Supporting Information for

N-heterocyclic carbene-stabilized Cu_9 Clusters with Combined Thermally Activated Delayed Fluorescence and Phosphorescence

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I. Experimental section

Chemicals and materials

Copper powder (Cu, 99%), copper(II) trifluoroacetate hydrate ($Cu(CF_3CO_2)_2 \cdot H_2O$, 99%), Tert-butyl acetylene ($^tBuC{\equiv}CH$, 96%), 2-bromopyridine (98%) were purchased from Shanghai Aladdin Biochemical Technology Co., Ltd. Imidazole (99%), phenylacetylene (PhC≡CH, 97%), potassium carbonate (K_2CO_3, 99%), magnesium sulfate ($MgSO_4$, 99%), sodium chloride (NaCl, 99.9%), sodium carbonate anhydrous (Na_2CO_3, 99%) were purchased from Shanghai Macklin Biochemical Technology Co., Ltd. dichloromethane (DCM, 99%), diethyl ether (Et_2O, 99%), ethanol (EtOH, 99%), were purchased by Guangzhou Biohonor Biotechnology Co., Ltd..

Synthesis of 1,3-di(pyridine-2-yl)-1H-imidazol-3-ium hexafluorophosphate $[H(py)_2im](PF_6)$

Cation! *The synthesis of the ligand at elevated temperatures may cause unexpected hazard. It is crucial to follow established safety protocols and maintain a secure laboratory environment.*

1,3-di(pyridin-2-yl)-1H-imidazol-3-ium hexafluorophosphate was synthesized following a previously reported procedure. Imidazole (5.8 g, 84.6 mmol), 2-bromopyridine (2.7 ml, 28.6 mmol) and potassium carbonate (7.8 g, 56.4 mmol) were added into a 200 ml round bottom flask. The mixture was heated to 190°C and stirred for about 19 h. Upon cooling to RT, the resulting solid was dissolved in 200 ml of water, then extracted with 3×200 ml of dichloromethane. The organic phase obtained was then subjected to wash with 3×200 ml of saturated sodium carbonate solution, followed by a wash with 200 ml of saturated aqueous sodium chloride solution. The obtained organic phase was dehydrated with anhydrous magnesium sulfate. After filtration, the obtained solution was rotary evaporated to dryness to obtain 3.3 g of a yellow oil (yield ~79.7%). ^{1}H NMR (d_6-DMSO): δ = 8.55 (s, 1H), 8.47–8.48 (d, 1H), 7.95–7.99 (m, 2H), 7.79 (d, J = 7.5 Hz, 1H), 7.34 (dd, J = 4.4, 3.9 Hz, 1H), 7.13 (s, 1H).

Next, the obtained yellow oil (2.5 g, 17.2 mmol) was combined with 2-bromopyridine (4.1 g, 25.8 mmol) in a 50 ml round bottom flask. The mixture was stirred under N_2 atmosphere at 160°C for 24 hours. After cooling to RT, the crude product was washed with a substantial quantity of Et_2O, followed by a 10 ml methanol wash. The isolated solid was dissolved in water, and a saturated aqueous solution of ammonium hexafluorophosphate was added dropwise, resulting in the immediate formation of a large amount of white solid. After stirring for 30 min, the obtained solid was filtered by suction, and subsequently vacuum-dried at 50°C overnight. Yield: 4.17 g, 65.9 %. ^{1}H NMR (d_6-DMSO, Fig. S1): δ = 10.78 (s, 1H), 8.73 (s, 2H), 8.73 (d, 2H), 8.27 (m, 4H), 7.71 (t, 2H).

II. Supporting figures

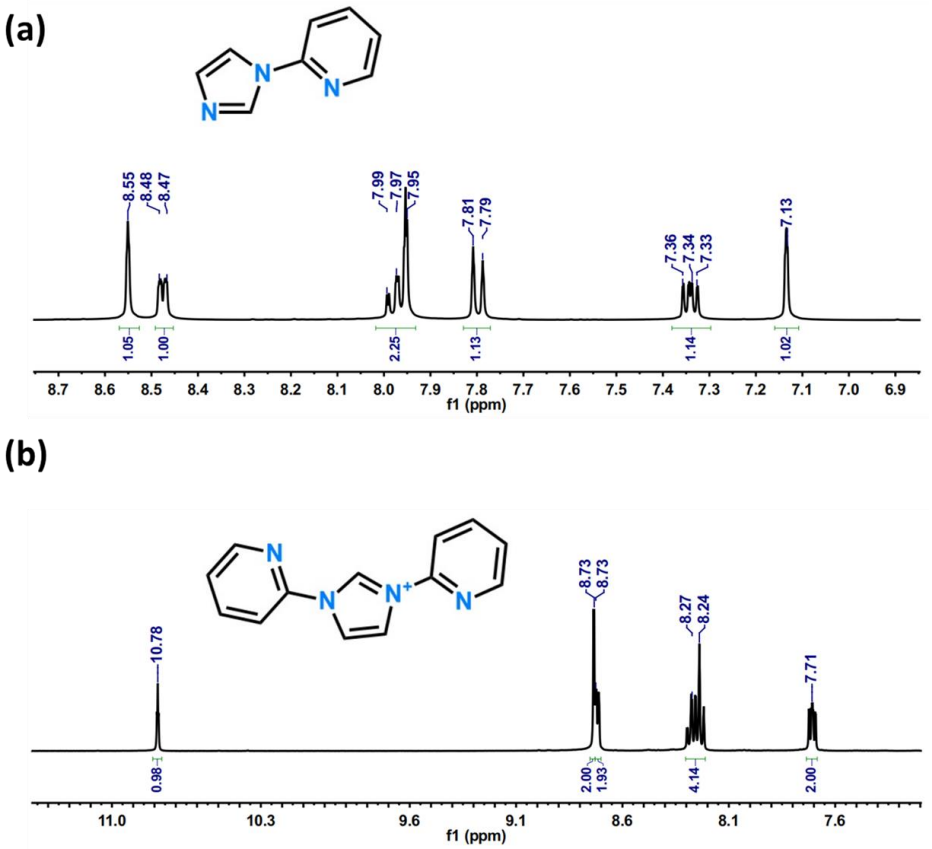

Figure S1. ^{1}H NMR for (a) 2-(1H-imidazol-1-yl)pyridine and (b) [H(py)$_2$im](PF$_6$).

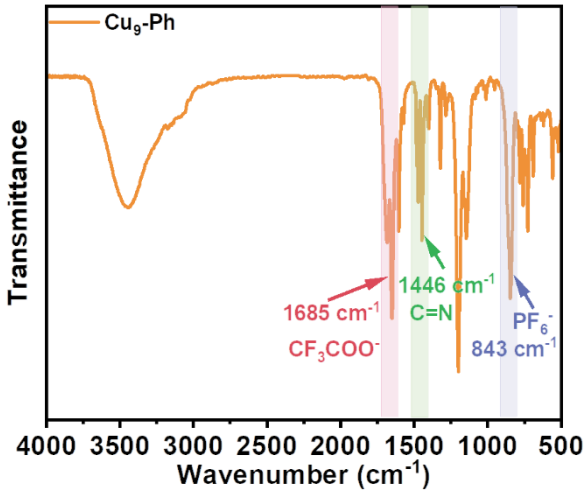

Figure S2. FT-IR spectra of **Cu9-Ph**.

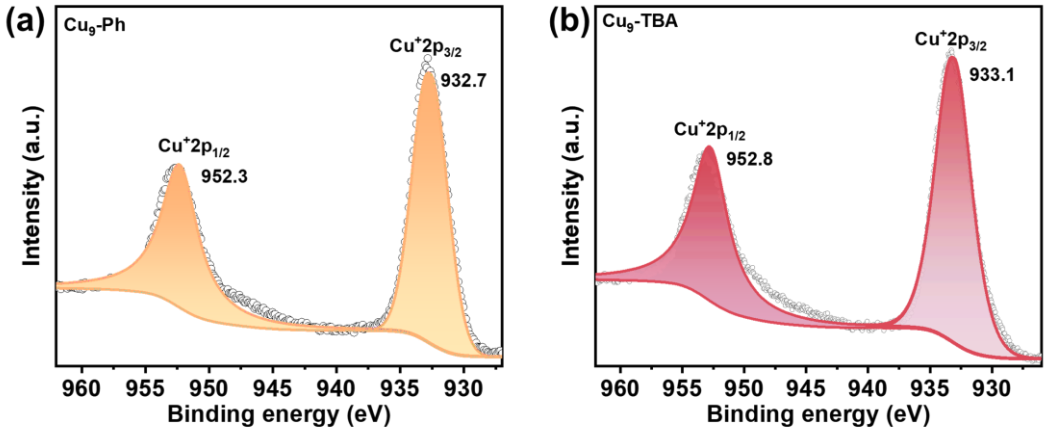

Figure S3. (a-b) X-ray photoelectron spectrum of **Cu9-Ph**; (c-d) X-ray photoelectron spectrum of **Cu9-TBA**.

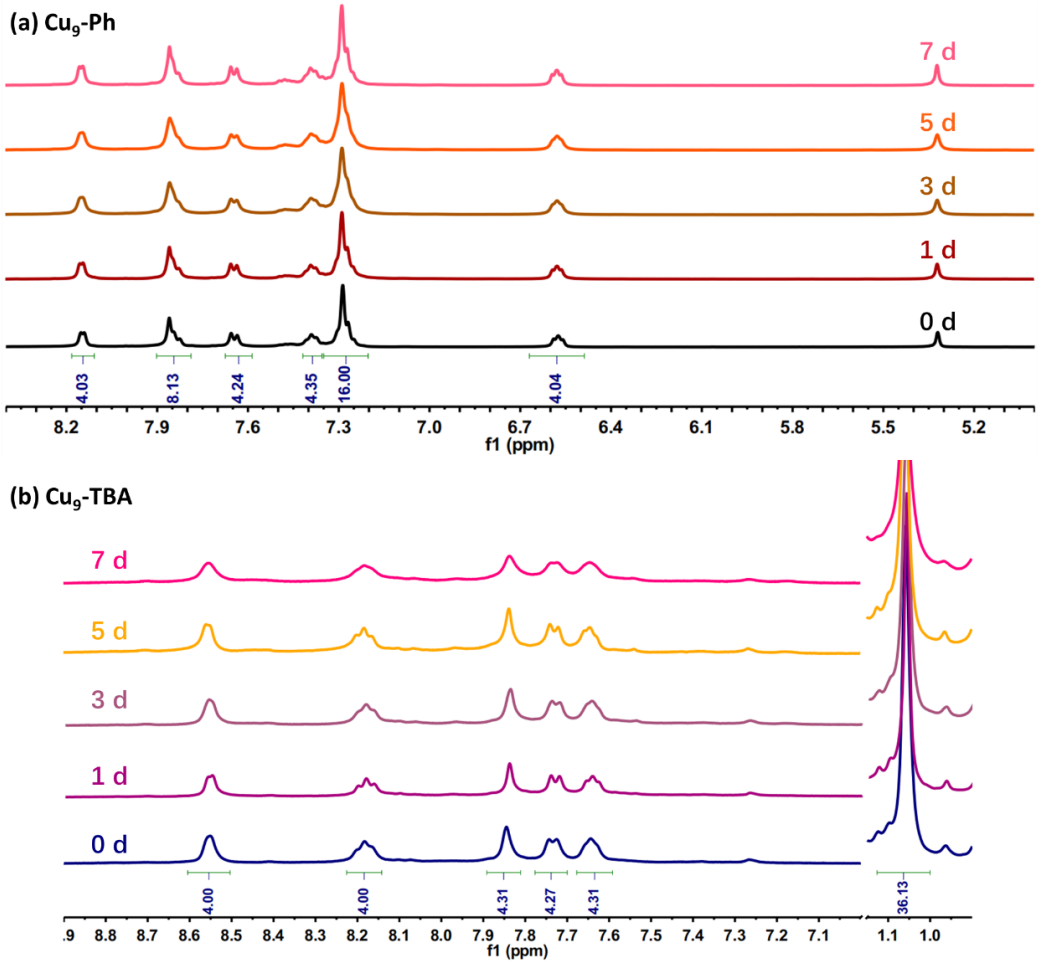

Figure S4. Stability check: (a) The ^{1}HNMR spectrum of **Cu$_9$-Ph** in CD_2Cl_2 at room temperature; (b) The ^{1}HNMR spectrum of **Cu$_9$-TBA** in CD_2Cl_2 at room temperature.

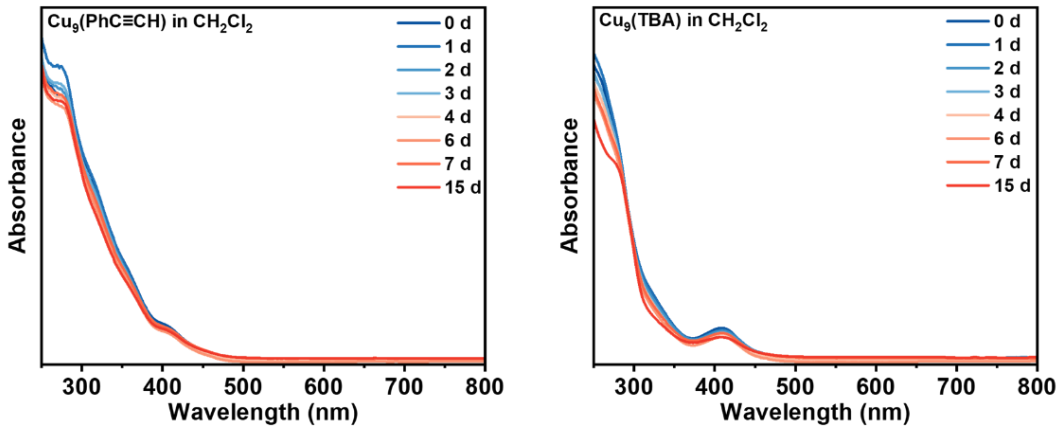

Figure S5. Stability check: (a) The UV-vis spectrum of **Cu$_9$-Ph** in CD_2Cl_2 at room temperature; (b) The UV-vis spectrum of **Cu$_9$-TBA** in CD_2Cl_2 at room temperature.

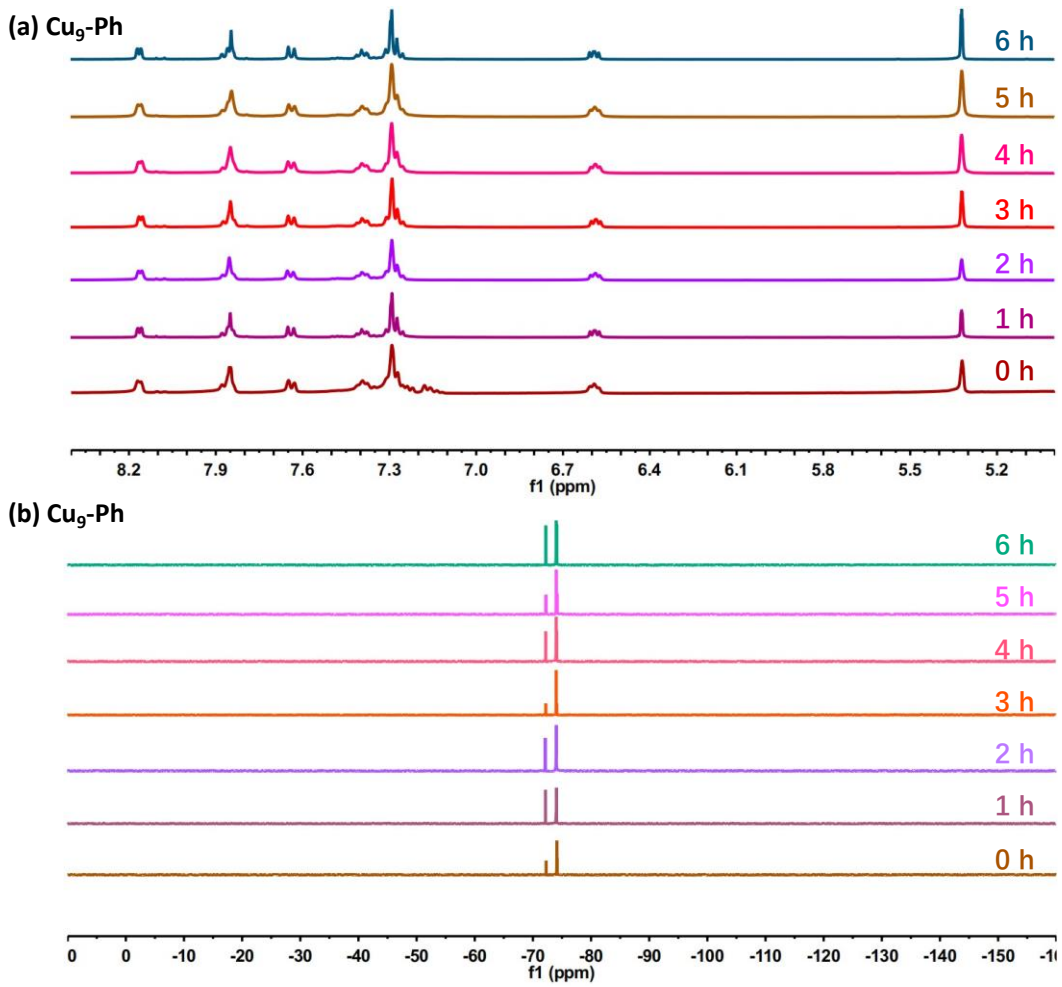

Figure S6. Stability check: Place **Cu9-Ph** in an oven at 50°C for heating, take a portion of the solid and dissolve it in CD_2Cl_2 every hour, and then perform (a) ^{1}H NMR spectrum test and (b) ^{19}F NMR spectrum.

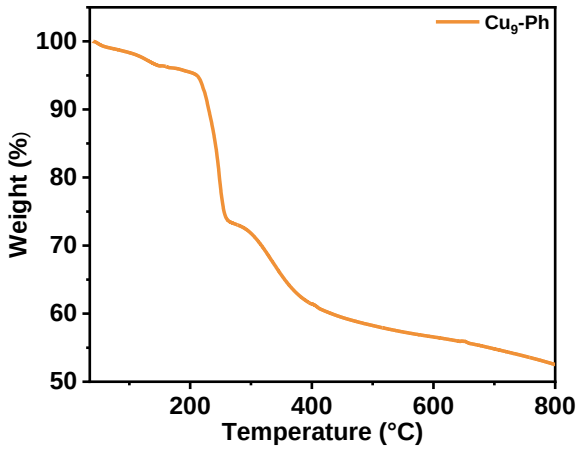

Figure S7. TG curves of **Cu9-Ph**.

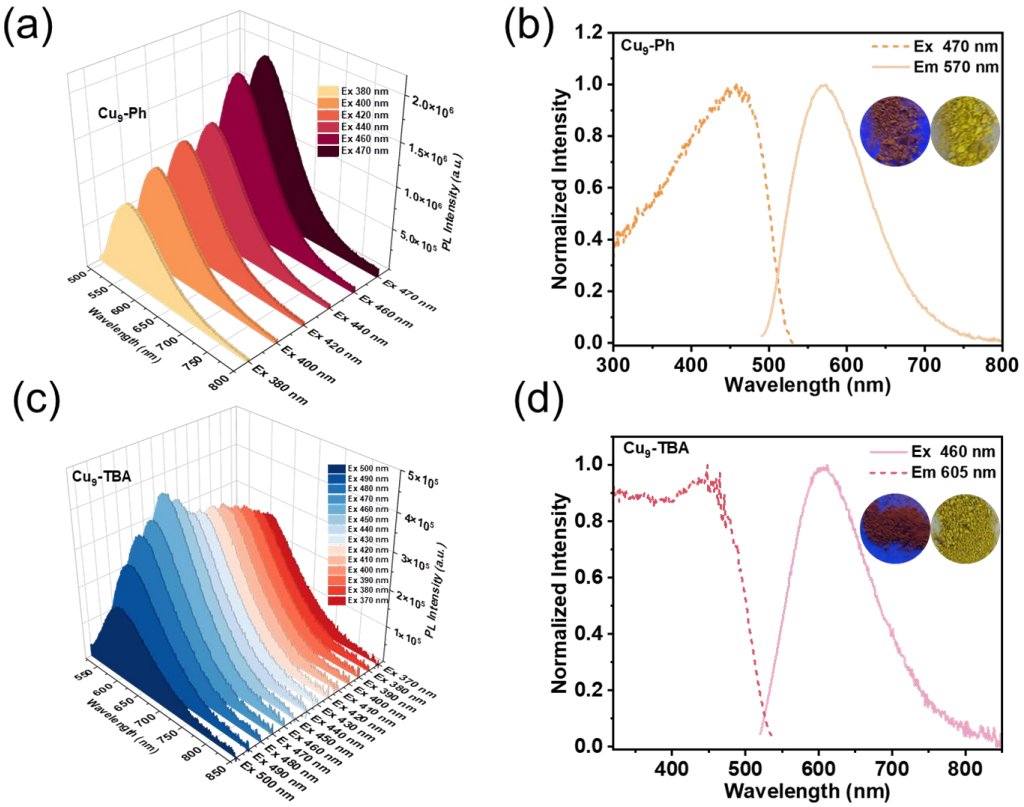

Figure S8. (a) Emission spectrum of **Cu9-Ph** in the solid state under different excitation wavelengths; (b) Normalized excitation and emission spectra of **Cu9-Ph** in the solid state; (c) Emission spectrum of **Cu9-TBA** in the solid state under various excitation wavelengths; (d) Normalized excitation and emission spectra of **Cu9-TBA** in the solid state.

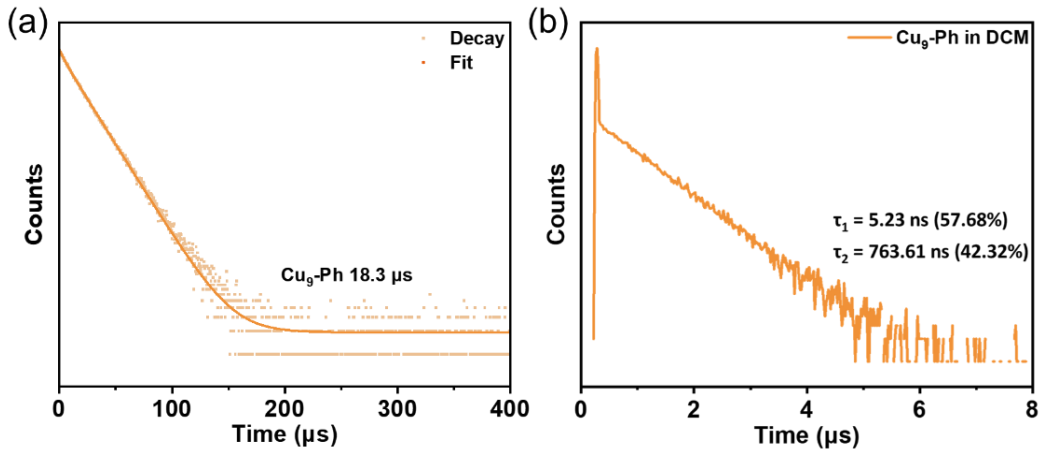

Figure S9. (a) The PL decay profiles for **Cu9-Ph** crystals under ambient conditions; (b) The PL decay profiles for **Cu9-Ph** in DCM under ambient conditions.

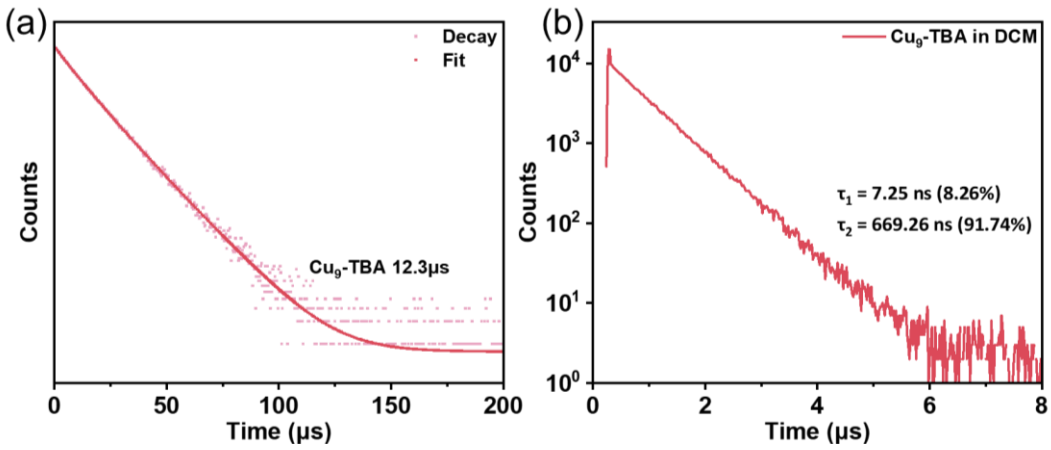

Figure S10. (a) The PL decay profiles for **Cu9-TBA** crystals under ambient conditions; (b) The PL decay profiles for **Cu9-TBA** dissolved in DCM under ambient conditions.

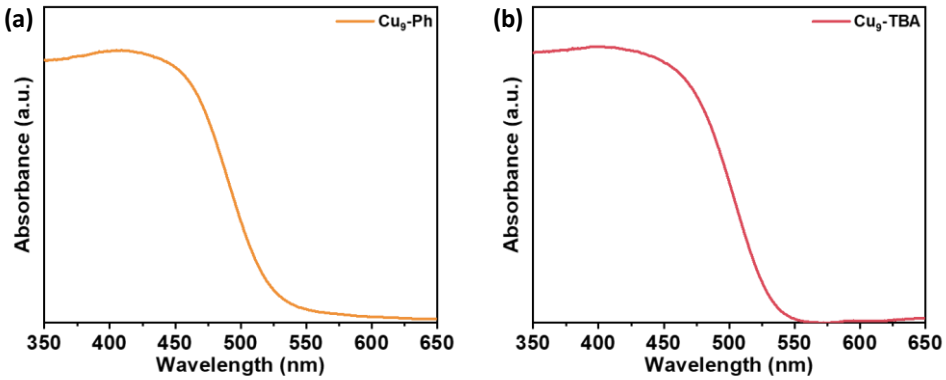

Figure S11. (a) UV-vis diffuse reflectance spectra of **Cu9-Ph**; (b) UV-vis diffuse reflectance spectra of **Cu9-TBA**.

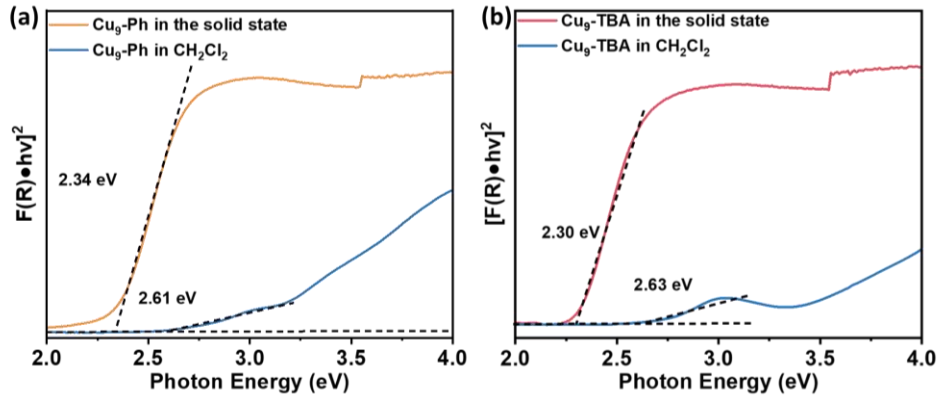

Figure S12. (a) UV-vis absorption spectra of **Cu9-Ph**; (b) UV-vis absorption spectra of **Cu9-TBA**.

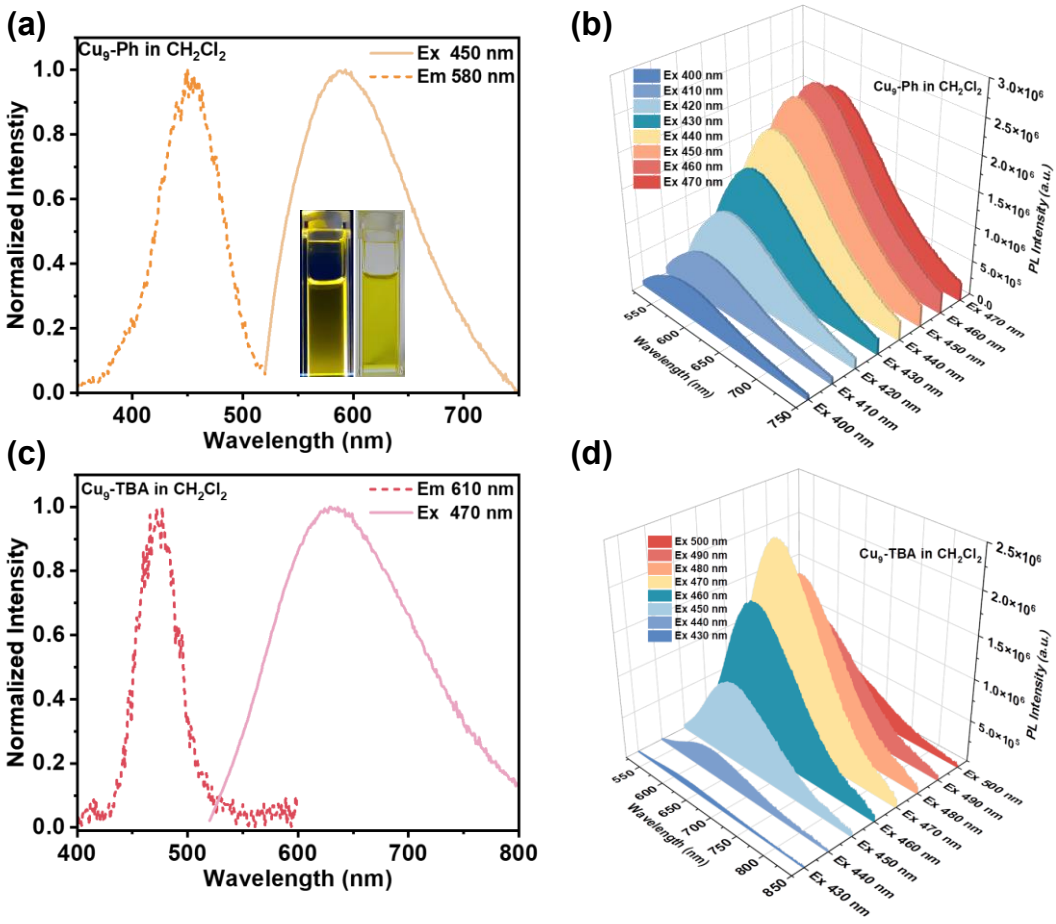

Figure S13. (a) Normalized excitation and emission spectra of **Cu9-Ph** in DCM; (b) Emission spectrum of **Cu9-Ph** in DCM under different excitation wavelengths; (c) Normalized excitation and emission spectra of **Cu9-TBA** in DCM; (d) Emission

spectrum of **Cu$_9$-TBA** in DCM under different excitation wavelengths.

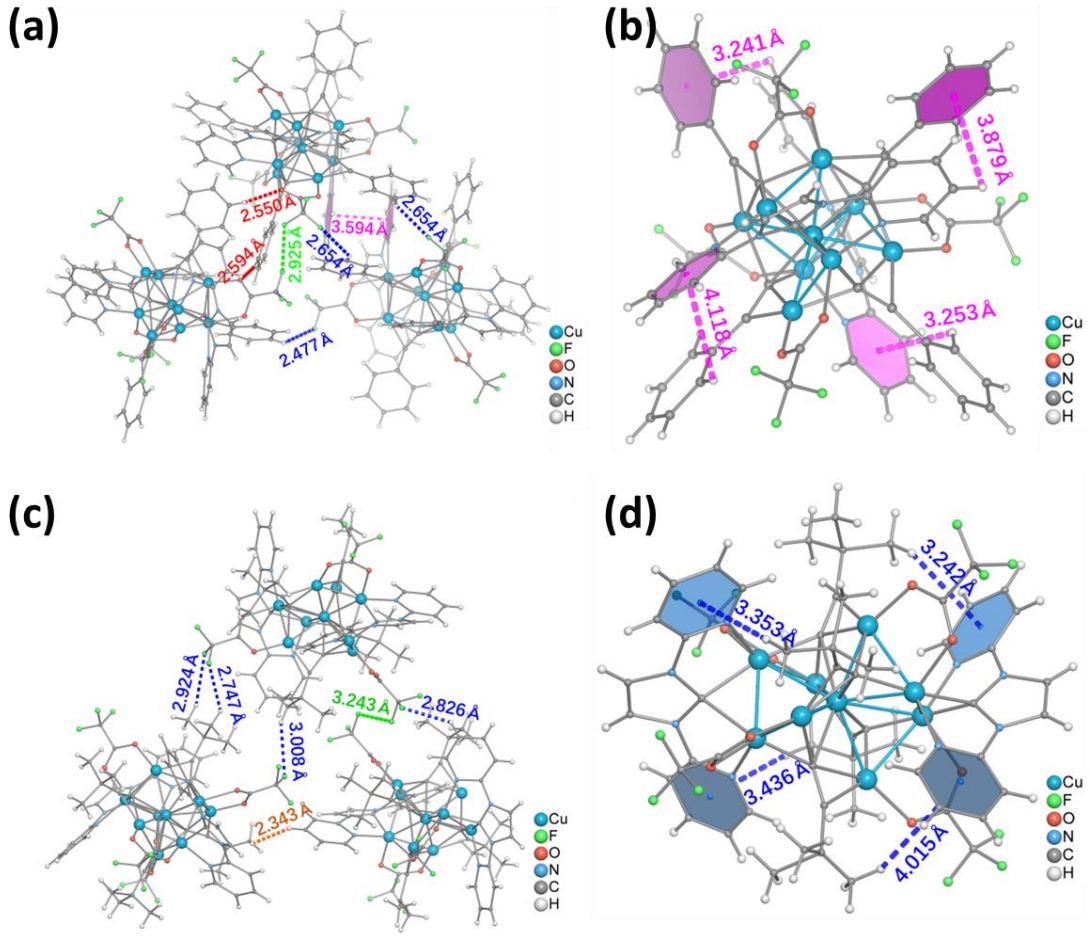

Figure S14. The intercluster and intracluster interactions in (a-b) **Cu$_9$-Ph** and (c-d) **Cu$_9$-TBA**.

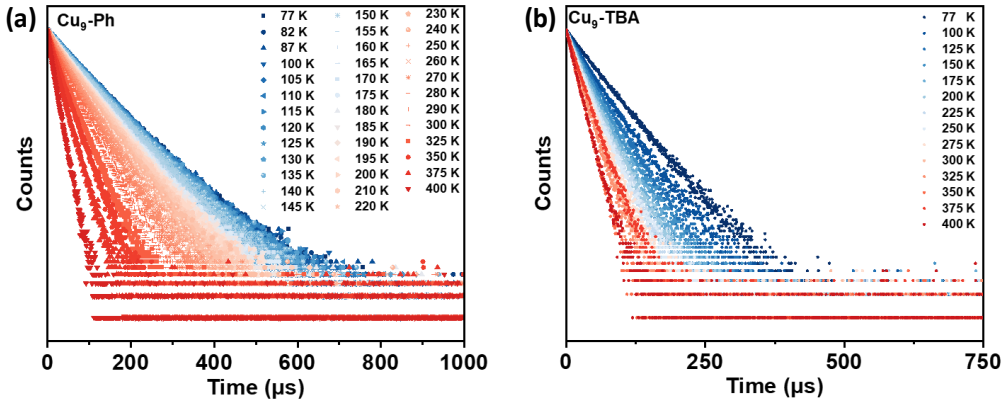

Figure S15. (a) Temperature-dependent solid-state of **Cu9-Ph** in the range of 77-400 K; (b) Temperature-dependent solid-state of **Cu9-TBA** in the range of 77-400 K.

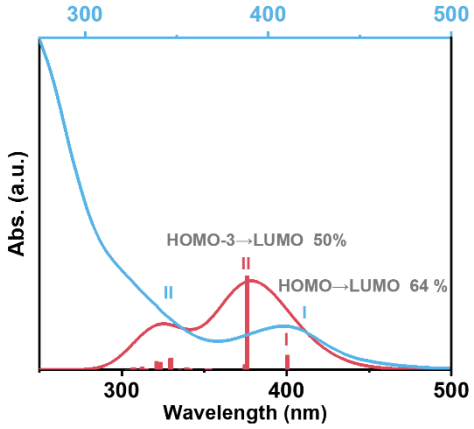

Figure S16. Experimental (blue line) and simulated (red line) optical absorption spectra of **Cu9-TBA**.

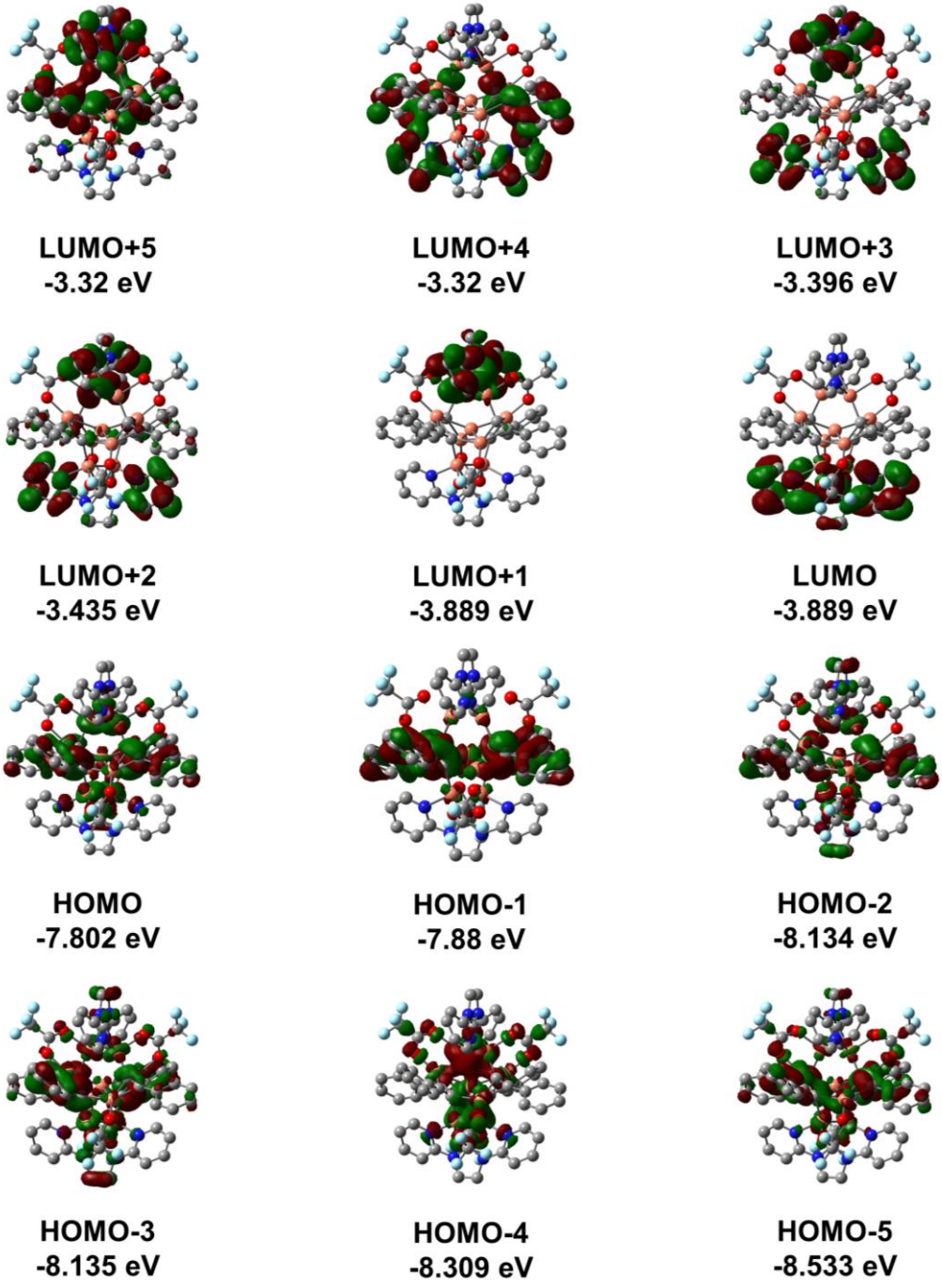

Figure S17. The frontier molecular orbital diagram of **Cu_9-Ph**.

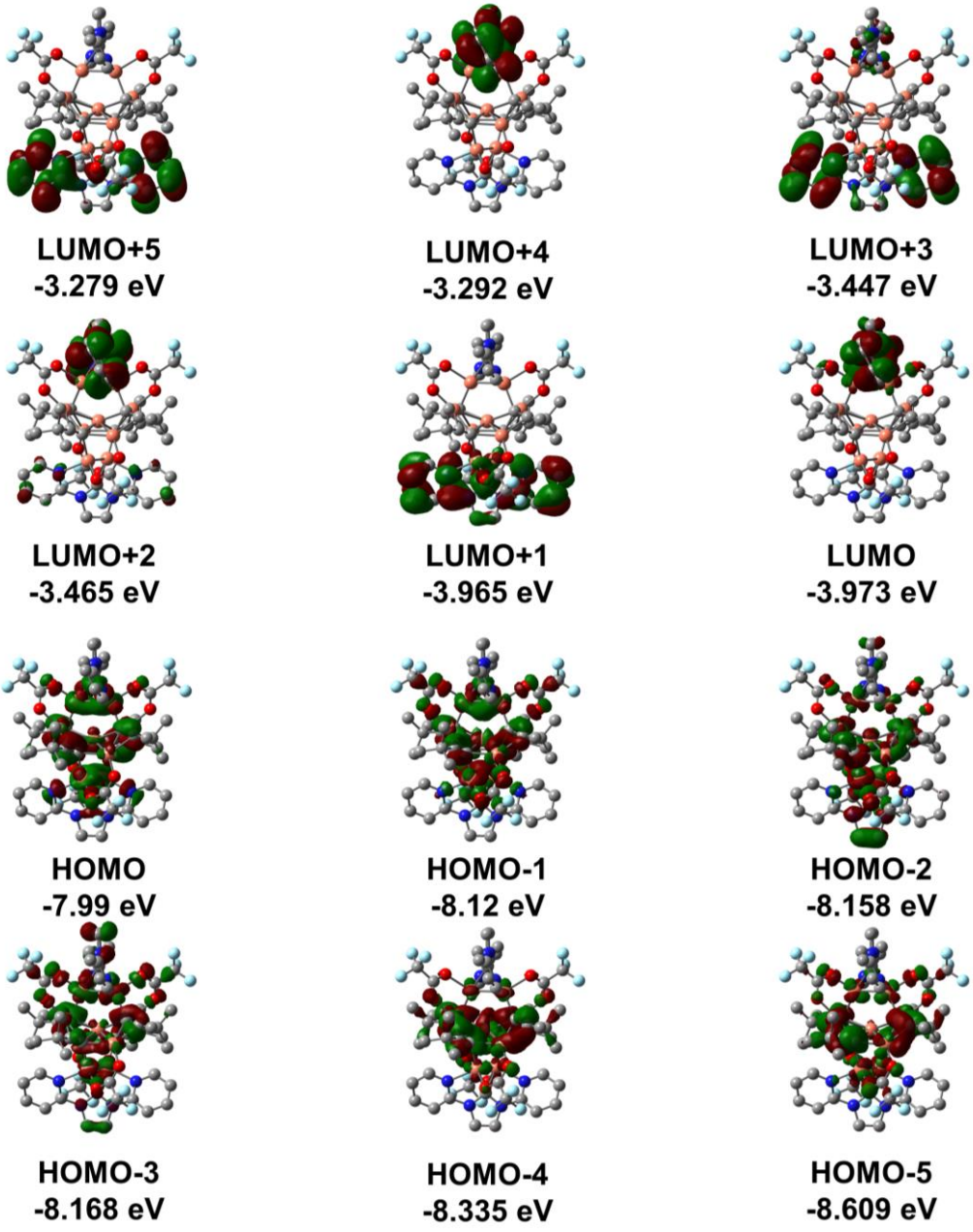

Figure S18. Frontier orbitals of the **Cu_9-TBA** cluster.

Table S1. Calculated vertical/adiabatic excitation energy of S1 state of two copper clusters.

	vertical excitation energy	**adiabatic excitation energy**
Cu_9-Ph	2.40 eV	2.48 eV
Cu_9-TBA	1.89 eV	2.30 eV

Table S2. Crystallographic data and structure refinement parameters for **Cu_9-Ph** and **Cu_9-TBA**.

Compounds	**Cu_9-Ph**	**Cu_9-TBA**
Formula	$C_{161}H_{114}N_{16}O_{16}F_{36}P_2Cl_2Cu_{18}$	$C_{65.3}H_{64.6}N_8O_8F_{18}PCl_{0.6}Cu_9$
Crystal system	orthorhombic	monoclinic
Space group	*Pbcn*	$P2_1/c$
Z	4	4
***a* (Å)**	26.0267(6)	22.2619(3)
***b* (Å)**	26.6509(6)	21.6279(5)
***c* (Å)**	23.8837(6)	18.4909(4)
***α* (deg.)**	90	90
***β* (deg.)**	90	108.627(2)
***γ* (deg.)**	90	90
***V* (Å^3)**	16566.6(7)	8436.6(3)
Goodness-of-fit on F^2	1.060	1.043
R_1, wR_2 ($I>2\sigma(I)$)	0.0700, 0.1870	0.0936, 0.2675
R_1, wR_2 (all data)	0.0825, 0.1940	0.1304, 0.2829

Table S3. PL decay lifetime of **Cu_9-Ph** and **Cu_9-TBA** at 298 K in the solid state.

Sample	A_1 (%)	τ_1 (μs)	A_2 (%)	τ_2 (μs)	A_3 (%)	τ_3 (μs)	τ_{ave} (μs)
Cu_9-Ph	12.88	4.73	87.12	18.4	-	-	18.3
Cu_9-TBA	4.0	3.38	45.0	9.31	51.0	14.2	12.3

Table S4. PL decay lifetime of **Cu_9-Ph** and **Cu_9-TBA** at 298 K in DCM.

Sample	A_1 (%)	τ_1 (ns)	A_2 (%)	τ_2 (ns)	τ_{ave} (ns)
Cu_9-Ph	57.68	5.23	42.32	763.61	326
Cu_9-TBA	8.26	7.25	91.74	669.26	614

Cartesian coordinates of the fully optimized S_0/S_1 geometries of **Cu_9-Ph** and **Cu_9-TBA**

Cu_9-Ph S_0 state

Cu 0.00020000 0.00000000 -0.00020000

Cu -2.43160000 0.14640000 -1.29180000

Cu -2.43240000 -0.14470000 1.29180000

Cu -0.82060000 2.23340000 -1.03210000

Cu 0.82150000 1.03150000 2.23330000

Cu 2.43280000 1.29040000 0.14650000

Cu 2.43150000 -1.29320000 -0.14570000

Cu 0.82120000 -1.03350000 -2.23320000

Cu -0.82330000 -2.23300000 1.03130000

C -0.64320000 -0.44240000 2.14140000

C 0.64220000 -2.14270000 -0.44200000

C 0.64370000 2.14110000 0.44230000

C -0.64210000 0.44190000 -2.14160000

O -3.62340000 1.61840000 -2.33090000

N -3.27690000 -1.77690000 -1.90670000

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O -3.62550000 -1.61520000 2.33060000

N -3.27410000 1.78020000 1.90650000

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C 0.15480000 3.30350000 0.50690000

O 2.13820000 2.05540000 3.29940000

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F 3.36090000 -4.36750000 -4.19790000

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Cu_9-TBA S_0 state

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Cu 0.82460000 -1.75140000 -1.71710000

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O 3.70290000 -2.69180000 -0.89150000

N 3.38280000 -1.41140000 2.32060000

O 2.19230000 -2.92320000 -2.55840000

C -0.34610000 -0.82430000 -3.24370000

O -3.68710000 -0.97160000 2.64510000

N -3.48380000 2.20030000 1.27050000

C -4.23890000 -0.06540000 -0.07020000

O -3.65880000 0.90700000 -2.72840000

N -3.41420000 -2.28040000 -1.44390000

O -2.14390000 2.57860000 -2.88070000

C 0.47590000 3.20480000 -0.87450000

O -2.11720000 -2.56960000 2.95270000

C 0.38980000 -3.25280000 0.82330000

C 3.13120000 3.24340000 2.01920000

C -0.40000000 1.21590000 4.63940000

C 4.73200000 0.70030000 -2.14290000

C 3.11320000 1.84160000 -3.28270000

N 5.07480000 -0.34590000 1.17490000

N 5.14720000 0.22770000 -0.87980000

C 3.29390000 -3.12240000 -1.98410000

C 2.84330000 -1.90450000 3.43580000

C 4.56780000 -0.81400000 2.40550000

C -0.21820000 -1.12890000 -4.68750000

C -3.23650000 -2.02200000 3.13350000

C -4.65350000 2.22030000 0.63800000

C -2.99950000 3.35240000 1.73560000

N -5.07360000 -1.10430000 -0.35910000

N -5.10000000 0.95660000 0.19650000

C -3.24280000 2.01250000 -3.11630000

C -2.90900000 -3.40130000 -1.95970000

C -4.59640000 -2.34300000 -0.83770000

C 0.39100000 4.64020000 -1.23310000

C 0.28090000 -4.69350000 1.15060000

C 3.96040000 4.32280000 2.74350000

C -0.75940000 2.69940000 4.82020000

C -1.41150000 0.33510000 5.39260000

C 1.01730000 0.97760000 5.17980000

C 5.50350000 0.51310000 -3.28430000

C 3.82580000 1.75490000 -4.47310000

H 2.14710000 2.33490000 -3.22760000

C 6.41560000 -0.27020000 0.83500000

C 6.46090000 0.08970000 -0.46470000

C 4.30280000 -3.96360000 -2.79190000

H 1.86580000 -2.36360000 3.31970000

C 3.48450000 -1.85120000 4.66800000

C 5.27650000 -0.66700000 3.59300000

C 1.20230000 -0.79620000 -5.16540000

C -1.24590000 -0.26880000 -5.44300000

C -0.49370000 -2.62010000 -4.93750000

C -4.18310000 -2.82280000 4.05000000

C -5.39800000 3.37430000 0.42200000

C -3.68220000 4.55730000 1.61580000

H -2.03240000 3.28980000 2.22620000

C -6.40670000 -0.73790000 -0.27090000

C -6.42290000 0.56570000 0.07760000

C -4.23570000 2.85110000 -3.94630000

H -1.93370000 -3.30280000 -2.42800000

C -3.58110000 -4.61730000 -1.91730000

C -5.33150000 -3.51500000 -0.69630000

C 1.53910000 5.37780000 -0.52330000

C 0.51020000 4.82120000 -2.75470000

C -0.96010000 5.20200000 -0.76680000

C -1.14460000 -5.18920000 0.86940000

C 1.29030000 -5.45390000 0.27350000

F 3.28400000 5.47780000 2.78440000

F 4.20380000 3.93840000 4.00570000

F 5.13010000 4.54760000 2.14850000

H -0.69100000 2.96070000 5.88230000

H -1.78500000 2.89960000 4.49250000

H -0.06590000 3.34110000 4.26580000

H -1.16670000 -0.72690000 5.28490000

H -2.42680000 0.49160000 5.01430000

H -1.39470000 0.58860000 6.45880000

H 1.74610000 1.59950000 4.65040000

H 1.30510000 -0.07280000 5.07580000

H 1.04700000 1.23700000 6.24440000

H 6.41940000 -0.06690000 -3.25650000

C 5.03670000 1.06880000 -4.47000000

H 3.43320000 2.20240000 -5.37990000

H 7.21070000 -0.50480000 1.52480000

H 7.30370000 0.28500000 -1.10840000

F 3.70070000 -4.81660000 -3.61980000

F 5.05830000 -3.12850000 -3.53390000

F 5.11870000 -4.65600000 -1.99760000

H 3.02070000 -2.28980000 5.54510000

C 4.71960000 -1.21390000 4.74350000

H 6.21710000 -0.12770000 3.62460000

H 1.94470000 -1.39420000 -4.62770000

H 1.42500000 0.26420000 -5.01520000

H 1.28660000 -1.01540000 -6.23610000

H -1.05520000 0.79840000 -5.28650000

H -2.26500000 -0.48560000 -5.10740000

H -1.18010000 -0.47860000 -6.51680000

H 0.21270000 -3.24770000 -4.38350000

H -0.37660000 -2.83520000 -6.00560000

H -1.51800000 -2.88520000 -4.65460000

F -4.68890000 -3.85730000 3.35260000

F -5.20260000 -2.08630000 4.48790000

F -3.53760000 -3.31570000 5.10940000

H -6.31680000 3.35200000 -0.15340000

C -4.89810000 4.56410000 0.93900000

H -3.26220000 5.46720000 2.03070000

H -7.21770000 -1.41410000 -0.48940000

H -7.25070000 1.22740000 0.27720000

F -3.61650000 3.68860000 -4.77760000

F -4.98620000 3.58630000 -3.10010000

F -5.05840000 2.08390000 -4.66020000

H -3.14540000 -5.49930000 -2.37460000

C -4.80900000 -4.67130000 -1.26430000

H -6.26590000 -3.53130000 -0.14600000

H 1.45950000 5.28230000 0.56400000

H 1.50050000 6.44290000 -0.77920000

H 2.51280000 4.98330000 -0.83160000

H 1.48460000 4.47770000 -3.11860000

H 0.42350000 5.88600000 -2.99900000

H -0.28530000 4.28280000 -3.28010000

H -1.78960000 4.67660000 -1.25050000

H -1.02100000 6.26470000 -1.02830000

H -1.06400000 5.11100000 0.31880000

H -1.40310000 -5.05870000 -0.18530000

H -1.87350000 -4.65000000 1.48250000

H -1.21080000 -6.25700000 1.10820000

H 1.23630000 -6.52540000 0.49820000

H 2.31270000 -5.11040000 0.46120000

H 1.07270000 -5.31180000 -0.79050000

H 5.61030000 0.95290000 -5.38450000

H 5.24250000 -1.12920000 5.69120000

H -5.44920000 5.48900000 0.79870000

H -5.35370000 -5.60710000 -1.18490000

C 0.60250000 -4.91910000 2.63660000

H 0.49970000 -5.98480000 2.87040000

H -0.09060000 -4.36170000 3.27630000

Cu_9-Ph S_1 state

Cu -0.00380000 0.00000000 0.00000000

Cu -2.47250000 0.54800000 -1.19640000

Cu -2.47250000 -0.54800000 1.19650000

Cu -0.91340000 2.40810000 -0.06580000

Cu 0.80430000 0.17970000 2.44800000

Cu 2.44160000 1.14740000 0.62470000

Cu 2.44160000 -1.14730000 -0.62470000

Cu 0.80420000 -0.17970000 -2.44790000

Cu -0.91350000 -2.40800000 0.06570000

C -0.63920000 -1.14940000 1.75100000

C 0.66430000 -1.86700000 -1.20470000

C 0.66440000 1.86700000 1.20470000

C -0.63930000 1.14940000 -1.75100000

O -3.54690000 2.36290000 -1.78890000

N -3.19150000 -1.04600000 -2.29780000

C -4.08320000 -0.00010000 0.00000000

O -3.54680000 -2.36280000 1.78900000

N -3.19170000 1.04610000 2.29770000

O -2.21650000 3.77240000 -0.62570000

C 0.20900000 2.95320000 1.65860000

O 2.12360000 0.66570000 3.83460000

C -0.16490000 -1.65020000 2.81590000

O 3.62110000 1.53970000 2.38410000

N 3.28090000 2.44440000 -0.90510000

C 4.08180000 0.00000000 0.00010000

O 3.62110000 -1.53940000 -2.38420000

N 3.28090000 -2.44450000 0.90510000

O 2.12350000 -0.66560000 -3.83460000

C -0.16510000 1.65020000 -2.81590000

O -2.21660000 -3.77230000 0.62570000

C 0.20900000 -2.95320000 -1.65850000

C -3.20700000 3.46950000 -1.35430000

C -2.64460000 -1.64800000 -3.36440000

C -4.46850000 -1.34710000 -1.97080000

N -4.93610000 -0.68410000 -0.85210000

N -4.93630000 0.68370000 0.85210000

C -3.20700000 -3.46940000 1.35440000

C -4.46870000 1.34680000 1.97080000

C -2.64490000 1.64830000 3.36420000

C -0.02600000 4.12080000 2.45430000

C 3.19380000 1.25160000 3.51270000

C 0.09480000 -2.54400000 3.89750000

C 4.43890000 1.97050000 -1.36010000

C 2.73740000 3.49590000 -1.52070000

N 4.92440000 -0.85070000 0.64710000

N 4.92440000 0.85070000 -0.64700000

C 3.19380000 -1.25140000 -3.51280000

C 2.73740000 -3.49600000 1.52070000

C 4.43880000 -1.97060000 1.36010000

C 0.09460000 2.54380000 -3.89770000

C -0.02590000 -4.12080000 -2.45420000

C -4.05480000 4.69390000 -1.75360000

H -1.61760000 -1.36960000 -3.58390000

C -3.32540000 -2.55980000 -4.14590000

C -5.23140000 -2.26450000 -2.70150000

C -6.25800000 -0.42280000 -0.52570000

C -6.25810000 0.42190000 0.52590000

C -4.05480000 -4.69380000 1.75370000

C -5.23190000 2.26420000 2.70140000

C -3.32590000 2.56000000 4.14570000

H -1.61780000 1.37010000 3.58380000

C -0.90370000 5.13450000 2.03490000

C 0.64730000 4.24640000 3.68480000

C 4.05300000 1.65710000 4.72660000

C -0.46790000 -3.83650000 3.85560000

C 0.89600000 -2.16670000 4.99090000

C 5.12170000 2.51090000 -2.44210000

C 3.34310000 4.12190000 -2.60380000

H 1.78990000 3.84010000 -1.11570000

C 6.25170000 -0.53700000 0.41050000

C 6.25170000 0.53690000 -0.41030000

C 4.05300000 -1.65670000 -4.72670000

H 1.78990000 -3.84020000 1.11560000

C 3.34300000 -4.12200000 2.60370000

C 5.12160000 -2.51100000 2.44220000

C -0.46810000 3.83640000 -3.85570000

C 0.89560000 2.16650000 -4.99110000

C -0.90370000 -5.13450000 -2.03480000

C 0.64750000 -4.24670000 -3.68460000

F -3.32520000 5.50350000 -2.54160000

F -5.15570000 4.35360000 -2.41480000

F -4.41420000 5.39120000 -0.66910000

H -2.83610000 -3.02420000 -4.99420000

C -4.65190000 -2.87090000 -3.79930000

H -6.24320000 -2.51020000 -2.39720000

H -7.08750000 -0.82900000 -1.08230000

H -7.08770000 0.82790000 1.08260000

F -3.32530000 -5.50340000 2.54160000

F -5.15570000 -4.35340000 2.41490000

F -4.41430000 -5.39110000 0.66920000

H -6.24370000 2.50970000 2.39710000

C -4.65240000 2.87080000 3.79910000

H -2.83660000 3.02460000 4.99390000

H -1.43770000 5.02900000 1.09460000

C -1.09250000 6.25660000 2.83250000

C 0.44330000 5.37070000 4.47300000

H 1.31960000 3.46130000 4.01580000

F 5.19580000 2.23480000 4.36780000

F 4.34520000 0.57800000 5.46630000

F 3.37120000 2.51690000 5.49750000

H -1.08190000 -4.12830000 3.00980000

C -0.23180000 -4.72580000 4.89380000

C 1.12030000 -3.06770000 6.02340000

H 1.34000000 -1.17530000 5.01230000

H 6.04360000 2.06800000 -2.80340000

C 4.55380000 3.61640000 -3.06800000

H 2.86720000 4.97410000 -3.07640000

H 7.07070000 -1.11170000 0.81350000

H 7.07070000 1.11160000 -0.81340000

F 5.19600000 -2.23410000 -4.36790000

F 4.34480000 -0.57770000 -5.46660000

F 3.37130000 -2.51690000 -5.49740000

H 2.86710000 -4.97420000 3.07630000

C 4.55370000 -3.61660000 3.06800000

H 6.04350000 -2.06800000 2.80350000

H -1.08200000 4.12820000 -3.00990000

C -0.23210000 4.72560000 -4.89410000

C 1.11990000 3.06750000 -6.02370000

H 1.33970000 1.17510000 -5.01250000

H -1.43790000 -5.02890000 -1.09460000

C -1.09250000 -6.25670000 -2.83230000

C 0.44360000 -5.37100000 -4.47270000

H 1.32000000 -3.46150000 -4.01560000

H -5.21870000 -3.59140000 -4.38050000

H -5.21940000 3.59130000 4.38020000

H -1.77020000 7.03860000 2.50230000

C -0.42310000 6.37820000 4.04870000

H 0.96690000 5.46230000 5.42030000

H -0.67620000 -5.71630000 4.86160000

C 0.55910000 -4.34400000 5.97900000

H 1.73330000 -2.77110000 6.86970000

H 5.05010000 4.06770000 -3.92170000

H 5.05000000 -4.06780000 3.92170000

H -0.67650000 5.71620000 -4.86180000

C 0.55870000 4.34380000 -5.97920000

H 1.73280000 2.77080000 -6.87000000

H -1.77030000 -7.03860000 -2.50210000

C -0.42290000 -6.37840000 -4.04850000

H 0.96730000 -5.46270000 -5.41990000

H -0.57570000 7.25800000 4.66750000

H 0.73340000 -5.04160000 6.79340000

H 0.73290000 5.04140000 -6.79380000

H -0.57550000 -7.25820000 -4.66720000

Cu_9-TBA S_1 state

Cu 0.18580000 0.17430000 0.00930000

Cu -1.02200000 0.94570000 -2.07120000

Cu -2.71520000 1.06900000 -0.08090000

Cu -2.59810000 -1.66270000 0.27170000

Cu -0.36340000 -1.33630000 2.16020000

Cu 2.41550000 -0.07830000 -1.50960000

Cu 2.68450000 0.50770000 0.98110000

Cu 0.63220000 2.35070000 1.18950000

Cu 0.78810000 -2.21810000 -0.66230000

C 0.43260000 -0.55860000 -1.92050000

C 0.90070000 0.33490000 1.95990000

C -0.85390000 -2.60690000 0.61140000

C -0.92540000 2.04710000 -0.21800000

O -2.26650000 1.93340000 -3.23480000

C 0.09000000 -0.58210000 -3.13160000

O -3.86910000 1.96510000 -1.64260000

N -3.86900000 1.38650000 1.64100000

C -4.30360000 -0.66930000 -0.18880000

O -3.21620000 -1.58180000 2.30940000

N -2.93690000 -2.34740000 -1.65390000

O -1.48730000 -2.17230000 3.63060000

C 0.69930000 0.22410000 3.19730000

O 3.46720000 -1.62650000 -2.47840000

N 2.80170000 1.95220000 -2.40470000

C 4.16650000 0.52320000 -0.50760000

O 3.65180000 2.17990000 1.86920000

N 3.97180000 -1.18370000 1.61810000

O 1.89570000 3.59290000 2.04280000

C -0.82590000 3.29100000 -0.05470000

O 2.41740000 -3.22200000 -1.26720000

C -0.23150000 -3.69490000 0.62880000

C -3.39950000 2.22250000 -2.76310000

C -0.03220000 -0.86270000 -4.58010000

C -5.09680000 0.86770000 1.53220000

C -3.58350000 2.12740000 2.71490000

N -4.87260000 -1.14540000 -1.33980000

N -5.30130000 0.08050000 0.39800000

C -2.70040000 -2.04870000 3.34910000

C -2.25490000 -3.32950000 -2.28900000

C -4.20380000 -2.08800000 -2.10170000

C 0.69570000 0.40290000 4.66660000

C 3.27600000 -2.78840000 -2.07750000

C 3.98070000 2.42270000 -2.00440000

C 2.01960000 2.75770000 -3.12630000

N 5.23410000 -0.17590000 -0.02960000

N 4.74630000 1.51270000 -1.24280000

C 3.10220000 3.25410000 2.16920000

C 3.75420000 -2.15380000 2.50680000

C 5.07860000 -1.24400000 0.88190000

C -0.97650000 4.76270000 -0.07290000

C 0.23370000 -5.07730000 0.85620000

C -4.30400000 2.98050000 -3.75420000

C 0.72240000 0.22250000 -5.36680000

C 0.61540000 -2.23240000 -4.85060000

C -1.50470000 -0.86690000 -5.01690000

C -6.10100000 1.08440000 2.47520000

C -4.51270000 2.40380000 3.70670000

H -2.57080000 2.51880000 2.75790000

C -6.18350000 -0.70590000 -1.46010000

C -6.44410000 0.05800000 -0.37580000

C -3.68410000 -2.44950000 4.46770000

H -1.25870000 -3.52190000 -1.90620000

C -2.75380000 -4.03980000 -3.35360000

C -4.78310000 -2.76320000 -3.17560000

C -0.69770000 0.84870000 5.13700000

C 1.72950000 1.49520000 4.99670000

C 1.07720000 -0.90880000 5.37080000

C 4.25130000 -3.86770000 -2.59160000

C 4.44890000 3.69820000 -2.29940000

C 2.40350000 4.03720000 -3.51010000

H 1.05600000 2.34830000 -3.41500000

C 6.43690000 0.36290000 -0.45390000

C 6.12890000 1.43250000 -1.21900000

C 4.02310000 4.36150000 2.71930000

H 2.83180000 -2.07150000 3.07460000

C 4.64510000 -3.20070000 2.71160000

C 6.02040000 -2.26100000 0.98170000

C -2.12160000 5.11650000 -1.03680000

C -1.30820000 5.25950000 1.34420000

C 0.33370000 5.41310000 -0.54310000

C 1.59990000 -5.04740000 1.55890000

C -0.80570000 -5.76980000 1.75570000

F -3.66090000 4.03890000 -4.26280000

F -4.63870000 2.16940000 -4.76850000

F -5.42590000 3.41300000 -3.18180000

H 0.69760000 -0.02950000 -6.43280000

H 1.76990000 0.29000000 -5.05390000

H 0.24150000 1.19900000 -5.24460000

H 0.09640000 -3.02570000 -4.30340000

H 1.66980000 -2.22950000 -4.55770000

H 0.55200000 -2.45720000 -5.92110000

H -1.96960000 0.10770000 -4.83990000

H -2.07560000 -1.63150000 -4.48400000

H -1.55610000 -1.08760000 -6.08940000

H -7.07270000 0.61510000 2.36470000

C -5.79730000 1.87260000 3.57450000

H -4.23890000 3.01580000 4.55900000

H -6.81160000 -0.94350000 -2.30320000

H -7.32360000 0.63080000 -0.12490000

F -3.24910000 -3.51350000 5.14070000

F -3.79060000 -1.42220000 5.32980000

F -4.89880000 -2.71840000 3.99270000

H -2.14330000 -4.80090000 -3.82770000

C -4.05930000 -3.74960000 -3.81730000

H -5.79490000 -2.52850000 -3.48930000

H -1.44790000 0.07870000 4.94100000

H -0.99900000 1.77870000 4.64380000

H -0.66830000 1.03100000 6.21710000

H 1.46010000 2.44810000 4.53060000

H 2.72940000 1.21210000 4.65200000

H 1.76430000 1.63800000 6.08260000

H 0.36730000 -1.70590000 5.13110000

H 1.06340000 -0.75070000 6.45490000

H 2.08920000 -1.22440000 5.09440000

F 5.16510000 -4.12480000 -1.63520000

F 4.90110000 -3.47970000 -3.68540000

F 3.61130000 -5.00800000 -2.86420000

H 5.39680000 4.05280000 -1.90920000

C 3.64030000 4.51260000 -3.08410000

H 1.74380000 4.64350000 -4.12190000

H 7.39540000 -0.03410000 -0.15900000

H 6.76630000 2.11200000 -1.76220000

F 3.39040000 5.14320000 3.59390000

F 4.43260000 5.12920000 1.69240000

F 5.10410000 3.85710000 3.31260000

H 4.43530000 -3.95910000 3.45810000

C 5.79470000 -3.25260000 1.92940000

H 6.88140000 -2.29810000 0.32360000

H -1.89830000 4.78720000 -2.05660000

H -2.26300000 6.20320000 -1.04870000

H -3.05990000 4.64820000 -0.72310000

H -2.24310000 4.81930000 1.70780000

H -1.43100000 6.34830000 1.32750000

H -0.50050000 5.01770000 2.04390000

H 1.15610000 5.17430000 0.13890000

H 0.20790000 6.50160000 -0.56650000

H 0.59920000 5.07700000 -1.55020000

H 1.53210000 -4.52950000 2.52240000

H 2.34800000 -4.55270000 0.93270000

H 1.92760000 -6.07610000 1.74670000

H -0.48380000 -6.79780000 1.95630000

H -1.78590000 -5.80550000 1.26910000

H -0.91270000 -5.24470000 2.71030000

H -6.55070000 2.05510000 4.33480000

H -4.49110000 -4.29430000 -4.64960000

H 3.96950000 5.51400000 -3.34410000

H 6.50490000 -4.06610000 2.04140000

C 0.36000000 -5.81710000 -0.48520000

H 0.67200000 -6.85020000 -0.29530000

H 1.10930000 -5.34100000 -1.12490000

H -0.60040000 -5.84770000 -1.01120000