782897	7.266893445
C	-0.084713716	2.315973436	6.308723578
H	-0.729811220	3.053084492	5.847380555
C	1.275271544	2.348812990	6.073872863
H	1.683704722	3.122044522	5.438328764
C	13.270441668	3.383519023	1.005083383
H	13.182203478	4.148856055	0.247304055
C	12.155296185	3.020139795	1.725611591
H	11.191168681	3.491013607	1.554839526
N	12.180662720	2.048216082	2.694127710
C	13.374605447	1.453679632	2.956859023
H	13.367116901	0.699993654	3.738647509
C	14.529234220	1.785665165	2.268569182
H	15.459510255	1.293526858	2.516564242
C	14.496355803	2.745781887	1.260971604
C	15.743110419	2.979276596	0.502194533
H	16.546038520	2.319637374	0.790692597
C	15.965262150	3.893010592	-0.460554681
H	15.173034648	4.579837517	-0.723760005
C	17.190345900	4.035844597	-1.272676803
C	17.193292359	4.987650033	-2.287607170
H	16.368236393	5.678188301	-2.365795421
C	18.235306287	5.047080253	-3.196309024
H	18.206865285	5.763020758	-4.008185343

C	19.331218664	4.214421444	-3.048457779
H	20.157941961	4.287231376	-3.744686818
C	19.374771116	3.311147811	-1.990576614
H	20.244258285	2.681726526	-1.854318277
C	18.308585535	3.210227354	-1.120098614
H	18.339654061	2.495162933	-0.310516442
C	6.019090529	5.244046190	6.631137888
H	5.106342924	5.752501985	6.361535944
C	7.234178173	5.691351849	6.172242786
H	7.330131026	6.590133371	5.579285602
N	8.396116101	5.037572663	6.455138085
C	8.338643430	3.901968007	7.226610780
H	9.285154571	3.400101755	7.402345200
C	7.167077757	3.441507610	7.764317255
H	7.179710859	2.572850863	8.406087600
C	5.969814231	4.137704793	7.481717553
C	4.707691138	3.836810307	8.107214428
H	3.898202938	4.499773926	7.842850069
C	4.508820121	2.851779058	9.019180295
H	5.322865252	2.188917015	9.263195196
C	3.312864504	2.656807929	9.784184803
C	3.376096121	1.705484234	10.813130699
H	4.270510502	1.102507746	10.918820255
C	2.336980471	1.587677149	11.697313702
H	2.441128067	0.887641383	12.509315447
C	1.198530207	2.379037997	11.549212760
H	0.375810284	2.295371771	12.246550103
C	1.098065107	3.288362444	10.497437946
H	0.198266178	3.877812251	10.383898046
C	2.145236068	3.437712425	9.622289692
H	2.084929209	4.157408380	8.817022733
C	13.882838019	6.504736758	3.382803268
H	14.245535471	7.279598039	2.723151129
C	12.586686135	6.571643072	3.849936247
H	11.912818332	7.380686980	3.581472875
N	12.067394235	5.628107707	4.684216290
C	12.880667328	4.615188373	5.104193745
H	12.446067759	3.891349896	5.787129651
C	14.187169866	4.505060533	4.677306945
H	14.799808686	3.694773275	5.047331406
C	14.702090921	5.440674342	3.774696053
C	16.079434946	5.232204468	3.297974446
H	16.565615062	4.381357853	3.746071077
C	16.751023848	5.969303999	2.396192447
H	16.260835690	6.824750561	1.953798123
C	18.165522995	5.791380214	2.017925166
C	18.780619526	6.792212775	1.268590158
H	18.184979678	7.616400254	0.894564731
C	20.150461882	6.766511800	1.056767887
H	20.621858161	7.564815474	0.499676284
C	20.912449392	5.732955765	1.578420198
H	21.986670423	5.719215148	1.442463789

C	20.300683343	4.705937884	2.289999797
H	20.895291190	3.897396218	2.695144360
C	18.939411860	4.733769776	2.507836892
H	18.475527410	3.941752622	3.077798059

STC(S$_{ALP\Sigma}$/T$_{BLPP}$)

Ag	10.462153995	1.437709433	3.795970799
Ag	10.176305039	5.541658454	5.551502103
C	6.333089597	2.653032561	4.268553991
H	5.823584671	3.562293592	3.986869613
C	7.670653040	2.514782021	3.959681226
H	8.206247040	3.309083501	3.448782220
N	8.388570510	1.400600111	4.296922331
C	7.718552948	0.382416649	4.907987622
H	8.306222222	-0.507602973	5.116632739
C	6.379894161	0.466951990	5.246019518
H	5.904591812	-0.376068745	5.727930486
C	5.666055431	1.633458511	4.957220484
C	4.259194909	1.868138567	5.342101215
H	3.813074792	2.723355752	4.864720925
C	3.541449274	1.185477484	6.249751695
H	4.013921159	0.347469794	6.743959271
C	2.119320793	1.374648084	6.598545702
C	1.537045390	0.430318133	7.443513496
H	2.159493993	-0.330872790	7.898026905
C	0.168282906	0.412810188	7.645908183
H	-0.253044062	-0.361294322	8.269469222
C	-0.641150186	1.352572762	7.026874256
H	-1.717479105	1.331460405	7.158140006
C	-0.066292738	2.327608546	6.215232087
H	-0.696368457	3.061208225	5.727557998
C	1.298171267	2.345205499	6.007197588
H	1.724767268	3.103673631	5.365376759
C	13.277991546	3.379413904	1.064649305
H	13.174760230	4.151860485	0.316160699
C	12.176875187	3.004187546	1.798771325
H	11.208553530	3.472715849	1.646990060
N	12.220673600	2.023688563	2.757806095
C	13.420414945	1.431059818	2.998495763
H	13.427095491	0.670704752	3.773999883
C	14.562320022	1.774017720	2.294145964
H	15.498635081	1.283773830	2.522284468
C	14.509391978	2.742617968	1.294613650
C	15.738799900	2.985465519	0.513928165
H	16.550058045	2.327690939	0.782437427
C	15.935827248	3.901660455	-0.445876770
H	15.134490171	4.585806822	-0.688175406
C	17.139047987	4.054996982	-1.285629760
C	17.111088907	5.007572022	-2.299561326
H	16.278775646	5.690782931	-2.356314051
C	18.129667691	5.075230704	-3.233734312

H	18.076560097	5.791947016	-4.043509597
C	19.234219627	4.249345867	-3.114752861
H	20.042537399	4.328258753	-3.831860536
C	19.309746874	3.344644106	-2.059613581
H	20.186050375	2.720071540	-1.946597439
C	18.266248286	3.236252265	-1.162715274
H	18.319684552	2.520128335	-0.355371516
C	6.036917399	5.222325903	6.638677923
H	5.133650391	5.738991402	6.344076640
C	7.273787355	5.655624871	6.206360536
H	7.398232751	6.552149134	5.612669384
N	8.413388288	4.982032288	6.520135922
C	8.336812530	3.855081019	7.292549546
H	9.275464806	3.351054501	7.489463015
C	7.148566608	3.409249309	7.812674742
H	7.145496692	2.544539472	8.462276910
C	5.967927503	4.118003524	7.494516605
C	4.694629790	3.836839015	8.091323288
H	3.892730705	4.503266316	7.806383671
C	4.472264160	2.850242402	9.021886561
H	5.279951893	2.181638727	9.286791951
C	3.284760297	2.684078565	9.749827283
C	3.325451953	1.731431742	10.808866853
H	4.214569302	1.118709851	10.936895362
C	2.277990294	1.648851441	11.677712078
H	2.355230302	0.967593890	12.509036888
C	1.146730263	2.461528490	11.490763228
H	0.312989493	2.398956186	12.184659225
C	1.058089867	3.361975100	10.416574953
H	0.162974612	3.956261768	10.287650812
C	2.111157461	3.488039356	9.552761675
H	2.067443287	4.196203385	8.732580543
C	13.916720974	6.480287816	3.465830374
H	14.262541852	7.264664498	2.808489967
C	12.629178010	6.533514687	3.956912312
H	11.946020553	7.340216298	3.705843388
N	12.126000456	5.576241351	4.785446533
C	12.951238406	4.565619758	5.182655591
H	12.530584086	3.832410817	5.864385296
C	14.252221519	4.469597572	4.732449468
H	14.873778458	3.658597914	5.084612070
C	14.748207554	5.415774542	3.829719591
C	16.116252083	5.220150392	3.320272901
H	16.617072787	4.368313750	3.750332494
C	16.760956452	5.965965737	2.412067949
H	16.253090070	6.819758673	1.986864536
C	18.165488546	5.804951494	1.994803925
C	18.750179081	6.816580752	1.234708018
H	18.135880867	7.636416437	0.881741274
C	20.113854723	6.806417585	0.985531247
H	20.562060338	7.612395758	0.420349958
C	20.900019812	5.778043095	1.481001736

H	21.970061242	5.776060321	1.316541903
C	20.318572339	4.740815422	2.202956971
H	20.932552359	3.936616242	2.587258338
C	18.963378297	4.752365599	2.456848865
H	18.522259053	3.952483416	3.034034900

CI(T$_{BLPP}$/T$_{ALPP}$)

Ag	10.454490820	1.448870110	3.785460291
Ag	10.169720804	5.556990412	5.541320415
C	6.326440485	2.669090207	4.262090329
H	5.816630436	3.579370274	3.984430307
C	7.662910595	2.530460193	3.951020304
H	8.197980656	3.325800258	3.441300262
N	8.380670635	1.414330107	4.284950331
C	7.710510618	0.394960028	4.894490379
H	8.297850638	-0.495880035	5.100420393
C	6.372870497	0.479200035	5.234670402
H	5.897740449	-0.364460030	5.715560439
C	5.659280427	1.647560127	4.949420380
C	4.257390330	1.880330144	5.337180396
H	3.809770291	2.736900213	4.864070376
C	3.534600270	1.183780090	6.257530495
H	4.008120307	0.345630025	6.748380494
C	2.116440163	1.371510106	6.606820500
C	1.534100117	0.424570035	7.450400579
H	2.157100164	-0.337070027	7.902890626
C	0.165920013	0.406870030	7.653370588
H	-0.254890017	-0.368650029	8.275440617
C	-0.644090052	1.348470104	7.037140559
H	-1.720230134	1.327110102	7.169360575
C	-0.069890006	2.325680181	6.227620497
H	-0.700360056	3.060610234	5.742570439
C	1.294320100	2.344130179	6.018480440
H	1.720180132	3.104430238	5.378510409
C	13.277151001	3.384140261	1.054680082
H	13.176461006	4.155210320	0.304380023
C	12.173910947	3.011960234	1.787580136
H	11.206470847	3.481480267	1.633210126
N	12.214740941	2.033100155	2.748440214
C	13.413301057	1.439550113	2.992450230
H	13.417591044	0.680560054	3.769270287
C	14.557141123	1.780040138	2.290220178
H	15.492451169	1.289310098	2.521430196
C	14.507511124	2.746600212	1.288790097
C	15.740091198	2.985800229	0.511510037
H	16.549261263	2.327450179	0.784890063
C	15.943161221	3.899320301	-0.450500033
H	15.144541152	4.584480354	-0.698710055
C	17.151201336	4.046530310	-1.284950101
C	17.131371318	4.995770385	-2.302160179
H	16.301601230	5.681550428	-2.365630180

C	18.155031421	5.057070389	-3.231270246
H	18.108261413	5.771110450	-4.043830310
C	19.256471478	4.228320327	-3.103700238
H	20.068791523	4.302340334	-3.816770296
C	19.323801504	3.327110257	-2.045080156
H	20.197661529	2.700390205	-1.925230146
C	18.275301398	3.224900248	-1.153360087
H	18.322741397	2.511510192	-0.343210028
C	6.034520438	5.228380400	6.644060502
H	5.130050393	5.744940465	6.354340509
C	7.268890560	5.664620461	6.208660499
H	7.389580545	6.563130515	5.617330430
N	8.411090653	4.992800383	6.515550495
C	8.336370667	3.863420297	7.285290557
H	9.276050711	3.358970257	7.478330554
C	7.149880555	3.414640265	7.806920574
H	7.149000533	2.548000196	8.453450657
C	5.967020440	4.121400318	7.495580569
C	4.693570361	3.835740295	8.095760598
H	3.890100297	4.500880345	7.815270621
C	4.474440343	2.850680222	9.022960685
H	5.285280406	2.184270167	9.284070710
C	3.286500253	2.677050208	9.757410763
C	3.333960256	1.722960133	10.809470856
H	4.226180324	1.114420087	10.931270843
C	2.288110174	1.628380124	11.681070924
H	2.371270183	0.941940070	12.507470947
C	1.153140087	2.433380187	11.502660879
H	0.321310023	2.361940179	12.196910949
C	1.059920079	3.337510257	10.434710809
H	0.161740015	3.927850305	10.309890808
C	2.111650162	3.473200268	9.569000749
H	2.062770160	4.184580324	8.752400665
C	13.910381060	6.488770475	3.452250268
H	14.257411108	7.271850566	2.793990214
C	12.622130957	6.543690500	3.941820304
H	11.939760916	7.350580552	3.689080286
N	12.117970933	5.588260448	4.772090369
C	12.942541007	4.577670351	5.171290398
H	12.521120968	3.845670295	5.853800428
C	14.243861101	4.480280343	4.722990362
H	14.864741169	3.669710282	5.077410391
C	14.741311157	5.424810402	3.819510296
C	16.110451242	5.227090403	3.313660254
H	16.609471262	4.375990334	3.747220286
C	16.758911287	5.970280437	2.405040184
H	16.253661264	6.823550545	1.975690154
C	18.165131404	5.805890466	1.994150153
C	18.754741436	6.814190511	1.233580093
H	18.143421378	7.633990582	0.875380066
C	20.119491572	6.800950549	0.990470074
H	20.571531606	7.604450585	0.424810033

C	20.901761599	5.772770426	1.492510114
H	21.972531706	5.768490440	1.332770103
C	20.315371558	4.738730363	2.215030171
H	20.926261606	3.934650301	2.604460202
C	18.959121437	4.753430367	2.462980188
H	18.514191429	3.956020304	3.040660236

[A···B]_{CT} complex-1

Ag	10.465874428	1.416986323	3.822730800
Ag	10.153078762	5.611432538	5.506913152
C	6.341422922	2.669567398	4.271524585
H	5.834464026	3.580100888	3.989704833
C	7.678236256	2.526660044	3.965941711
H	8.218690537	3.318608480	3.455564949
N	8.389721153	1.406782547	4.301234316
C	7.711726720	0.390653099	4.908933785
H	8.292289779	-0.504488425	5.115087372
C	6.374949158	0.483415194	5.246665411
H	5.892696120	-0.356387895	5.726607384
C	5.667831561	1.653187525	4.957843590
C	4.261406013	1.888158363	5.340774409
H	3.816557005	2.747365291	4.873264000
C	3.546705253	1.195789952	6.246812486
H	4.016625011	0.352911598	6.730818371
C	2.124141513	1.388394765	6.598013085
C	1.540364263	0.438096334	7.432243926
H	2.160182272	-0.332368699	7.873522558
C	0.172295739	0.426552420	7.640560318
H	-0.249912768	-0.352429528	8.257047527
C	-0.632832462	1.380527132	7.038834508
H	-1.708086976	1.366790532	7.176816577
C	-0.054181877	2.361035027	6.237695714
H	-0.680134944	3.106514344	5.763616665
C	1.309415219	2.370035988	6.021287673
H	1.738659837	3.134135089	5.388459153
C	13.275544577	3.352440242	1.056541685
H	13.174106537	4.114996389	0.297612723
C	12.171297447	2.982921055	1.789626814
H	11.201734076	3.445886980	1.627814254
N	12.214669555	2.013782439	2.759915428
C	13.415135079	1.428277150	3.011417165
H	13.422422009	0.676492305	3.794684390
C	14.559321810	1.764361913	2.308176898
H	15.494895438	1.276676976	2.545185159
C	14.507305221	2.722116646	1.299410647
C	15.739719187	2.964265525	0.521610073
H	16.554036929	2.313440079	0.797144199
C	15.931652992	3.880688541	-0.446381735
H	15.125601475	4.556956025	-0.693449838
C	17.138863674	4.040122243	-1.281418044
C	17.108283685	4.993809545	-2.293674991

H	16.271150890	5.671022817	-2.356905497
C	18.133510735	5.072198587	-3.219485903
H	18.078301831	5.788380096	-4.029868735
C	19.246070499	4.258561664	-3.091001540
H	20.060702255	4.347770428	-3.799251507
C	19.321426556	3.352600641	-2.037436895
H	20.203456179	2.737600748	-1.917073508
C	18.271009717	3.230859705	-1.150407727
H	18.327483513	2.513588456	-0.344314636
C	6.044719588	5.233345734	6.647414057
H	5.138259265	5.741510074	6.357185630
C	7.268456582	5.667963750	6.213479399
H	7.382499148	6.560551464	5.614149281
N	8.427393811	5.014503382	6.514384241
C	8.343110956	3.881952984	7.289085605
H	9.283344361	3.372535451	7.481555996
C	7.161722483	3.431186658	7.810542634
H	7.154802433	2.565116048	8.455914930
C	5.963867285	4.130432733	7.509801996
C	4.714044911	3.840341083	8.096690892
H	3.904909857	4.495764249	7.826348629
C	4.481300877	2.780796243	9.066194625
H	5.283962141	2.107215403	9.311397423
C	3.327702846	2.642708398	9.763890433
C	3.304860502	1.660958726	10.830517929
H	4.172436564	1.026365384	10.956339874
C	2.257267575	1.596114907	11.663451756
H	2.306766556	0.898151489	12.481907876
C	1.124505993	2.438653925	11.479188534
H	0.279900868	2.377152485	12.150240849
C	1.088202233	3.352968371	10.411552373
H	0.207068501	3.965106325	10.269002447
C	2.146544523	3.472438449	9.572372243
H	2.122891681	4.182745376	8.759484391
C	13.902695237	6.481185036	3.418804324
H	14.253819105	7.255731563	2.752687533
C	12.611129203	6.541748367	3.899090029
H	11.930583554	7.346205791	3.633907493
N	12.103586942	5.599854351	4.742383697
C	12.927554549	4.591771173	5.156655202
H	12.506019837	3.866514777	5.846127040
C	14.230696547	4.486458868	4.714804804
H	14.853516049	3.680805472	5.079097741
C	14.731079357	5.422640087	3.802897972
C	16.104167104	5.224483179	3.306199406
H	16.606548034	4.379320595	3.746539606
C	16.753581520	5.968678352	2.391319470
H	16.247256632	6.820099939	1.960058703
C	18.164439293	5.806248983	1.987793174
C	18.754358999	6.813777912	1.227481394
H	18.143227064	7.631838154	0.865316935
C	20.120036360	6.802448068	0.988327785

H	20.571556265	7.605864177	0.422123700
C	20.903276316	5.776760634	1.493572834
H	21.974557026	5.774341077	1.334704595
C	20.316146167	4.743687389	2.217440134
H	20.926553394	3.940758800	2.610164548
C	18.959118050	4.757335844	2.462433421
H	18.515199617	3.960006152	3.040700940

Transition-1

Ag	10.245380768	1.489290112	3.595670278
Ag	10.177570778	5.779630468	5.479110444
C	6.228230480	2.787210216	4.430820341
H	5.718620459	3.702170284	4.172600323
C	7.489810579	2.563930199	3.917890300
H	7.964860615	3.297400251	3.272370252
N	8.211290628	1.434280111	4.210360326
C	7.601090574	0.487870038	4.981260382
H	8.175900630	-0.418610034	5.155830395
C	6.339750510	0.665520053	5.528810401
H	5.927170430	-0.118150008	6.149330469
C	5.639700446	1.852910142	5.295200394
C	4.339290336	2.191590170	5.923600441
H	3.820270295	2.946820229	5.353240396
C	3.461610265	1.159290089	6.455260484
H	3.921140300	0.276510020	6.864820550
C	2.028370157	1.292880097	6.673850535
C	1.403190106	0.288330024	7.423240557
H	2.011330152	-0.482230035	7.880970622
C	0.029360003	0.243680016	7.535300560
H	-0.413420033	-0.579240047	8.074420626
C	-0.756300061	1.224620095	6.941210514
H	-1.837490139	1.189340091	7.017740551
C	-0.145490014	2.253950174	6.229590465
H	-0.753650058	3.017370230	5.759700436
C	1.230720096	2.294030175	6.096450475
H	1.683850129	3.095790239	5.528880411
C	13.227271018	3.432250262	1.055820083
H	13.175041011	4.243170327	0.343110024
C	12.089480929	3.068620237	1.741140133
H	11.146210841	3.584910273	1.584480119
N	12.062820926	2.036750155	2.648750205
C	13.233680995	1.383950105	2.891870220
H	13.191901022	0.582160047	3.623470276
C	14.410041119	1.718550134	2.239980175
H	15.320281181	1.182410092	2.470130193
C	14.426391109	2.733880209	1.286380097
C	15.685561229	2.962960230	0.545250040
H	16.476701272	2.277580176	0.807010063
C	15.912741203	3.909640300	-0.403290030
H	15.122221144	4.608940356	-0.634090047
C	17.118731338	4.064740315	-1.240320096

C	17.085681308	5.027100388	-2.247360171
H	16.250831224	5.711540438	-2.296810176
C	18.102831366	5.100820393	-3.185400247
H	18.044091369	5.819500428	-3.993620306
C	19.210771466	4.275030327	-3.073240234
H	20.019161523	4.361030334	-3.790660293
C	19.288821459	3.360740260	-2.024940157
H	20.166751545	2.736300210	-1.917640146
C	18.244931386	3.241980248	-1.126890085
H	18.300491399	2.515490192	-0.327650026
C	6.080050478	5.203440398	6.611340520
H	5.153130395	5.680850433	6.326140495
C	7.293560539	5.772100435	6.271410496
H	7.370730563	6.709690493	5.736070449
N	8.478340668	5.174540399	6.562490528
C	8.453270631	3.991310309	7.258760573
H	9.420120699	3.541620272	7.467520575
C	7.277100534	3.395720263	7.652460615
H	7.307210560	2.470010191	8.209080625
C	6.056000483	3.997430308	7.299750537
C	4.749110365	3.389760261	7.598850567
H	3.947120305	4.096710315	7.449610571
C	4.602810356	2.589550199	8.813680661
H	5.399980400	1.917070148	9.083930688
C	3.447270265	2.591830202	9.688190727
C	3.468030264	1.716240132	10.781650844
H	4.325270335	1.069380081	10.922100836
C	2.414700188	1.685250131	11.671000893
H	2.463600188	1.014190079	12.516010968
C	1.310790101	2.508640194	11.477990900
H	0.474840038	2.472380191	12.164840955
C	1.275010099	3.377960259	10.393450806
H	0.411560033	4.013230307	10.240300772
C	2.333860177	3.428120261	9.507710752
H	2.296880175	4.112270317	8.670890647
C	13.965831057	6.534100486	3.375850260
H	14.358881110	7.312360566	2.736620209
C	12.665000981	6.629820501	3.829360295
H	12.020100923	7.464470556	3.565880276
N	12.105550931	5.690780444	4.645900360
C	12.887610980	4.643470357	5.051770388
H	12.426660977	3.916830300	5.715700459
C	14.195851072	4.499600345	4.632920356
H	14.777791155	3.659350282	4.989260383
C	14.752921148	5.440660425	3.756500288
C	16.136181216	5.213660403	3.298130252
H	16.609291289	4.359770337	3.755080288
C	16.829191318	5.945570452	2.405720182
H	16.348641277	6.802130509	1.955310152
C	18.250331428	5.766380452	2.045320159
C	18.867171439	6.757520496	1.281140099
H	18.271451421	7.574320609	0.890190070

C	20.238331552	6.730420536	1.070670082
H	20.707951595	7.520190592	0.498980040
C	21.003261605	5.705280430	1.609110124
H	22.077901692	5.690350434	1.468890113
C	20.391261555	4.690270359	2.340980177
H	20.986461603	3.888730300	2.760860210
C	19.027401442	4.718900361	2.556160194
H	18.563961448	3.932110303	3.135100240

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Ag	10.251800799	1.490890117	3.603090279
Ag	10.177370802	5.788410471	5.491090435
C	6.234880491	2.789900214	4.434870341
H	5.726640458	3.705800287	4.177450322
C	7.496860595	2.566410199	3.923680303
H	7.973660621	3.300650252	3.280350250
N	8.216720622	1.435660110	4.214970323
C	7.604390577	0.488280039	4.983100384
H	8.178020620	-0.419090035	5.156770399
C	6.342120483	0.666060052	5.528850406
H	5.927620442	-0.118420010	6.147000449
C	5.643730448	1.854630143	5.296180431
C	4.381060339	2.308040180	6.081720455
H	3.844940295	3.007960230	5.431580431
C	3.481110267	1.219010091	6.529080499
H	3.938210304	0.334780028	6.938180551
C	2.047500158	1.354310104	6.744110510
C	1.418780107	0.349070026	7.489490585
H	2.024500157	-0.423320034	7.947310611
C	0.044600006	0.306000025	7.597310608
H	-0.400850030	-0.517520040	8.133270640
C	-0.737930059	1.289200098	7.002960524
H	-1.819380138	1.255230099	7.076130551
C	-0.123650011	2.319160178	6.295390481
H	-0.729390054	3.084330239	5.825280473
C	1.252950097	2.357620182	6.166360451
H	1.708830132	3.159820242	5.601650432
C	13.230050997	3.432050265	1.057730079
H	13.175781013	4.239470324	0.341250025
C	12.093130929	3.068270233	1.744170134
H	11.148430845	3.581030277	1.584650123
N	12.068850954	2.040330155	2.656210202
C	13.241401003	1.392010109	2.902850224
H	13.201481035	0.593220047	3.637820277
C	14.417121088	1.727070131	2.249990171
H	15.328731189	1.194450092	2.482780191
C	14.430941134	2.738050210	1.291740101
C	15.689471214	2.966640229	0.549450040
H	16.482091260	2.284190177	0.814310064
C	15.914531250	3.908790303	-0.403600032
H	15.122681157	4.605450352	-0.637800050

C	17.120011311	4.061330313	-1.241780096
C	17.085471330	5.018420383	-2.253700174
H	16.249981260	5.701740446	-2.306230176
C	18.101971400	5.088360391	-3.192610244
H	18.042021386	5.802770437	-4.004520309
C	19.210861479	4.264460328	-3.076720236
H	20.018761518	4.347630334	-3.794990291
C	19.290481488	3.355810259	-2.023730156
H	20.169141574	2.732920212	-1.913640148
C	18.247161392	3.240520248	-1.124640087
H	18.303821405	2.518200193	-0.321770026
C	6.079710482	5.207510401	6.620280493
H	5.152700396	5.685180426	6.335910482
C	7.293230544	5.778060452	6.283240465
H	7.370350561	6.717270534	5.750820418
N	8.478170643	5.180110397	6.572960511
C	8.453190672	3.994690307	7.265160549
H	9.420130700	3.544750271	7.472950568
C	7.277270558	3.397280261	7.656100613
H	7.307580561	2.469640190	8.209450626
C	6.056070440	3.999160310	7.304470586
C	4.711000364	3.274980250	7.440460567
H	3.927980302	4.038440312	7.371970584
C	4.583980351	2.528550197	8.733130676
H	5.381600434	1.856260141	9.002550689
C	3.427180263	2.526880193	9.605910756
C	3.447380265	1.648210126	10.696780815
H	4.305230329	1.002100078	10.836740842
C	2.392650182	1.613230124	11.584230906
H	2.441110186	0.939840072	12.427310966
C	1.287960098	2.435580189	11.391810892
H	0.450970038	2.396150187	12.077170943
C	1.252750094	3.307950252	10.309810797
H	0.388680028	3.942440304	10.157090772
C	2.312960179	3.362130260	9.426020708
H	2.276360174	4.048600314	8.591110668
C	13.965621079	6.541300524	3.387110263
H	14.359111090	7.319570553	2.748200211
C	12.665470997	6.638520492	3.842140296
H	12.021450907	7.474290551	3.580130273
N	12.105380906	5.699150440	4.657750358
C	12.886260996	4.650240359	5.061560389
H	12.424710959	3.923270302	5.724710442
C	14.193801092	4.504930345	4.641330358
H	14.774701131	3.663170281	4.995730385
C	14.751271120	5.446030410	3.765360292
C	16.133101246	5.216790402	3.303910254
H	16.605761253	4.361800335	3.759250290
C	16.824831268	5.947660438	2.409690187
H	16.344371240	6.804960549	1.960600152
C	18.244491428	5.766040456	2.044910158
C	18.860421466	6.755950533	1.278550099

H	18.264801410	7.573690570	0.889450069
C	20.230741563	6.726440540	1.063520083
H	20.699791576	7.515300570	0.490150041
C	20.995641611	5.700120422	1.599560120
H	22.069721723	5.683320420	1.455760114
C	20.384391564	4.686320363	2.333610178
H	20.979591613	3.883840300	2.751620209
C	19.021371467	4.717330361	2.553310199
H	18.558481448	3.931480302	3.133880243

Reactant2

Ag	10.291867243	1.561653186	3.622903051
Ag	10.181832825	5.604017653	5.684439577
C	6.268132772	2.777514344	4.432280341
H	5.750886248	3.685692779	4.167139065
C	7.533586184	2.573459401	3.925162259
H	8.005225832	3.307496477	3.277071267
N	8.277317026	1.460406073	4.232045560
C	7.672563582	0.515959375	5.011669394
H	8.263475496	-0.378217532	5.195134432
C	6.406958349	0.686396916	5.564553572
H	6.009430081	-0.090229621	6.204521063
C	5.689918626	1.854987851	5.316685732
C	4.396376200	2.277693425	5.993389819
H	3.772706537	2.727471618	5.229773766
C	3.640185731	1.347269686	6.965273844
H	3.983900388	0.309190371	6.931508684
C	2.120374760	1.333390844	6.884230295
C	1.470186020	0.299020706	7.553367835
H	2.059278569	-0.466374572	8.042747569
C	0.090186864	0.222891542	7.567156237
H	-0.377765403	-0.616076435	8.061559132
C	-0.670852461	1.197280057	6.938052701
H	-1.754731204	1.146130531	6.945874312
C	-0.031665956	2.241238950	6.284678134
H	-0.618082715	3.002798170	5.786008642
C	1.353828611	2.315954263	6.262795861
H	1.824718520	3.151193234	5.761222138
C	13.254322664	3.421391953	1.038516368
H	13.198575217	4.207756187	0.301527647
C	12.119803315	3.077462603	1.736501313
H	11.173324348	3.582787452	1.570098278
N	12.092614452	2.081475131	2.682818890
C	13.272622037	1.446200622	2.942379299
H	13.231394526	0.675121043	3.704319146
C	14.443353674	1.763453331	2.277817295
H	15.357271994	1.243173965	2.527237387
C	14.459967247	2.744916026	1.286993688
C	15.714128704	2.959478085	0.550433299
H	16.510390230	2.297240656	0.848402371
C	15.954470215	3.857460978	-0.420410247

H	15.164297614	4.540751755	-0.693511386
C	17.176902840	3.988704963	-1.223837897
C	17.178472962	4.907898630	-2.266711055
H	16.341309315	5.580016608	-2.372008967
C	18.226780553	4.952811443	-3.173733947
H	18.193888483	5.636958673	-4.010009057
C	19.338151680	4.144746830	-2.995503784
H	20.169840141	4.213310341	-3.688661849
C	19.385466476	3.272881924	-1.909700862
H	20.263822973	2.663531666	-1.749112993
C	18.309573880	3.181464094	-1.043725938
H	18.339997232	2.491851791	-0.215006955
C	6.041234110	5.202720479	6.583904585
H	5.148602342	5.685165662	6.209215924
C	7.287311538	5.750709873	6.336771136
H	7.430315181	6.677929645	5.793498987
N	8.437726420	5.118903068	6.704856882
C	8.327316021	3.954501327	7.422802610
H	9.267684154	3.481533730	7.691803356
C	7.109498563	3.385921175	7.726250731
H	7.077767084	2.462171944	8.286443905
C	5.937381011	3.986333958	7.246799156
C	4.611478533	3.285395633	7.220094015
H	3.824807223	4.029086490	7.166252188
C	4.234736162	2.164683750	8.197446558
H	5.124478696	1.650476365	8.570985263
C	3.341100206	2.473547799	9.383789823
C	3.438923812	1.659345137	10.509285166
H	4.222407025	0.913114859	10.556322832
C	2.540500093	1.795416526	11.554741075
H	2.628053686	1.153726394	12.420482357
C	1.533034428	2.746621940	11.487476243
H	0.808964146	2.835047310	12.288155712
C	1.444012522	3.578632845	10.382031426
H	0.656111652	4.319133736	10.326400715
C	2.339674306	3.443195082	9.334593114
H	2.245214553	4.087726939	8.472269258
C	13.833085198	6.490524856	3.446390376
H	14.167945491	7.272435413	2.778590490
C	12.550710285	6.541157329	3.951949926
H	11.859829539	7.342914414	3.707664689
N	12.059395827	5.593633185	4.806711547
C	12.904788867	4.588549272	5.193570279
H	12.497204115	3.858562376	5.887263798
C	14.196268751	4.493505816	4.720437748
H	14.825442720	3.684550153	5.064092910
C	14.682554491	5.437146582	3.805002208
C	16.044528722	5.249815508	3.294298754
H	16.555172808	4.405133289	3.725734515
C	16.697049673	6.002262745	2.385461859
H	16.185466139	6.852275080	1.957644967
C	18.101021210	5.849229342	1.979491150

C	18.685420486	6.852240790	1.200650943
H	18.065457641	7.657234958	0.825967786
C	20.055478270	6.854551442	0.963150600
H	20.501313701	7.653024612	0.384110471
C	20.848176528	5.849352269	1.483939972
H	21.920673817	5.858238849	1.326427659
C	20.269948835	4.817313412	2.222553034
H	20.890408842	4.028241383	2.625610141
C	18.914801414	4.813985236	2.465077836
H	18.479711615	4.014551166	3.048703174

CI(S$_{BRPP}$/S$_{BRP\Sigma}$)

Ag	10.255743117	1.634975572	3.536944457
Ag	10.183683992	5.603898165	5.707054020
C	6.228919468	2.801137790	4.420789120
H	5.699917747	3.707136512	4.173706007
C	7.486299646	2.612738079	3.890464662
H	7.939704852	3.357011799	3.242404675
N	8.241588460	1.503426199	4.173255735
C	7.658605421	0.545815555	4.951257561
H	8.258719092	-0.345608106	5.116037197
C	6.401482793	0.698697778	5.527811102
H	6.021577821	-0.088028413	6.165128738
C	5.673295898	1.864731613	5.304218474
C	4.386587378	2.281283295	5.999234158
H	3.757379034	2.735490881	5.243202962
C	3.636032828	1.343903325	6.972285389
H	3.976360137	0.308853518	6.930981729
C	2.117722249	1.335058075	6.901300442
C	1.469887749	0.296426664	7.565075935
H	2.059622556	-0.473889202	8.045609677
C	0.090331070	0.222936581	7.584666871
H	-0.377325165	-0.618221910	8.074975098
C	-0.671309025	1.204011462	6.966247106
H	-1.754324759	1.155355715	6.978379236
C	-0.034096832	2.251809927	6.318309835
H	-0.621344088	3.018158100	5.828237991
C	1.350646911	2.323797178	6.290859242
H	1.820329064	3.161467629	5.793492319
C	13.216221109	3.508074012	0.945404096
H	13.158623340	4.291505165	0.203976980
C	12.081517129	3.158818202	1.640302758
H	11.133188265	3.656260808	1.466047722
N	12.059891189	2.166042053	2.590846652
C	13.238651662	1.533723226	2.862504068
H	13.196085862	0.764838087	3.627914820
C	14.412542487	1.852660206	2.206062342
H	15.327315481	1.335870224	2.464767759
C	14.426176633	2.836185432	1.209079350
C	15.672893149	3.053634408	0.489020787
H	16.468676246	2.398896034	0.806428122

C	15.926935430	3.959449489	-0.513989555
H	15.147902486	4.642734049	-0.820323306
C	17.138478222	4.046137808	-1.259572946
C	17.212356816	4.951262515	-2.356902793
H	16.401636580	5.641352061	-2.517464595
C	18.273859813	4.926809075	-3.205822054
H	18.291532587	5.582416638	-4.069515716
C	19.390863713	4.071376203	-2.961219369
H	20.243587023	4.099525099	-3.631678466
C	19.386334591	3.227875410	-1.837835470
H	20.243547441	2.602482005	-1.627724982
C	18.275726909	3.194906149	-1.003545838
H	18.255280505	2.537348007	-0.148841082
C	6.039778872	5.197794251	6.606528182
H	5.148691249	5.687046357	6.238400155
C	7.286621967	5.744737843	6.365197956
H	7.429989207	6.677111431	5.832424524
N	8.434188605	5.107998683	6.726668775
C	8.324223509	3.936184561	7.430455836
H	9.262941350	3.458697689	7.695529928
C	7.107122028	3.365847122	7.726747681
H	7.074760669	2.436059772	8.276200198
C	5.935959111	3.974810753	7.255414056
C	4.610168581	3.274190193	7.227229653
H	3.823605355	4.018177808	7.185124501
C	4.238459130	2.146522530	8.199219407
H	5.126841891	1.627941420	8.560074846
C	3.354530794	2.449358483	9.391882689
C	3.454250034	1.629984807	10.513401848
H	4.232422715	0.878385179	10.553449294
C	2.563339780	1.768704468	11.565103476
H	2.650730196	1.124059003	12.428724186
C	1.562795356	2.727492156	11.507036275
H	0.845187445	2.819217967	12.311674042
C	1.472218860	3.564052942	10.405425188
H	0.689975080	4.310671346	10.357390499
C	2.359553219	3.425735376	9.352719869
H	2.264225171	4.074633633	8.494038764
C	13.854949690	6.453777994	3.480494902
H	14.195874408	7.230545689	2.810441049
C	12.571242997	6.514810440	3.981426368
H	11.886702483	7.319919440	3.729806852
N	12.073024681	5.574549942	4.836406159
C	12.908179941	4.565421417	5.230988021
H	12.494097791	3.839949217	5.925294020
C	14.202263747	4.459484735	4.764224096
H	14.824786963	3.647372318	5.113647406
C	14.695151132	5.396986950	3.847606507
C	16.061092552	5.201625865	3.338405847
H	16.570078143	4.358573952	3.775989769
C	16.711765087	5.949910393	2.425022362
H	16.199301425	6.797563497	1.993414486

C	18.119096211	5.796859103	2.018562582
C	18.699592012	6.796245846	1.234311156
H	18.078955154	7.599466741	0.856409093
C	20.077569885	6.797261390	0.995155415
H	20.521695597	7.593383690	0.412470324
C	20.867217278	5.799769155	1.518861638
H	21.938906778	5.808462267	1.361296085
C	20.289050916	4.766280034	2.267539271
H	20.912275504	3.980600201	2.674376307
C	18.940385493	4.761217565	2.511291869
H	18.509141913	3.964547583	3.100191771

STC(S$_{BRP\Sigma}$/T$_{ARPP}$)

Ag	10.252430785	1.690270129	3.515250269
Ag	10.153260799	5.624020448	5.664600458
C	6.214530504	2.808290214	4.415980338
H	5.669780415	3.704190286	4.164920320
C	7.472780596	2.637060203	3.881910300
H	7.911610620	3.384450258	3.226940248
N	8.247650609	1.541300118	4.167420323
C	7.682740613	0.579710046	4.955460382
H	8.297560649	-0.301340021	5.122380392
C	6.425850506	0.717210055	5.537450436
H	6.061060476	-0.071250007	6.181800468
C	5.676960451	1.869240145	5.308340395
C	4.385590340	2.269380173	6.004220436
H	3.747400286	2.706660209	5.245610406
C	3.652700281	1.330730103	6.989970546
H	4.009720306	0.299690026	6.959150522
C	2.133790166	1.293760098	6.925680537
C	1.510180115	0.251700020	7.607590564
H	2.118150163	-0.500350038	8.094460622
C	0.132530013	0.150950012	7.637570572
H	-0.314870025	-0.692970054	8.142070646
C	-0.652420048	1.108060085	7.011330521
H	-1.734440136	1.037820082	7.031440526
C	-0.039830002	2.159430169	6.345060486
H	-0.645490048	2.907090225	5.848620470
C	1.343410106	2.259010172	6.307400476
H	1.793210138	3.099240237	5.795900446
C	13.194131028	3.601270275	0.920840069
H	13.135351024	4.397220338	0.193800012
C	12.062490931	3.246270251	1.619710126
H	11.115430876	3.753250288	1.462720112
N	12.041050945	2.237530174	2.556120199
C	13.221571038	1.598240125	2.804230218
H	13.183591034	0.818170062	3.557700275
C	14.387901084	1.920390148	2.141530166
H	15.301361189	1.395390107	2.383560181
C	14.403601085	2.917730223	1.159820087
C	15.653361217	3.128060240	0.438700031

H	16.433121250	2.449610186	0.743860056
C	15.941171250	4.051610311	-0.548600044
H	15.189661186	4.767260367	-0.845680067
C	17.160091302	4.106720317	-1.283800098
C	17.287641329	5.025180385	-2.360800183
H	16.513751247	5.754770462	-2.515160192
C	18.356881426	4.969360382	-3.201650248
H	18.412811439	5.638460425	-4.051030311
C	19.423301485	4.064680312	-2.962370229
H	20.283811585	4.063780313	-3.622250279
C	19.367241505	3.204310247	-1.856730140
H	20.192451567	2.536740194	-1.650220127
C	18.249041400	3.206320248	-1.035390079
H	18.188961420	2.534770194	-0.195110017
C	6.007680462	5.210600399	6.566700503
H	5.111960394	5.683950459	6.188670458
C	7.250630559	5.764080436	6.313760499
H	7.386330550	6.687120501	5.762510420
N	8.404570661	5.143540396	6.688160493
C	8.303050651	3.985510304	7.415420587
H	9.246000693	3.521350270	7.689530592
C	7.091130556	3.409950262	7.721210582
H	7.066830525	2.490310192	8.288100653
C	5.914690472	3.998280309	7.238300570
C	4.597410356	3.281330255	7.221290538
H	3.799890293	4.013190307	7.169860542
C	4.245090324	2.161030168	8.207820654
H	5.143650396	1.661830127	8.574070684
C	3.358180259	2.465970187	9.398460733
C	3.472670265	1.663900126	10.531070811
H	4.263920330	0.926460069	10.580710812
C	2.579920200	1.801780137	11.581340910
H	2.679220205	1.170720090	12.453560962
C	1.562460123	2.741920210	11.510830899
H	0.843260065	2.831940219	12.314550967
C	1.456890114	3.561510272	10.397990777
H	0.661370049	4.293390332	10.340220814
C	2.346340182	3.424380264	9.346660736
H	2.239290170	4.059440314	8.478970653
C	13.836121087	6.421740492	3.435020262
H	14.180391105	7.175980529	2.741140208
C	12.547110980	6.494580523	3.922470302
H	11.861280913	7.287300584	3.637360280
N	12.044540922	5.581650442	4.806280368
C	12.881991012	4.591340354	5.242780403
H	12.464900966	3.888870299	5.958670446
C	14.180041108	4.476330347	4.792390370
H	14.803101121	3.680490284	5.176130396
C	14.678561108	5.382400391	3.847460295
C	16.049681215	5.170520398	3.363570257
H	16.551601285	4.345400333	3.840960295
C	16.716161280	5.876540444	2.430530187

H	16.211801227	6.706020490	1.956320150
C	18.127831393	5.707680460	2.051970160
C	18.719621423	6.676850494	1.237830095
H	18.103351389	7.462820581	0.818940063
C	20.097961572	6.672190506	1.020850076
H	20.550201582	7.445620574	0.414350030
C	20.882291580	5.696350458	1.596550123
H	21.956281678	5.701570421	1.455690114
C	20.294881550	4.693360362	2.374000182
H	20.912141622	3.925340301	2.821060218
C	18.940411476	4.695570360	2.596460201
H	18.500561410	3.922120299	3.208680246

CI(T_{ARPP}/T_{BRPP})

Ag	10.258280786	1.616110123	3.547040275
Ag	10.187740771	5.602120447	5.709520462
C	6.234370470	2.797620217	4.424720341
H	5.709200416	3.705650286	4.176980323
C	7.491880561	2.604360198	3.896710298
H	7.949160614	3.347030256	3.249570248
N	8.242290625	1.491940116	4.180490324
C	7.654590606	0.536360042	4.957170382
H	8.250840648	-0.357510027	5.122790393
C	6.397140471	0.694080056	5.531500420
H	6.013070450	-0.091320007	6.167920466
C	5.673840422	1.862950143	5.306770432
C	4.387450339	2.283240177	5.999900445
H	3.760360287	2.739530213	5.243390402
C	3.633360282	1.346700101	6.970920535
H	3.971280305	0.311120027	6.929100557
C	2.115270163	1.341520101	6.897390510
C	1.463930113	0.303280022	7.558200600
H	2.050980160	-0.468990036	8.038870604
C	0.084210008	0.232600019	7.574570592
H	-0.386240029	-0.608270049	8.062620609
C	-0.674040050	1.216100093	6.955800513
H	-1.757140136	1.169630091	6.965410530
C	-0.033300002	2.263530176	6.310790491
H	-0.617850047	3.031770233	5.820460462
C	1.351610104	2.332680180	6.286570472
H	1.824060139	3.170010243	5.791320470
C	13.221791017	3.489650267	0.959780074
H	13.165430994	4.275840328	0.221230016
C	12.087040946	3.140640244	1.654330130
H	11.139760858	3.641050280	1.482520115
N	12.063940930	2.144850166	2.601470202
C	13.241401003	1.508770117	2.869880222
H	13.197851038	0.737340058	3.632730280
C	14.415481115	1.827230139	2.213240171
H	15.329261160	1.307370103	2.469200190
C	14.430321097	2.814320215	1.219910095

C	15.676681211	3.033270233	0.498510041
H	16.472811290	2.376890183	0.811270062
C	15.927961240	3.942990304	-0.500170038
H	15.146891175	4.627010356	-0.799920062
C	17.138131293	4.036490309	-1.251220094
C	17.204851336	4.948330380	-2.342780179
H	16.391281269	5.637280412	-2.495180189
C	18.262551401	4.932720382	-3.196840244
H	18.274951400	5.593900419	-4.056300314
C	19.381491508	4.079520315	-2.962730229
H	20.231231581	4.114130317	-3.636550278
C	19.383281503	3.229400250	-1.845070143
H	20.242941533	2.604770199	-1.642530128
C	18.277481396	3.188070247	-1.006600079
H	18.263141381	2.524810194	-0.156070013
C	6.044250473	5.196340400	6.611470486
H	5.153610396	5.687490443	6.244830505
C	7.291510559	5.742550436	6.370810516
H	7.435370570	6.675960524	5.839990436
N	8.438520662	5.103890394	6.730320521
C	8.327610667	3.930630300	7.431640558
H	9.265850714	3.451570264	7.695480608
C	7.110010542	3.361020258	7.727620612
H	7.076980568	2.430170188	8.275200635
C	5.939270438	3.972240306	7.258020572
C	4.611990353	3.274180250	7.228590538
H	3.827390296	4.020220310	7.186840570
C	4.236330324	2.146030168	8.198900631
H	5.122840395	1.624630126	8.559670660
C	3.352050259	2.449370188	9.391010711
C	3.448800265	1.628140126	10.511410818
H	4.224790323	0.874260067	10.550880826
C	2.557740196	1.767890133	11.562830872
H	2.642760204	1.121800088	12.425620932
C	1.560030120	2.729640208	11.505570877
H	0.842350065	2.822330217	12.310000942
C	1.472410115	3.568020274	10.405050795
H	0.692410052	4.317000332	10.357650801
C	2.359880182	3.428640263	9.352630702
H	2.266880175	4.079080315	8.494880632
C	13.856631045	6.461360522	3.481690266
H	14.197141100	7.242380579	2.816430219
C	12.573960957	6.520200481	3.985350308
H	11.890010899	7.327880541	3.740420290
N	12.076260917	5.574790453	4.835040374
C	12.910880968	4.561760352	5.221310401
H	12.497310956	3.832150293	5.911510435
C	14.203791112	4.457130341	4.751520366
H	14.825891145	3.641910278	5.094370389
C	14.696441107	5.400770409	3.840280297
C	16.059821256	5.208510403	3.327840257
H	16.568551255	4.361690335	3.758360288

C	16.713071308	5.968160447	2.414950187
H	16.201811260	6.819560549	1.990100154
C	18.118931373	5.816550424	2.008880157
C	18.701861441	6.820550534	1.231900092
H	18.082981399	7.627520597	0.859130064
C	20.079371522	6.820610542	0.993790074
H	20.525091592	7.620060573	0.416920032
C	20.867271625	5.817740438	1.511130115
H	21.939071670	5.825510453	1.354270103
C	20.287041577	4.780150368	2.252170175
H	20.908741605	3.990540309	2.653770203
C	18.938091457	4.775830366	2.495010191
H	18.504981416	3.975810306	3.077940239

[A···B]ᴄᴛ complex-2

Ag	10.191537089	1.443004899	3.421779723
Ag	10.211119663	5.652296663	5.654584667
C	6.204261502	2.754300217	4.399344524
H	5.690001177	3.670697012	4.154074928
C	7.448286252	2.528492104	3.849263726
H	7.904240927	3.258747447	3.186945391
N	8.180055941	1.399792518	4.129497047
C	7.595627560	0.465742767	4.936073222
H	8.177795931	-0.436068718	5.108864925
C	6.347965299	0.652324161	5.529987820
H	5.961965739	-0.118661129	6.182605399
C	5.641617232	1.833199613	5.298493359
C	4.366025408	2.275775518	5.997908093
H	3.727338716	2.711098165	5.239259644
C	3.617703493	1.355334141	6.992920709
H	3.959203432	0.325303131	6.978507985
C	2.100080262	1.344676115	6.924011248
C	1.448203791	0.286858287	7.557838960
H	2.034527711	-0.486858219	8.037536866
C	0.064800014	0.204171712	7.554852442
H	-0.408862234	-0.643247390	8.029195392
C	-0.694178187	1.189706954	6.934411433
H	-1.776711555	1.133290172	6.927820953
C	-0.052562837	2.252937937	6.309196398
H	-0.636852955	3.021181867	5.817554961
C	1.333996042	2.336768990	6.309946454
H	1.804410116	3.186364154	5.833802555
C	13.224523106	3.486827085	0.998405775
H	13.189277943	4.299582807	0.287049907
C	12.053023845	3.028100002	1.557578648
H	11.095338333	3.473205819	1.300130762
N	12.004672655	1.993982632	2.467700819
C	13.196868568	1.423038671	2.821837061
H	13.138464333	0.607005088	3.535840498
C	14.406115312	1.856080152	2.311733726
H	15.323580178	1.379688916	2.630526357

C	14.456072132	2.902012240	1.374570322
C	15.744052302	3.298045477	0.858441605
H	16.578672934	2.768947430	1.281184873
C	16.001176828	4.195685183	-0.258546500
H	15.235839150	4.908478878	-0.514379786
C	17.092587918	4.161758248	-1.052541237
C	17.194943604	5.081693435	-2.206253915
H	16.445545803	5.848911253	-2.278750536
C	18.140098304	4.949405854	-3.129398985
H	18.145465643	5.591157535	-4.002260468
C	19.223173423	3.968021430	-2.987712618
H	20.014272137	3.937784353	-3.725995352
C	19.238729541	3.136242749	-1.848070451
H	20.054970366	2.439174175	-1.708353613
C	18.216041272	3.199164856	-0.897607680
H	18.224001738	2.553202522	-0.033574354
C	6.045599028	5.207434681	6.586860992
H	5.153601903	5.707018830	6.236056217
C	7.294923964	5.761994843	6.345861766
H	7.423244367	6.708306747	5.833119599
N	8.448186772	5.121961305	6.691973427
C	8.341528769	3.932954076	7.372153574
H	9.279166030	3.451051062	7.634311528
C	7.124579427	3.351194294	7.662293892
H	7.099639197	2.410631820	8.193720303
C	5.944858656	3.970112818	7.215664643
C	4.608153115	3.278395470	7.196767353
H	3.835270226	4.036100258	7.155247629
C	4.231001102	2.163210849	8.188080755
H	5.117710397	1.641167470	8.534693071
C	3.359714307	2.463419532	9.388223905
C	3.459497816	1.627639689	10.501940715
H	4.217122508	0.854092620	10.519744725
C	2.589975991	1.777156895	11.575407722
H	2.672564494	1.122335621	12.433237380
C	1.614078072	2.765823427	11.545481796
H	0.916132170	2.869123832	12.365670389
C	1.526118917	3.619249797	10.451957384
H	0.765270509	4.388933375	10.427190566
C	2.390922228	3.469288849	9.378741472
H	2.297599978	4.131705547	8.529509144
C	13.863436476	6.398357314	3.297155629
H	14.190631743	7.150387613	2.592789949
C	12.600805537	6.505779131	3.853979865
H	11.930049137	7.324952604	3.608241259
N	12.114876939	5.596613617	4.752308824
C	12.939369860	4.568987627	5.128945995
H	12.543661485	3.867323397	5.857408464
C	14.212157827	4.416800409	4.608423529
H	14.828675993	3.597967023	4.954127898
C	14.692778142	5.325252529	3.653775559
C	16.050259235	5.097740333	3.111733090

H	16.541040177	4.231526660	3.522929726
C	16.750205792	5.933893521	2.319276750
H	16.262678391	6.817258046	1.934252469
C	18.176862946	5.805450402	1.971634662
C	18.770498958	6.797857826	1.197721259
H	18.161289524	7.596490066	0.791431503
C	20.173479769	6.796358720	0.992396173
H	20.624305606	7.589491221	0.410376724
C	20.943448066	5.812655785	1.542815560
H	22.018822491	5.812664622	1.414737939
C	20.342217513	4.775543743	2.301879096
H	20.962945972	3.999262028	2.732056373
C	18.998222026	4.768415725	2.509822042
H	18.552587842	3.984997680	3.106000275

Transition-2

Ag	10.168820779	1.352560104	3.396710263
Ag	10.275700772	5.621820446	5.643340444
C	6.259300487	2.758420211	4.401200338
H	5.766840466	3.687000286	4.158280321
C	7.493760569	2.508740192	3.849780298
H	7.967210638	3.226770250	3.184730245
N	8.204750632	1.369120103	4.129810320
C	7.607080596	0.454270034	4.944630378
H	8.179390607	-0.454960034	5.116470392
C	6.370390508	0.667490053	5.537980407
H	5.971170460	-0.093010008	6.195150498
C	5.681440412	1.853880145	5.300660392
C	4.416420338	2.307850178	6.004370458
H	3.768450290	2.745870212	5.252470406
C	3.679000285	1.387480109	7.007590561
H	4.041580312	0.363120026	7.008080526
C	2.164850166	1.348090102	6.931690509
C	1.531720116	0.282800021	7.564210571
H	2.131010165	-0.476110037	8.052540629
C	0.155270014	0.169890012	7.548640589
H	-0.301610024	-0.687740052	8.021610642
C	-0.617420048	1.132920086	6.919430531
H	-1.698550128	1.053710079	6.902400548
C	0.003730001	2.204240168	6.297040508
H	-0.593830046	2.956580226	5.796500427
C	1.383500108	2.318420177	6.309310488
H	1.839100140	3.177190247	5.834700463
C	13.188731039	3.450650263	1.119590085
H	13.152911031	4.299420328	0.452210037
C	12.018140904	2.937240226	1.611600125
H	11.054180832	3.368590260	1.351430104
N	11.965160895	1.858880145	2.466080187
C	13.161080998	1.297560099	2.825620218
H	13.094461022	0.443390034	3.492940267
C	14.368461123	1.781960136	2.380260184

H	15.287891194	1.309240099	2.700570210
C	14.423851111	2.880620224	1.505830114
C	15.714671217	3.380200261	1.094590085
H	16.545151249	2.779980215	1.433240108
C	15.942761216	4.232580326	-0.069110004
H	15.142731154	4.884210375	-0.374730027
C	17.023821334	4.207990321	-0.895010070
C	17.049921309	5.101120394	-2.056760156
H	16.264121246	5.835340450	-2.145300168
C	18.002801361	5.010280383	-2.983240229
H	17.977941408	5.659260424	-3.852140297
C	19.105691470	4.079960315	-2.837640220
H	19.887791525	4.057930312	-3.587220275
C	19.167351467	3.242260247	-1.701770129
H	20.003211539	2.565760200	-1.578410123
C	18.156841419	3.281600252	-0.741240057
H	18.191001398	2.627300201	0.117500009
C	6.123530485	5.228760402	6.574220482
H	5.234390404	5.735090466	6.224760453
C	7.370040569	5.771270420	6.328410506
H	7.506690592	6.719440531	5.819840425
N	8.519320630	5.117460393	6.655430510
C	8.401300663	3.933140304	7.337860560
H	9.338670742	3.439800267	7.582450570
C	7.183530566	3.372440258	7.646140598
H	7.152370546	2.435540188	8.183730654
C	6.010080440	3.998400305	7.206820556
C	4.666590359	3.326930258	7.198110563
H	3.899350300	4.092340316	7.144790558
C	4.279240328	2.222030170	8.201770624
H	5.163640395	1.707230133	8.569920665
C	3.381140260	2.530190196	9.375650707
C	3.467480264	1.702290131	10.491010824
H	4.243120325	0.947130071	10.532580819
C	2.566570196	1.831640143	11.532640886
H	2.643650201	1.177260091	12.390380955
C	1.570680119	2.793170217	11.473350862
H	0.844540065	2.874500220	12.272270922
C	1.496290117	3.642260281	10.380550788
H	0.715920053	4.391200338	10.329720773
C	2.393140184	3.511980271	9.335900711
H	2.307750180	4.167870320	8.480600678
C	13.836141090	6.360940513	3.184170243
H	14.144591100	7.110940571	2.468570189
C	12.613170980	6.498900515	3.806870294
H	11.950050926	7.338170552	3.608010278
N	12.144190924	5.597730446	4.722010362
C	12.963130977	4.548790349	5.041520388
H	12.580680979	3.850440299	5.781320449
C	14.195821067	4.369600334	4.456470341
H	14.805171157	3.532730274	4.768060367
C	14.660141136	5.266450406	3.484600270

C	15.978941223	4.980370385	2.863660220
H	16.492651257	4.165890318	3.331290255
C	16.722011282	5.886450452	2.159510164
H	16.233251268	6.778010504	1.792390140
C	18.152701401	5.789150420	1.889450143
C	18.774591456	6.819420529	1.173820090
H	18.167471373	7.627900599	0.782760061
C	20.165871576	6.826830545	1.002440079
H	20.635151570	7.638760586	0.462370034
C	20.927161630	5.814520447	1.523200119
H	22.004231699	5.820360447	1.407880109
C	20.315071567	4.757570364	2.218700169
H	20.922881592	3.961440307	2.631010205
C	18.964011458	4.739350363	2.394880182
H	18.513051422	3.926960303	2.945890226

STC(T$_{BRPP}$/S$_0$)

Ag	10.146710960	1.230928629	3.354469081
Ag	10.361677364	5.602298409	5.654876244
C	6.270184181	2.739733904	4.361020465
H	5.794615392	3.682184741	4.116069725
C	7.505597682	2.466625499	3.808228237
H	7.997755596	3.180449121	3.144744506
N	8.197353581	1.306010615	4.089705082
C	7.577558221	0.395894894	4.907322959
H	8.135619287	-0.526996092	5.079792223
C	6.340466275	0.635174013	5.500069091
H	5.923454865	-0.120152033	6.159728908
C	5.672744496	1.841401230	5.263208608
C	4.422080868	2.314754809	5.973887679
H	3.776584623	2.772247623	5.227329025
C	3.677780658	1.398014488	6.975589413
H	4.024133539	0.365360314	6.963021930
C	2.163457149	1.382495455	6.909808395
C	1.517345116	0.317957108	7.543939908
H	2.112053824	-0.454550779	8.026287457
C	0.134285326	0.222090410	7.534399371
H	-0.331390733	-0.635875136	8.007116636
C	-0.633190218	1.201988708	6.911061116
H	-1.719432457	1.135587214	6.899046993
C	0.000835952	2.273005132	6.287698255
H	-0.591799434	3.038626745	5.792245154
C	1.388137024	2.370061944	6.293091523
H	1.854433818	3.228905797	5.818738995
C	13.135246565	3.514664200	1.257077912
H	13.083708775	4.426779682	0.671230521
C	11.960879216	2.908511289	1.656079738
H	10.983619173	3.323825972	1.402079093
N	11.935944860	1.762135627	2.427115676
C	13.144074723	1.204443228	2.759886857
H	13.088788295	0.296814175	3.362697549

C	14.352564744	1.779470431	2.382904086
H	15.286759231	1.318263672	2.693348094
C	14.372712745	2.966724247	1.646471901
C	15.687906013	3.674320305	1.400555729
H	16.484616123	2.954695460	1.571530507
C	15.826221887	4.264713217	0.034395108
H	15.049370211	4.939509319	-0.282302621
C	16.904242093	4.171570951	-0.827656745
C	16.928260654	5.038401688	-1.990720942
H	16.150925523	5.788783594	-2.083684780
C	17.911126907	4.946495273	-2.925631273
H	17.893831436	5.597427227	-3.797866650
C	18.983974987	4.029854982	-2.761357504
H	19.780488508	3.997789011	-3.502026246
C	19.025637271	3.195796712	-1.620963668
H	19.859105726	2.511873202	-1.484158342
C	18.008977283	3.249395128	-0.667610367
H	18.037177615	2.599664951	0.201264878
C	6.182888827	5.218655900	6.560333760
H	5.294222157	5.746054225	6.227039989
C	7.438896848	5.751935818	6.311988231
H	7.582382148	6.712499683	5.819595469
N	8.591439922	5.074539742	6.619503344
C	8.460856757	3.872436038	7.284951460
H	9.397156523	3.361024306	7.515945796
C	7.230644169	3.322400749	7.593688390
H	7.190094480	2.373496733	8.118534112
C	6.055526764	3.973845645	7.176913257
C	4.701836046	3.322778545	7.176601149
H	3.942805298	4.101369890	7.134118270
C	4.304134827	2.213452133	8.176191360
H	5.185646326	1.679537954	8.532483650
C	3.417444825	2.522964688	9.357903848
C	3.496774464	1.679350784	10.469971636
H	4.266446167	0.911790450	10.502297063
C	2.595142333	1.809214246	11.518464281
H	2.665352231	1.143879056	12.373681339
C	1.605073920	2.786096578	11.469778122
H	0.878576661	2.866729914	12.273945027
C	1.537724822	3.650225229	10.380853530
H	0.761684995	4.410113959	10.337933816
C	2.435484376	3.520113487	9.328984152
H	2.354910578	4.186656001	8.475790139
C	13.863373927	6.282039286	3.085399362
H	14.129961043	6.991567444	2.307248446
C	12.667767520	6.464086526	3.771162080
H	11.992171266	7.296773862	3.562123779
N	12.237426135	5.601266461	4.749657588
C	13.081642232	4.568534609	5.092940775
H	12.733405131	3.902254747	5.884787248
C	14.291454773	4.361767891	4.452831453
H	14.914845311	3.533648556	4.775363806

C	14.691656869	5.191980345	3.392091149
C	15.953921247	4.810895355	2.636447480
H	16.547820260	4.231063444	3.339517495
C	16.769615538	5.943167088	2.114476186
H	16.248568409	6.803310362	1.715261958
C	18.177335343	5.883820230	1.914022997
C	18.830011396	6.938755978	1.205831673
H	18.223933157	7.746854564	0.801415692
C	20.209682531	6.945625016	1.055582826
H	20.687646165	7.760213168	0.518423600
C	20.979285801	5.918516106	1.588475085
H	22.061216415	5.926480594	1.482733231
C	20.359343488	4.855823625	2.273454001
H	20.967332957	4.056936469	2.691274630
C	18.999375739	4.826929542	2.429220198
H	18.543347454	4.002457978	2.966664794

Product3

Ag	10.192569566	1.137142767	3.373558097
Ag	10.385328147	5.640917606	5.680876786
C	6.301593179	2.658491205	4.348097713
H	5.823623301	3.585754512	4.075065944
C	7.533019541	2.370873321	3.810737056
H	8.021242705	3.063226634	3.131597489
N	8.219628821	1.226301963	4.120568033
C	7.604126676	0.342824061	4.952094815
H	8.157289783	-0.570483195	5.152760775
C	6.370493009	0.592550913	5.534505300
H	5.957966588	-0.142261758	6.209562905
C	5.706995229	1.785400101	5.266613451
C	4.448716687	2.274675237	5.958838090
H	3.813854730	2.711744608	5.197188740
C	3.691452661	1.380019233	6.967922058
H	4.030650674	0.349186528	6.976152617
C	2.176079709	1.371397534	6.892711101
C	1.520153322	0.334215242	7.546868692
H	2.101695137	-0.426754143	8.050075774
C	0.141499547	0.254473818	7.537443146
H	-0.336708182	-0.577920305	8.031390314
C	-0.608274261	1.222433757	6.889458937
H	-1.689553422	1.167408033	6.875795792
C	0.036481188	2.265816603	6.245079959
H	-0.542887067	3.021433136	5.731133860
C	1.417864641	2.346438164	6.252347838
H	1.893272687	3.182271777	5.760015614
C	13.215941862	3.426115204	1.279953234
H	13.178192315	4.334647425	0.697821852
C	12.039119183	2.818035198	1.650518837
H	11.074271522	3.234009437	1.375991057
N	11.996779817	1.682784858	2.418035820
C	13.185624980	1.120858396	2.766741481

H	13.121791016	0.218817491	3.366374865
C	14.397613445	1.691010501	2.416669352
H	15.319206898	1.234484054	2.748962633
C	14.434698398	2.880649720	1.699861609
C	15.758032159	3.602338250	1.610805608
H	16.541974016	2.864534108	1.729686542
C	16.104278495	4.625495396	0.503752387
H	15.198543426	5.038263488	0.078120964
C	17.028432796	4.279849364	-0.647409020
C	16.941357897	5.075054457	-1.795525277
H	16.173169647	5.833569399	-1.848062857
C	17.824663948	4.926090140	-2.836419191
H	17.744321824	5.556974484	-3.711882015
C	18.847658769	3.970624744	-2.764095827
H	19.559375181	3.879310834	-3.573937846
C	18.945566932	3.154105519	-1.632614516
H	19.733999757	2.417432071	-1.562163101
C	18.038226180	3.307222300	-0.574364546
H	18.127355186	2.679853603	0.299081921
C	6.186089978	5.196927618	6.525123629
H	5.302758157	5.713085847	6.178998474
C	7.435488259	5.741075037	6.294842306
H	7.567588839	6.696061798	5.801102576
N	8.582309022	5.088511767	6.627206894
C	8.457432240	3.896428421	7.292519065
H	9.390049884	3.401516505	7.545348313
C	7.237938930	3.330781271	7.582967259
H	7.204326438	2.390269831	8.110775685
C	6.066404531	3.962127756	7.146030843
C	4.714316707	3.299529539	7.140313771
H	3.958655988	4.074372283	7.080636019
C	4.306997374	2.207982737	8.152497554
H	5.181619906	1.680322290	8.522169615
C	3.414477601	2.534006829	9.328423860
C	3.482820081	1.707396691	10.445479672
H	4.241977958	0.938006150	10.489526111
C	2.583060131	1.856142346	11.486129752
H	2.641986315	1.204720178	12.346507187
C	1.609941377	2.839177586	11.425033910
H	0.889504658	2.939371636	12.225568278
C	1.553884223	3.686453953	10.329989648
H	0.792148613	4.452271446	10.277490079
C	2.446663113	3.534168033	9.285622734
H	2.375012000	4.188664064	8.429546768
C	13.928432513	6.259831146	3.130482068
H	14.198866271	6.943691879	2.339379972
C	12.729437943	6.452079706	3.797960151
H	12.058949466	7.272135475	3.555632949
N	12.294444613	5.617377474	4.781461585
C	13.128555119	4.597741695	5.153296768
H	12.773913491	3.948542056	5.948201098
C	14.339613766	4.377350272	4.537257169

H	14.954775174	3.556215388	4.873616014
C	14.746944408	5.186622563	3.471720651
C	15.991859975	4.752186452	2.722000762
H	16.702708642	4.408732959	3.464334083
C	16.643220017	5.629462665	1.626173540
H	16.196005074	6.614215540	1.526210539
C	18.152764108	5.778194334	1.682828955
C	18.746372392	6.894276302	1.055102296
H	18.113183555	7.664431504	0.635137362
C	20.106262511	7.001380772	0.975273659
H	20.547548234	7.856141308	0.481528990
C	20.930312616	6.003411007	1.519343581
H	22.006130228	6.081424592	1.447536445
C	20.375267913	4.923632011	2.144912238
H	21.007470099	4.157599698	2.573845748
C	18.978838634	4.799034873	2.225232820
H	18.560500735	3.929886155	2.707899728