Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Intramolecular rearrangements guided by adaptive coordination-driven reactions toward highly luminescent polynuclear Cu(I) assemblies

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Supporting Information

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I. Experimental Section

All experiments were performed under an atmosphere of dry argon using standard Schlenk techniques. Commercially available reagents ($[Cu(CH_3CN)_4].PF_6$, KCN, dppm, CuCN, $K[Au(CN)_2]$ and $K_2[Pt(CN)_4]$) were obtained from Sigma-Aldrich. The precursor **A** was synthesized according to synthetic procedure that has been improved considering the previously reported procedure.[S1] ^1H, and $^{31}P\{^1H\}$ NMR spectra were recorded on Bruker DPX200, AV300 or AV400 spectrometers. ^1H NMR chemical shifts were reported in parts per million (ppm) relative to Me_4Si as external standard. $^{31}P\{^1H\}$ NMR downfield chemical shifts were expressed with a positive sign, in ppm, relative to 85% H_3PO_4 respectively. FT-IR measurements have been performed on a Perkin Elmer Frontier spectrometer using UATR (Universal Attenuated Total Reflectance) accessory. Spectra have been recorded between 650 cm^{-1} and 4000 cm^{-1}, on pure samples. UV-vis solid-state absorption measurements have been recorded on a Perkin-Elmer Lambda 650 spectrometer using a 60 mm integrating sphere. Spectra have been recorded between 800 nm and 200 nm, on pellets.

Steady-state emission spectra and luminescence quantum yield measurements were recorded on a *Horiba Jobin-Yvon* (*HJY*) Fluorolog-3 (FL3-2iHR550) fluorescence spectrofluorometer equipped with a IR R928P PMT / *HJY* FL-1073 detector and with an integrating sphere. High temperature measurements were performed using a Peltier effect F3004 (*HJY*) heating system (allowing temperature measurements between 263 K and 383 K). Low temperature measurements were allowed by using a OptistatCF (*Oxford Inst.*) in the range of 77 K to 300 K. Excited-state lifetimes in the range 77 K and 383 K were measured with a delta hub (TCSPC: Time-Correlated-Single-Photon-Counting) + delta diode system allowing to measure excited-state lifetimes between 500 ps et 10 µs and with a pulsed xenon source (FL-1035) allowing to measure excited-state lifetimes longer than 10 µs.

Solid sample was placed in a quartz sample holders inside the integrating sphere and the cryostat and maintained at the desired temperature until equilibrium was reached before recording the spectrum.

The experimental data were then fitted according to the following equation[s2]

$$\tau(\mathrm{obs}) = \frac{1 + \frac{1}{3}\exp(-\frac{\Delta E_{\mathrm{ST}}}{k_{\mathrm{B}}T})}{\frac{1}{\tau(\mathrm{T_1})} + \frac{1}{3\tau(\mathrm{S_1})}\exp(-\frac{\Delta E_{\mathrm{ST}}}{k_{\mathrm{B}}T})} \qquad \text{equation (S1)}$$

where τ(obs), $\tau(S_1)$, $\tau(T_1)$, k_B, T and ΔE_{ST} represent the observed lifetime, singlet state decay lifetime, triplet state decay lifetime, Boltzmann constant, temperature and singlet-triplet energy difference, respectively.

Synthesis of derivative 1

To a dichloromethane solution (10 ml) of the derivative **A** (0.11 g, 0.05 mmol) was added a methanol suspension (4 ml) of CuCN (0.005 g, 0.05 mmol). This reaction mixture was stirred overnight at room temperature along the appearance of few amount of white precipitate. This crude solution was then filtered over cotton and was after left upon n-pentane vapour diffusion under argon, affording after crystallization the derivative **1** together with the derivative **A**. Bulk crystalline sample was collected upon filtration and dried under air on paper affording batches of colourless crystals in an overall yield of 80 %. Crystals of derivative **1** were manually separated from those of derivative **A** under air upon UV-Vis excitation (λ_{lamp} = 365 nm, crystals of derivative **1** are green-light emitters while those of derivative **A** are blue-light emitters).

The amount of derivative **1** finally obtained as pure colorless polycrystalline powder after manual separation was variable depending of the experiments performed (despite similar experimental conditions were applied). A mean yield of 20 % (ca. 0.023 g, 0.01 mmol) can be estimated for the synthesis of the air-stable colourless compound **1** after manual separation under UV-Vis irradiation (λ_{lamp} = 365 nm) of the crystals of green luminophore **1** from the crystals of the blue luminophore **A** (main compound).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.10 (broad s, 4H, P*CH*$_2$P), 3.40 (broad s, 4H, P*CH*$_2$P), 6.66 (broad s, 4H, H_{arom}), 6.84 (broad s, 4H, H_{arom}), 7.00-7.60 (broad m, 72H, H_{arom}).

^{31}P{^{1}H} NMR ($CDCl_3$, 161.98 MHz): δ = -144.6 (sept, ^{1}J(P,F) = 711 Hz, PF_6^-), -11.0 (broad m, dppm)

Elemental analysis, calcd. (%) for $C_{104}H_{90}Cl_2Cu_6F_{12}N_4P_{10}$: C 52.36, H 3.80, N 2.35; found: C 52.00, H 3.64, N 2.50.

IR (cm^{-1}): 686 (vs), 733 (s), 773 (m), 825 (vs), 999 (w), 1025 (w), 1148 (vw), 1192 (vw), 1310 (vw), 1435 (s), 1483 (m), 1586 (w), 1651 (w), 2141 (υ_{CN}, w), 3061 (vw), 3646 (vw).

Synthesis of derivative 2

To a 10:1 water/acetonitrile suspension (10ml) of $KAu(CN)_2$ (0.015 g, 0.052 mmol) was added one equivalent of the $[Cu_2(\mu_2\text{-dppm})_2(CH_3CN)_4](PF_6)_2$ complex **D** prepared in-situ in CH_2Cl_2 at room temperature from the reaction of $[Cu(CH_3CN)_4](PF_6)$ (0.039 g, 0.104 mmol) and dppm (0.040 g, 0.104 mmol). This reaction solution was stirred for one night at room temperature. The organic phase was collected and the crude solution was left upon n-pentane vapour diffusion affording after three weeks the derivative **2** that was collected and dried affording an air-stable colourless solid (0.044 g, 0.0087 mmol, 83% yield based on amount of Cu(I) ions introduced in the reaction, 33% yield based on amount of Au(I) ions introduced in the reaction).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.10 (broad s, 9H, P*CH*$_2$P), 3.80 (broad s, 9H, P*CH*$_2$P), 6.90-7.75 (broad m, 180H, H_{arom}).

$^{31}P\{^1H\}$ NMR ($CDCl_3$, 161.98 MHz): δ = -144.6 (sept, ^1J(P,F) = 711 Hz, PF_6^-), -14.5 (broad m, dppm), 30.4 (broad m, dppm), 34.4 (broad m, dppm), 37.0 (broad m, dppm). Signal at -14.5 ppm is assigned to the phosphorus atoms of the $Cu_2(\mu_2\text{-dppm})_2$ fragments while the other signals are assigned to the phosphorus atoms of the $Cu_2(\mu_2\text{-dppm})_1$ fragment.

Elemental analysis, calcd. (%) for $C_{235}H_{202}Cl_4Cu_{10}Au_2F_{12}N_{10}P_{20}$: C 58.91, H 4.25, N 2.29; found: C 58.86, H 4.20, N 2.26.

IR (cm^{-1}): 690 (vs), 737 (vs), 780 (s), 838 (vs), 999 (m), 1027 (w), 1101 (s), 1188 (vw), 1312 (w), 1368 (w), 1436 (s), 1484 (m), 1587 (w), 2124 (υ_{CN}, vw), 2149 (υ_{CN}, w), 3055 (w).

Synthesis of derivative 3

*Optimized synthesis was performed using a 1:1 potassium tetracyanoplatinate / complex **D** stoichiometry regarding the stoichiometry observed in the molecular structure determined for compound **3** accordingly to X-ray crystal structure diffraction analysis.*

To a methanol suspension (6ml) of $K_2Pt(CN)_4$ (0.032 g, 0.052 mmol) was added one equivalent of the $[Cu_2(\mu_2\text{-dppm})_2(CH_3CN)_4](PF_6)_2$ complex **D** prepared in-situ in CH_2Cl_2 at room temperature from the reaction of $[Cu(CH_3CN)_4](PF_6)$ (0.039 g, 0.104 mmol) and dppm (0.040 g, 0.104 mmol). This reaction solution was stirred for one night at room temperature along the appearance of few amount of white precipitate. This crude solution was then filtered over cotton and was after left upon n-pentane vapour diffusion affording after one week of crystallization the derivative **3** that was collected and dried affording an air-stable colourless solid (0.051 g,

0.0083 mmol, 87 % yield based on amount of Cu(I) ions introduced in the reaction, 64% yield based on amount of Pt(II) ions introduced in the reaction).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.25 (broad s, 8H, PCH_2P), 3.10 (broad s, 10H, PCH_2P), 3.40 (broad s, 2H, PCH_2P) 6.51-6.75 (broad m, 88H, H_{arom}), 6.78-7.80 (broad m, 112H, H_{arom}).

^{31}P{^{1}H} NMR ($CDCl_3$, 161.98 MHz): δ = δ = -143.8 (sept, ^{1}J(P,F) = 719 Hz, PF_6^-), from -21.0 to -12.0 (broad m, dppm), 3.0 (bd with ^{2}J(P,P)= 79 Hz and with satellites corresponding to ^{1}J(P,Pt)= 2590 Hz, P atom linked to the Pt(II) center of the [$Pt_1Cu_1(\mu_2$-dppm)$_1$] fragments).

Elemental analysis, calcd. (%) for $C_{260}H_{226}Cl_6Cu_{11}F_{18}N_{10}P_{23}Pt_4$: C 50.07, H 3.65, N 2.25; found: C 50.27, H 3.80, N 2.02.

IR (cm^{-1}): 691 (vs), 735 (vs), 787 (m), 832 (vs), 997 (s), 1026 (w), 1188 (vw), 1188 (vw), 1434 (s), 1481 (m), 1580 (w), 2121 (υ_{CN}, w), 2137 (υ_{CN}, vw), 3056 (vw).

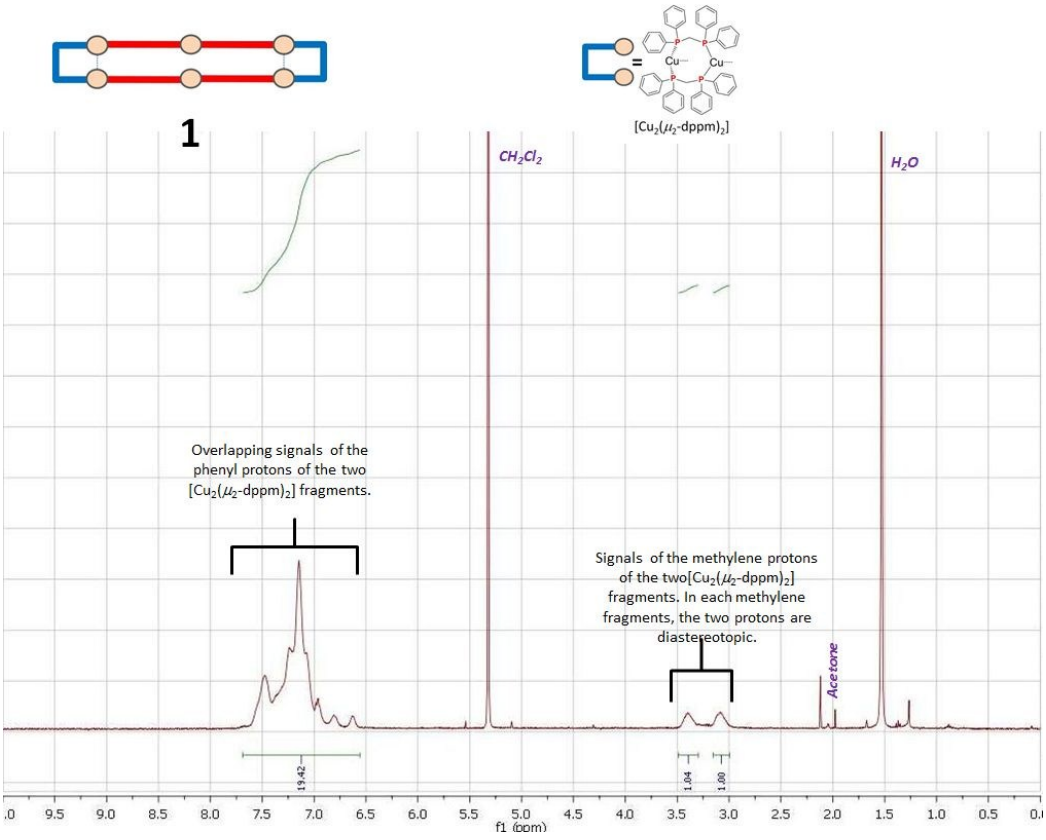


Fig. S1. ^{1}H NMR spectrum of **1** in CD_2Cl_2 at 400 MHz at 298K

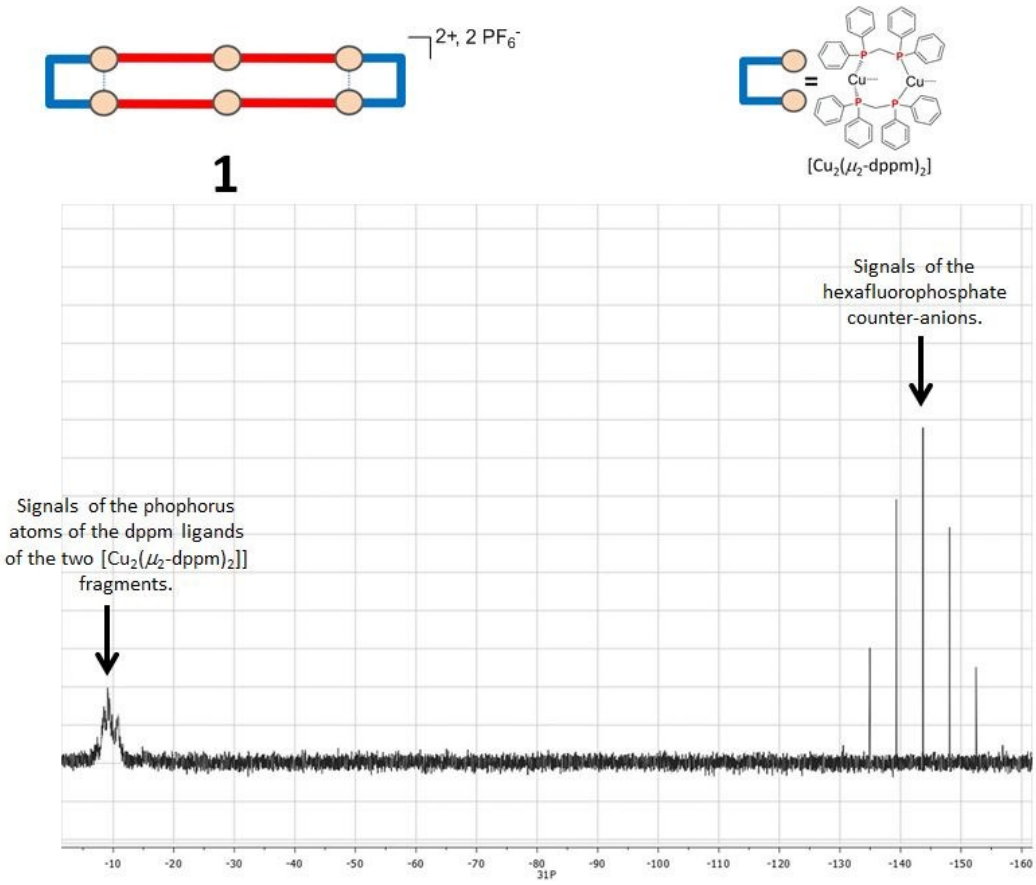


Fig. S2. $^{31}P\{^{1}H\}$ NMR spectrum of **1** in CD_2Cl_2 at 162 MHz at 298K

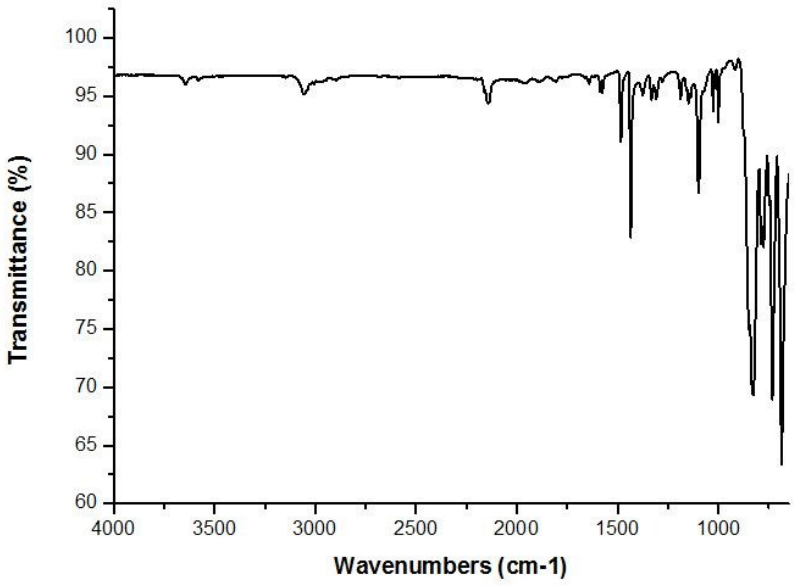


Fig. S3. IR spectrum of **1** in the solid state at 298K

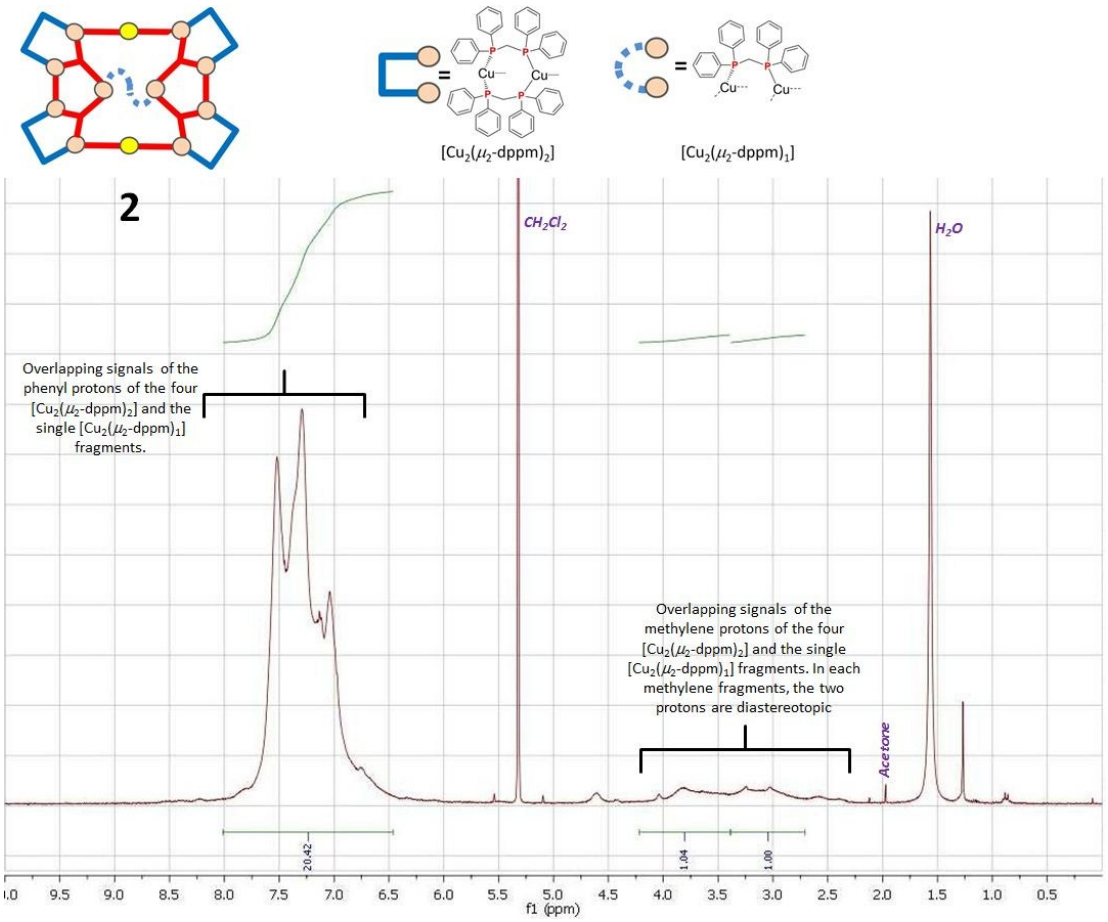


Fig. S4. ^{1}H NMR spectrum of **2** in CD_2Cl_2 at 400 MHz at 298K

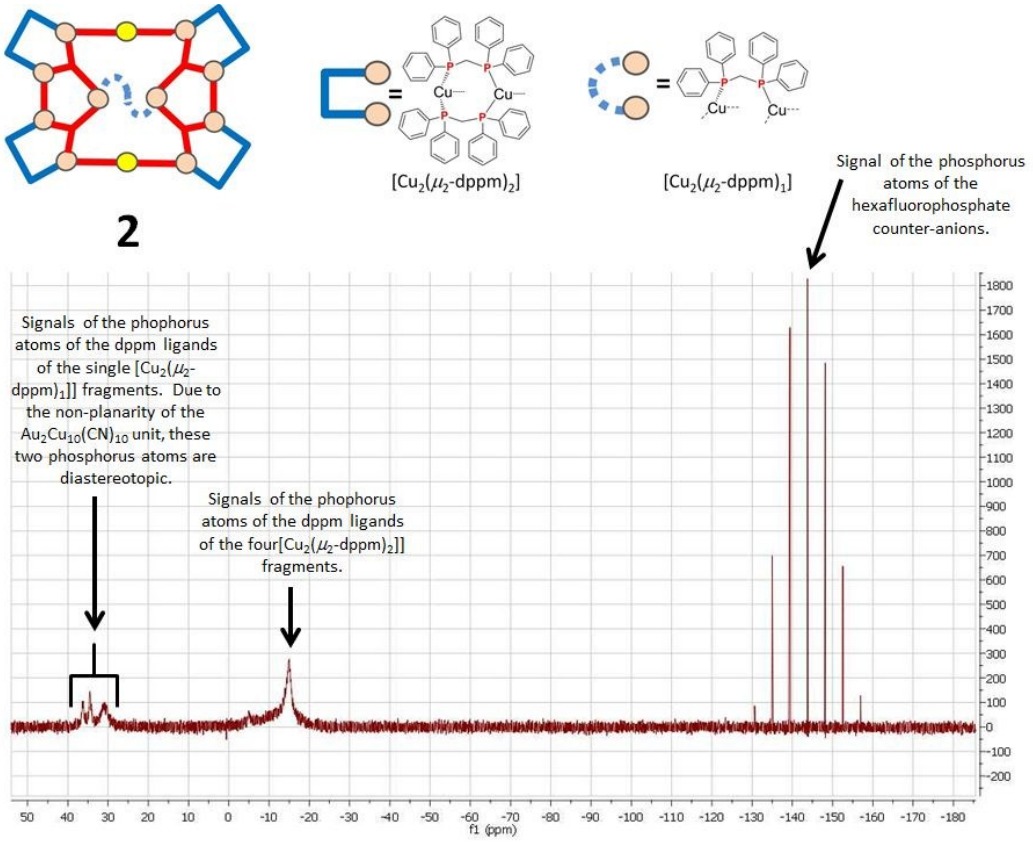


Fig. S5. $^{31}P\{^{1}H\}$ NMR spectrum of **2** in CD_2Cl_2 at 162 MHz at 298K

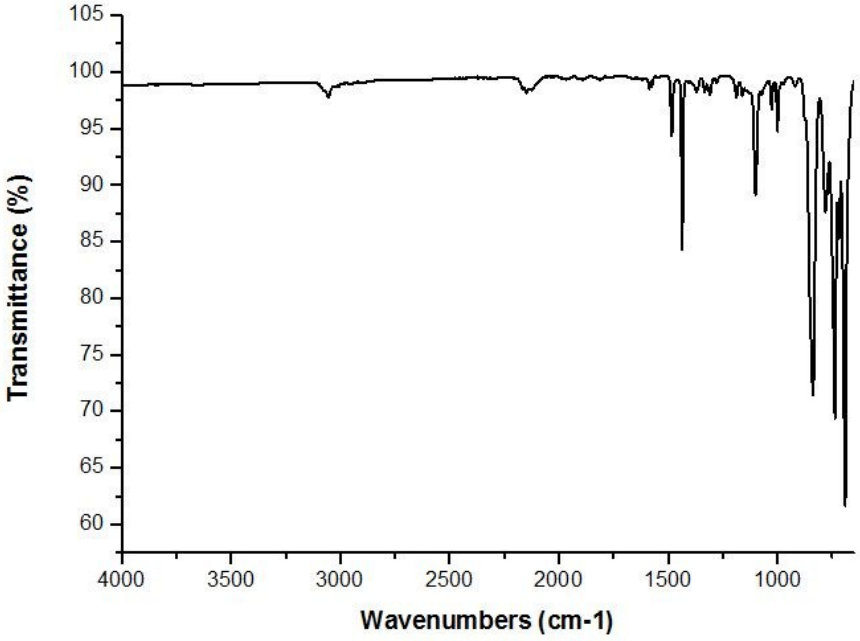


Fig. S6. IR spectrum of **2** in the solid state at 298K

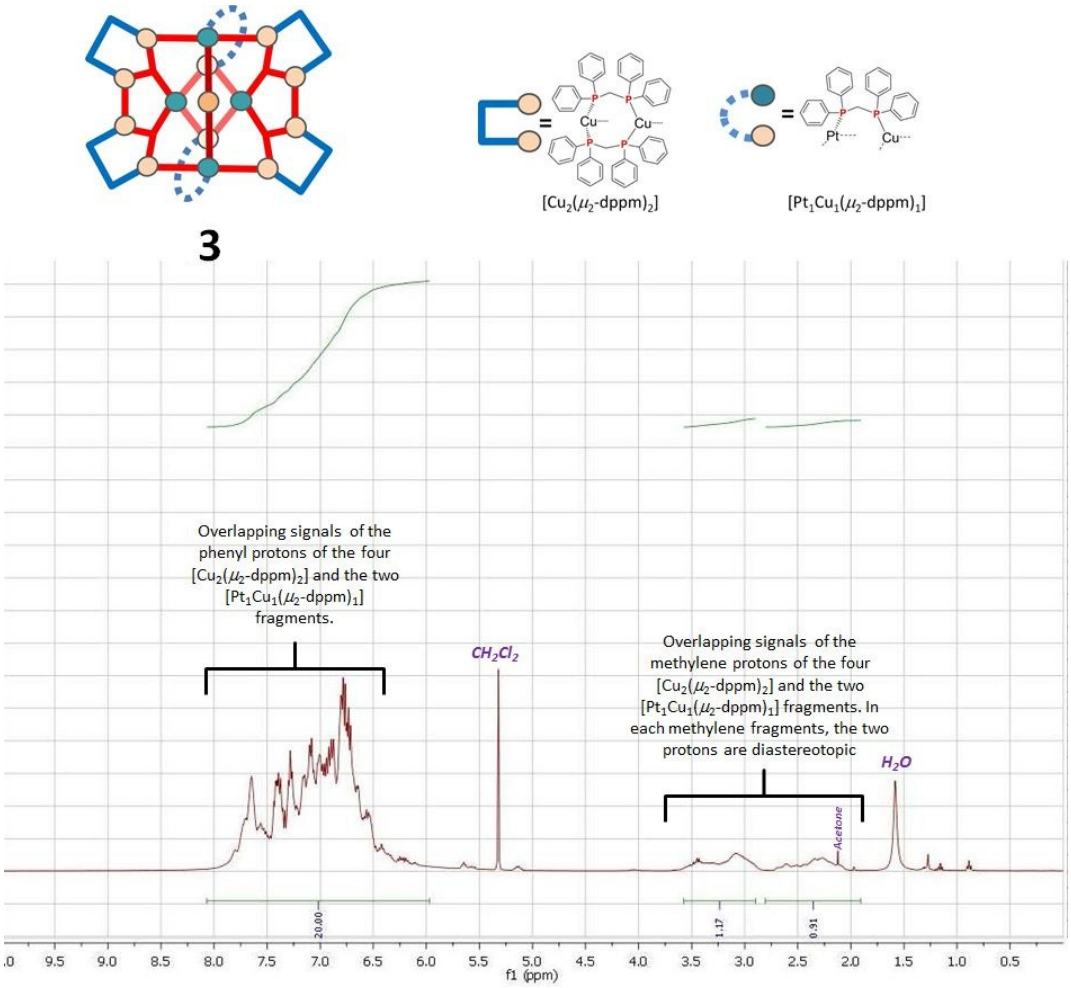


Fig. S7. ^{1}H NMR spectrum of **3** in CD_2Cl_2 at 400 MHz at 298K

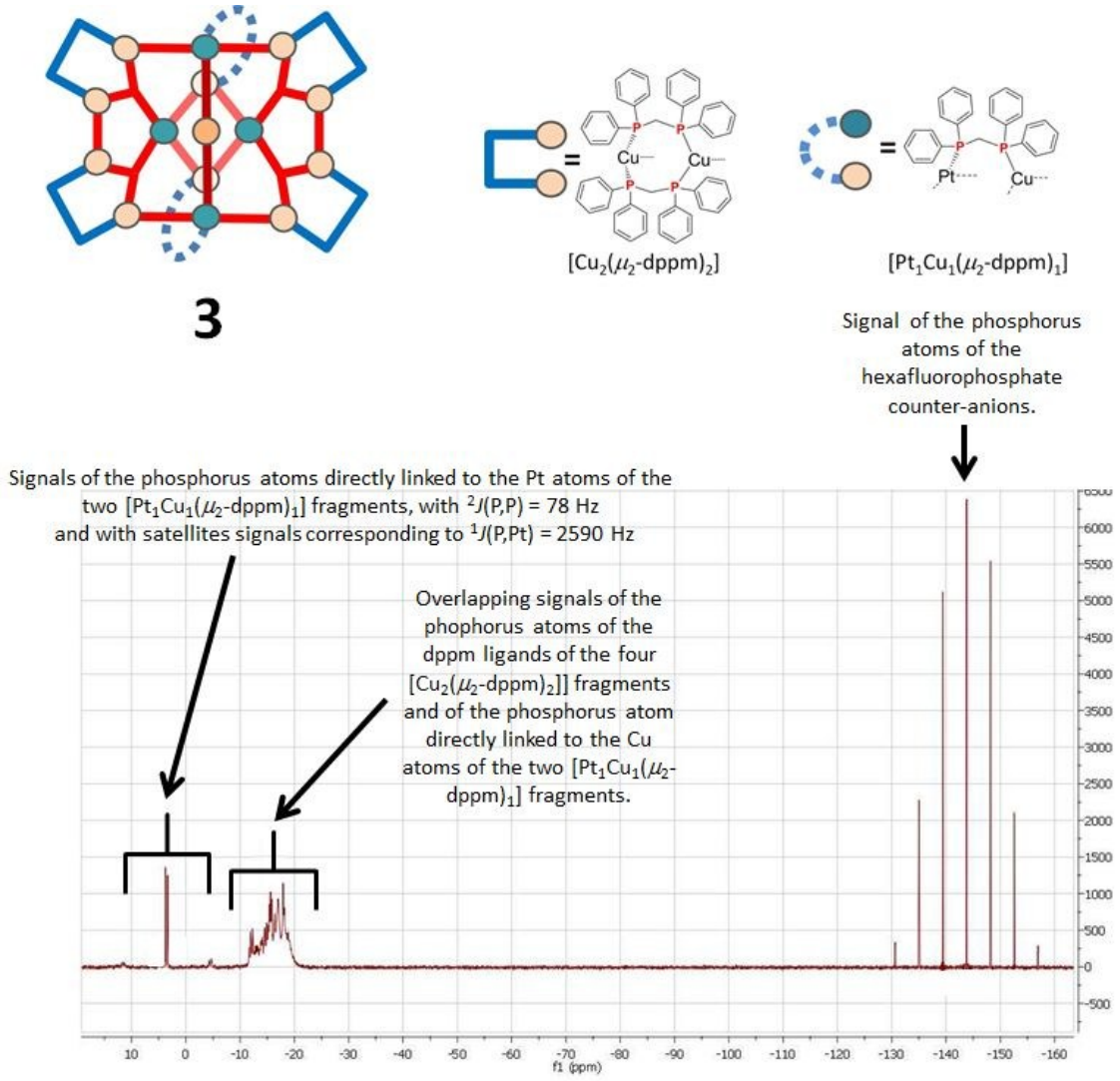


Fig. S8. $^{31}P\{^{1}H\}$ NMR spectrum of **3** in CD_2Cl_2 at 162 MHz at 298K

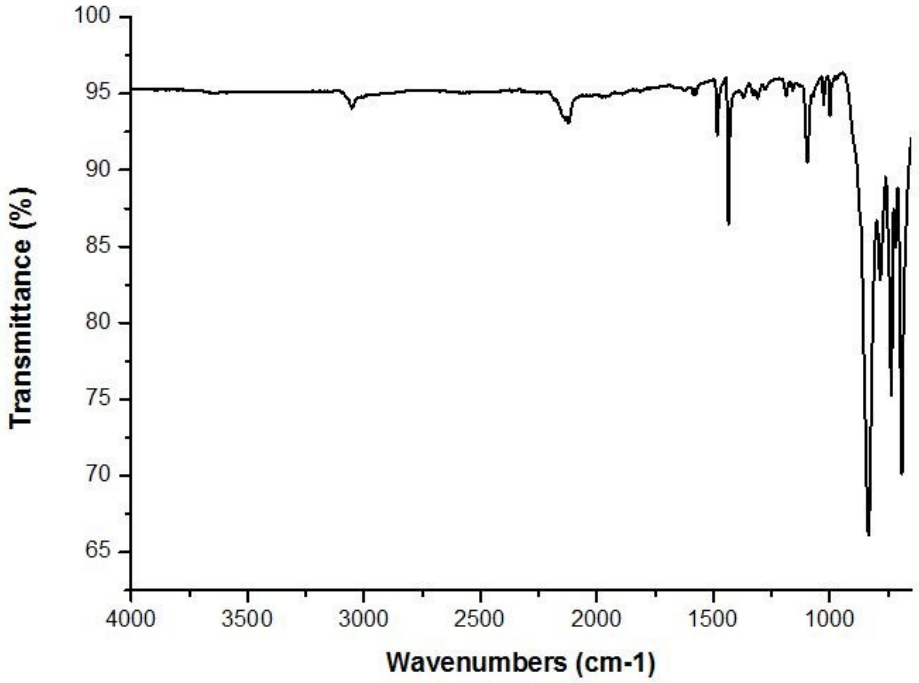


Fig. S9. IR spectrum of **3** in the solid state at 298K

II. X-ray Crystallographic Study

Single crystals of **1**, **2** and **3** suitable for X-ray crystal analyses were obtained by slow diffusion of vapors of n-pentane into crude mother solutions. Reference single crystal data collection for **1**, **2** and **3** were performed at 100 K for **1** and at 150 K for **2** and **3** with a D8 Venture Bruker AXS (Centre de Diffractométrie, Université de Rennes 1, France) with Mo-*K*α radiation (λ = 0.71073 Å). Temperature dependant single crystal data collections for **1** were performed at 100 K, 125 K, 150 K, 175 K, 200 K, 225 K and 250 K with a D8 Venture Bruker AXS (Centre de Diffractométrie, Université de Rennes 1, France) with Mo-*K*α radiation (λ = 0.71073 Å). Reflections were indexed, Lorentz-polarization corrected and integrated by the *DENZO* program of the KappaCCD software package. The data merging process was performed using the SCALEPACK program.[s3] Structure determinations were performed by direct methods with the solving program SIR97,[s4] that revealed all the non-hydrogen atoms. SHELXL program[s5] was used to refine the structures by full-matrix least-squares based on F^2. All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were included in idealised positions and refined with isotropic displacement parameters.

In the crystal lattices of the coordination complexes studied, dichloromethane solvent molecules were found in addition to the cationic coordination complexes and their counter-anions. These solvent molecules in most cases have a strong tendency to leave the bulk crystal via evaporation once the crystals are removed from their mother solution, a process that induce a rapid degradation of the single-crystal integrity of the crystals investigated. In order to slow down this process, single crystals of all these derivatives were always coated in paratone oil once removed from the mother solution, mounted at low temperature as quickly as possible on the diffractometer goniometer and X-ray data collection was performed at low temperature.

The included dichloromethane solvent molecules (for derivatives **1**, **2** and **3**) were found to be highly disordered and a correct modelling of the disorder of these solvent molecules was not always possible leading to rather high anisotropic displacement parameters for some of their atoms. We have therefore proceeded to a 'squeeze' treatment[s6] in order to remove the scattering contribution of these molecules which cannot be satisfactorily modelled (4 CH_2Cl_2 molecules for derivative **1**, 12 CH_2Cl_2 molecules for derivative **2** and 23 CH_2Cl_2 molecules for derivative **3**). As a result, since these disordered molecules occupy a significant volume of the unit cell, several ALERTs A appear in the checkcif reports since " VERY LARGE Solvent Accessible VOIDs" are present in the structure resolution. For the temperature dependant X-ray crystal structures of derivative **1**, included PF_6^- were also removed along the 'squeeze' treatment.[S6]

Concerning derivative **1**, in the asymetric unit, two phenyl ring of the dppm ligands were found disordered over two neighboring positions and the relatives occupancies were ponderated. The cyano carbon and nitrogen atoms are disordered and had to be modelled with isotropic parameters. Their relative occupancies and special coordinates were refined without constraints.

Concerning temperature dependence of the X-ray structure of the derivative **1**, measurements were performed on the same single crystal from 100 K to 250 K every 25 K. In order to keep a reasonable time for such data collection, time exposure for each frame collected was significantly shorter than the one time exposure applied for the data collection of the reference X-ray structure of the derivative **1** at 100 K (see above). As a result, the intrinsic quality of these temperature dependent the X-ray structures is lower than the one obtained for the reference X-ray structure of the derivative **1** at 100 K but is in complete agreement with the result obtained in this case. Nevertheless, the squeeze procedure in the case of the data treatment of the temperature dependent the X-ray structures of the derivative **1** also included the PF_6^- counter-anion that was not satisfactory modelled. In addition the quality of the modelling of the disordered phenyl rings was lower compared to the modelling of

these disorders in the case of reference X-ray structure of the derivative **1** at 100 K. As a consequence, several additional ALERTs appear in the different checkcif reports.

Concerning derivative **2**, one of the dppm ligands was found disordered over two neighboring positions and the relatives occupancies of all the carbon atoms involved were ponderated over these two position, with the exception of the phenyl ring containing the C(31), C(32), C(33) , C(34), C(35) and C(36) atoms. In this case, the modelling of the disorder over two positions lead to unstable refinements and therefore the carbon atoms of this phenyl ring were modelled being located on one single position associated with isotropic parameters and fairly high displacement parameters resultings in ALERTs A in the checkcif report. In the case of these atoms associated with the disordered dppm ligand, it was necessary to apply isotropic displacement parameters in these ponderations, implying several ALERTs in the checkcif report. As a consequence of this disorded, several atoms of the neighboring dppm ligands and of a PF_6^- counter anion are also disordered inducing quite large anisotropy factors that implied several ALERTs in the checkcif report. A correct modelling of these disorders was not realized as it induced a significant increase of the number of parameters refined and/or instable refinement cycles. For the same reasons, the C and N atoms of the CN^- fragments located between two Cu(I) centers were assigned arbitrarily while the CN^-fragments connecting the Cu(I) and the Au(I) metal centers were defined with the C atoms linked to the Au(I) centers and the N atoms linked to the Cu(I) centers. [s7]

Concerning derivative **3**, equal relative occupancies for C and N atoms have been modelled at the atomic position determined for the peripheral cyano ligands located between two Cu(I) metal centers. In the case of the atom involved, it was necessary to apply isotropic displacement parameters to some of the atoms in these ponderations, implying several ALERTs in the checkcif report. For the other cyano ligands, C atoms have been assigned to the atoms directly connected to the Pt(II) metal centres and N atoms have been assigned to the atoms directly connected to the Cu(I) metal centres.[s7] In addition, in the case of the derivative **3**, two phenyl rings of the dppm ligands were found disordered over two neighboring positions and the relatives occupancies were ponderated. In the case of the atom involved, it was necessary to apply isotropic displacement parameters to some of the atoms in these ponderations, implying several ALERTs in the checkcif report.

Table S1 gives the crystallographic data for the derivatives **1**, **2** and **3** after the 'squeeze' treatment. Table S2 give the crystallographic data for the derivatives **1**, **2** and **3** before 'squeeze' treatment.

Atomic scattering factors for all atoms were taken from International Tables for X-ray Crystallography.[S7] CCDC reference numbers 1895178, 1895184 and 1895185 contain the supplementary crystallographic data for the reference measurements of the X-ray crystal structures of the derivative **1** (100K), **2** (150K) and **3** (150K) respectively. CCDC reference numbers 1895179, 1895180, 1895182, 1895187, 1895183, 1895186 and 1895181 contain the supplementary crystallographic data for the temperature dependence of the X-ray crystal structures of the derivative **1** (100K, 125K, 150K, 175K, 200K, 225 K and 250K) These data can be obtained free of charge from the Cambridge Crystallographic Data Centre.

Table S1. Crystal data and structure refinement for derivatives **1**, **2** and **3** after the 'squeeze' treatment

	1 . 2PF$_6$	**2 . 2PF$_6$**	**3 . 3PF$_6$**
Molecular formula	$C_{104}H_{88}Cu_6F_{12}N_4P_{10}$	$C_{235}H_{198}Au_2Cu_{10}F_{12}N_{10}P_{20}$	$C_{266}H_{200}Cu_{11}F_{18}N_{16}P_{23}Pt_4$
CCDC number	1895178	1895184	1895185
Molecular weight	2312.72	5038.77	6174.19
a(Å)	16.377(1)	17.168(2)	51.162(3)
b (Å)	20.497(2)	17.670(2)	51.162
c (Å)	17.822(1)	86.943(11)	26.3704(17)
α (°)	90	90	90
β (°)	104.396(2)	94.106(7)	90
γ (°)	90	90	120
V (Å^3)	5794.6(7)	26307(5)	59777(5)
Z	2	4	6
*D*c (g cm^{-3})	1.325	1.272	1.029
Crystal system	Monoclinic	Monoclinic	Trigonal
Space group	P21/n	P21/n	P-31c
Temperature (K)	100(2)	150(2)	150(2)
Wavelength Mo-*K*α (Å)	0.71073	0.71073	0.71073
Crystal size (mm)	0.21 * 0.14 * 0.08	0.4 * 0.06 * 0.03	0.40 * 0.1 * 0.08
μ (mm^{-1})	1.281	2.078	2.108
F(000)	2344	10136	18396
θ limit (°)	2.37 – 27.45	0.94 – 27.56	3.96– 27.72
Index ranges *hkl*	-21 ≤*h*≤ 20, -26 ≤*k*≤ 26, -23 ≤*l*≤ 19	-20 ≤*h*≤ 22, -22 ≤*k*≤ 22, -112 ≤*l*≤ 107	-47 ≤*h*≤ 66, -66 ≤*k*≤ 43, -31 ≤*l*≤ 34
Reflections collected	51524	229731	325355
Independant reflections	13256	60238	46598
Reflections [$I>2\sigma(I)$]	10139	26080	28111
Data/restraints/parameters	13256/ 0 / 673	60238/ 0 / 1984	46598/ 0 / 1453
Goodness-of-fit on F^2	1.076	0.942	0.955
Final *R* indices [$I>2\sigma(I)$]	R1= 0.0546 wR2= 0.1569	R1= 0.0906 wR2= 0.2233	R1= 0.0566 wR2= 0.1329
R indices (all data)	R1= 0.0683 wR2= 0.1644	R1= 0.1847 wR2= 0.2551	R1= 0.1078 wR2= 0.1471
Largest diff peak and hole (e Å^{-3})	1.070 and -0.641	1.934 and -1.540	2.172 and -0.768

Table S2. Crystal data and structure refinement for derivatives **1**, **2** and **3** before the 'squeeze' treatment

	1 . $2PF_6.4CH_2Cl_2$	**2. $2PF_6.12CH_2Cl_2$**	**3. $3PF_6.23CH_2Cl_2$**
Molecular formula	$C_{108}H_{94}Cl_8Cu_6F_{12}N_4P_{10}$	$C_{247}H_{215}Au_2Cl_{24}Cu_{10}F_{12}N_{10}P_{20}$	$C_{289}H_{220}Cl_{46}Cu_{11}F_{18}N_{16}P_{23}Pt_4$
Molecular weight	2650.42	6050.82	8081.12
a(Å)	16.377(1)	17.168(2)	51.162(3)
b (Å)	20.497(2)	17.670(2)	51.162
c (Å)	17.822(1)	86.943(11)	26.3704(17)
α (°)	90	90.00	90
β (°)	104.396(2)	94.106(7)	90
γ (°)	90	90.00	120
V (Å^3)	5794.6(7)	26307(5)	59777(5)
Z	2	4	6
Dc (g cm^{-3})	1.519	1.528	1.347
Crystal system	Monoclinic	Monoclinic	Trigonal
Space group	P21/n	P21/n	P-31c
Temperature (K)	100(2)	150(2)	150(2)
Wavelength Mo-$K\alpha$ (Å)	0.71073	0.71073	0.71073
Crystal size (mm)	0.21 * 0.14 * 0.08	0.4 * 0.06 * 0.03	0.40 * 0.1 * 0.08
μ (mm^{-1})	1.470	2.327	2.424
F(000)	2676	12124	23916
θ limit (°)	2.37 – 27.45	0.94 – 27.56	3.96– 27.72
Index ranges hkl	-21 ≤h≤ 20, -26 ≤k≤ 26, -23 ≤l≤ 19	-20 ≤h≤ 22, -22 ≤k≤ 22, -112 ≤l≤ 107	-47 ≤h≤ 66, -66 ≤k≤ 43, -31 ≤l≤ 34
Reflections collected	51524	229731	325355
Independant reflections	13256	60238	46598
Reflections [I>2σ(I)]	10279	27070	27293
Data/restraints/parameters	13256/ 0 / 756	60238/ 0 / 2834	46598/ 0 / 1453
Goodness-of-fit on F^2	1.020	1.757	1.284
Final R indices [I>2σ(I)]	R1= 0.0723 wR2= 0.2067	R1= 0.1559 wR2= 0.3571	R1= 0.1329 wR2= 0.3250
R indices (all data)	R1= 0.0925 wR2= 0.2280	R1= 0.3060 wR2= 0.4893	R1= 0.2050 wR2= 0.3793
Largest diff peak and hole (e Å^{-3})	2.007 and -0.937	6.721 and -4.814	7.614 and -3.477

Table S3. Crystal data and structure refinement for derivative **1** at 100 K, 125 K, 150 K, 175 K, 200K, 225 K and 250K after the 'squeeze' treatments

	100K	**125K**	**150K**	**175K**
Molecular formula	$C_{104}H_{88}Cu_6N_4P_8$	$C_{104}H_{88}Cu_6N_4P_8$	$C_{104}H_{88}Cu_6N_4P_8$	$C_{104}H_{88}Cu_6N_4P_8$
CCDC number	1895179	1895180	1895182	1895187
Molecular weight	2022.78	2022.78	2022.78	2022.78
a (Å)	16.4642(7)	16.4868(6)	16.5201(7)	16.5640(7)
b (Å)	20.4801(8)	20.5016(8)	20.5304(9)	20.5580(9)
c (Å)	17.7355(8)	17.7554(8)	17.7924(9)	17.8345(9)
α (°)	90	90	90	90
β (°)	104.421(2)	104.513(2)	104.643(2)	104.804(2)
γ (°)	90	90	90	90
V (Å^3)	5791.8(4)	5809.9(4)	5838.5(5)	5871.5(5)
Z	2	2	2	2
*D*c (g cm^{-3})	1.160	1.156	1.151	1.144
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	P21/n	P21/n	P21/n	P21/n
Temperature (K)	100(2)	125(2)	150(2)	175(2)
Wavelength Mo-*K*α (Å)	0.71073	0.71073	0.71073	0.71073
Crystal size (mm)	0.24*0.14*0.11	0.24*0.14*0.11	0.24*0.14*0.11	0.24*0.14*0.11
μ (mm^{-1})	1.232	1.229	1.223	1.216
F(000)	2068	2068	2068	2068
θ limit (°)	1.51 –27.42	1.51 –27.45	1.50 –27.45	1.50 –27.43
Index ranges *hkl*	$-18 \le h \le 21$, $-20 \le k \le 26$, $-22 \le l \le 22$	$-21 \le h \le 18$, $-20 \le k \le 26$, $-22 \le l \le 22$	$-18 \le h \le 21$, $-20 \le k \le 26$, $-23 \le l \le 22$	$-18 \le h \le 21$, $-20 \le k \le 26$, $-23 \le l \le 23$
Reflections collected	38859	38932	39101	39488
Independant reflections	13039	13089	13156	13243
Reflections [$I>2\sigma(I)$]	8227	7860	7494	7163
Data/restraints/parameters	13039 / 0 / 484	13089 / 0 / 484	13156 / 0 / 484	13243 / 0 / 484
Goodness-of-fit on F^2	1.083	1.104	1.097	1.061
Final *R* indices [$I>2\sigma(I)$]	R1= 0.1089 wR2= 0.2932	R1= 0.1016 wR2= 0.2817	R1= 0.0938 wR2= 0.2656	R1= 0.0889 wR20.2483
R indices (all data)	R1= 0.1436 wR2= 0.3096	R1= 0.1418 wR2= 0.3001	R1= 0.1393 wR2= 0.2841	R1= 0.1394 wR2= 0.2672
Largest diff peak and hole (e Å^{-3})	0.809 and -1.038	0.790 and -1.003	0.813 and -0.868	0.703 and -0.888

	200K	**225K**	**250K**
Molecular formula	$C_{104}H_{88}Cu_6N_4P_8$	$C_{104}H_{88}Cu_6N_4P_8$	$C_{104}H_{88}Cu_6N_4P_8$
CCDC number	1895183	1895186	1895181
Molecular weight	2022.78	2022.78	2022.78
a (Å)	16.6264(8)	16.6665(14)	16.668(3)
b (Å)	20.5858(11)	20.6256(18)	20.655(4)
c (Å)	17.9032(11)	18.0048(19)	18.088(4)
α (°)	90	90	90
β (°)	105.128(3)	105.255(5)	105.289(11)
γ (°)	90	90	90
V (Å^3)	5915.3(6)	5971.2(10)	6007(2)
Z	2	2	2
*D*c (g cm^{-3})	1.136	1.125	1.118
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	P21/n	P21/n	P21/n
Temperature (K)	200(2)	225(2)	250(2)
Wavelength Mo-*K*α (Å)	0.71073	0.71073	0.71073
Crystal size (mm)	0.24*0.14*0.11	0.24*0.14*0.11	0.24*0.14*0.11
μ (mm^{-1})	1.207	1.195	1.188
F(000)	2068	2068	2068
θ limit (°)	1.49 –27.42	1.48 –27.47	1.48 –27.87
Index ranges *hkl*	$-19 \le h \le 21$, $-20 \le k \le 26$,	$-19 \le h \le 21$, $-20 \le k \le 26$,	$-19 \le h \le 21$, $-20 \le k \le 26$,

	-23 ≤ *l* ≤ 23	-23 ≤ *l* ≤ 23	-23 ≤ *l* ≤ 23
Reflections collected	39645	40087	40465
Independant reflections	13319	13467	13778
Reflections [$I>2\sigma(I)$]	6324	5864	5516
Data/restraints/parameters	13319 / 0 / 484	13467 / 0 / 484	13778 / 0 / 484
Goodness-of-fit on F^2	0.904	0.897	0.869
Final *R* indices [$I>2\sigma(I)$]	R1= 0.0690	R1= 0.0691	R1= 0.0706
	wR2= 0.1665	wR2= 0.1665	wR2= 0.1704
R indices (all data)	R1= 0.1327	R1= 0.1438	R1= 0.1540
	wR2= 0.1868	wR2= 0.1893	wR2= 0.1937
Largest diff peak and hole (e Å^{-3})	0.855 and -0.506	0.996 and -0.579	0.901 and -0.710

Table S4. Intermetallic distances [Å] and angles [°] for the derivatives **1** (at different temperatures), **2** (at 150K), and **3** (at 150 K)

	1 $_{100K}$	**1** $_{125K}$	**1** $_{150K}$	**1** $_{175K}$	**1** $_{200K}$	**1** $_{225K}$	**1** $_{250K}$	**2**	**3**
Cu(1)-Cu(2)	2.873(4)	2.877(4)	2.880(1)	2.886(1)	2.898(9)	2.905(9)	2.908(1)	2.952(2)	
Cu(3)-Cu(3)	3.769(5)	3.778(5)	3.782(1)	3.791(1)	3.793(9)	3.794(9)	3.797(1)		
Cu(3)-Cu(4)								2.959(2)	
Cu(5)-Cu(6)								3.012(1)	
Cu(7)-Cu(8)								2.912(2)	
Cu(9)-Cu(10)								6.339(2)	
Cu(1)-Cu(1)									6.382(8)
Cu(2)-Cu(3)									3.036(1)
Cu(4)-Cu(5)									3.179(1)
Cu(1)-Cu(2)'	9.783(5)	9.778(5)	9.776(1)	9.772(1)	9.769(1)	9.779(1)	9.781(2)		
Au(1)-Au(2)								11.095(1)	
Pt(2)-Pt(2)'									9.368(4)
Pt(3)-Pt(3)'									6.573(5)
Cu-Pt									2.945(1)
Cu(1)-Cu(2)-Cu(1)'	123.37(1)	123.27(1)	123.22(3)	123.05(3)	122.86(2)	122.63(2)	122.50(2)		
Cu(2)'-Cu(1)-Cu(2)	56.63(1)	56.73(1)	56.78(2)	56.95(2)	57.14(2)	57.37(2)	57.50(2)		

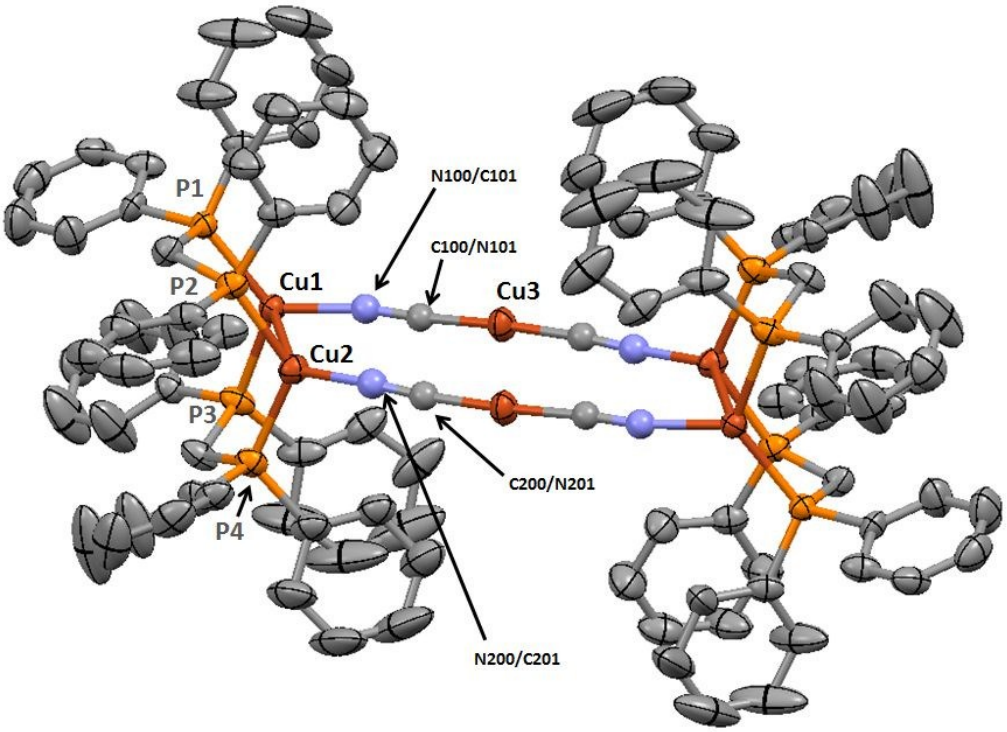


Fig. S10. ORTEP views of the molecular structure of the derivative **1,** Hydrogen atoms have been omitted for clarity. Only one position over the two positions modelled for the disordered phenyl ring has been shown, as well as for the modelled cyano fragments located between two Cu(I) metal centers

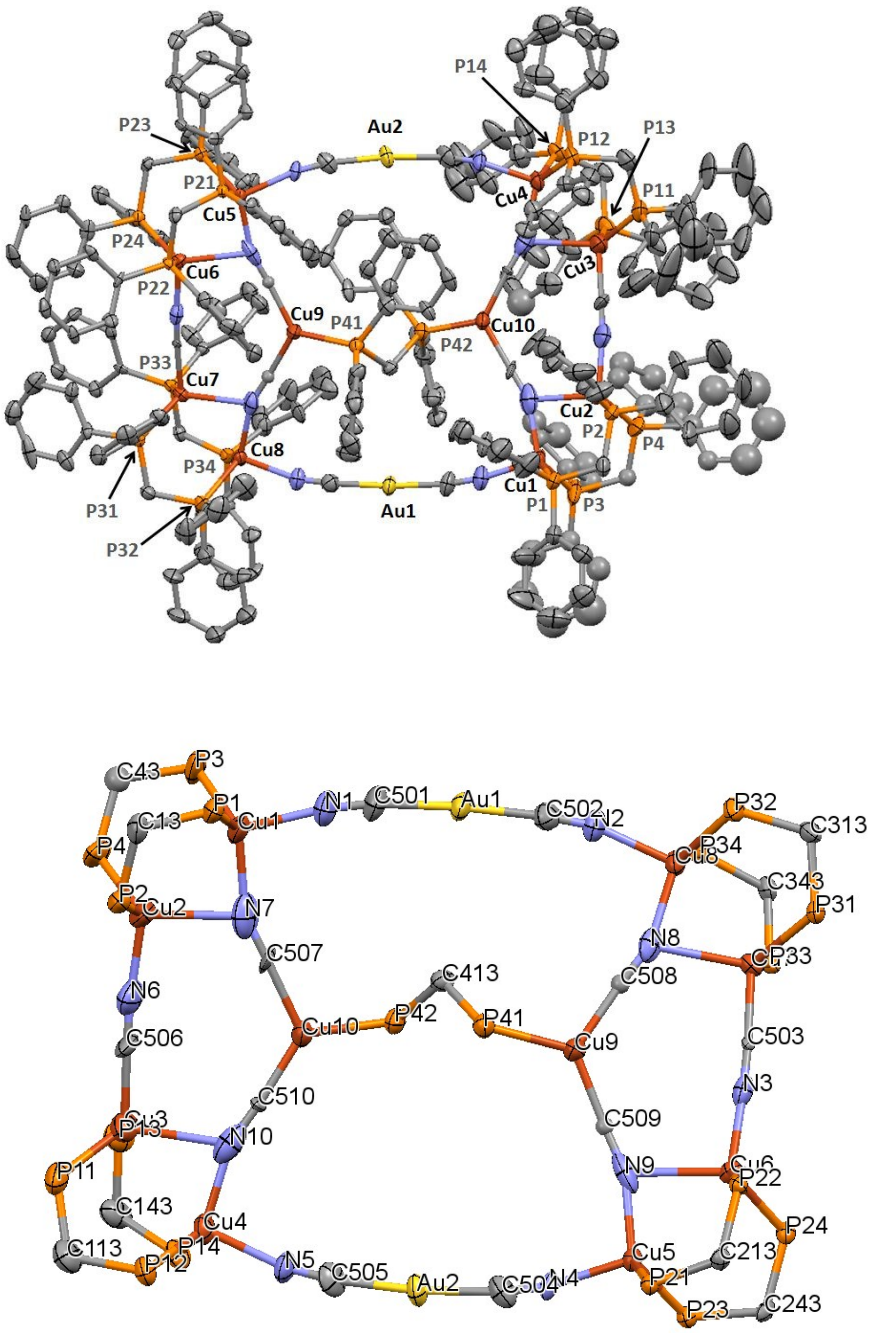


Fig. S11. Detailed and simplified ORTEP views of the molecular structure of the derivative **2,** Hydrogen atoms have been omitted for clarity. Only one position over the two positions modelled for the disordered phenyl ring has been shown

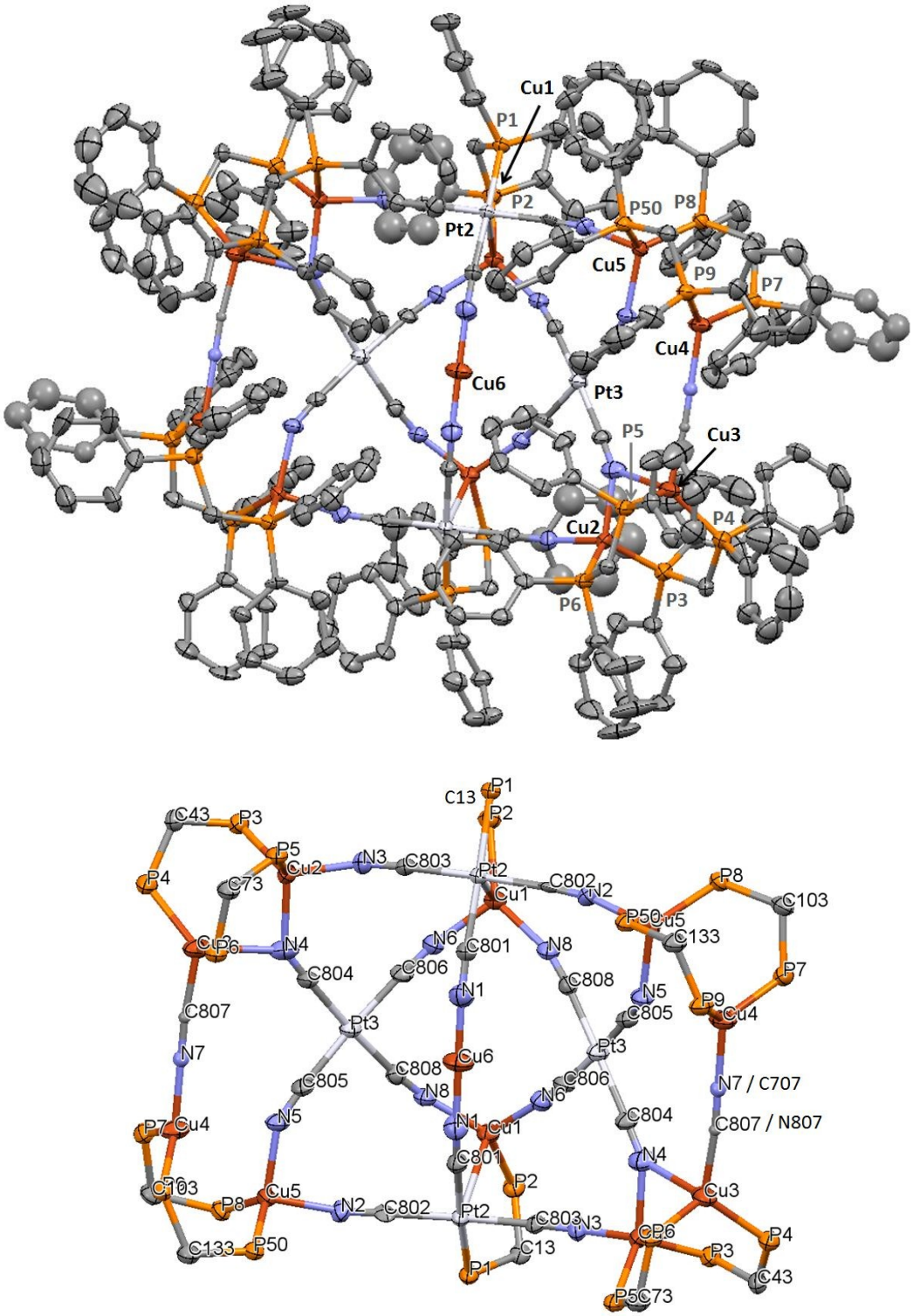


Fig. S12. Detailed and simplified ORTEP views of the molecular structure of the derivative **3,** Hydrogen atoms have been omitted for clarity. Only one position over the two positions modelled for the disordered phenyl ring has been shown, as well as for the modelled cyano fragments located between two Cu(I) metal centers

III. Photophysical study

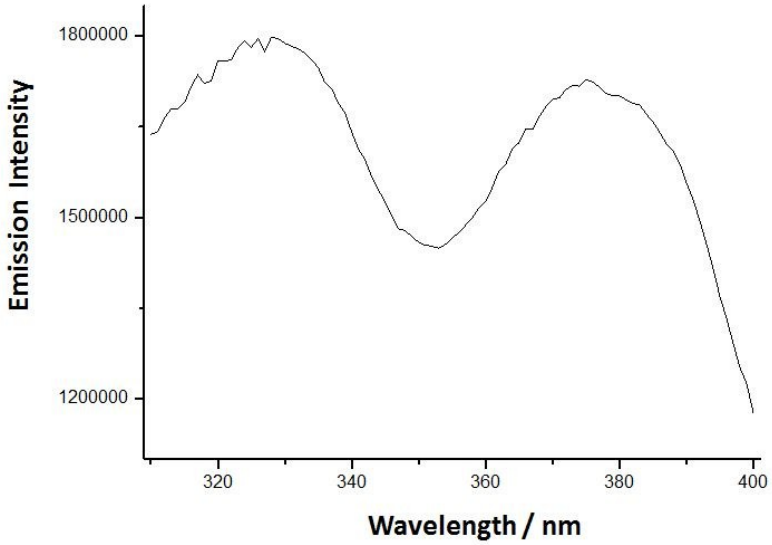


Fig. S13. RT solid state excitation spectrum of **1** at 298K

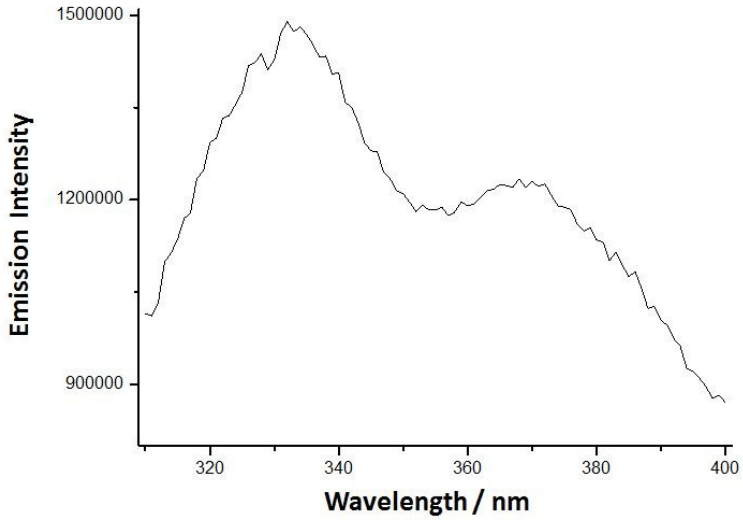


Fig. S14. RT solid state excitation spectrum of **2** at 298K

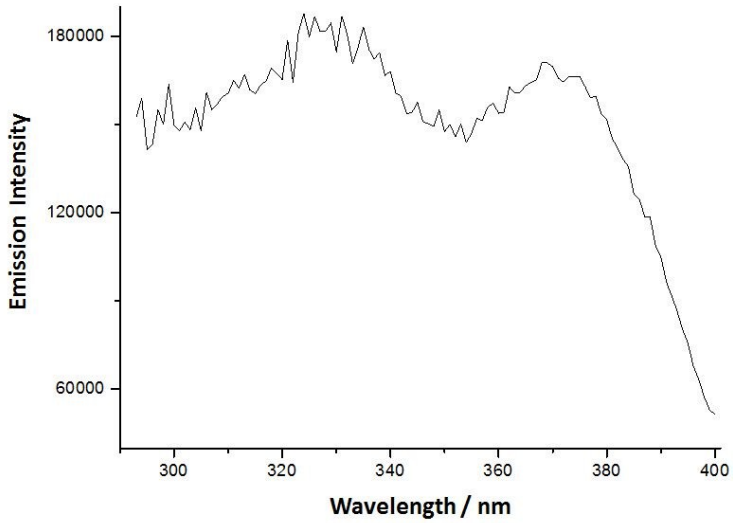


Fig. S15. RT solid state excitation spectrum of **3** at 298K

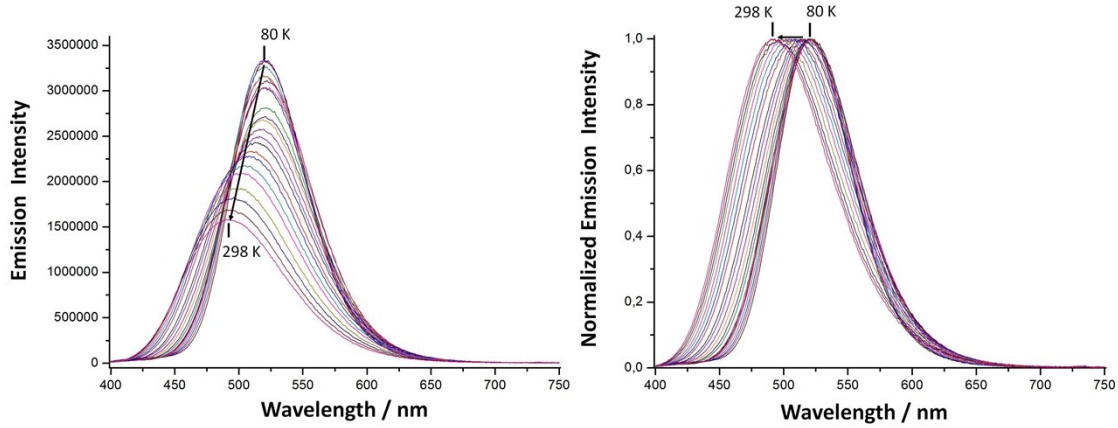


Fig. S16. Temperature-dependent non-normalized (left) and normalized (right) solid state emission spectra of **1** (λ_{exc} = 365 nm), from 80 K to 298 K (measurements were performed every 10 K)

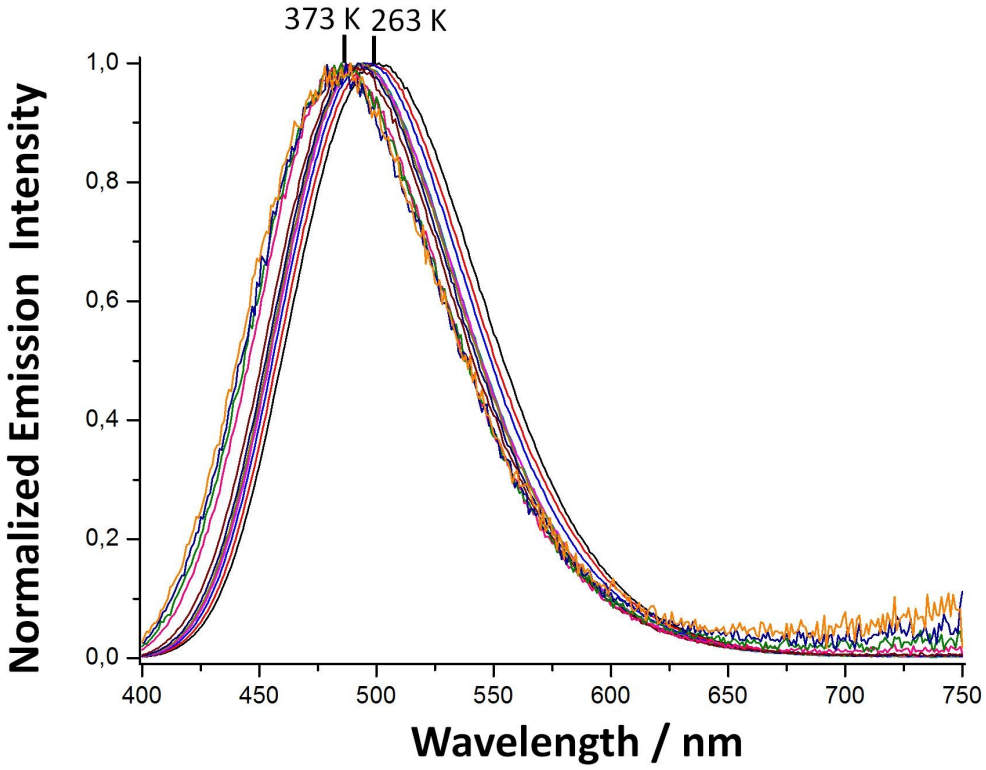


Fig. S17. Temperature-dependent normalized solid state emission spectra of **1** (λ_{exc} = 365 nm), from 263 K to 373 K (measurements were performed every 10 K)

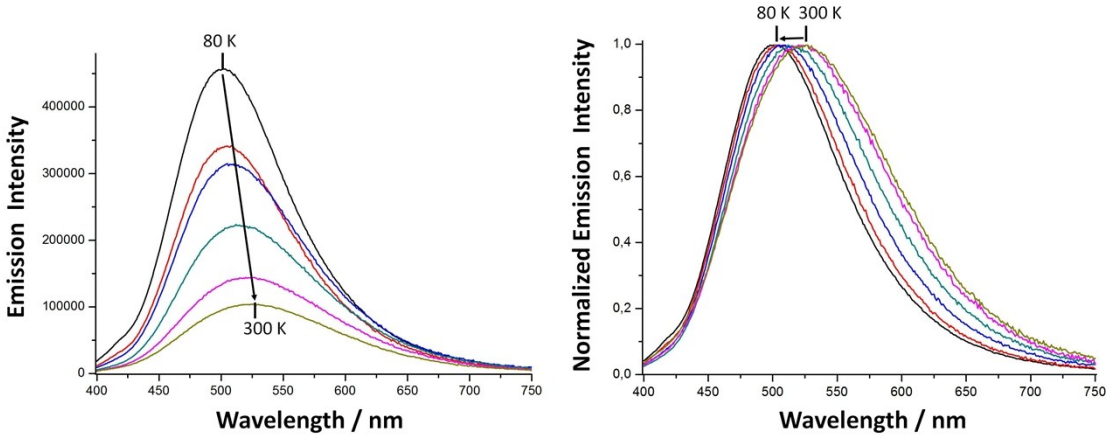


Fig. S18. Temperature-dependent non-normalized (left) and normalized (right) solid state emission spectra of **2** (λ_{exc} = 330 nm), from 80 K to 300 K (measurements were performed every 50 K)

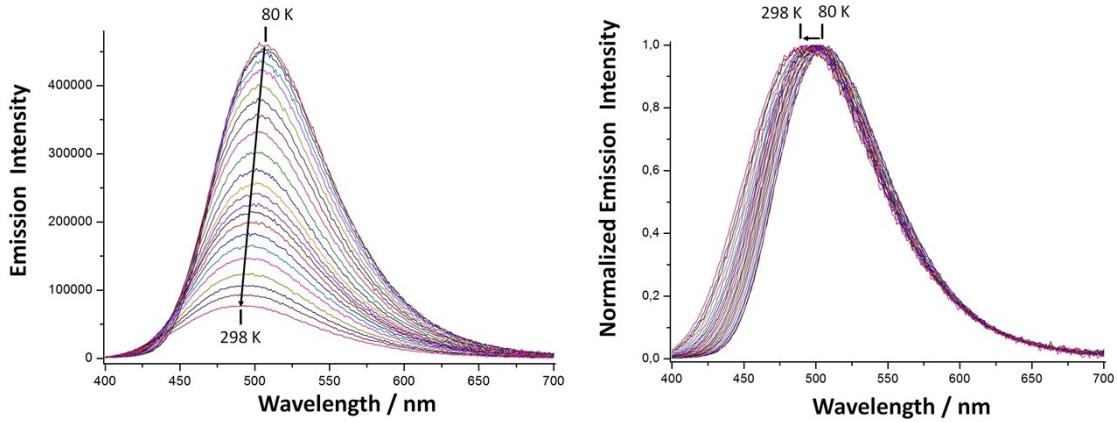


Fig. S19. Temperature-dependent non-normalized (left) and normalized (right) solid state emission spectra of **3** (λ_{exc} = 385 nm), from 80 K to 298 K (measurements were performed every 10 K)

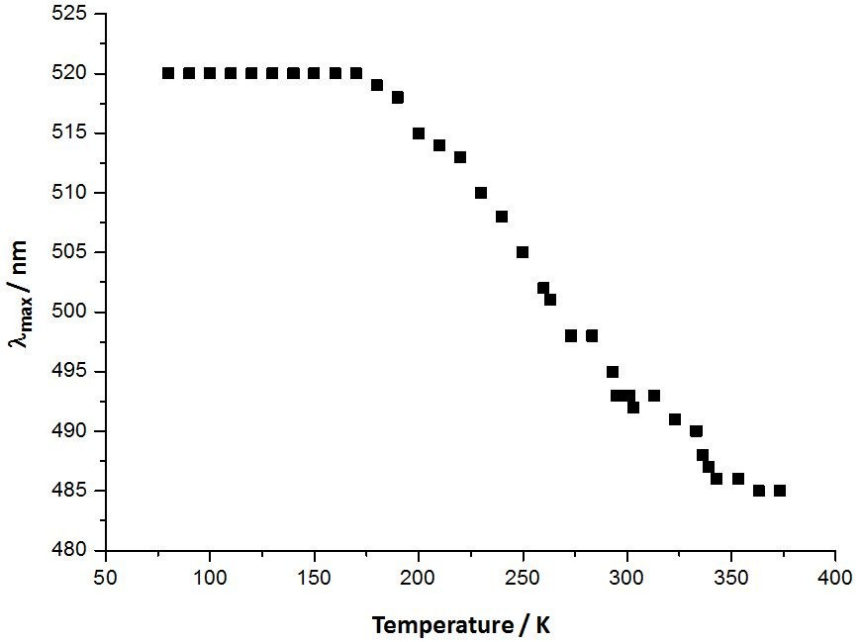


Fig. S20: A plot of emission peak maximum (λ_{em}) of the solid-state emission spectra of **1** against temperature

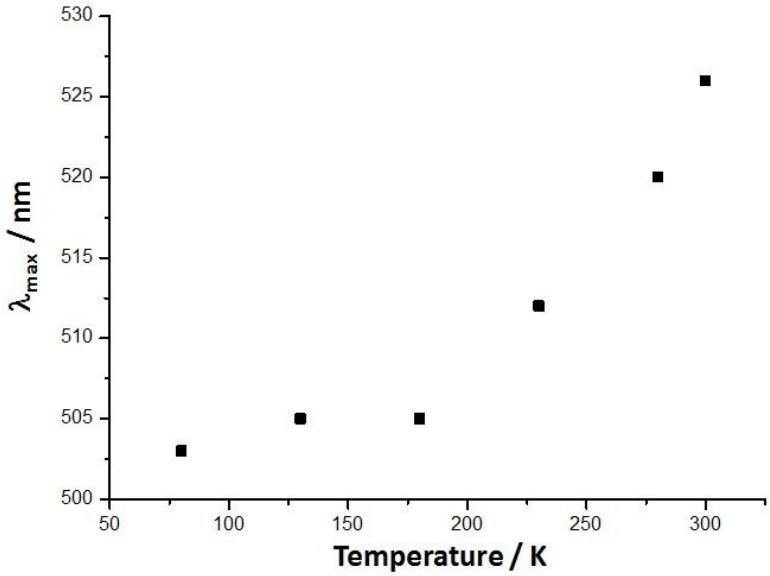


Fig. S21: A plot of emission peak maximum (λ_{em}) of the solid-state emission spectra of **2** against temperature

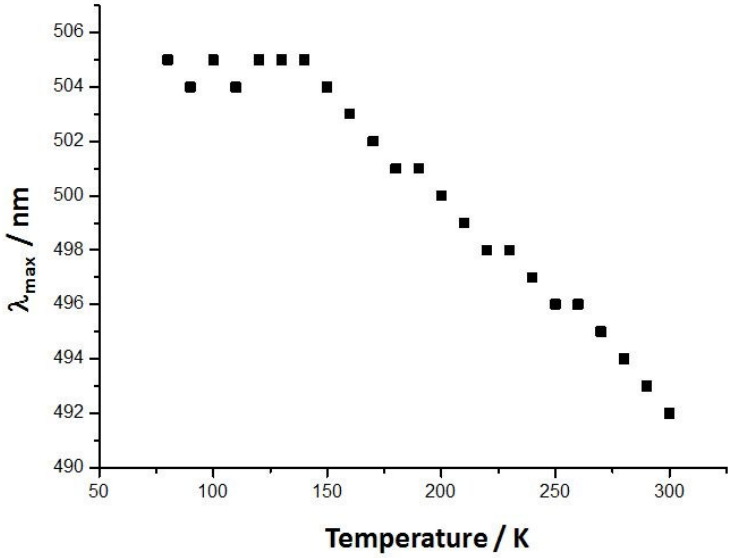


Fig. S22: A plot of emission peak maximum (λ_{em}) of the solid-state emission spectra of **3** against temperature

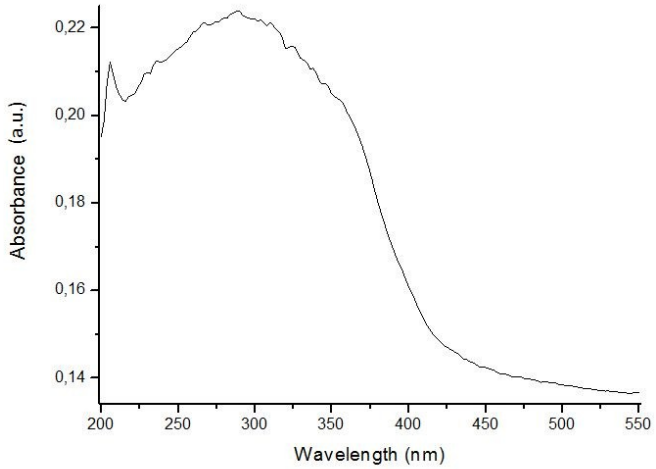


Fig. S23: Solid state UV-Vis absorption spectrum of **1** at room temperature

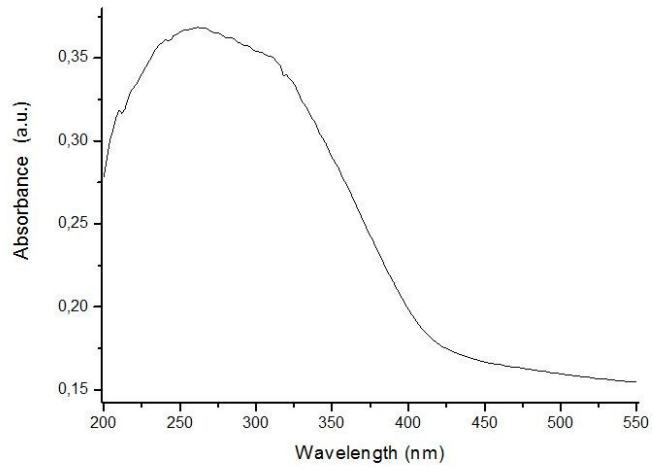


Fig. S24: Solid state UV-Vis absorption spectrum of **2** at room temperature

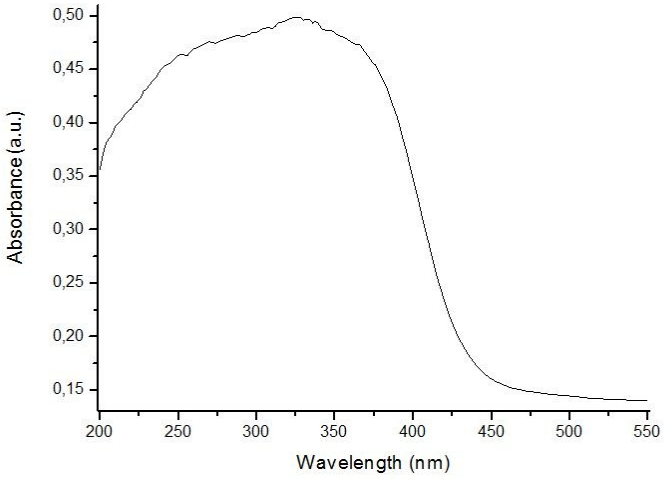
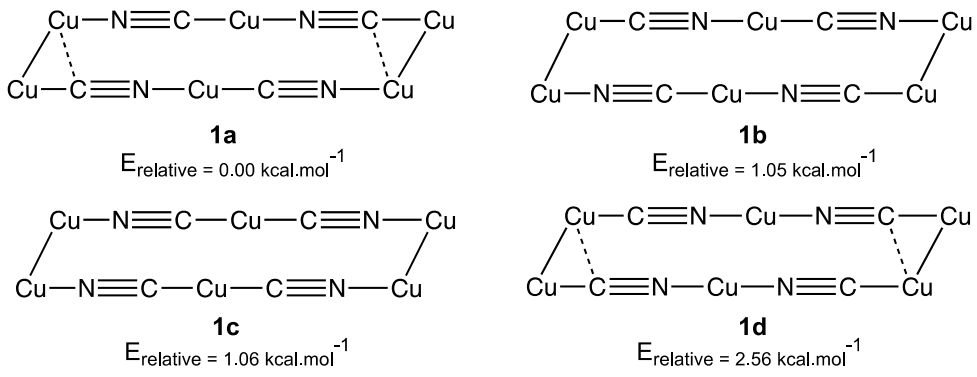


Fig. S25: Solid state UV-Vis absorption spectrum of **3** at room temperature

IV. Computational details

DFT calculations were carried out using the Gaussian 09 program,[1] and using ADF for the spin-orbit coupling calculations.[2] The different isomers of **1** (**1a**, **1b**, **1c**, **1d**) in their ground states configuration (S_0) (see Scheme S1) were fully optimized imposing a C_i symmetry following the X-Ray characterization using PBE0[3] functional and SVP[4] atomic basis set. Harmonic vibrational frequency calculations were not possible because of the size of the systems (2240 basis functions). Tighter criteria of energy convergence were applied to ensure high quality of calculations (10^{-10} u.a.). The relative energies (see Scheme S1) of those four isomers are small and do not allow excluding the existence any of these isomers on the thermodynamic point of view.



Scheme S1

Taking into account the enormous computational cost that a complete excited states investigation of each isomer would generate, we have focused our efforts at a first stage on the study of the excited state properties of **1a**, which is the most stable isomer, and of **1c**, which presents a nitrogen-only coordination sphere for the bridging bi-coordinated Cu atoms (most probable scenario on the synthetic mechanism point of view). It has to be emphasized that the most stable S_0 arrangement **1a** is diverging more importantly from the X-Ray geometry than **1c** (bent Cu-NC-Cu-CN-Cu chains (167-174 °) not observed experimentally). The isomer **1c**'s metrics better compare to the experimental X-Ray structures. The first excited-state S_x and T_x (x = 1, 2, 3) geometries of **1a** and **1c** were optimized using analytic TD-DFT gradients. A careful check of the optimization procedure was done to avoid jumps between potential energy surfaces. At that stage, the isomer **1a** was excluded from the rest of the computational study since its first triplet excited state is much higher in energy than the one of **1c** (+ 3.39 kcal.mol^{-1}) and its associative emission energy of 478 nm diverges strongly from the experimental measurements (~ 520 nm). Thus, only the isomer **1c** was considered for the rest of the study and the use of labelling **1** in the main text stands and hereafter for the **1c** isomer.

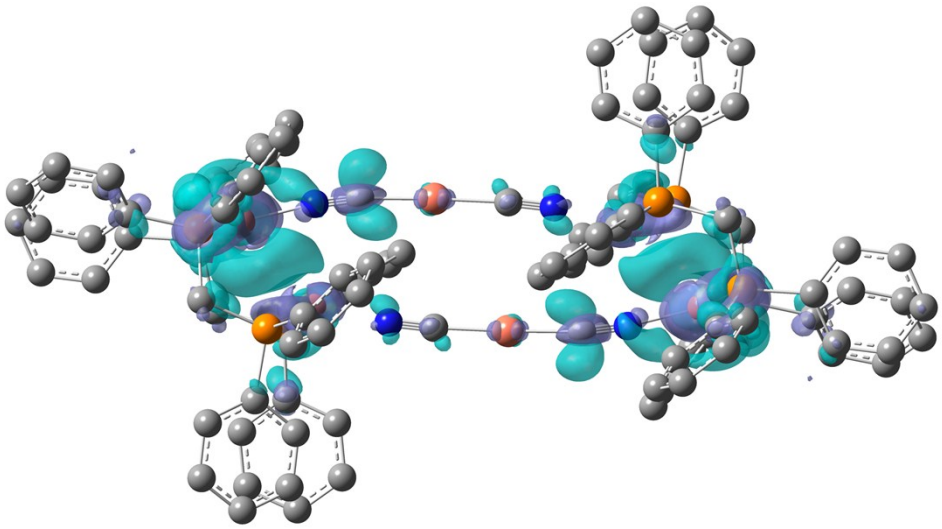


Fig. S26. Isosurface plots of the electronic charge-density difference between the first singlet excited state and the ground state (purple = density depletion, blue = density increase) of **1** (± 8.10^{-4} e.borh^{-3})

Table S5. Energetics associated with **1** (**1c**) optimized excited states: relative energies compare to S_0 and S_1 and emission energies. Experimental data are given for sake of comparison

	E_{rel/S_0} (eV)	E_{rel/S_1} (cm^{-1})	$E_{emission}$ (eV)	$E_{emission}$ (nm)
First relaxed singlet excited states				
S_1	3.055	0	2.502	496
S_2	3.100	364	2.492	497
S_3	3.119	524	2.511	494
First relaxed triplet excited states				
T_1	2.843	-1703	2.212	560
$T_{1\text{-const}}$	2.988	-533	2.412	514
T_2	3.090	290	2.598	477
Experimental data				
S_1	-	0	2.546	487
T_1	-	-1023	2.375	522

DFT 2-component spin-orbit coupling calculations were performed with the ADF2019 package on the optimized S_x and T_x structures.[2] For these calculations, the same hybrid functional PBE0 was used, with an all-electron triple-zeta Slater basis set with two additional polarization function. Calculations relying on the Tamm-Dancoff approximation (TDA) of the full TD-DFT equations were used to evaluate the lifetime of the excited states and the oscillator strengths.[5]

The iso-surface representations were done using the GaussView 5.0 program.[6]

Table S6. Cartesian coordinates of the optimized geometries of **1** in S_0, S_1, S_2, S_3, T_1, T_1-const, T_2 states

S_0

E_{rel/S_0} = 0.000 eV

Cu	2.800226	-2.933459	4.413707
Cu	2.708866	-0.356368	3.190781
Cu	-0.224789	-1.809196	0.613761
P	4.880599	-3.630523	3.710545
P	4.917066	-0.738069	2.668617
P	2.259876	-2.398102	6.572548
P	1.929057	0.335142	5.238502
C	0.799725	-2.450168	2.061398
C	1.218041	1.112196	0.831948
N	1.496822	-2.702892	2.963168
N	1.792320	0.612014	1.713524
C	5.968885	-4.658557	4.765817
C	6.490548	-5.883238	4.332133
H	6.269356	-6.251772	3.328360
C	7.299434	-6.639773	5.179966
H	7.702604	-7.593255	4.830864
C	7.596788	-6.182011	6.461457
H	8.236533	-6.774143	7.119952
C	7.068534	-4.968981	6.904540
H	7.284582	-4.609605	7.913079
C	6.249391	-4.217226	6.067148
H	5.817239	-3.285402	6.443741
C	4.922155	-4.429788	2.071722
C	6.075467	-4.466097	1.274810
H	7.001678	-3.994354	1.612124

C	6.055100	-5.113188	0.042895
H	6.957130	-5.135179	-0.572805
C	4.887970	-5.737234	-0.401460
H	4.878149	-6.250910	-1.365832
C	3.739023	-5.708300	0.385825
H	2.824821	-6.198369	0.042886
C	3.753621	-5.051409	1.615751
H	2.847137	-5.014196	2.225019
C	5.862534	-2.072447	3.532643
H	6.843974	-2.250443	3.065545
H	6.038925	-1.720884	4.562428
C	5.237845	-1.055938	0.894537
C	6.485281	-0.793045	0.313326
H	7.288374	-0.350230	0.909130
C	6.703847	-1.079380	-1.031931
H	7.677694	-0.868822	-1.480398
C	5.679582	-1.628378	-1.805054
H	5.854951	-1.855396	-2.859641
C	4.433534	-1.881845	-1.233921
H	3.629011	-2.307689	-1.838459
C	4.208856	-1.589761	0.110719
H	3.228745	-1.779369	0.554512
C	5.868937	0.778936	3.042270
C	7.144674	0.780484	3.620395
H	7.645778	-0.155598	3.876902
C	7.798634	1.985865	3.876438
H	8.794267	1.975790	4.326215
C	7.187442	3.196459	3.557053
H	7.702378	4.138587	3.759004
C	5.916935	3.202439	2.980981
H	5.430444	4.148769	2.734365
C	5.258236	2.002588	2.728330
H	4.258301	2.015854	2.284655
C	3.240241	-3.110794	7.942727
C	3.186568	-4.504335	8.098195
H	2.577051	-5.108801	7.419878
C	3.898007	-5.128740	9.117305
H	3.842382	-6.213746	9.230571
C	4.682845	-4.371950	9.988973
H	5.240109	-4.862274	10.790599
C	4.750033	-2.989181	9.836279
H	5.357428	-2.390564	10.519310
C	4.029914	-2.358268	8.819783
H	4.087131	-1.271165	8.732852
C	0.537564	-2.683497	7.111455
C	-0.410993	-3.089708	6.166721
H	-0.115100	-3.227774	5.123440
C	-1.730532	-3.317708	6.556544
H	-2.467070	-3.638374	5.816294
C	-2.105054	-3.144408	7.887099
H	-3.137278	-3.330667	8.193249
C	-1.160236	-2.744429	8.834133
H	-1.451446	-2.619366	9.879687
C	0.158168	-2.518133	8.450931
H	0.898581	-2.228413	9.201976
C	2.532826	-0.577534	6.724838
H	3.626457	-0.438130	6.726513
H	2.126285	-0.170739	7.664856
C	0.113526	0.434052	5.433091
C	-0.700642	0.088273	4.349552
H	-0.245998	-0.249101	3.416015
C	-2.088774	0.179371	4.458046
H	-2.718922	-0.091091	3.606810
C	-2.667684	0.609574	5.649496
H	-3.754926	0.674407	5.738567
C	-1.859584	0.961265	6.732792
H	-2.312133	1.304638	7.665872
C	-0.474967	0.880518	6.624315
H	0.147499	1.179511	7.472104
C	2.472414	2.060284	5.536738
C	3.441267	2.420567	6.479764
H	3.896432	1.673075	7.132611
C	3.839143	3.751738	6.607828
H	4.591416	4.020627	7.352976
C	3.276622	4.733484	5.796240
H	3.585146	5.775958	5.903593
C	2.314172	4.380413	4.849151

H	1.866527	5.146403	4.211363
C	1.916919	3.053619	4.715578
H	1.163960	2.786740	3.968728
Cu	-2.800226	2.933459	-4.413707
Cu	-2.708866	0.356368	-3.190781
Cu	0.224789	1.809196	-0.613761
P	-4.880599	3.630523	-3.710545
P	-4.917066	0.738069	-2.668617
P	-2.259876	2.398102	-6.572548
P	-1.929057	-0.335142	-5.238502
C	-0.799725	2.450168	-2.061398
C	-1.218041	-1.112196	-0.831948
N	-1.496822	2.702892	-2.963168
N	-1.792320	-0.612014	-1.713524
C	-5.968885	4.658557	-4.765817
C	-6.490548	5.883238	-4.332133
H	-6.269356	6.251772	-3.328360
C	-7.299434	6.639773	-5.179966
H	-7.702604	7.593255	-4.830864
C	-7.596788	6.182011	-6.461457
H	-8.236533	6.774143	-7.119952
C	-7.068534	4.968981	-6.904540
H	-7.284582	4.609605	-7.913079
C	-6.249391	4.217226	-6.067148
H	-5.817239	3.285402	-6.443741
C	-4.922155	4.429788	-2.071722
C	-6.075467	4.466097	-1.274810
H	-7.001678	3.994354	-1.612124
C	-6.055100	5.113188	-0.042895
H	-6.957130	5.135179	0.572805
C	-4.887970	5.737234	0.401460
H	-4.878149	6.250910	1.365832
C	-3.739023	5.708300	-0.385825
H	-2.824821	6.198369	-0.042886
C	-3.753621	5.051409	-1.615751
H	-2.847137	5.014196	-2.225019
C	-5.862534	2.072447	-3.532643
H	-6.843974	2.250443	-3.065545
H	-6.038925	1.720884	-4.562428
C	-5.237845	1.055938	-0.894537
C	-6.485281	0.793045	-0.313326
H	-7.288374	0.350230	-0.909130
C	-6.703847	1.079380	1.031931
H	-7.677694	0.868822	1.480398
C	-5.679582	1.628378	1.805054
H	-5.854951	1.855396	2.859641
C	-4.433534	1.881845	1.233921
H	-3.629011	2.307689	1.838459
C	-4.208856	1.589761	-0.110719
H	-3.228745	1.779369	-0.554512
C	-5.868937	-0.778936	-3.042270
C	-7.144674	-0.780484	-3.620395
H	-7.645778	0.155598	-3.876902
C	-7.798634	-1.985865	-3.876438
H	-8.794267	-1.975790	-4.326215
C	-7.187442	-3.196459	-3.557053
H	-7.702378	-4.138587	-3.759004
C	-5.916935	-3.202439	-2.980981
H	-5.430444	-4.148769	-2.734365
C	-5.258236	-2.002588	-2.728330
H	-4.258301	-2.015854	-2.284655
C	-3.240241	3.110794	-7.942727
C	-3.186568	4.504335	-8.098195
H	-2.577051	5.108801	-7.419878
C	-3.898007	5.128740	-9.117305
H	-3.842382	6.213746	-9.230571
C	-4.682845	4.371950	-9.988973
H	-5.240109	4.862274	-10.790599
C	-4.750033	2.989181	-9.836279
H	-5.357428	2.390564	-10.519310
C	-4.029914	2.358268	-8.819783
H	-4.087131	1.271165	-8.732852
C	-0.537564	2.683497	-7.111455
C	0.410993	3.089708	-6.166721
H	0.115100	3.227774	-5.123440
C	1.730532	3.317708	-6.556544
H	2.467070	3.638374	-5.816294

C	2.105054	3.144408	-7.887099
H	3.137278	3.330667	-8.193249
C	1.160236	2.744429	-8.834133
H	1.451446	2.619366	-9.879687
C	-0.158168	2.518133	-8.450931
H	-0.898581	2.228413	-9.201976
C	-2.532826	0.577534	-6.724838
H	-3.626457	0.438130	-6.726513
H	-2.126285	0.170739	-7.664856
C	-0.113526	-0.434052	-5.433091
C	0.700642	-0.088273	-4.349552
H	0.245998	0.249101	-3.416015
C	2.088774	-0.179371	-4.458046
H	2.718922	0.091091	-3.606810
C	2.667684	-0.609574	-5.649496
H	3.754926	-0.674407	-5.738567
C	1.859584	-0.961265	-6.732792
H	2.312133	-1.304638	-7.665872
C	0.474967	-0.880518	-6.624315
H	-0.147499	-1.179511	-7.472104
C	-2.472414	-2.060284	-5.536738
C	-3.441267	-2.420567	-6.479764
H	-3.896432	-1.673075	-7.132611
C	-3.839143	-3.751738	-6.607828
H	-4.591416	-4.020627	-7.352976
C	-3.276622	-4.733484	-5.796240
H	-3.585146	-5.775958	-5.903593
C	-2.314172	-4.380413	-4.849151
H	-1.866527	-5.146403	-4.211363
C	-1.916919	-3.053619	-4.715578
H	-1.163960	-2.786740	-3.968728

S_1

E_{rel/S_0} = 3.055 eV

Cu	2.430078	-1.148425	4.156799
Cu	3.850225	0.812808	3.232171
Cu	-1.002228	-1.449831	0.618855
P	3.955288	-2.788750	3.574116
P	5.814800	-0.353965	3.246676
P	2.974309	-0.903800	6.405047
P	3.330775	1.857526	5.189291
C	0.137364	-1.517668	2.113611
C	2.159017	1.549049	0.730444
N	0.911069	-1.507320	2.987859
N	2.900532	1.340866	1.608089
C	3.863635	-4.372880	4.451268
C	2.603954	-4.992297	4.519215
H	1.732262	-4.508156	4.068055
C	2.463373	-6.221860	5.153535
H	1.483185	-6.702267	5.195456
C	3.572701	-6.839661	5.735518
H	3.461438	-7.806384	6.232249
C	4.821224	-6.222609	5.683518
H	5.690185	-6.703670	6.138213
C	4.970789	-4.991777	5.046263
H	5.958158	-4.527807	5.011919
C	3.800291	-3.195081	1.808755
C	4.023498	-4.502849	1.351235
H	4.271505	-5.300839	2.054485
C	3.929535	-4.785977	-0.008983
H	4.109968	-5.803943	-0.361835
C	3.604225	-3.776277	-0.914392
H	3.526726	-4.003715	-1.980298
C	3.374311	-2.478113	-0.458866
H	3.114338	-1.685791	-1.164380
C	3.467799	-2.183336	0.897726
H	3.275467	-1.168424	1.254400
C	5.632244	-2.110644	3.863435
H	6.390010	-2.778141	3.423564
H	5.768295	-2.099124	4.957744
C	6.670360	-0.547445	1.636696
C	7.840432	-1.304840	1.490258
H	8.275879	-1.830559	2.344663
C	8.478714	-1.377558	0.255658
H	9.392546	-1.966855	0.149978
C	7.959474	-0.687641	-0.841310

H	8.467199	-0.740162	-1.807375
C	6.801902	0.073908	-0.699805
H	6.398406	0.622862	-1.553960
C	6.157003	0.145627	0.534943
H	5.249372	0.744721	0.648000
C	7.131896	0.278303	4.364609
C	8.077683	-0.530634	5.012047
H	8.058318	-1.617448	4.899017
C	9.068233	0.042868	5.807840
H	9.803248	-0.596108	6.303386
C	9.129293	1.428037	5.963046
H	9.910014	1.874194	6.583569
C	8.192952	2.239481	5.324748
H	8.229531	3.324605	5.444803
C	7.196911	1.667669	4.534500
H	6.455621	2.307515	4.045891
C	3.991983	-2.076185	7.363217
C	3.371852	-3.239579	7.850368
H	2.303072	-3.399428	7.686331
C	4.104710	-4.182437	8.562597
H	3.604768	-5.073096	8.949665
C	5.469148	-3.990328	8.787846
H	6.040991	-4.727700	9.355912
C	6.096765	-2.849342	8.292495
H	7.161902	-2.685567	8.472834
C	5.366307	-1.895009	7.583817
H	5.884180	-1.000133	7.230847
C	1.416907	-0.790766	7.348231
C	0.190565	-0.986366	6.704430
H	0.154715	-1.202594	5.632854
C	-0.997631	-0.904729	7.429835
H	-1.952445	-1.056941	6.921952
C	-0.965745	-0.631185	8.795198
H	-1.897324	-0.571005	9.362873
C	0.256458	-0.439296	9.442306
H	0.283169	-0.231567	10.514506
C	1.445623	-0.519340	8.724472
H	2.398874	-0.384450	9.243183
C	3.798150	0.731607	6.590113
H	4.886868	0.585631	6.502990
H	3.581256	1.154659	7.583827
C	1.545156	2.175617	5.439716
C	0.651090	1.822188	4.422156
H	1.036290	1.374555	3.501908
C	-0.715948	2.049776	4.581459
H	-1.406354	1.781640	3.777887
C	-1.195624	2.625842	5.756446
H	-2.266142	2.805771	5.882256
C	-0.306992	2.986044	6.771455
H	-0.681096	3.445685	7.689234
C	1.059268	2.770252	6.612289
H	1.751005	3.078851	7.401136
C	4.088140	3.452267	5.704320
C	4.982068	3.602645	6.772057
H	5.244511	2.756181	7.409690
C	5.555547	4.846692	7.042416
H	6.246127	4.951010	7.882908
C	5.244139	5.950990	6.253342
H	5.691311	6.923878	6.469782
C	4.356750	5.808855	5.184249
H	4.107341	6.670706	4.560821
C	3.789893	4.569600	4.907137
H	3.102252	4.466841	4.061830
Cu	-2.827517	1.966746	-3.944876
Cu	-3.617815	-0.802665	-3.577692
Cu	0.870632	1.834718	-0.609214
P	-4.919263	2.421513	-3.093057
P	-5.870283	-0.367018	-3.819890
P	-2.604107	1.740902	-6.233570
P	-2.391747	-1.189501	-5.495968
C	-0.461070	2.046718	-1.921062
C	-2.092463	-1.329320	-0.912634
N	-1.311885	2.096446	-2.715886
N	-2.724389	-1.188604	-1.881334
C	-5.428145	4.162043	-3.344425
C	-5.318216	5.083765	-2.293754
H	-4.993647	4.752669	-1.304434

C	-5.633580	6.425238	-2.499989
H	-5.549962	7.132732	-1.671733
C	-6.059328	6.862060	-3.753237
H	-6.312401	7.913018	-3.910838
C	-6.158653	5.952725	-4.805323
H	-6.486555	6.287144	-5.792213
C	-5.837330	4.611551	-4.608029
H	-5.905893	3.923851	-5.454920
C	-5.250256	2.102400	-1.327803
C	-6.523649	2.292275	-0.769917
H	-7.349476	2.659542	-1.385260
C	-6.742254	2.023359	0.576867
H	-7.736082	2.169947	1.005814
C	-5.692958	1.566152	1.378109
H	-5.869805	1.355405	2.435711
C	-4.426074	1.382034	0.830468
H	-3.602435	1.021839	1.452174
C	-4.202106	1.650995	-0.520231
H	-3.211299	1.504404	-0.953804
C	-6.209978	1.446128	-3.981310
H	-7.230193	1.704255	-3.656881
H	-6.104496	1.704063	-5.046924
C	-6.944309	-0.921668	-2.446191
C	-8.341954	-0.903019	-2.551489
H	-8.823654	-0.574477	-3.476583
C	-9.127685	-1.324209	-1.482696
H	-10.216573	-1.311690	-1.570948
C	-8.525179	-1.773253	-0.305892
H	-9.144943	-2.109853	0.528703
C	-7.136502	-1.801787	-0.200817
H	-6.662563	-2.158792	0.716413
C	-6.344222	-1.379516	-1.268187
H	-5.254734	-1.400862	-1.184908
C	-6.654588	-1.083357	-5.311428
C	-7.622963	-0.417724	-6.076659
H	-7.941643	0.594770	-5.817095
C	-8.202983	-1.045542	-7.178903
H	-8.960814	-0.519845	-7.764815
C	-7.827288	-2.342740	-7.525389
H	-8.287166	-2.833434	-8.386354
C	-6.865104	-3.011753	-6.769627
H	-6.562147	-4.026696	-7.036357
C	-6.278363	-2.384735	-5.672568
H	-5.518355	-2.916409	-5.092831
C	-3.785049	2.729606	-7.232546
C	-3.469924	4.072701	-7.487828
H	-2.511451	4.482721	-7.158852
C	-4.363799	4.891466	-8.173567
H	-4.097187	5.932046	-8.372702
C	-5.588273	4.385618	-8.610223
H	-6.284595	5.025772	-9.156871
C	-5.914194	3.055052	-8.353470
H	-6.866717	2.646371	-8.699325
C	-5.020962	2.231382	-7.666935
H	-5.307291	1.191520	-7.489997
C	-0.978338	2.191698	-6.934298
C	0.059614	2.544816	-6.066134
H	-0.112186	2.549333	-4.986926
C	1.311692	2.886013	-6.579118
H	2.118233	3.164143	-5.896917
C	1.530203	2.876141	-7.954364
H	2.509811	3.147814	-8.354998
C	0.495280	2.527240	-8.825282
H	0.663668	2.527486	-9.904769
C	-0.755621	2.188475	-8.319585
H	-1.566399	1.936786	-9.009581
C	-2.874393	0.001778	-6.814504
H	-3.952246	-0.155239	-6.976385
H	-2.347619	-0.163811	-7.767205
C	-0.568537	-1.080346	-5.425893
C	0.031139	-0.686806	-4.226526
H	-0.591008	-0.465921	-3.358042
C	1.418592	-0.564307	-4.146281
H	1.875754	-0.237131	-3.208564
C	2.209457	-0.844947	-5.257520
H	3.296295	-0.747936	-5.197050
C	1.614584	-1.252785	-6.454295

H	2.234398	-1.478576	-7.325056
C	0.231420	-1.372796	-6.539705
H	-0.224116	-1.703981	-7.477227
C	-2.701376	-2.840484	-6.218189
C	-3.082313	-3.058330	-7.547070
H	-3.215796	-2.221694	-8.236039
C	-3.301154	-4.356176	-8.010781
H	-3.593864	-4.515839	-9.051275
C	-3.144267	-5.443727	-7.154072
H	-3.314338	-6.458659	-7.520870
C	-2.768951	-5.233483	-5.826058
H	-2.646438	-6.082869	-5.149997
C	-2.552283	-3.940322	-5.358880
H	-2.260212	-3.782890	-4.315685

S_2

E_{rel/S_0} = 3.100 eV

Cu	5.720209	-0.281166	-0.458951
Cu	4.334283	-0.173957	1.987918
Cu	0.757878	-0.519919	-1.089081
P	6.552050	1.865826	-0.581892
P	5.103020	1.995604	2.113626
P	7.093529	-2.089562	-0.142213
P	5.397796	-2.167835	2.408080
C	2.628617	-0.542854	-0.849577
C	1.245610	-0.116367	2.513417
N	3.783015	-0.493363	-0.684634
N	2.408121	-0.156990	2.459128
C	8.257627	2.198947	-1.164725
C	8.507998	2.954006	-2.317057
H	7.680121	3.392603	-2.878143
C	9.817628	3.158685	-2.751340
H	10.000425	3.753444	-3.649375
C	10.886761	2.617212	-2.041482
H	11.911616	2.787402	-2.379394
C	10.643873	1.852856	-0.899930
H	11.475397	1.413651	-0.344489
C	9.338016	1.634925	-0.470929
H	9.170002	1.007736	0.409280
C	5.515775	3.056674	-1.495526
C	5.615019	4.442866	-1.310727
H	6.324253	4.858609	-0.590480
C	4.817514	5.307087	-2.054924
H	4.898590	6.385864	-1.903401
C	3.922836	4.797242	-2.997689
H	3.304022	5.479363	-3.585664
C	3.822502	3.421336	-3.190848
H	3.125594	3.018993	-3.929782
C	4.611125	2.552488	-2.437310
H	4.517710	1.472253	-2.575412
C	6.611523	2.477541	1.163940
H	6.810634	3.559414	1.221896
H	7.460981	1.950291	1.627543
C	3.884191	3.288909	1.676982
C	3.986052	4.589602	2.188701
H	4.779738	4.842019	2.897461
C	3.066318	5.563393	1.808344
H	3.148758	6.575060	2.212787
C	2.039906	5.245499	0.917481
H	1.320201	6.011689	0.618441
C	1.929396	3.950779	0.413698
H	1.123556	3.699198	-0.280273
C	2.844505	2.970821	0.796687
H	2.750511	1.953779	0.411136
C	5.529007	2.372007	3.852438
C	6.747597	2.926576	4.262089
H	7.518579	3.188639	3.534189
C	6.991889	3.163467	5.616065
H	7.944390	3.600866	5.924582
C	6.022951	2.853896	6.568012
H	6.214933	3.045658	7.626333
C	4.806332	2.299898	6.166064
H	4.044680	2.051805	6.908796
C	4.561060	2.054302	4.818617
H	3.608772	1.610723	4.512486
C	8.865146	-1.969878	-0.576095

C	9.169950	-1.677025	-1.913718
H	8.364264	-1.515129	-2.635982
C	10.493346	-1.596989	-2.334402
H	10.717296	-1.373065	-3.379770
C	11.530678	-1.796042	-1.422150
H	12.570147	-1.734330	-1.752710
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H	12.045617	-2.237596	0.628031
C	9.910289	-2.166120	0.334345
H	9.706358	-2.402997	1.380950
C	6.587476	-3.670597	-0.909997
C	5.307238	-3.771911	-1.466034
H	4.634015	-2.911247	-1.441570
C	4.891457	-4.969601	-2.046181
H	3.891557	-5.043004	-2.479908
C	5.751527	-6.065399	-2.080580
H	5.428181	-7.000852	-2.543612
C	7.032811	-5.965680	-1.535456
H	7.712693	-6.820161	-1.573132
C	7.452849	-4.772308	-0.954376
H	8.465250	-4.694527	-0.548309
C	7.084808	-2.399960	1.678331
H	7.702637	-1.611668	2.139067
H	7.524006	-3.372921	1.949513
C	4.481456	-3.680042	1.956781
C	3.119450	-3.559633	1.656261
H	2.644537	-2.576587	1.683257
C	2.371663	-4.689620	1.327373
H	1.307789	-4.585772	1.100014
C	2.977419	-5.943362	1.287582
H	2.392535	-6.828609	1.026304
C	4.335613	-6.069953	1.582286
H	4.815351	-7.050706	1.550549
C	5.084272	-4.945559	1.917617
H	6.144913	-5.066547	2.149473
C	5.746585	-2.320667	4.201533
C	6.404535	-1.252067	4.828666
H	6.675389	-0.357651	4.258992
C	6.702606	-1.307119	6.187256
H	7.217291	-0.468676	6.662037
C	6.328774	-2.421435	6.938898
H	6.557573	-2.463893	8.006330
C	5.654004	-3.475843	6.327129
H	5.350685	-4.346013	6.914011
C	5.361935	-3.429462	4.964007
H	4.829889	-4.261072	4.497337
Cu	-5.080140	0.259180	0.491017
Cu	-4.150087	-0.045117	-1.913069
Cu	-0.629010	-0.041539	2.399696
P	-6.116645	-1.802852	0.577018
P	-5.651950	-1.680396	-2.465916
P	-6.898643	1.608188	-0.010736
P	-4.887583	2.087005	-2.243581
C	-2.480317	0.050850	2.102433
C	-1.092313	-0.439379	-1.442729
N	-3.583412	0.119398	1.725071
N	-2.228472	-0.346912	-1.696955
C	-7.448320	-2.024503	1.785732
C	-7.168888	-1.665835	3.115668
H	-6.186649	-1.260643	3.378106
C	-8.136100	-1.830646	4.101170
H	-7.909898	-1.558422	5.134604
C	-9.392571	-2.342721	3.769397
H	-10.150998	-2.473392	4.544887
C	-9.679209	-2.686595	2.449514
H	-10.661132	-3.087424	2.187986
C	-8.713827	-2.527677	1.456557
H	-8.956315	-2.807759	0.429850
C	-4.902055	-3.108209	0.929610
C	-5.257455	-4.230606	1.693517
H	-6.262064	-4.320006	2.112545
C	-4.324035	-5.239281	1.917132
H	-4.605803	-6.114028	2.507591
C	-3.036738	-5.132117	1.391370
H	-2.308380	-5.926347	1.571892
C	-2.680196	-4.012178	0.640285
H	-1.672450	-3.920798	0.228252

C	-3.604572	-2.997841	0.411252
H	-3.319506	-2.114996	-0.166442
C	-6.830894	-2.116471	-1.080071
H	-7.176321	-3.159963	-1.151083
H	-7.706330	-1.450821	-1.161751
C	-4.961623	-3.302215	-2.971520
C	-5.770155	-4.410698	-3.257127
H	-6.858075	-4.346530	-3.166527
C	-5.197464	-5.605035	-3.684337
H	-5.834494	-6.463852	-3.908259
C	-3.813277	-5.700619	-3.838581
H	-3.367070	-6.637407	-4.180826
C	-3.005198	-4.599605	-3.565199
H	-1.922339	-4.668554	-3.693250
C	-3.575401	-3.402298	-3.132853
H	-2.942526	-2.536729	-2.919310
C	-6.832812	-1.273178	-3.817092
C	-8.143302	-1.767204	-3.898504
H	-8.547025	-2.418692	-3.119508
C	-8.953421	-1.439902	-4.984727
H	-9.970828	-1.834689	-5.040824
C	-8.464913	-0.620613	-6.002907
H	-9.101162	-0.370158	-6.855016
C	-7.164689	-0.124033	-5.929766
H	-6.775392	0.522572	-6.719460
C	-6.355180	-0.444300	-4.840817
H	-5.339304	-0.041813	-4.780692
C	-8.642698	1.091267	0.116670
C	-9.242815	1.111415	1.387414
H	-8.679822	1.470265	2.252885
C	-10.560337	0.697727	1.550158
H	-11.018284	0.735407	2.541066
C	-11.296033	0.242708	0.454274
H	-12.333950	-0.072948	0.582752
C	-10.703417	0.200942	-0.806026
H	-11.274773	-0.144302	-1.671020
C	-9.384544	0.621937	-0.978613
H	-8.958148	0.598515	-1.984234
C	-6.790662	3.100896	1.031528
C	-5.793082	3.204130	2.006913
H	-5.071408	2.394946	2.151257
C	-5.713136	4.346269	2.803020
H	-4.931952	4.421765	3.562519
C	-6.626705	5.383553	2.630718
H	-6.565557	6.275769	3.258366
C	-7.626108	5.282732	1.660884
H	-8.347575	6.092584	1.529998
C	-7.711357	4.146169	0.862815
H	-8.507745	4.068702	0.117310
C	-6.674210	2.185255	-1.744252
H	-7.206562	1.491733	-2.415032
H	-7.108190	3.190314	-1.866635
C	-4.051059	3.347629	-1.211467
C	-3.008267	2.939145	-0.371598
H	-2.714760	1.886277	-0.355778
C	-2.351727	3.869166	0.435065
H	-1.536682	3.542352	1.086026
C	-2.735990	5.209126	0.408190
H	-2.226974	5.937968	1.044042
C	-3.769407	5.623424	-0.434676
H	-4.066777	6.674382	-0.461063
C	-4.420568	4.699356	-1.247883
H	-5.214053	5.036112	-1.920942
C	-4.909813	2.892843	-3.898334
C	-6.069394	3.235192	-4.605408
H	-7.059072	3.084007	-4.170140
C	-5.979721	3.781201	-5.887442
H	-6.892932	4.049426	-6.424386
C	-4.735899	3.991784	-6.476841
H	-4.668940	4.422280	-7.478592
C	-3.574510	3.649756	-5.780422
H	-2.595039	3.811571	-6.236731
C	-3.660640	3.098297	-4.506768
H	-2.745470	2.823925	-3.972688

S_3

E_{rel/S_0} = 3.119 eV

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Cu	3.186455	0.397893	3.524320
Cu	-0.516012	-1.063180	0.888797
P	4.474146	-3.310383	3.814500
P	5.102498	-0.535748	2.665563
P	2.448393	-1.662264	6.844659
P	2.768360	1.119420	5.657656
C	0.565526	-1.417091	2.393364
C	1.610099	1.923201	1.294460
N	1.296950	-1.645318	3.273758
N	2.270383	1.492800	2.151851
C	5.364920	-4.507569	4.880690
C	5.353737	-5.880755	4.606194
H	4.841818	-6.260240	3.719201
C	6.006939	-6.772596	5.456828
H	5.995680	-7.840919	5.228298
C	6.679202	-6.305503	6.583843
H	7.199271	-7.005649	7.241698
C	6.682863	-4.940407	6.871032
H	7.197011	-4.566449	7.759102
C	6.020199	-4.049064	6.032455
H	6.014232	-2.986986	6.292798
C	4.211603	-4.211517	2.249767
C	5.272383	-4.631046	1.434430
H	6.307247	-4.414965	1.712492
C	5.017808	-5.343465	0.266512
H	5.849172	-5.665395	-0.364784
C	3.704670	-5.653579	-0.092589
H	3.509706	-6.220138	-1.006318
C	2.645975	-5.245240	0.715235
H	1.617414	-5.489264	0.439291
C	2.897497	-4.520127	1.879670
H	2.065902	-4.184206	2.504109
C	5.786425	-2.056261	3.459207
H	6.621421	-2.485685	2.883702
H	6.177757	-1.743916	4.440722
C	5.052531	-0.950265	0.883681
C	6.221044	-1.028958	0.114185
H	7.193662	-0.811538	0.564464
C	6.147312	-1.366158	-1.234890
H	7.061690	-1.422765	-1.830365
C	4.908838	-1.622918	-1.825376
H	4.852150	-1.885467	-2.884744
C	3.743503	-1.538052	-1.065685
H	2.772736	-1.732753	-1.528129
C	3.812480	-1.197308	0.284682
H	2.897821	-1.118868	0.876104
C	6.456732	0.684165	2.808635
C	7.760594	0.365295	3.207950
H	8.035639	-0.662091	3.457058
C	8.732852	1.362189	3.291701
H	9.747303	1.103185	3.603881
C	8.413545	2.681009	2.975765
H	9.177414	3.459200	3.042145
C	7.116292	3.005730	2.578320
H	6.859674	4.039320	2.335278
C	6.141106	2.015812	2.499067
H	5.123390	2.278484	2.194398
C	3.316023	-2.719348	8.057030
C	3.031726	-4.091907	8.011467
H	2.348406	-4.483704	7.252114
C	3.609069	-4.962722	8.929867
H	3.375858	-6.028905	8.887015
C	4.489564	-4.475708	9.896705
H	4.942949	-5.159073	10.618521
C	4.789430	-3.115874	9.940200
H	5.476041	-2.729582	10.697333
C	4.203706	-2.238147	9.026544
H	4.440929	-1.173831	9.090746
C	0.769225	-1.518750	7.554561
C	-0.334728	-1.561602	6.696420
H	-0.182072	-1.678902	5.620281
C	-1.625051	-1.453013	7.214132
H	-2.484198	-1.488870	6.540418
C	-1.817644	-1.306508	8.586031

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C	-0.718997	-1.271056	9.446538
H	-0.869429	-1.167847	10.523724
C	0.570579	-1.381178	8.935276
H	1.424968	-1.377668	9.617906
C	3.214217	0.006340	7.060434
H	4.304770	-0.143619	6.996581
H	2.975794	0.452204	8.039334
C	1.053953	1.649014	6.007001
C	0.087468	1.512367	5.005716
H	0.363584	1.080107	4.041861
C	-1.222350	1.932281	5.237689
H	-1.972181	1.827091	4.449751
C	-1.572205	2.483587	6.467556
H	-2.598391	2.811468	6.650350
C	-0.609088	2.626139	7.468690
H	-0.879960	3.066004	8.431220
C	0.700431	2.217169	7.238604
H	1.451006	2.355494	8.021967
C	3.748220	2.637373	5.953871
C	4.714555	2.767505	6.956952
H	4.916831	1.949836	7.652028
C	5.433880	3.956051	7.088829
H	6.183286	4.048979	7.878352
C	5.193867	5.021047	6.224330
H	5.754923	5.951927	6.334237
C	4.233342	4.895990	5.219355
H	4.039297	5.729312	4.539859
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H	2.771707	3.617566	4.284847
Cu	-2.563248	2.093707	-3.887486
Cu	-3.113286	-0.381554	-3.326756
Cu	0.476991	2.428641	-0.118361
P	-4.687930	2.878661	-3.432248
P	-5.370772	-0.117387	-3.580602
P	-2.655025	1.960237	-6.197814
P	-2.008933	-0.864178	-5.263600
C	-0.675488	2.758332	-1.563722
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C	-5.174139	4.470377	-4.148029
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H	-7.559563	6.055407	-5.994963
C	-6.336582	4.653627	-4.908576
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C	-4.921231	3.052586	-1.638095
C	-5.760336	4.051571	-1.120361
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H	-6.619157	4.917916	0.653225
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H	-5.483553	3.328801	2.194498
C	-4.482388	2.263883	0.603167
H	-3.978337	1.564176	1.273750
C	-4.274945	2.163301	-0.769093
H	-3.608783	1.395255	-1.169717
C	-5.869779	1.622758	-4.049880
H	-6.889754	1.861756	-3.709421
H	-5.839991	1.696047	-5.149828
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C	-8.582148	-0.660680	-1.037014
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C	-7.965301	-1.184640	0.100554
H	-8.568178	-1.457311	0.970038
C	-6.584738	-1.367678	0.121649
H	-6.100513	-1.785691	1.007371
C	-5.815353	-1.023944	-0.989928
H	-4.731886	-1.169571	-0.975450

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H	-7.680773	0.327236	-5.540014
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C	-7.240418	-2.750844	-6.913337
H	-7.672182	-3.397765	-7.680590
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H	-5.721653	-4.176399	-6.334161
C	-5.602959	-2.360131	-5.182093
H	-4.740012	-2.702134	-4.602740
C	-3.917406	2.765766	-7.238455
C	-3.756390	4.131866	-7.527166
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C	-5.837069	4.138528	-8.756656
H	-6.577058	4.669226	-9.360122
C	-6.013844	2.788426	-8.461340
H	-6.890560	2.254334	-8.835437
C	-5.061866	2.101802	-7.707210
H	-5.217916	1.037540	-7.515620
C	-1.067610	2.569631	-6.858500
C	-0.102980	3.101716	-5.996223
H	-0.290301	3.160416	-4.920342
C	1.110168	3.561229	-6.507768
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C	0.400563	2.968147	-8.740339
H	0.594127	2.922243	-9.814554
C	-0.811833	2.507217	-8.236767
H	-1.565779	2.111878	-8.923328
C	-2.722144	0.172249	-6.630196
H	-3.779053	-0.131501	-6.704779
H	-2.240405	0.007027	-7.606781
C	-0.226031	-0.447202	-5.245725
C	0.328664	0.054753	-4.062621
H	-0.309456	0.183148	-3.184858
C	1.682572	0.386212	-4.007591
H	2.108625	0.773100	-3.078337
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H	3.546238	0.486858	-5.094545
C	1.940052	-0.286046	-6.315044
H	2.570560	-0.421196	-7.196983
C	0.591243	-0.628255	-6.370016
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C	-2.012403	-2.544065	-6.017403
C	-2.529532	-2.858239	-7.280301
H	-2.937854	-2.082287	-7.930638
C	-2.531812	-4.178606	-7.734349
H	-2.934631	-4.407972	-8.723917
C	-2.018576	-5.197625	-6.936104
H	-2.019197	-6.229296	-7.295340
C	-1.504612	-4.894138	-5.673446
H	-1.102595	-5.688908	-5.040593
C	-1.509719	-3.581081	-5.214882
H	-1.118816	-3.353797	-4.217921

T_1

E_{rel/S_0} = 2.843 eV

Cu	2.435881	-1.174251	4.125617
Cu	3.822185	0.807171	3.242009
Cu	-1.065373	-1.538448	0.662054
P	3.986506	-2.763770	3.532832
P	5.820516	-0.309312	3.252909
P	2.971077	-0.961961	6.379913
P	3.281120	1.828643	5.213878
C	0.096434	-1.614610	2.140362
C	2.166153	1.630618	0.735502
N	0.886152	-1.598308	3.000070
N	2.892545	1.397571	1.618379
C	3.933019	-4.380875	4.357568
C	2.690234	-5.036241	4.391109
H	1.812432	-4.565263	3.937657

C	2.573429	-6.284063	4.993762
H	1.606207	-6.791696	5.007898
C	3.689718	-6.885684	5.579543
H	3.597171	-7.866572	6.051704
C	4.921117	-6.233628	5.562279
H	5.795849	-6.701332	6.019945
C	5.046774	-4.984282	4.956113
H	6.021710	-4.493602	4.949940
C	3.850006	-3.125810	1.754625
C	4.150009	-4.404269	1.260223
H	4.442956	-5.206403	1.941273
C	4.072085	-4.654343	-0.107487
H	4.310713	-5.650018	-0.488380
C	3.687903	-3.640571	-0.984957
H	3.622702	-3.842372	-2.056868
C	3.383692	-2.371595	-0.493252
H	3.078029	-1.575862	-1.176284
C	3.461241	-2.110158	0.871511
H	3.215607	-1.117331	1.257095
C	5.655794	-2.071610	3.848161
H	6.422548	-2.726198	3.404226
H	5.785310	-2.072791	4.943322
C	6.694767	-0.466818	1.649429
C	7.884934	-1.193023	1.507002
H	8.327111	-1.712669	2.361669
C	8.533551	-1.241455	0.276722
H	9.462775	-1.806690	0.173859
C	8.004745	-0.557587	-0.819582
H	8.520555	-0.590922	-1.782216
C	6.827129	0.173111	-0.681940
H	6.415848	0.716813	-1.535724
C	6.171355	0.219633	0.548320
H	5.247174	0.793400	0.658162
C	7.113465	0.338302	4.387969
C	8.065102	-0.458834	5.041462
H	8.065523	-1.544971	4.920076
C	9.035404	0.125887	5.853917
H	9.775127	-0.503908	6.354190
C	9.070294	1.510672	6.019793
H	9.835136	1.965711	6.653491
C	8.127904	2.310535	5.375630
H	8.143904	3.395150	5.504336
C	7.151819	1.727441	4.568980
H	6.405797	2.358632	4.076585
C	4.006178	-2.124337	7.331981
C	3.408949	-3.312509	7.786915
H	2.347084	-3.496141	7.603699
C	4.155531	-4.250946	8.490437
H	3.673236	-5.161770	8.852069
C	5.511600	-4.029343	8.738473
H	6.094292	-4.763956	9.299021
C	6.116966	-2.863393	8.274855
H	7.175286	-2.677258	8.472760
C	5.372334	-1.913291	7.575155
H	5.872612	-0.999557	7.246106
C	1.405634	-0.890001	7.313303
C	0.186122	-1.088890	6.657527
H	0.159206	-1.283860	5.581680
C	-1.007383	-1.037995	7.376887
H	-1.956788	-1.193426	6.859908
C	-0.987867	-0.791421	8.747676
H	-1.923743	-0.755304	9.310301
C	0.227500	-0.596272	9.406445
H	0.244775	-0.410008	10.482774
C	1.422081	-0.645964	8.694808
H	2.370235	-0.509391	9.222399
C	3.761152	0.687924	6.595515
H	4.853537	0.568111	6.514749
H	3.526327	1.085377	7.595822
C	1.492349	2.127351	5.470518
C	0.600772	1.781842	4.448045
H	0.988118	1.345456	3.523324
C	-0.767342	2.001296	4.609150
H	-1.456269	1.738429	3.802561
C	-1.250456	2.562067	5.789944
H	-2.321834	2.736113	5.916705
C	-0.364324	2.914392	6.809802

H	-0.741006	3.362194	7.732345
C	1.002862	2.705785	6.649270
H	1.692272	3.008232	7.442560
C	4.025470	3.424441	5.740511
C	4.866966	3.588021	6.847761
H	5.101254	2.748402	7.505117
C	5.423743	4.836458	7.132345
H	6.074073	4.951341	8.002980
C	5.146988	5.931664	6.317965
H	5.580872	6.908079	6.545460
C	4.312265	5.776238	5.209283
H	4.091295	6.630870	4.565521
C	3.762384	4.532211	4.918313
H	3.116087	4.418425	4.042316
Cu	-2.805716	1.964909	-3.957606
Cu	-3.654966	-0.794913	-3.536305
Cu	0.893499	1.926349	-0.618846
P	-4.893334	2.454497	-3.116699
P	-5.898120	-0.326265	-3.794814
P	-2.586648	1.694325	-6.240990
P	-2.421644	-1.221025	-5.440874
C	-0.439849	2.106847	-1.934797
C	-2.154237	-1.371740	-0.866259
N	-1.292595	2.128765	-2.728717
N	-2.777566	-1.200997	-1.835664
C	-5.368457	4.200311	-3.394395
C	-5.216919	5.138300	-2.363328
H	-4.881481	4.817651	-1.374121
C	-5.505058	6.482727	-2.588585
H	-5.389497	7.203061	-1.775377
C	-5.944315	6.906485	-3.841765
H	-6.176042	7.960030	-4.014207
C	-6.084706	5.980749	-4.874604
H	-6.423590	6.304800	-5.861247
C	-5.791162	4.636055	-4.658276
H	-5.892037	3.934898	-5.490743
C	-5.229559	2.168356	-1.346783
C	-6.495018	2.405507	-0.788997
H	-7.309530	2.792625	-1.407306
C	-6.719410	2.158605	0.561039
H	-7.707046	2.341999	0.990141
C	-5.683755	1.676537	1.365486
H	-5.865212	1.483275	2.425642
C	-4.424549	1.445610	0.817892
H	-3.611691	1.065968	1.442199
C	-4.194724	1.692585	-0.536018
H	-3.209796	1.509806	-0.969395
C	-6.202161	1.489926	-3.989702
H	-7.217124	1.774231	-3.670664
H	-6.090689	1.726171	-5.059694
C	-6.989697	-0.836382	-2.417833
C	-8.386183	-0.788989	-2.529301
H	-8.857172	-0.463492	-3.460959
C	-9.185047	-1.177669	-1.457955
H	-10.273049	-1.142904	-1.550994
C	-8.597071	-1.622632	-0.272277
H	-9.227271	-1.933768	0.564378
C	-7.209778	-1.679551	-0.160849
H	-6.747331	-2.033498	0.763404
C	-6.404356	-1.289894	-1.230792
H	-5.315928	-1.333669	-1.142807
C	-6.686480	-1.053692	-5.278744
C	-7.643021	-0.386213	-6.057157
H	-7.948606	0.634276	-5.813567
C	-8.227475	-1.022040	-7.152404
H	-8.976047	-0.494781	-7.748717
C	-7.867972	-2.329036	-7.478780
H	-8.331355	-2.825926	-8.334292
C	-6.917523	-2.999881	-6.709928
H	-6.627320	-4.022544	-6.960920
C	-6.326355	-2.365019	-5.619732
H	-5.575694	-2.898391	-5.029457
C	-3.756515	2.681479	-7.254354
C	-3.424978	4.016704	-7.529372
H	-2.461668	4.419884	-7.206049
C	-4.308544	4.835917	-8.227753
H	-4.029299	5.870126	-8.442154

C	-5.538800	4.338405	-8.657717
H	-6.227021	4.978709	-9.214356
C	-5.880817	3.015778	-8.381646
H	-6.837836	2.613361	-8.722414
C	-4.997929	2.191628	-7.682380
H	-5.296629	1.157861	-7.490812
C	-0.956671	2.109372	-6.953672
C	0.086315	2.470323	-6.094831
H	-0.084357	2.501638	-5.015894
C	1.341653	2.785212	-6.616586
H	2.152172	3.069663	-5.941745
C	1.558429	2.741029	-7.991437
H	2.540648	2.991955	-8.399145
C	0.518502	2.384229	-8.853145
H	0.685719	2.357582	-9.932491
C	-0.735714	2.071877	-8.338713
H	-1.550138	1.813842	-9.022045
C	-2.882027	-0.051939	-6.786979
H	-3.961462	-0.196288	-6.949863
H	-2.353957	-0.246125	-7.733549
C	-0.598243	-1.127915	-5.358787
C	-0.005194	-0.704171	-4.166496
H	-0.632448	-0.454082	-3.309660
C	1.382326	-0.588758	-4.078509
H	1.833934	-0.236385	-3.147297
C	2.180018	-0.908239	-5.174284
H	3.267013	-0.816890	-5.107879
C	1.591749	-1.347586	-6.363184
H	2.216882	-1.603771	-7.221645
C	0.208402	-1.459391	-6.456747
H	-0.242318	-1.814333	-7.387872
C	-2.744280	-2.883425	-6.130172
C	-3.122811	-3.124842	-7.455708
H	-3.245097	-2.301357	-8.162350
C	-3.353578	-4.429714	-7.893183
H	-3.644249	-4.607944	-8.931229
C	-3.211093	-5.500778	-7.013484
H	-3.390516	-6.521292	-7.359760
C	-2.838181	-5.266919	-5.688761
H	-2.726848	-6.103298	-4.994794
C	-2.609646	-3.966672	-5.247636
H	-2.319714	-3.790644	-4.206830

$\mathbf{T}_{\mathbf{1\text{-}const}}$

E_{rel/S_0} = 2.988 eV

Cu	2.581322	-1.489683	3.994813
Cu	3.777224	0.591426	3.173416
Cu	-0.996699	-1.427988	0.563596
P	4.400821	-2.903850	3.787902
P	5.887238	-0.273258	3.281880
P	2.743639	-1.153362	6.292996
P	3.260692	1.626949	5.160862
C	0.187452	-1.621605	2.012533
C	2.047458	1.328162	0.697535
N	0.971726	-1.715204	2.872485
N	2.772663	1.091032	1.579929
C	4.587687	-4.457318	4.727933
C	3.606690	-5.440219	4.515844
H	2.785854	-5.251530	3.816642
C	3.683031	-6.663382	5.172756
H	2.919908	-7.424858	4.994092
C	4.736833	-6.920398	6.051531
H	4.800777	-7.884731	6.561269
C	5.709590	-5.947374	6.271122
H	6.541612	-6.148704	6.949153
C	5.634979	-4.715052	5.621306
H	6.413996	-3.973752	5.804044
C	4.598063	-3.478809	2.061333
C	5.736285	-4.222698	1.715616
H	6.501450	-4.452721	2.462564
C	5.895572	-4.683453	0.412810
H	6.788380	-5.253863	0.146053
C	4.912628	-4.429827	-0.546087
H	5.038209	-4.804115	-1.565001
C	3.771944	-3.710438	-0.199045
H	2.994165	-3.517745	-0.942583

C	3.614624	-3.228598	1.101371
H	2.724215	-2.658102	1.364415
C	5.883990	-1.902509	4.185770
H	6.802348	-2.478918	3.986086
H	5.847513	-1.690516	5.267651
C	6.688246	-0.677929	1.683448
C	8.056343	-0.957615	1.570634
H	8.701434	-0.929024	2.453242
C	8.607381	-1.255465	0.326344
H	9.676173	-1.467562	0.242346
C	7.798749	-1.272570	-0.811232
H	8.236613	-1.504213	-1.785633
C	6.439381	-0.982034	-0.704742
H	5.803193	-0.990153	-1.593405
C	5.885653	-0.675176	0.537212
H	4.823851	-0.430720	0.625136
C	7.177440	0.658018	4.190372
C	8.125793	0.074174	5.044117
H	8.119752	-1.000821	5.238939
C	9.100757	0.861512	5.655381
H	9.836601	0.397229	6.316633
C	9.144533	2.235188	5.416389
H	9.913960	2.848070	5.892118
C	8.203564	2.823702	4.572931
H	8.224728	3.900065	4.388693
C	7.221148	2.041379	3.969919
H	6.475616	2.512467	3.322088
C	3.517741	-2.320359	7.464854
C	2.825952	-3.514824	7.728835
H	1.866057	-3.710213	7.242658
C	3.339142	-4.440248	8.629421
H	2.784834	-5.358382	8.836337
C	4.555609	-4.196628	9.270862
H	4.953481	-4.922265	9.984028
C	5.257872	-3.024837	9.000809
H	6.205254	-2.823072	9.506487
C	4.745204	-2.088629	8.101388
H	5.301996	-1.164161	7.934793
C	1.063597	-0.946243	6.986156
C	-0.070145	-1.228505	6.221301
H	0.024446	-1.517716	5.171482
C	-1.338280	-1.131416	6.797236
H	-2.221420	-1.354251	6.194213
C	-1.476699	-0.753340	8.129529
H	-2.470215	-0.681288	8.578380
C	-0.344251	-0.469917	8.896203
H	-0.449409	-0.177970	9.943691
C	0.922627	-0.569888	8.330822
H	1.802464	-0.371963	8.949135
C	3.610631	0.445771	6.550120
H	4.693962	0.246660	6.506988
H	3.373218	0.864159	7.542106
C	1.512009	2.118278	5.386987
C	0.589519	1.749073	4.402216
H	0.932344	1.180566	3.535296
C	-0.750778	2.113798	4.527194
H	-1.465174	1.827390	3.751477
C	-1.173778	2.848217	5.633003
H	-2.223067	3.137708	5.730954
C	-0.255734	3.223448	6.615626
H	-0.586475	3.805657	7.479105
C	1.084063	2.865421	6.493203
H	1.801939	3.181245	7.255169
C	4.164568	3.129270	5.711833
C	5.096419	3.147468	6.756806
H	5.307506	2.249080	7.339254
C	5.775549	4.323481	7.078348
H	6.492728	4.324011	7.902559
C	5.539704	5.490668	6.356812
H	6.068714	6.411794	6.612620
C	4.622268	5.478672	5.304792
H	4.432617	6.390054	4.732828
C	3.942059	4.308184	4.982448
H	3.223212	4.312536	4.157771
Cu	-2.901018	2.099672	-3.959878
Cu	-3.699451	-0.651742	-3.563521
Cu	0.798416	1.735052	-0.650850

P	-4.991671	2.557391	-3.117753
P	-5.956594	-0.235345	-3.790157
P	-2.728865	1.857133	-6.255842
P	-2.508921	-1.066081	-5.500243
C	-0.517453	2.070544	-1.959308
C	-2.124143	-1.218125	-0.931407
N	-1.365156	2.187569	-2.750910
N	-2.776677	-1.049070	-1.881165
C	-5.493512	4.296193	-3.388441
C	-5.281729	5.239132	-2.372031
H	-4.883039	4.923335	-1.404756
C	-5.592414	6.580616	-2.581951
H	-5.429479	7.304558	-1.780128
C	-6.115539	6.996881	-3.805368
H	-6.365715	8.048199	-3.965410
C	-6.317383	6.066499	-4.823467
H	-6.723910	6.384750	-5.786167
C	-6.001379	4.724103	-4.622740
H	-6.154210	4.019105	-5.443719
C	-5.327827	2.267656	-1.349027
C	-6.597948	2.495023	-0.797874
H	-7.413241	2.872765	-1.421011
C	-6.824387	2.254062	0.552843
H	-7.815114	2.430224	0.977905
C	-5.785182	1.791525	1.364300
H	-5.966819	1.605728	2.425691
C	-4.520908	1.573493	0.823291
H	-3.705202	1.215895	1.456161
C	-4.289553	1.810281	-0.532336
H	-3.299206	1.640860	-0.960392
C	-6.284103	1.574553	-3.993001
H	-7.302951	1.847740	-3.676429
H	-6.172826	1.807254	-5.063861
C	-7.022947	-0.753290	-2.396848
C	-8.421138	-0.709290	-2.487855
H	-8.906460	-0.380145	-3.410951
C	-9.203350	-1.106685	-1.407627
H	-10.292713	-1.074405	-1.484412
C	-8.596838	-1.556905	-0.233196
H	-9.213878	-1.874639	0.610761
C	-7.208034	-1.610028	-0.141880
H	-6.731695	-1.967236	0.774026
C	-6.419127	-1.211252	-1.220951
H	-5.329291	-1.249889	-1.148155
C	-6.760955	-0.983696	-5.255174
C	-7.710884	-0.321107	-6.045267
H	-7.999519	0.709647	-5.825533
C	-8.311470	-0.975196	-7.121093
H	-9.054868	-0.451216	-7.726712
C	-7.975729	-2.295953	-7.415035
H	-8.452678	-2.807386	-8.254383
C	-7.032226	-2.962283	-6.633544
H	-6.761262	-3.996146	-6.858728
C	-6.424059	-2.309272	-5.563809
H	-5.679802	-2.840466	-4.963412
C	-3.925341	2.846694	-7.236143
C	-3.620265	4.196039	-7.470682
H	-2.666213	4.608787	-7.132045
C	-4.517494	5.017676	-8.148103
H	-4.258437	6.063156	-8.330795
C	-5.736543	4.508803	-8.596452
H	-6.435720	5.151231	-9.136785
C	-6.053182	3.172434	-8.359760
H	-7.001133	2.761541	-8.715596
C	-5.155647	2.345277	-7.682598
H	-5.434299	1.300600	-7.523967
C	-1.117989	2.293225	-6.997739
C	-0.052872	2.626205	-6.154888
H	-0.196434	2.626582	-5.071480
C	1.189576	2.954625	-6.698719
H	2.017489	3.217677	-6.036396
C	1.371245	2.951279	-8.079449
H	2.343299	3.213495	-8.504137
C	0.309161	2.621820	-8.924983
H	0.448909	2.627610	-10.008547
C	-0.932452	2.296304	-8.388457
H	-1.764811	2.059997	-9.057892

C	-3.023826	0.114182	-6.815719
H	-4.107263	-0.040051	-6.939064
H	-2.530997	-0.062520	-7.784600
C	-0.682933	-0.971151	-5.488951
C	-0.038531	-0.628113	-4.297711
H	-0.628665	-0.431195	-3.401710
C	1.352499	-0.521239	-4.260092
H	1.845621	-0.232187	-3.327962
C	2.102126	-0.766494	-5.407709
H	3.191192	-0.678218	-5.380301
C	1.462535	-1.124772	-6.597692
H	2.049564	-1.321897	-7.497675
C	0.076289	-1.228902	-6.639650
H	-0.413181	-1.519006	-7.573617
C	-2.849927	-2.724186	-6.190991
C	-3.266775	-2.958108	-7.505909
H	-3.409528	-2.130472	-8.203933
C	-3.510615	-4.260606	-7.943232
H	-3.831760	-4.433316	-8.973203
C	-3.343940	-5.336148	-7.073392
H	-3.534400	-6.354674	-7.419664
C	-2.933366	-5.109415	-5.758400
H	-2.804661	-5.949533	-5.071936
C	-2.691076	-3.811616	-5.317883
H	-2.373852	-3.640008	-4.284310

$\mathbf{T_2}$

E_{rel/S_0} = 3.090 eV

Cu	2.807610	-2.921711	4.384635
Cu	2.755786	-0.344209	3.164306
Cu	-0.155975	-1.808371	0.529608
P	4.903403	-3.622695	3.731972
P	4.972553	-0.732253	2.687736
P	2.232000	-2.387890	6.534993
P	1.942604	0.348755	5.198701
C	0.853319	-2.434919	1.994206
C	1.290127	1.127554	0.793233
N	1.534793	-2.684108	2.908802
N	1.863808	0.626148	1.674424
C	5.965614	-4.655054	4.809703
C	6.461307	-5.897408	4.395934
H	6.237830	-6.274298	3.395744
C	7.248160	-6.660730	5.258262
H	7.631445	-7.627621	4.923971
C	7.549401	-6.192503	6.535014
H	8.172307	-6.789796	7.204885
C	7.046932	-4.961656	6.958438
H	7.266520	-4.593319	7.962990
C	6.249837	-4.202618	6.106438
H	5.838946	-3.255620	6.468480
C	4.978409	-4.422875	2.094726
C	6.152833	-4.475295	1.330052
H	7.075965	-4.017073	1.693599
C	6.157607	-5.122024	0.097882
H	7.076023	-5.156729	-0.492491
C	4.994628	-5.729836	-0.378884
H	5.004443	-6.243468	-1.343280
C	3.824903	-5.685098	0.376338
H	2.913829	-6.162494	0.008116
C	3.814613	-5.028531	1.606537
H	2.892303	-4.979019	2.190568
C	5.894422	-2.068191	3.574726
H	6.884782	-2.251072	3.128694
H	6.050075	-1.714943	4.607260
C	5.334138	-1.055509	0.922429
C	6.598197	-0.803688	0.373221
H	7.388601	-0.364785	0.988556
C	6.850119	-1.096297	-0.964782
H	7.836854	-0.894166	-1.388225
C	5.842749	-1.641250	-1.762496
H	6.044530	-1.873687	-2.811141
C	4.580437	-1.883752	-1.223327
H	3.789341	-2.308045	-1.846509
C	4.322084	-1.584539	0.113773
H	3.329257	-1.765517	0.532179
C	5.920742	0.782419	3.080084

C	7.186516	0.780307	3.679847
H	7.680452	-0.157260	3.944774
C	7.839595	1.983762	3.946821
H	8.827457	1.970854	4.413353
C	7.237450	3.196121	3.617007
H	7.751735	4.136758	3.827400
C	5.976726	3.205775	3.019879
H	5.497169	4.153496	2.765195
C	5.318872	2.007815	2.756178
H	4.326728	2.024164	2.295449
C	3.189095	-3.108689	7.916856
C	3.144102	-4.504339	8.054733
H	2.556602	-5.105835	7.354658
C	3.836943	-5.134582	9.083073
H	3.788619	-6.221306	9.182288
C	4.594457	-4.381409	9.981562
H	5.137254	-4.876422	10.790206
C	4.653067	-2.996381	9.846614
H	5.239197	-2.400758	10.550521
C	3.951313	-2.359743	8.820946
H	4.000843	-1.271193	8.747908
C	0.500134	-2.662274	7.048473
C	-0.440995	-3.041454	6.085229
H	-0.132688	-3.166425	5.043870
C	-1.768226	-3.258614	6.454421
H	-2.499119	-3.557691	5.699697
C	-2.157631	-3.102314	7.782868
H	-3.195899	-3.280667	8.072877
C	-1.220250	-2.729662	8.748197
H	-1.523291	-2.617913	9.791895
C	0.105704	-2.513522	8.385428
H	0.839915	-2.244761	9.150173
C	2.514679	-0.569305	6.694200
H	3.609159	-0.438369	6.715063
H	2.094743	-0.160295	7.627320
C	0.124356	0.455663	5.361577
C	-0.672600	0.114429	4.263892
H	-0.203406	-0.223078	3.337647
C	-2.062042	0.210200	4.349088
H	-2.678809	-0.056004	3.486805
C	-2.659437	0.640798	5.531251
H	-3.747847	0.709174	5.601945
C	-1.868571	0.988333	6.628533
H	-2.335552	1.332040	7.554349
C	-0.482629	0.902572	6.543364
H	0.126382	1.197822	7.402180
C	2.487883	2.070919	5.509971
C	3.448909	2.422886	6.464111
H	3.894738	1.670353	7.117621
C	3.850609	3.751852	6.602389
H	4.596567	4.014350	7.356111
C	3.299895	4.739570	5.789903
H	3.611341	5.780326	5.905196
C	2.345499	4.394756	4.831688
H	1.907204	5.165499	4.193134
C	1.944332	3.070169	4.688034
H	1.197562	2.809693	3.932779
Cu	-2.807034	2.890199	-4.398316
Cu	-2.706431	0.299526	-3.260827
Cu	0.286859	1.827907	-0.642832
P	-4.926089	3.506321	-3.733123
P	-4.900385	0.635799	-2.644076
P	-2.216187	2.479183	-6.571454
P	-1.947237	-0.321861	-5.343055
C	-0.769815	2.459246	-2.070464
C	-1.145713	-1.127498	-0.926294
N	-1.493788	2.701895	-2.953377
N	-1.727293	-0.644381	-1.812412
C	-6.029274	4.475021	-4.828748
C	-6.584308	5.699550	-4.438523
H	-6.382206	6.104291	-3.444684
C	-7.402415	6.409396	-5.317510
H	-7.832502	7.362857	-5.002117
C	-7.674919	5.905370	-6.587152
H	-8.321632	6.461275	-7.269958
C	-7.113707	4.692120	-6.987146
H	-7.310533	4.297085	-7.986231

C	-6.286662	3.986790	-6.118070
H	-5.830101	3.053383	-6.460361
C	-5.001498	4.354188	-2.120488
C	-6.157299	4.378639	-1.327034
H	-7.066455	3.865269	-1.649501
C	-6.161617	5.067259	-0.117576
H	-7.065277	5.079387	0.496035
C	-5.017752	5.746130	0.306307
H	-5.027841	6.292627	1.252458
C	-3.866497	5.729421	-0.477983
H	-2.970217	6.261486	-0.150732
C	-3.855400	5.029521	-1.683840
H	-2.945476	5.000619	-2.288702
C	-5.878915	1.932897	-3.522117
H	-6.861468	2.100617	-3.053487
H	-6.052921	1.561579	-4.545384
C	-5.150892	1.018247	-0.872043
C	-6.369047	0.756117	-0.231098
H	-7.185791	0.275039	-0.776440
C	-6.539493	1.093770	1.109083
H	-7.490631	0.884794	1.604578
C	-5.496473	1.692939	1.817127
H	-5.634395	1.961311	2.867578
C	-4.279028	1.944855	1.186653
H	-3.459758	2.409416	1.740634
C	-4.102113	1.601906	-0.153094
H	-3.144864	1.790578	-0.644064
C	-5.854331	-0.901681	-2.905670
C	-7.111760	-0.948741	-3.519930
H	-7.597415	-0.037272	-3.875620
C	-7.769634	-2.168897	-3.679950
H	-8.752209	-2.194683	-4.157089
C	-7.181499	-3.347232	-3.225118
H	-7.701394	-4.300310	-3.347755
C	-5.927946	-3.307098	-2.613542
H	-5.459867	-4.229141	-2.261429
C	-5.264153	-2.093953	-2.459002
H	-4.276202	-2.071552	-1.989439
C	-3.167092	3.262257	-7.921747
C	-3.197405	4.664706	-7.940267
H	-2.677775	5.233715	-7.163568
C	-3.880985	5.342294	-8.944555
H	-3.893238	6.434512	-8.950064
C	-4.553154	4.628611	-9.937927
H	-5.089327	5.160954	-10.727046
C	-4.536150	3.235712	-9.922524
H	-5.055498	2.671823	-10.701083
C	-3.843713	2.552432	-8.921073
H	-3.832022	1.460331	-8.941002
C	-0.479041	2.756061	-7.067592
C	0.472808	3.032134	-6.079890
H	0.167452	3.089884	-5.032005
C	1.806675	3.233422	-6.433385
H	2.545805	3.450820	-5.658944
C	2.192672	3.166552	-7.770387
H	3.236490	3.332856	-8.047336
C	1.244373	2.900933	-8.759862
H	1.544069	2.860935	-9.809740
C	-0.088233	2.699182	-8.412627
H	-0.829701	2.513268	-9.194633
C	-2.501214	0.669119	-6.807343
H	-3.592476	0.530604	-6.867566
H	-2.054057	0.285452	-7.738214
C	-0.135634	-0.470818	-5.500326
C	0.676299	-0.178151	-4.399533
H	0.222273	0.134500	-3.457367
C	2.062684	-0.291261	-4.503719
H	2.692093	-0.061700	-3.640028
C	2.642117	-0.690250	-5.706239
H	3.728588	-0.771701	-5.790602
C	1.835961	-0.987719	-6.806492
H	2.288343	-1.305808	-7.748528
C	0.452022	-0.882885	-6.704699
H	-0.170288	-1.133837	-7.567865
C	-2.598892	-1.950915	-5.637960
C	-4.026746	-2.131153	-6.010249
H	-4.656647	-1.256773	-6.188770

C	-4.557922	-3.380768	-6.128555
H	-5.604130	-3.500893	-6.419078
C	-3.758832	-4.558673	-5.861649
H	-4.177334	-5.556280	-5.996530
C	-2.390659	-4.388676	-5.371512
H	-1.809120	-5.274637	-5.106192
C	-1.839922	-3.150165	-5.243391
H	-0.819636	-3.031938	-4.872557

Table S7. Spin-orbit coupling energy (in cm^{-1}) between states of **1** at the geometries of T_1, $T_{1\text{-const}}$ and S_1

Geometry	S_0/T_1	S_0/S_1	S_1/T_1
1-T_1	26	-	6
1-$T_{1\text{-const}}$	34	-	34
1-S_1	-	26	5

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