

**Supplementary Information:**

**QM/MM studies on luminescence mechanism of dinuclear copper iodide  
complexes with thermally activated delayed fluorescence**

Qian Wang,<sup>a</sup> Yuan-Jun Gao,<sup>a</sup> Ting-Ting Zhang,<sup>\*a,b</sup> Juan Han,<sup>\*a</sup> and Ganglong Cui<sup>a</sup>

<sup>a</sup>Key Laboratory of Theoretical and Computational Photochemistry, Ministry of Education,  
Chemistry College, Beijing Normal University, Beijing 100875, P. R. China

<sup>b</sup>Key Laboratory of Magnetic Molecules and Magnetic Information Materials of Ministry of  
Education, School of Chemistry and Materials Science, Shanxi Normal University, Linfen  
041000, P. R. China

E-mail: zhangtt@bnu.edu.cn and hanjuan@bnu.edu.cn

## Table of Contents

### 1 □ Additional Figures

**Figure S1.** ONIOM clusters of complexes **1** and **2** used in our present studies.

**Figure S2.** Frontier molecular orbitals and related orbital energies (in eV) at the  $T_1$  minimum of complexes **1** (left) and **2** (right) in crystal.

**Figure S3.** Frontier molecular orbitals and related orbital energies (in eV) at the  $S_0$  and  $S_1$  minima of complex **2** in crystal.

**Figure S4.** Selected molecular orbitals of complexes **1** and **2** at their  $S_0$  minima in crystal.

**Figure S5.** Calculated Huang-Rhys factors of each vibrational mode of complexes **1** and **2** in crystal.

### 2、 Additional Tables

**Table S1.** Selected Geometric Parameters of Complexes **1** and **2** in Crystal (Length in Å and Angles in °).

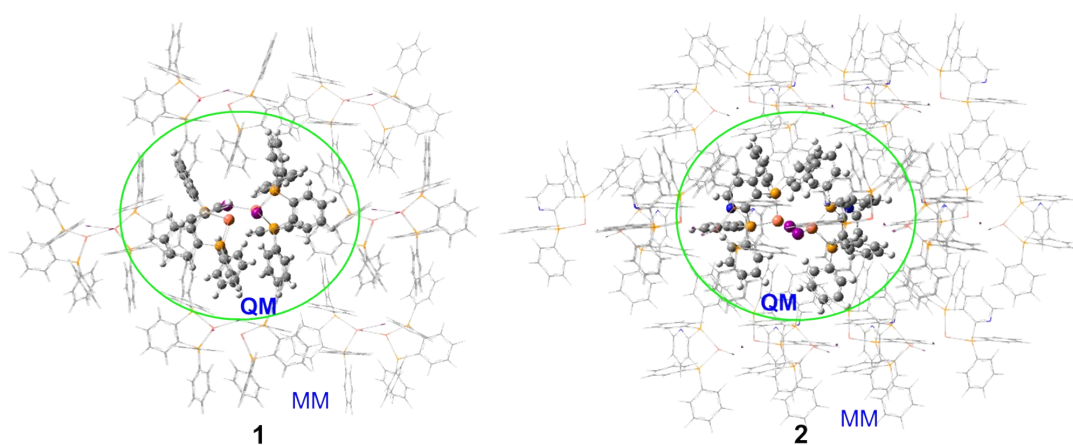
**Table S2.** Relative Energies (eV) of Optimized Structures for **1** and **2** in Crystal. (Ground State Energy as Reference).

**Table S3.** Calculated Vertical Excitation Energies (E/eV), Wavelength ( $\lambda$ /nm), Oscillator Strengths ( $f$ ), and Main Configurations, and State Assignments in Crystals.

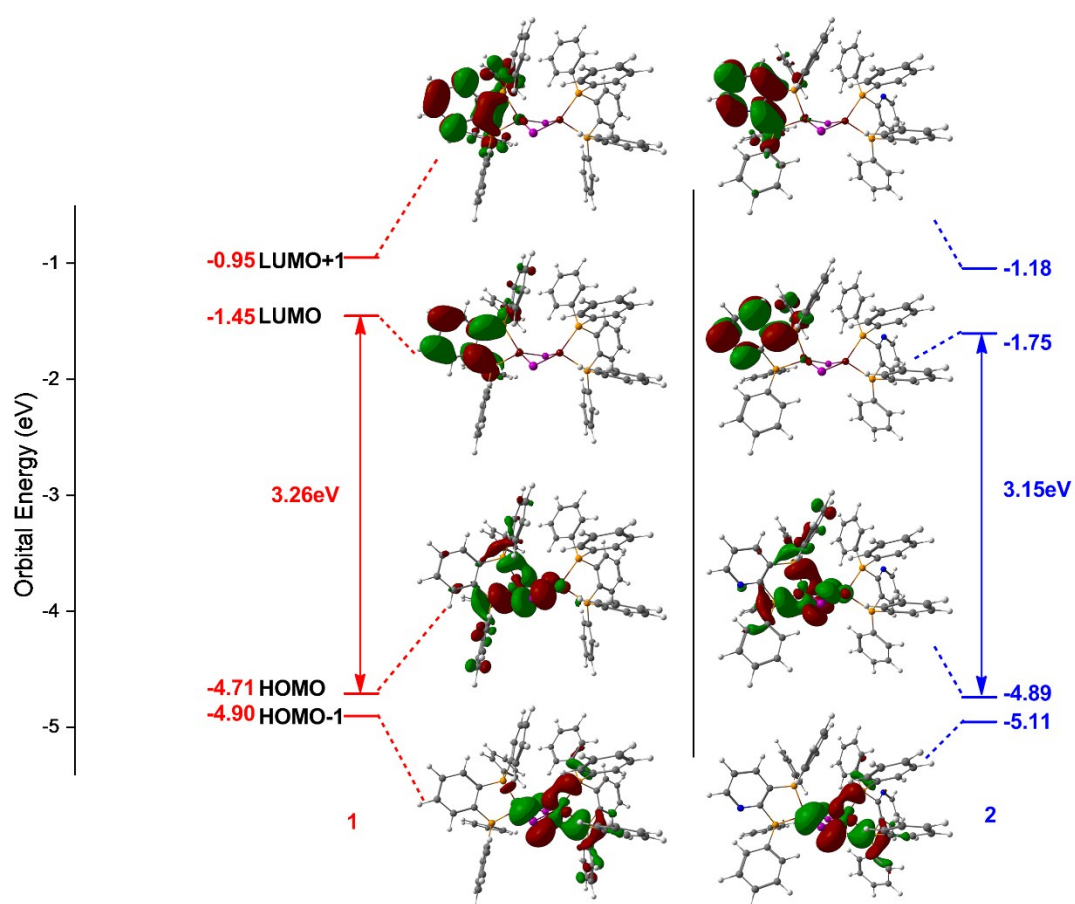
**Table S4.** Temperature Dependence of Intersystem Crossing Rates and Reverse Intersystem Crossing Rates ( $s^{-1}$ ) (ISC from  $S_1$  to  $T_1$  and rISC from  $T_1$  to  $S_1$ ).

### 3、 Cartesian coordinates of optimized structures

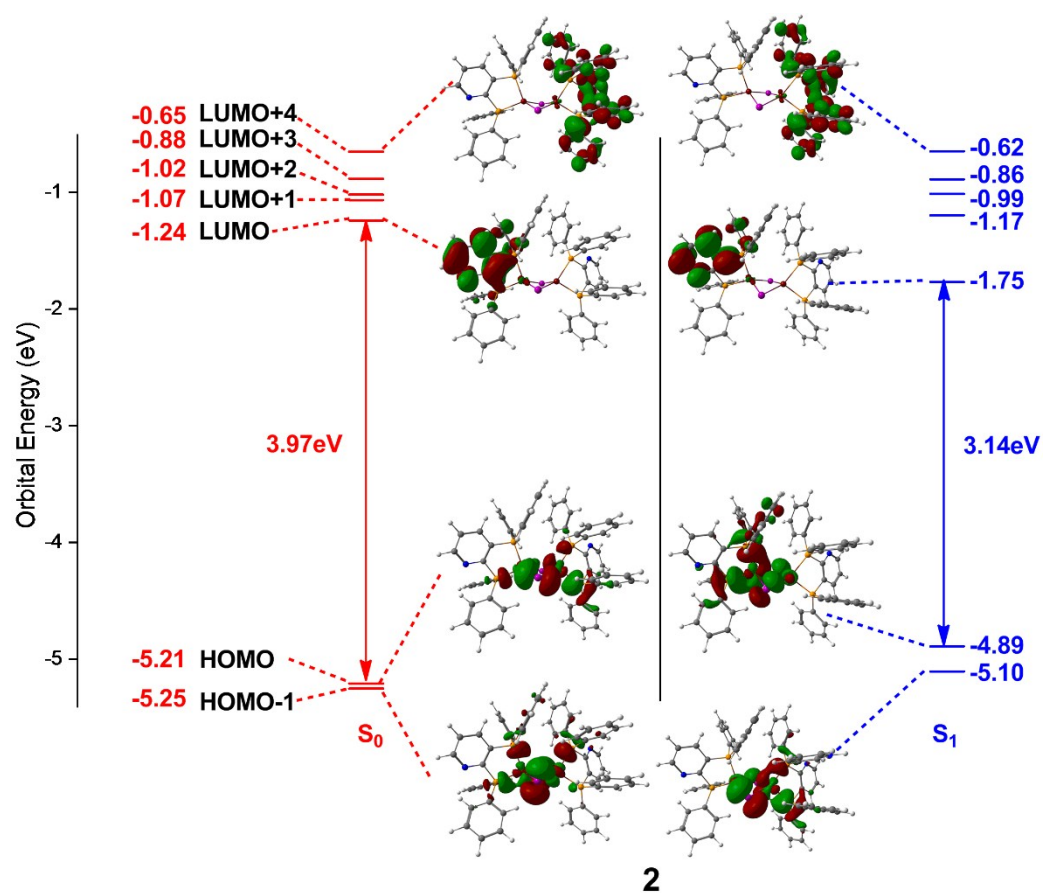
## 1、Additional Figures



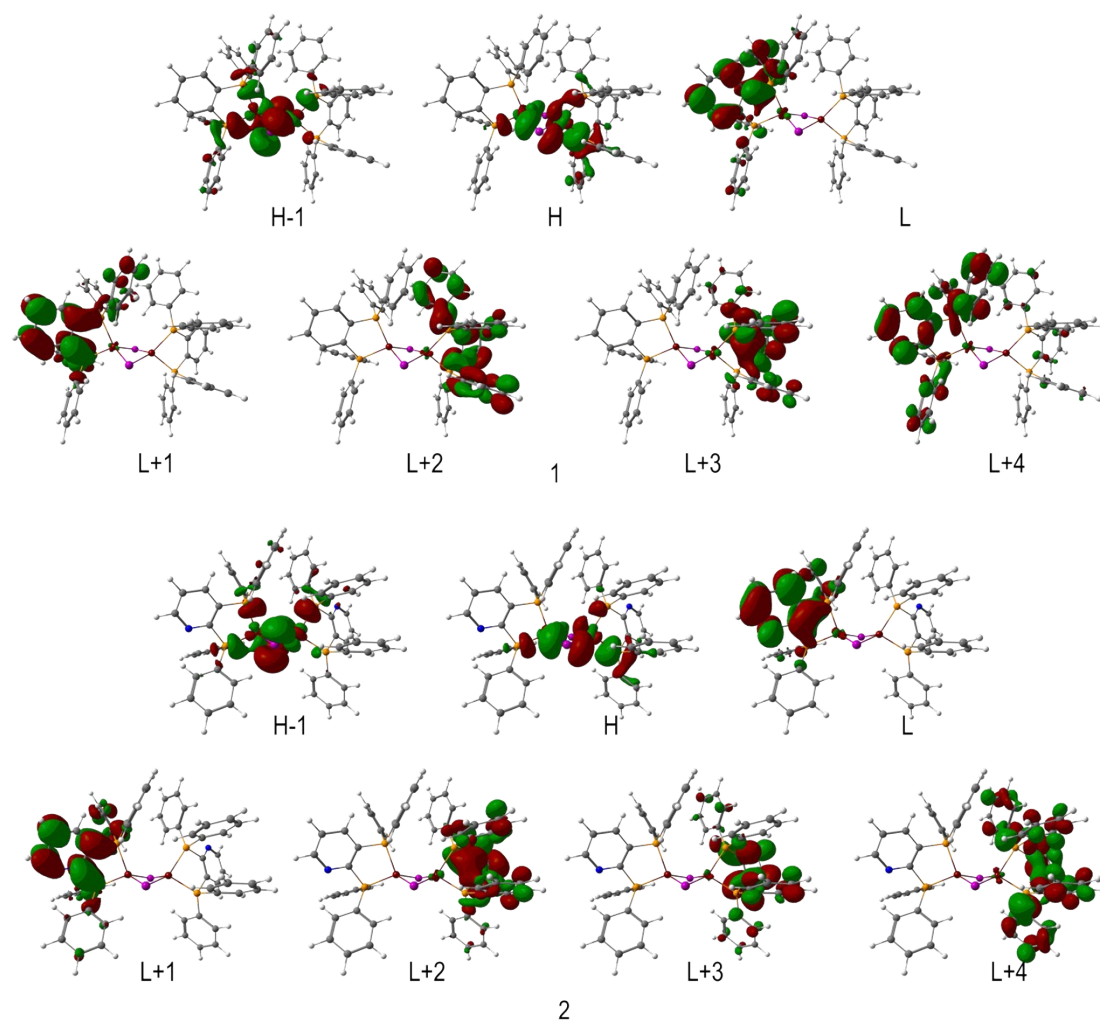
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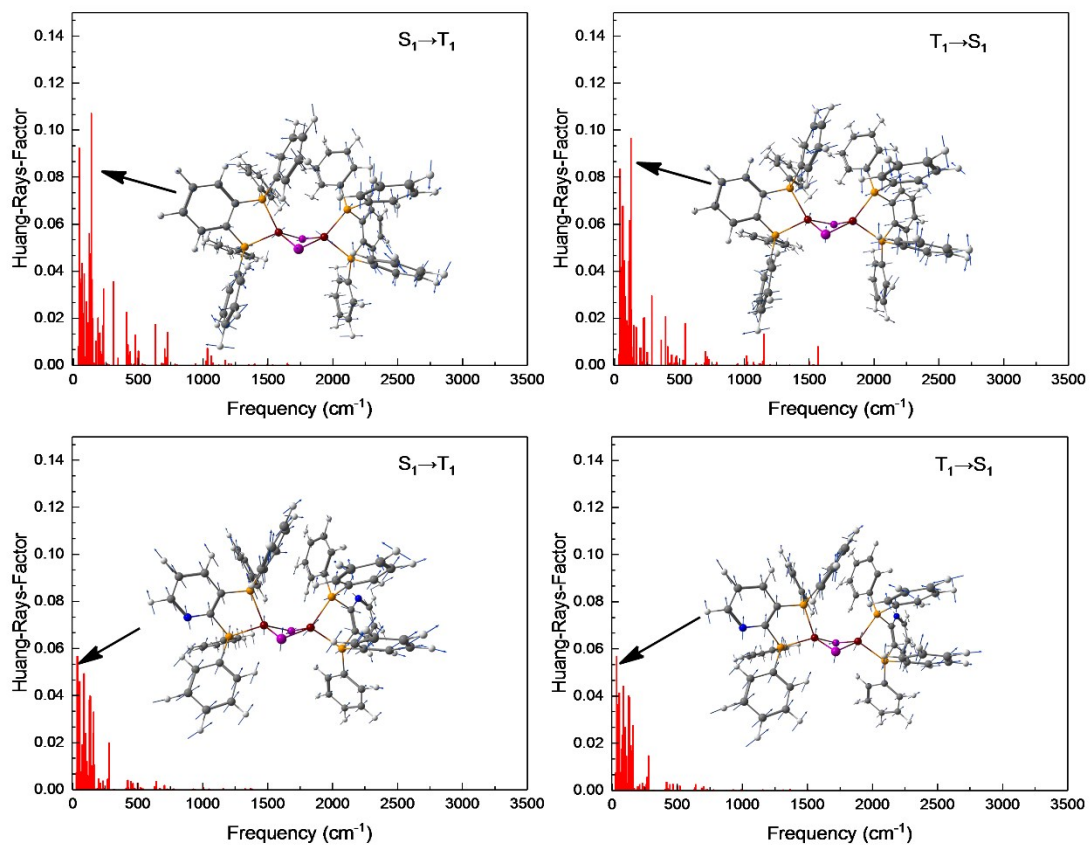
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**Figure S3.** Frontier molecular orbitals and related orbital energies (in eV) at the  $S_0$  and  $S_1$  minima of complex **2** in crystal.



**Figure S4.** Selected molecular orbitals of complexes **1** and **2** at their  $S_0$  minima in crystal (ONIOM calculations).



**Figure S5.** Calculated Huang-Rhys factors of each vibrational mode of complexes **1** and **2** in crystal.

## 2 □ Additional Tables

**Table S1.** Selected Geometric Parameters of Complexes **1** and **2** in Crystal (Length in Å and Angles in °).

In Crystal								
	<b>1</b>				<b>2</b>			
	EXP.(1)	S <sub>0</sub>	S <sub>1</sub>	T <sub>1</sub>	EXP.(2)	S <sub>0</sub>	S <sub>1</sub>	T <sub>1</sub>
<b>Distances</b>								
<b>Cu1-I1</b>	<b>2.570</b>	2.616	2.607	2.610	<b>2.670</b>	2.713	2.698	2.704
<b>Cu1-I2</b>	<b>2.649</b>	2.695	2.683	2.686	<b>2.601</b>	2.638	2.623	2.625
<b>Cu2-I1</b>	<b>2.679</b>	2.728	2.685	2.684	<b>2.627</b>	2.691	2.664	2.662
<b>Cu2-I2</b>	<b>2.626</b>	2.677	2.673	2.675	<b>2.645</b>	2.716	2.685	2.690
<b>Cu1-P1</b>	<b>2.263</b>	2.286	2.281	2.281	<b>2.295</b>	2.314	2.303	2.302
<b>Cu1-P2</b>	<b>2.274</b>	2.298	2.304	2.3	<b>2.285</b>	2.325	2.327	2.323
<b>Cu2-P3</b>	<b>2.273</b>	2.308	2.303	2.317	<b>2.270</b>	2.305	2.310	2.311
<b>Cu2-P4</b>	<b>2.277</b>	2.302	2.329	2.326	<b>2.272</b>	2.291	2.295	2.299
<b>Cu...Cu</b>	<b>2.812</b>	2.783	2.918	2.934	<b>2.834</b>	2.805	2.925	2.943
<b>I...I</b>	<b>4.340</b>	4.475	4.308	4.301	<b>4.342</b>	4.499	4.345	4.345
<b>Bond Angles</b>								
<b>I-Cu-I<sup>a</sup></b>	<b>111.0</b>	113.3	108.0	107.7	<b>111.0</b>	113.5	109.0	108.9
<b>Cu-I-Cu<sup>a</sup></b>	<b>64.6</b>	62.6	66.0	66.8	<b>65.1</b>	62.9	66.5	66.9
<b>P-Cu-P<sup>a</sup></b>	<b>88.0</b>	88.3	87.5	87.2	<b>89.0</b>	90.0	88.2	88.2
<b>Torsion Angles</b>								
<b>Cu-P-C-C<sup>a,b</sup></b>	<b>23.0</b>	22.3	22.7	22.8	<b>20.0</b>	20.0	20.8	20.9
<b>Cu-I-Cu-I<sup>a</sup></b>	<b>22.1</b>	22.7	25.5	25.5	<b>22.0</b>	21.4	23.2	22.5
<b>Cu-I-I-Cu</b>	<b>142.9</b>	141.5	137.7	137.9	<b>143.1</b>	144.1	141.6	142.7

<sup>a</sup>Average values. <sup>b</sup>Torsion angle around the P-C axis in the five-membered ring CuP2C2

**Table S2.** Relative energy (eV) of PBE1PBE/6-31g\*(C/N/O/H)&6-31+G\*(P)&SDD(Cu/I) Optimized Structures for Complexes **1** and **2** in Crystal (Ground State Energy as Reference).

In Crystal						
	<b>1</b>			<b>2</b>		
	At S <sub>0</sub>	At S <sub>1</sub>	At T <sub>1</sub>	At S <sub>0</sub>	At S <sub>1</sub>	At T <sub>1</sub>
<b>S<sub>1</sub></b>	3.32	2.89	2.91	3.17	2.75	2.76
<b>T<sub>1</sub></b>	3.10	2.76	2.74	3.06	2.67	2.66
<b>T<sub>2</sub></b>	3.17	3.20	3.24	3.16	3.18	3.19

**Table S3.** Vertical Excitation Energy (E/eV), Wavelength ( $\lambda$ /nm), Oscillator Strength ( $f$ ) and Major Contribution of Calculated Transition for Complexes **1** and **2** in Crystal, Which were Computed by TD-PBE1PBE.

In Crystal						
	State	E (eV)	$\lambda$ (nm)	$f$	Contribution	Assignment
<b>1</b>	<b>1</b>	3.32	374	0.0226	H-1-> L(50.7%) H-> L(40.5%)	(M+X)LCT
	<b>2</b>	3.37	367	0.0170	H-1-> L+1(45.8%) H-> L+1(41.1%)	(M+X)LCT
	<b>3</b>	3.38	367	0.0153	H-> L+2 (71.4%)	(M+X)LCT
	<b>4</b>	3.49	356	0.0061	H-> L(33.8%)	(M+X)LCT
	<b>5</b>	3.52	353	0.0083	H-> L+3 (54.1%)	(M+X)LCT
	<b>6</b>	3.59	345	0.0038	H-1-> L+1(37.4%) H-> L+1(51.9%)	(M+X)LCT
	<b>7</b>	3.66	338	0.0090	H-1-> L+2(74.3%)	(M+X)LCT
	<b>8</b>	3.74	331	0.0639	H-> L+4(60.5%) H-1-> L+4(23.9%)	(M+X)LCT
	<b>9</b>	3.78	328	0.0101	H-> L+5(29.4%)	(M+X)LCT
	<b>10</b>	3.79	327	0.0219	H-1-> L+3 (55.2%)	(M+X)LCT
	<b>11</b>	3.82	325	0.0088	H-2-> L(68.0%)	(M+X)LCT
	<b>26</b>	4.25	291	0.0511	H-> L+1(38.7%)	(M+X)LCT
<b>2</b>	<b>1</b>	3.17	392	0.0040	H-1 -> L(57.6%) H -> L(31.0%)	(M+X)LCT
	<b>2</b>	3.32	374	0.0046	H-1 -> L+1(42.7%) H -> L+1(26.1%)	(M+X)LCT
	<b>3</b>	3.32	373	0.0070	H -> L+2(59.0%)	(M+X)LCT
	<b>4</b>	3.36	369	0.0045	H -> L(60.1%)	(M+X)LCT
	<b>5</b>	3.47	357	0.0173	H -> L+3(75.3%)	(M+X)LCT
	<b>6</b>	3.52	352	0.0025	H -> L+1 (47.0%)	(M+X)LCT
	<b>7</b>	3.52	352	0.0094	H-1-> L+2(39.9%) H -> L+2(24.2%)	(M+X)LCT
	<b>8</b>	3.60	345	0.0046	H-2 -> L(76.8%)	(M+X)LCT
	<b>9</b>	3.65	339	0.0088	H-1-> L+3 (65.8%) H -> L+3(20.5%)	(M+X)LCT
	<b>10</b>	3.74	332	0.0470	H -> L+4 (74.2%)	(M+X)LCT
	<b>11</b>	3.77	329	0.0026	H-2 -> L+1 (77.3%)	(M+X)LCT
	<b>28</b>	4.26	291	0.0320	H-1 -> L+7 (33.7%)	(M+X)LCT

Note:

(M+X)LCT: Metal-To-Ligand Charge Transfer Combined With The Halide-To-Ligand Charge-Transfer.



**Table S4.** Temperature Dependence of Intersystem Crossing Rates and Reverse Intersystem Crossing Rates ( $s^{-1}$ ) (ISC from  $S_1$  to  $T_1$  and rISC from  $T_1$  to  $S_1$ ).

	In Crystal			
	1		2	
	$k_{ISC}$	$k_{rISC}$	$k_{ISC}$	$k_{rISC}$
<b>275</b>	$5.08 \times 10^8$	$2.18 \times 10^5$	$1.43 \times 10^9$	$1.36 \times 10^7$
<b>300</b>	$8.25 \times 10^8$	$6.27 \times 10^5$	$2.34 \times 10^9$	$3.36 \times 10^7$
<b>325</b>	$1.24 \times 10^9$	$1.53 \times 10^6$	$3.54 \times 10^9$	$7.20 \times 10^7$
<b>350</b>	$1.75 \times 10^9$	$3.28 \times 10^6$	$5.03 \times 10^9$	$1.38 \times 10^8$
<b>375</b>	$2.36 \times 10^9$	$6.34 \times 10^6$	$6.81 \times 10^9$	$2.42 \times 10^8$

### 3、Cartesian coordinates of optimized structures

#### Crystal

##### $S_0(1)$

I	-0.04312900	-0.91245600	-2.17657900
I	0.17686000	-0.73856400	2.28932800
Cu	-1.29399800	-0.38328800	0.05956700
Cu	1.48701900	-0.29692200	-0.00335000
P	-2.63822900	1.45096200	0.29544300
P	-3.15156100	-1.66281400	0.49715700
P	3.45997500	-1.40262100	-0.46349100
P	2.57757900	1.71215500	-0.27197100
C	-3.69116400	1.88813600	-1.13581000
C	-5.07829500	2.03895300	-1.05626800
C	-5.80772100	2.40165300	-2.18527700
C	-5.16150300	2.60543800	-3.39987200
C	-3.78536900	2.40910600	-3.49594000
C	-3.05107200	2.05669300	-2.36977500
C	-2.10449600	3.08122100	0.93413700
C	-2.87538200	4.24612400	0.83699100
C	-2.39567900	5.44688300	1.35303300
C	-1.13090600	5.50415300	1.93323400
C	-0.34957600	4.35486700	2.00515500
C	-0.83882100	3.14646300	1.52182400
C	-4.02450500	-0.56217500	1.68375700
C	-4.88597100	-1.03967000	2.67391100
C	-5.55171700	-0.15491700	3.51466100
C	-5.35949300	1.21131400	3.37759400
C	-4.49402700	1.70180100	2.41138200
C	-3.82148800	0.83015600	1.55567700
C	-4.36791200	-1.74271500	-0.86967600
C	-5.70474800	-2.07162800	-0.63054900
C	-6.64363400	-1.97159500	-1.64637600
C	-6.25374800	-1.54611000	-2.91767500
C	-4.91945300	-1.25457400	-3.17370200
C	-3.97791000	-1.34800000	-2.15081600
C	-3.18235500	-3.32721100	1.24117700
C	-2.76002700	-3.54789000	2.56018300
C	-2.64201300	-4.84709500	3.04513600
C	-2.91707600	-5.93830200	2.22650000
C	-3.32383400	-5.72393800	0.91378800
C	-3.46128900	-4.42949300	0.42619300

C	3.60175300	-2.90626900	-1.50026800
C	2.93925000	-2.95445900	-2.73392600
C	2.91029000	-4.13266400	-3.46812800
C	3.55194700	-5.27584000	-2.99816800
C	4.24057100	-5.22948600	-1.79159200
C	4.25475100	-4.05290100	-1.04516200
C	4.51343600	-1.75124200	0.99492500
C	3.86996800	-2.18452400	2.16158400
C	4.60576900	-2.44042400	3.31563500
C	5.98689200	-2.26588900	3.31566000
C	6.63517900	-1.84837700	2.15484100
C	5.90290900	-1.58981600	1.00058400
C	4.04301500	1.23330100	-1.29816700
C	4.77774200	2.18417700	-2.01531600
C	5.85357700	1.81078600	-2.81518000
C	6.18822200	0.46614600	-2.94278700
C	5.46497200	-0.49303400	-2.24279000
C	4.40416600	-0.12849100	-1.40382600
C	1.77922900	3.08732200	-1.19247400
C	1.72130400	4.40641100	-0.73183700
C	0.96112000	5.35812500	-1.40748100
C	0.26420500	5.01606700	-2.56095600
C	0.31558500	3.70513100	-3.02984100
C	1.05017900	2.74669000	-2.34137900
C	3.28566100	2.53173000	1.21220600
C	2.81265300	2.16025900	2.47578900
C	3.26863700	2.81110800	3.62181800
C	4.20248100	3.83539200	3.52121200
C	4.68960600	4.19842800	2.26916100
C	4.23619900	3.55403700	1.12483000
H	-5.58830600	1.85294400	-0.11623900
H	-6.88472000	2.51862000	-2.12090600
H	-5.73273100	2.91117000	-4.26864100
H	-3.28177400	2.51814300	-4.45271900
H	-1.97888600	1.89271100	-2.44514500
H	-3.84402000	4.21428800	0.34382000
H	-3.00483900	6.34401000	1.29335400
H	-0.75228600	6.44913800	2.30984700
H	0.65565400	4.38392500	2.41434500
H	-0.23233600	2.24653400	1.58475100
H	-5.03132500	-2.11015300	2.79343400
H	-6.23486000	-0.52235800	4.26948100

H	-5.85238200	1.89426400	4.05169400
H	-4.30923200	2.76914100	2.34554300
H	-6.01150800	-2.38985400	0.36065200
H	-7.67511400	-2.21905400	-1.42253100
H	-6.97992200	-1.44742400	-3.71892600
H	-4.61192600	-0.93119300	-4.16440000
H	-2.93898000	-1.09499600	-2.33951200
H	-2.50698200	-2.70756100	3.20109400
H	-2.30906800	-5.01707500	4.06380300
H	-2.79491900	-6.94514600	2.61274200
H	-3.52913200	-6.55800900	0.25343100
H	-3.77773100	-4.27023400	-0.60006400
H	2.41818700	-2.08061700	-3.10620000
H	2.37624400	-4.15922800	-4.41018100
H	3.51738300	-6.19414200	-3.57592700
H	4.75877000	-6.11088300	-1.42388200
H	4.76922100	-4.01387100	-0.09367800
H	2.78889600	-2.29866200	2.16875300
H	4.09736900	-2.76235000	4.22041500
H	6.55220300	-2.46274000	4.21903500
H	7.71296700	-1.71557100	2.14166100
H	6.41695500	-1.25615100	0.10316600
H	4.46465600	3.22333800	-1.98797900
H	6.40374900	2.56149500	-3.37443800
H	7.00144000	0.16237900	-3.59592800
H	5.71146600	-1.54537900	-2.36189400
H	2.24368300	4.69671500	0.17353300
H	0.90563800	6.36867300	-1.01674900
H	-0.32995400	5.76001600	-3.08187800
H	-0.23505600	3.42087200	-3.92333300
H	1.03109000	1.71571000	-2.67998500
H	2.08306600	1.35945200	2.56334800
H	2.88798700	2.52136900	4.59553600
H	4.54565500	4.34641100	4.41694400
H	5.43544300	4.97551700	2.16985500
H	4.62800100	3.85468700	0.15841700

**S<sub>1</sub>(1)**

I	0.01978400	-1.09816600	-2.03706500
I	0.21184100	-0.66408100	2.24432600
Cu	-1.32413900	-0.34916300	0.06724000
Cu	1.59178000	-0.29423700	-0.01475500

P	-2.67669300	1.47762600	0.25567800
P	-3.17573400	-1.64217300	0.52150100
P	3.57532200	-1.35069500	-0.51971600
P	2.70872600	1.72617200	-0.32512000
C	-3.71916200	1.86631700	-1.19566100
C	-5.10776800	2.00861300	-1.12986300
C	-5.83055100	2.33805700	-2.27318400
C	-5.17601200	2.51708600	-3.48714900
C	-3.79775200	2.32892300	-3.56814100
C	-3.07026200	2.00945500	-2.42795600
C	-2.15754000	3.12095300	0.86551900
C	-2.93756800	4.27693600	0.73735700
C	-2.47336200	5.49051900	1.23644400
C	-1.21597300	5.56898800	1.83057800
C	-0.42564700	4.42865600	1.93250700
C	-0.89950700	3.20816200	1.46556500
C	-4.06297700	-0.52094800	1.67501700
C	-4.93237800	-0.98251200	2.66602400
C	-5.61142600	-0.08391100	3.48082800
C	-5.42384500	1.28000700	3.31648900
C	-4.55026500	1.75497000	2.34973300
C	-3.86445100	0.86941900	1.51912400
C	-4.37167100	-1.75859500	-0.85911800
C	-5.70841000	-2.09293800	-0.62645000
C	-6.63729600	-2.02254700	-1.65381500
C	-6.23749400	-1.62190500	-2.92994000
C	-4.90291800	-1.32488800	-3.17895300
C	-3.97165400	-1.38811100	-2.14447700
C	-3.19873700	-3.29105900	1.29844300
C	-2.78980900	-3.48076100	2.62652400
C	-2.67087200	-4.76852300	3.14094900
C	-2.93189000	-5.87850400	2.34309900
C	-3.32569400	-5.69501600	1.02184500
C	-3.46380500	-4.41212000	0.50440900
C	3.56827400	-2.92259800	-1.44148700
C	2.96377900	-3.00609500	-2.70148500
C	2.94342400	-4.21099400	-3.38632300
C	3.55211100	-5.34335500	-2.84808100
C	4.19380800	-5.26017800	-1.61905500
C	4.18837700	-4.05835600	-0.91403400
C	4.51185900	-1.72223700	1.01546500
C	3.84390700	-2.18255300	2.15712100

C	4.54584900	-2.39133500	3.34115900
C	5.91878500	-2.15999400	3.38989000
C	6.59174100	-1.72828000	2.24828900
C	5.89030700	-1.49358800	1.06999800
C	4.07641000	1.25962300	-1.34761900
C	4.88733000	2.20866500	-2.02696400
C	5.96678700	1.83412600	-2.79041600
C	6.31005300	0.45731900	-2.93381200
C	5.55475700	-0.49438500	-2.27186200
C	4.44476800	-0.14357500	-1.48815900
C	1.68862300	2.97753000	-1.21000400
C	1.59822400	4.30748600	-0.78134500
C	0.85145200	5.23739600	-1.50263700
C	0.18410100	4.85862200	-2.66129800
C	0.25921900	3.53397400	-3.09311900
C	0.99611300	2.60364700	-2.37059900
C	3.25958700	2.63492100	1.17468400
C	2.77585400	2.27365900	2.43949500
C	3.20559200	2.94321000	3.58383900
C	4.13055300	3.97684100	3.48636400
C	4.63027700	4.32714900	2.23467800
C	4.20125500	3.66798500	1.09101100
H	-5.62388300	1.84310200	-0.18941900
H	-6.90865900	2.44927700	-2.22016000
H	-5.74235000	2.79895000	-4.36692200
H	-3.28701100	2.42166300	-4.52271400
H	-1.99493900	1.86142600	-2.48966100
H	-3.89979700	4.22802000	0.23324300
H	-3.08824600	6.38148400	1.15144500
H	-0.84885200	6.52382000	2.19281200
H	0.57609800	4.47177800	2.34829100
H	-0.28044100	2.31947100	1.54916900
H	-5.07394200	-2.05099400	2.80614400
H	-6.29998000	-0.43903800	4.23673500
H	-5.92690700	1.97472900	3.97036700
H	-4.36989900	2.82160200	2.26389600
H	-6.02353900	-2.39184500	0.36818000
H	-7.66910100	-2.27311200	-1.43517800
H	-6.95651300	-1.54670600	-3.74006800
H	-4.58841100	-1.02068600	-4.17341200
H	-2.93339200	-1.12929000	-2.32824400
H	-2.55275700	-2.62544800	3.25383400

H	-2.34984700	-4.91513700	4.16691700
H	-2.80997700	-6.87620400	2.75243500
H	-3.52134200	-6.54493000	0.37885500
H	-3.77185100	-4.27724700	-0.52785200
H	2.50527300	-2.13041500	-3.14256700
H	2.46149200	-4.26455600	-4.35343900
H	3.53698600	-6.27857300	-3.39794400
H	4.69460500	-6.13034100	-1.20437100
H	4.67975600	-3.98507100	0.04742000
H	2.77219500	-2.35924100	2.12541200
H	4.01838000	-2.72677400	4.23003500
H	6.45900700	-2.32439100	4.31564500
H	7.66446500	-1.56004700	2.27057500
H	6.41042400	-1.12887600	0.18798400
H	4.59102600	3.25260300	-1.99838100
H	6.53190700	2.58348300	-3.33572000
H	7.12575800	0.15712400	-3.58112600
H	5.80204900	-1.54831300	-2.39192600
H	2.10417600	4.62697400	0.12281700
H	0.78975000	6.26128100	-1.14702900
H	-0.39485000	5.58623900	-3.22171200
H	-0.26025800	3.22339800	-3.99671600
H	1.03032200	1.57383100	-2.70618600
H	2.05909800	1.46388800	2.53226000
H	2.81307000	2.65964300	4.55526700
H	4.45867500	4.49996200	4.38062500
H	5.37278900	5.10588200	2.13459300
H	4.60850900	3.95522400	0.12712400

**T<sub>1</sub>(1)**

I	0.02820900	-1.09348800	-2.03865500
I	0.21116500	-0.66922300	2.23712900
Cu	-1.33274500	-0.35458000	0.06195800
Cu	1.59965200	-0.28823700	-0.01778200
P	-2.67881800	1.47666600	0.25188400
P	-3.18511600	-1.64053000	0.51591700
P	3.59824100	-1.34214200	-0.52928500
P	2.72794000	1.72265500	-0.32346900
C	-3.71866200	1.87093900	-1.20011900
C	-5.10662800	2.01992900	-1.13554000
C	-5.82677800	2.35431200	-2.27910900
C	-5.17018500	2.53221700	-3.49214600

C	-3.79277100	2.33742200	-3.57211200
C	-3.06801600	2.01230300	-2.43174900
C	-2.15760700	3.11955100	0.86353000
C	-2.93597600	4.27684200	0.73682400
C	-2.47071000	5.48919500	1.23810600
C	-1.21355200	5.56541600	1.83291300
C	-0.42467500	4.42390700	1.93343300
C	-0.89973600	3.20453100	1.46447400
C	-4.07177000	-0.51813400	1.66910600
C	-4.94331900	-0.97797900	2.65903500
C	-5.62146200	-0.07815400	3.47332100
C	-5.43096700	1.28545000	3.30943100
C	-4.55512000	1.75867100	2.34382400
C	-3.87002800	0.87186500	1.51389300
C	-4.37953200	-1.75295700	-0.86618300
C	-5.71761500	-2.08354600	-0.63627100
C	-6.64454300	-2.00871700	-1.66506800
C	-6.24132100	-1.60718500	-2.93984700
C	-4.90532300	-1.31416600	-3.18620800
C	-3.97590800	-1.38204000	-2.15032000
C	-3.21296600	-3.28977200	1.29185800
C	-2.80525900	-3.48143500	2.61999500
C	-2.68887700	-4.76990300	3.13322300
C	-2.95111500	-5.87867100	2.33407200
C	-3.34355300	-5.69315500	1.01270600
C	-3.47929800	-4.40953500	0.49655000
C	3.58466600	-2.92057300	-1.43711600
C	2.98558500	-2.99547100	-2.70027900
C	2.95279400	-4.19972500	-3.38645600
C	3.54483300	-5.33883600	-2.84454800
C	4.18063800	-5.26519600	-1.61105000
C	4.18497500	-4.06445900	-0.90501300
C	4.49109600	-1.72751100	1.03492300
C	3.81741500	-2.18698900	2.17286600
C	4.51543700	-2.40001300	3.35874500
C	5.88946000	-2.17459500	3.41248100
C	6.56818400	-1.74332700	2.27404400
C	5.87076600	-1.50308700	1.09475600
C	4.11986800	1.26454200	-1.32965700
C	4.91401200	2.20550400	-2.01321800
C	5.98202900	1.83491900	-2.80394700
C	6.28573400	0.44755500	-2.97909300



C	5.52962200	-0.50376400	-2.34207900
C	4.44009100	-0.15224900	-1.50002200
C	1.72303900	2.98973800	-1.19633800
C	1.64292400	4.32079000	-0.76781800
C	0.89151600	5.25199200	-1.48183200
C	0.21101100	4.87492500	-2.63387400
C	0.27639700	3.54965400	-3.06540100
C	1.01521300	2.61655300	-2.34886300
C	3.27925000	2.60131100	1.19435000
C	2.76876500	2.24539400	2.44775100
C	3.17664500	2.91968100	3.59815600
C	4.10100500	3.95392400	3.51383200
C	4.62317900	4.30283100	2.27152200
C	4.21761600	3.63597900	1.12306100
H	-5.62440500	1.85573000	-0.19574900
H	-6.90440100	2.47079400	-2.22690000
H	-5.73429000	2.81816500	-4.37207100
H	-3.28080800	2.42929300	-4.52613300
H	-1.99360800	1.85718500	-2.49275100
H	-3.89816200	4.22997700	0.23241300
H	-3.08474200	6.38092600	1.15473000
H	-0.84573600	6.51925700	2.19717100
H	0.57642200	4.46586100	2.35103400
H	-0.28284600	2.31422800	1.54796500
H	-5.08726600	-2.04620200	2.79875100
H	-6.31145300	-0.43210700	4.22851400
H	-5.93352100	1.98129900	3.96264400
H	-4.37259700	2.82497600	2.25849100
H	-6.03526600	-2.38289700	0.35742100
H	-7.67743700	-2.25654500	-1.44848200
H	-6.95882700	-1.52830100	-3.75099100
H	-4.58822200	-1.00961700	-4.17974300
H	-2.93625900	-1.12653100	-2.33164000
H	-2.56669900	-2.62713400	3.24814600
H	-2.36873000	-4.91811800	4.15923400
H	-2.83100900	-6.87696500	2.74249900
H	-3.53978000	-6.54187900	0.36839200
H	-3.78598500	-4.27306100	-0.53590400
H	2.53904300	-2.11246800	-3.13919400
H	2.47409200	-4.24829500	-4.35567200
H	3.52081900	-6.27400700	-3.39442500
H	4.66836600	-6.14246500	-1.19587700

H	4.67032700	-3.99519900	0.05971300
H	2.74564200	-2.36221600	2.13710000
H	3.98461200	-2.73644000	4.24534500
H	6.42667100	-2.34376900	4.33910400
H	7.64181300	-1.58146900	2.29915200
H	6.39429200	-1.14155000	0.21314900
H	4.63118200	3.25213600	-1.95794000
H	6.55484400	2.58270000	-3.34103000
H	7.09234000	0.14697100	-3.63833700
H	5.75310100	-1.55768700	-2.49854400
H	2.15833100	4.63974600	0.13140700
H	0.83498300	6.27592100	-1.12577800
H	-0.37167900	5.60408500	-3.18842600
H	-0.25296800	3.24050200	-3.96364000
H	1.03838300	1.58533100	-2.68179000
H	2.05075400	1.43556400	2.52920900
H	2.76855900	2.63751900	4.56322700
H	4.41154200	4.47985700	4.41281600
H	5.36526200	5.08363000	2.18325100
H	4.64152300	3.91874000	0.16518900

**S<sub>0</sub> (2)**

I	0.15492900	-0.91660700	2.33043100
I	0.05715400	-1.01732700	-2.16615100
Cu	-1.27624600	-0.53307200	0.05763800
Cu	1.52855600	-0.49291500	0.05541400
P	-2.49355700	1.38601900	0.49204500
P	-3.25002700	-1.74663100	0.24411100
P	3.63803400	-1.33358500	-0.33930000
P	2.23168200	1.65282000	-0.33067800
N	-4.25448700	1.43057900	2.58925000
N	5.68727500	-0.09155500	-1.69569500
C	-1.95971800	2.91311300	1.35536500
C	-2.36599600	4.18983700	0.95399900
C	-1.84620600	5.32033100	1.58194700
C	-0.93091400	5.19007200	2.62300800
C	-0.53436200	3.92077100	3.03810100
C	-1.03877600	2.78977200	2.40348600
C	-3.44833100	1.99635900	-0.94166300
C	-4.80693500	2.31638100	-0.88504600
C	-5.47540000	2.77207200	-2.01714600
C	-4.79410600	2.89394100	-3.22558700

C	-3.44447700	2.55820400	-3.29197100
C	-2.76829800	2.12193000	-2.15793500
C	-4.05792800	-0.72847700	1.53824400
C	-4.95204900	-1.26098500	2.46386300
C	-5.48746500	-0.44101800	3.44516100
C	-5.09326500	0.88998600	3.47007100
C	-3.74653600	0.64589400	1.63940800
C	-4.40842200	-1.51044000	-1.15231900
C	-5.80421600	-1.54316400	-1.03349700
C	-6.61029400	-1.17492200	-2.10591500
C	-6.02919000	-0.71881100	-3.28833200
C	-4.64580700	-0.67214000	-3.40586000
C	-3.83960800	-1.09499200	-2.35738600
C	-3.46114900	-3.46116000	0.85172900
C	-4.56308700	-4.27257600	0.55670500
C	-4.64981000	-5.55483300	1.09324100
C	-3.63917000	-6.04443300	1.91757400
C	-2.52841300	-5.25245900	2.19588500
C	-2.43793000	-3.96946800	1.66288100
C	4.71452900	-1.70414400	1.10201900
C	4.12218500	-1.66183800	2.36968000
C	4.87116200	-1.94798600	3.50885300
C	6.21367500	-2.28700900	3.38912400
C	6.80793600	-2.34790400	2.13058400
C	6.06617100	-2.05385200	0.98984100
C	3.86255800	-2.75193000	-1.49272200
C	2.72942400	-3.55442100	-1.67551700
C	2.76736500	-4.68902600	-2.48112500
C	3.94487900	-5.02820900	-3.13612200
C	5.06973200	-4.21819500	-2.99297800
C	5.03892200	-3.08888200	-2.17791700
C	3.82771200	1.37057700	-1.22867700
C	4.45934500	2.38323900	-1.96427700
C	5.69388800	2.14729600	-2.54958700
C	6.27384100	0.89502100	-2.36930700
C	4.48104800	0.12022500	-1.15417300
C	2.85278800	2.64540700	1.07630600
C	2.71881200	2.18952600	2.38967700
C	3.26680000	2.92560400	3.44126900
C	3.95309600	4.10239900	3.17860500
C	4.05546600	4.57528400	1.87665400
C	3.50891000	3.85377800	0.83255900

C	1.35892600	2.91286400	-1.34347200
C	0.84833400	4.07789600	-0.75676400
C	0.15632500	5.01182200	-1.52231000
C	-0.04601500	4.79576300	-2.88087000
C	0.40509800	3.61376200	-3.46316500
C	1.09382900	2.67597600	-2.70013800
H	-3.07527400	4.30593100	0.13962200
H	-2.14603700	6.30852700	1.24569000
H	-0.51873900	6.07070200	3.10504300
H	0.18381700	3.81105500	3.84655400
H	-0.70540400	1.80311400	2.71224000
H	-5.34536500	2.19858700	0.04686600
H	-6.53047800	3.01597800	-1.94942300
H	-5.31332900	3.22772600	-4.11936000
H	-2.91747100	2.60214200	-4.23960500
H	-1.71729900	1.85066100	-2.22069200
H	-5.19709800	-2.31889700	2.42800700
H	-6.18767600	-0.82380400	4.17826600
H	-5.46003100	1.55788400	4.23736600
H	-6.26703400	-1.82199900	-0.09144700
H	-7.69143700	-1.21586000	-2.00335300
H	-6.64129400	-0.37041800	-4.11237800
H	-4.17681900	-0.26546400	-4.29483200
H	-2.75914600	-1.05059200	-2.45340400
H	-5.34678700	-3.92049000	-0.10731700
H	-5.50484500	-6.17209000	0.84685900
H	-3.71028800	-7.04030600	2.34159900
H	-1.72969000	-5.63444100	2.82529400
H	-1.57068600	-3.35094900	1.87887200
H	3.06689200	-1.41711300	2.46016800
H	4.40281800	-1.92056100	4.48878900
H	6.79430500	-2.51571300	4.27472100
H	7.84736200	-2.64696600	2.04277700
H	6.53584200	-2.09545500	0.01351300
H	1.79194600	-3.24563500	-1.23542800
H	1.87006100	-5.28846700	-2.60984400
H	3.98229400	-5.90651000	-3.77392600
H	5.97425000	-4.46586500	-3.53834500
H	5.90934900	-2.44615300	-2.10678500
H	3.96683100	3.34125200	-2.10804100
H	6.19044300	2.90698300	-3.14474500
H	7.24288800	0.66689400	-2.80786600

H	2.18653500	1.26226300	2.58545200
H	3.16256800	2.58696500	4.46526900
H	4.45253000	4.64380900	3.97235900
H	4.59079000	5.48632500	1.66738900
H	3.59495000	4.23248500	-0.17895300
H	0.97949500	4.26546700	0.30414900
H	-0.22855400	5.90483900	-1.04137600
H	-0.56634500	5.53893100	-3.47655100
H	0.21447600	3.41214500	-4.51274000
H	1.39448000	1.74172700	-3.15768500

**S<sub>1</sub>(2)**

I	0.18538000	-0.90599100	2.24408500
I	0.05125900	-1.09207300	-2.09472800
Cu	-1.33467400	-0.50009600	0.05209400
Cu	1.58979500	-0.48197000	0.02003300
P	-2.52837800	1.41962200	0.49227600
P	-3.30613100	-1.71944600	0.25210100
P	3.72859800	-1.26149900	-0.37396000
P	2.39421200	1.63102200	-0.37371800
N	-4.29439700	1.47556500	2.58021900
N	5.78864000	-0.10116100	-1.65326700
C	-1.97934300	2.93849800	1.35520600
C	-2.37614400	4.21708200	0.95098100
C	-1.83744000	5.34402700	1.56867500
C	-0.91315000	5.20828200	2.60108300
C	-0.52801900	3.93730800	3.02104200
C	-1.05226500	2.80979100	2.39689200
C	-3.45999100	2.02081900	-0.95809800
C	-4.81882400	2.34161200	-0.92094500
C	-5.47377800	2.78161900	-2.06686400
C	-4.77898300	2.88492600	-3.26922500
C	-3.42832200	2.54947900	-3.31541100
C	-2.76491800	2.13145000	-2.16727000
C	-4.11009200	-0.68768800	1.53635800
C	-5.00945900	-1.21164300	2.46209100
C	-5.54271700	-0.38477100	3.43819300
C	-5.13884400	0.94354000	3.46044400
C	-3.79041700	0.68514700	1.63323000
C	-4.44779300	-1.48875100	-1.15625600
C	-5.84453400	-1.51512100	-1.04984200
C	-6.63845800	-1.15341400	-2.13335400

C	-6.04415900	-0.71065800	-3.31424400
C	-4.65957000	-0.67010400	-3.41958000
C	-3.86569400	-1.08608700	-2.35940500
C	-3.52184500	-3.42783900	0.87277200
C	-4.62656500	-4.23722400	0.58264500
C	-4.72070900	-5.51316700	1.13275300
C	-3.71501300	-5.99858000	1.96566100
C	-2.60142600	-5.20892500	2.23935800
C	-2.50386200	-3.93219300	1.69285700
C	4.69566600	-1.67837100	1.12150200
C	4.09537700	-1.60230600	2.38218400
C	4.82215300	-1.91814000	3.52750700
C	6.15071000	-2.31209400	3.42036900
C	6.75287300	-2.39899900	2.16741500
C	6.03288600	-2.08526700	1.01841600
C	3.85899700	-2.73605200	-1.45991900
C	2.74377200	-3.57220900	-1.57356100
C	2.78607800	-4.72991800	-2.34430500
C	3.95107600	-5.05885800	-3.02750800
C	5.05713200	-4.21600200	-2.94743600
C	5.02517600	-3.06033800	-2.16993500
C	3.88155100	1.36834900	-1.30145100
C	4.56770500	2.43910900	-1.99117800
C	5.83709000	2.16799400	-2.49138200
C	6.42861900	0.93141000	-2.30877400
C	4.57920200	0.14608400	-1.19885200
C	2.84019000	2.63162500	1.07414300
C	2.72730000	2.18122900	2.39559000
C	3.27141000	2.92773100	3.43652500
C	3.95694100	4.10721600	3.16250100
C	4.05576000	4.56366800	1.85562700
C	3.49640400	3.84475500	0.81570500
C	1.32526800	2.77440100	-1.33943100
C	0.78961400	3.92243700	-0.73968000
C	0.11569400	4.87160800	-1.50464800
C	-0.05616400	4.67727000	-2.87064200
C	0.40971300	3.50533500	-3.46478700
C	1.09196000	2.56195300	-2.70529600
H	-3.08793600	4.33703600	0.13931400
H	-2.12598600	6.33398300	1.22829000
H	-0.48217300	6.08639300	3.07068000
H	0.20119900	3.82359300	3.81850300

H	-0.72377300	1.82299900	2.70864900
H	-5.36831800	2.23633800	0.00576400
H	-6.52910700	3.02705400	-2.01405800
H	-5.28816200	3.20518200	-4.17355700
H	-2.88988400	2.58009900	-4.25698100
H	-1.71056500	1.87000900	-2.21347500
H	-5.25968600	-2.26842200	2.43025200
H	-6.24842300	-0.75988300	4.16972000
H	-5.50209300	1.61546300	4.22534600
H	-6.31743900	-1.78399200	-0.10994400
H	-7.72050200	-1.18947700	-2.04062500
H	-6.64642100	-0.36807900	-4.14768400
H	-4.18108000	-0.27435200	-4.30833700
H	-2.78458300	-1.04799600	-2.44614100
H	-5.40647600	-3.88872300	-0.08767000
H	-5.57767100	-6.12927700	0.89041800
H	-3.79171900	-6.98986000	2.39936000
H	-1.80674000	-5.58848100	2.87522500
H	-1.63393100	-3.31616200	1.90401200
H	3.05439400	-1.30685100	2.46950200
H	4.34823900	-1.86684100	4.50363700
H	6.71395800	-2.55998300	4.31224600
H	7.78323100	-2.72964600	2.08850000
H	6.50805700	-2.13894700	0.04589900
H	1.81207100	-3.27536000	-1.11713700
H	1.90125100	-5.35525700	-2.42680700
H	3.99018100	-5.95403700	-3.64139900
H	5.94547700	-4.45097000	-3.52318200
H	5.86927200	-2.37849400	-2.15159600
H	4.06805800	3.37568900	-2.21150900
H	6.36851200	2.93012000	-3.05502300
H	7.41064900	0.70752100	-2.70813400
H	2.21120500	1.24949400	2.60599100
H	3.16846000	2.59857100	4.46413700
H	4.46043800	4.65419500	3.94986600
H	4.59743600	5.46830400	1.63651100
H	3.58459100	4.21068000	-0.19958400
H	0.91412100	4.09469200	0.32426000
H	-0.26817700	5.76565500	-1.02354300
H	-0.55672100	5.43429600	-3.46661000
H	0.25088500	3.32702000	-4.52383600
H	1.43440000	1.65149300	-3.17670300

**T<sub>1</sub> (2)**

I	0.19097100	-0.91239200	2.23890700
I	0.05093400	-1.07294800	-2.10059000
Cu	-1.34349700	-0.50681500	0.04978300
Cu	1.59963600	-0.48805700	0.02020100
P	-2.53354100	1.41220200	0.49804000
P	-3.31220000	-1.72423900	0.24623200
P	3.74396000	-1.25534700	-0.37124600
P	2.39576300	1.63200500	-0.37783000
N	-4.29875800	1.46176200	2.58730200
N	5.79674300	-0.07604400	-1.65600700
C	-1.98381700	2.92809900	1.36633100
C	-2.37849300	4.20864000	0.96614800
C	-1.83881600	5.33279400	1.58809200
C	-0.91556000	5.19242900	2.62079800
C	-0.53252400	3.91950900	3.03675100
C	-1.05779600	2.79479100	2.40842100
C	-3.46461800	2.02078700	-0.94976500
C	-4.82271900	2.34439700	-0.91125500
C	-5.47678200	2.79086900	-2.05517200
C	-4.78176600	2.89829600	-3.25704500
C	-3.43188000	2.55995800	-3.30477300
C	-2.76945100	2.13499300	-2.15859700
C	-4.11630200	-0.69735500	1.53444500
C	-5.01567600	-1.22450300	2.45827300
C	-5.54768000	-0.40140300	3.43827200
C	-5.14270900	0.92643700	3.46602600
C	-3.79596100	0.67496600	1.63666300
C	-4.45368800	-1.48735900	-1.16134300
C	-5.85047100	-1.51244900	-1.05530700
C	-6.64375400	-1.14532100	-2.13747400
C	-6.04865800	-0.69859300	-3.31647900
C	-4.66395300	-0.65933400	-3.42132800
C	-3.87069200	-1.08055900	-2.36269700
C	-3.52923800	-3.43485300	0.86025700
C	-4.63438600	-4.24258300	0.56723100
C	-4.72876500	-5.52086000	1.11188100
C	-3.72287800	-6.01002900	1.94237900
C	-2.60899200	-5.22181400	2.21913300
C	-2.51108000	-3.94286300	1.67785400
C	4.71956200	-1.68139900	1.11564600



C	4.11901300	-1.59983700	2.37614700
C	4.84066500	-1.92644600	3.52164200
C	6.16448700	-2.33550000	3.41478300
C	6.76696200	-2.42813500	2.16229200
C	6.05124000	-2.10525200	1.01331900
C	3.87125900	-2.72348400	-1.46645200
C	2.75371300	-3.55696300	-1.57669500
C	2.78842400	-4.71110300	-2.35330700
C	3.94785700	-5.03812900	-3.04666300
C	5.05594600	-4.19733200	-2.97044700
C	5.03154600	-3.04593700	-2.18634100
C	3.87164400	1.37271300	-1.31178400
C	4.54940900	2.43977500	-2.01716000
C	5.82446500	2.18793300	-2.50134600
C	6.43549100	0.95871800	-2.30283100
C	4.58868200	0.15458200	-1.19991600
C	2.82659500	2.61698300	1.09194000
C	2.71541500	2.16228800	2.41151500
C	3.26615000	2.90320300	3.45337100
C	3.95672600	4.08025700	3.18281000
C	4.05533900	4.54068500	1.87708500
C	3.49060200	3.82700900	0.83679400
C	1.33320500	2.79422800	-1.33005200
C	0.79316500	3.93563100	-0.72177500
C	0.11500000	4.88683100	-1.47989100
C	-0.05855400	4.69936600	-2.84690200
C	0.40952600	3.53257700	-3.44921100
C	1.09618400	2.58719100	-2.69614500
H	-3.08972000	4.33229300	0.15453800
H	-2.12584000	6.32427700	1.25091100
H	-0.48394400	6.06838400	3.09382900
H	0.19562500	3.80210800	3.83468000
H	-0.73109200	1.80640300	2.71696300
H	-5.37237500	2.23632300	0.01503900
H	-6.53159500	3.03821800	-2.00114600
H	-5.29025300	3.22385900	-4.15987900
H	-2.89352600	2.59357800	-4.24630800
H	-1.71608100	1.86983000	-2.20612200
H	-5.26662700	-2.28097600	2.42215400
H	-6.25321300	-0.77910200	4.16862400
H	-5.50457800	1.59517300	4.23435300
H	-6.32386300	-1.78453600	-0.11656600

H	-7.72588000	-1.18026000	-2.04510700
H	-6.65057500	-0.35213100	-4.14862200
H	-4.18475700	-0.26071200	-4.30843500
H	-2.78939700	-1.04314000	-2.44877500
H	-5.41444900	-3.89079600	-0.10122300
H	-5.58595000	-6.13575200	0.86704900
H	-3.79968600	-7.00312300	2.37191700
H	-1.81439100	-5.60430800	2.85332800
H	-1.64077400	-3.32784900	1.89095600
H	3.08102900	-1.29310200	2.46232900
H	4.36652000	-1.87236000	4.49747000
H	6.72341700	-2.59109400	4.30698100
H	7.79356700	-2.77031100	2.08425300
H	6.52533800	-2.16745600	0.04073400
H	1.82625500	-3.25977400	-1.11171000
H	1.90207400	-5.33472300	-2.43265900
H	3.98117800	-5.92999100	-3.66579800
H	5.93904700	-4.43083700	-3.55469300
H	5.87827700	-2.36720700	-2.17009700
H	4.04358800	3.37401000	-2.23535200
H	6.34840900	2.95418400	-3.06600400
H	7.42463600	0.74552800	-2.68964900
H	2.19528900	1.23247000	2.62028100
H	3.16372800	2.57096400	4.48007500
H	4.46510800	4.62136700	3.97108300
H	4.60111500	5.44327300	1.65874000
H	3.58065400	4.19554700	-0.17783600
H	0.91734500	4.10056900	0.34337300
H	-0.27206500	5.77635000	-0.99315900
H	-0.56480600	5.45724600	-3.43693400
H	0.24662500	3.35896700	-4.50838800
H	1.43832900	1.67831400	-3.17149100