Supporting Information

I. Experimental Section

All experiments were performed under an atmosphere of dry argon using standard Schlenk techniques. Commercially available reagents ($[Cu(CH_3CN)_4].PF_6$, CuCN, dppm) were used as received without further purification. Solvents were freshly distilled under argon from phosphorus pentoxide (dichloromethane, pentane). ^1H, ^{13}C and $^{31}P\{^1H\}$ NMR spectra were recorded on Bruker DPX200, AV300 or AV400 spectrometers. ^1H and ^{13}C 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. Elemental analyses were performed by the CRMPO, University of Rennes 1. The UV/Vis absorption spectra were recorded on a Hewlett-Packard 8452A diode array spectrophotometer. Steady-state emission spectra were recorded on a Spex Fluorolog-3 Model FL3-211 fluorescence spectrofluorometer equipped with a R2658P PMT detector. Excited-state lifetimes were measured with a conventional laser system. The excitation source used was the 355 nm output (third harmonic, 8 ns) of a Spectra-Physics Quanta-Ray Q-switched GCR-150 pulsed Nd:YAG laser (10 Hz). Luminescence decay signals were detected by a Hamamatsu R928 photomultiplier tube, recorded on a Tektronix Model TDS-620A (500 MHz, 2 GS s^{-1}) digital oscilloscope, and analyzed with a program for exponential fits. Luminescence quantum yield in solid state were measured on a Hamamatsu C9920-03 Absolute PL Quantum Yield Measurement System. Variable-temperature emission spectra were obtained using the Edinburgh Instruments FS5 Spectrofluorometer with an Oxford Instrument OptistatDN2 cryostat for temperatures in the range of 80 K to 405 K. Solid sample was placed in a quartz tube inside the cryostat and maintained at the desired temperature until equilibrium was reached before recording the spectrum. Variable-temperature excited state lifetimes were measured using the above mentioned conventional nanosecond pulsed laser system. Solid sample was placed in a quartz tube inside an Oxford Instrument OptistatDN2 cryostat for temperatures in the range of 80 K to 405 K. The experimental data were then fitted according to the following equation[1]

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

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. 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. Solid state ^{31}P NMR spectra were recorded at 14 T on a Bruker Avance III spectrometer, using a 2.5 mm MAS probe at a rf field strength of 40 kHz and a recycle interval of 75 s. Spectra were referenced with respect to H_3PO_4 1M used as an external reference. Spectra were recorded at a MAS rate of 25 kHz. A SPINAL64 ^1H decoupling was employed during acquisition with an rf field strength of ~ 60 kHz.

Synthesis of the derivative 2

To a dichloromethane solution (10 ml) of bis(diphenylphosphino)methane (dppm) (0.04 g, 0.10 mmol) and $[Cu(CH_3CN)_4].PF_6$ (0.04 g, 0.10 mmol) stirred for 30 minutes at room temperature was added a methanol suspension (5 ml) of copper cyanide (0.005 g, 0.05 mmol). This reaction mixture was stirred for one night at room temperature affording a colorless clear solution together with a small amount of white precipitate. This crude solution was then filtered over cotton and pentane vapour diffusion into the solution afforded after crystallization derivative **2** (0.030 g, 0.02 mmol, 56% yield) as an air-stable colorless polycrystalline solid.

^1H NMR (400 MHz, $CDCl_3$, ppm): δ = 3.10 (broad s, 8H, PCH_2P), 6.92 (broad s, 24H, H_{arom}), 7.22 (broad s, 32H, H_{arom}), 7.50 (broad s, 16H, H_{arom}), 7.75 (broad s, 8H, H_{arom}).

$^{31}P\{^1H\}$ NMR (161.98 MHz, $CDCl_3$, ppm): δ = −8.8 (broad s, P_{dppm}), −10.9 (broad s, P_{dppm}), -144.4 (sept, ^1J(P-F) = 711.0 Hz).

Elemental analysis, calcd. (%) for $C_{102}H_{90}Cl_2Cu_4F_{12}N_2P_{10}$: C 55.52, H 4.11, N 1.27; found: C 55.88, H 4.16, N 1.54.

IR (cm^{-1}): 690 (s), 715 (m), 739 (s), 771 (m), 832 (s), 998 (w), 1099 (m), 1189 (w), 1331 (w), 1435 (m), 1484 (w), 2117 (w), 3054 (w).

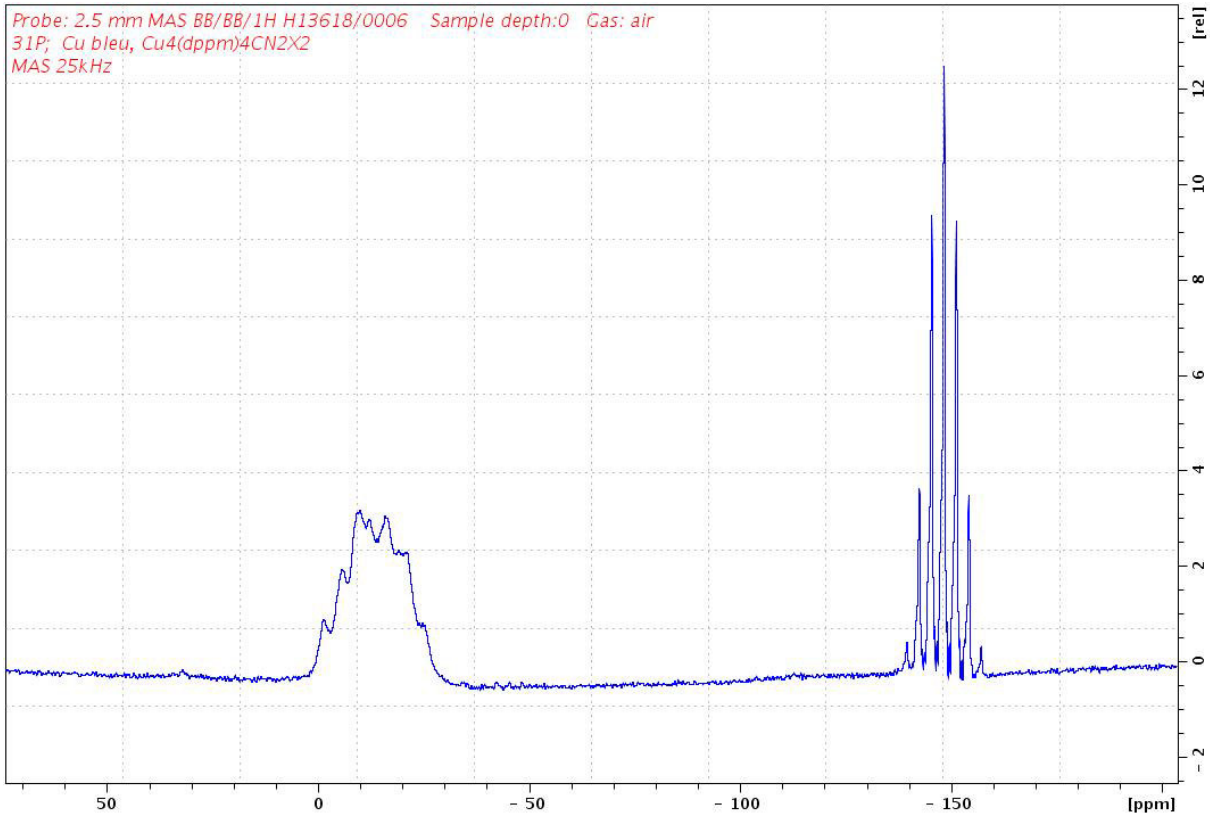


Fig. S1. ^{31}P CPMAS (Cross Polarization Magic Angle Spinning) NMR spectrum of **2**

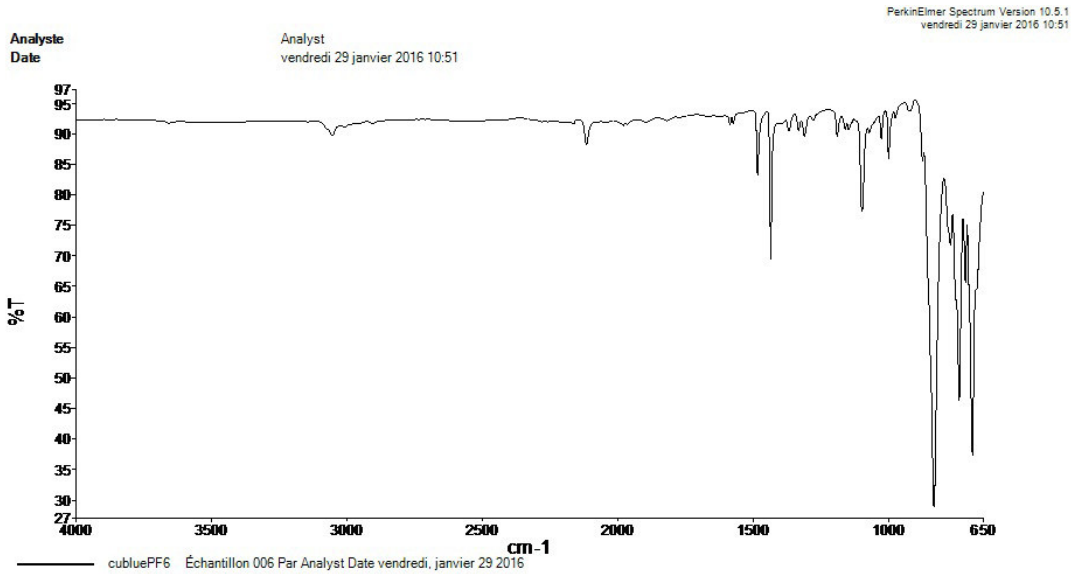


Fig. S2. IR spectrum of **2**.

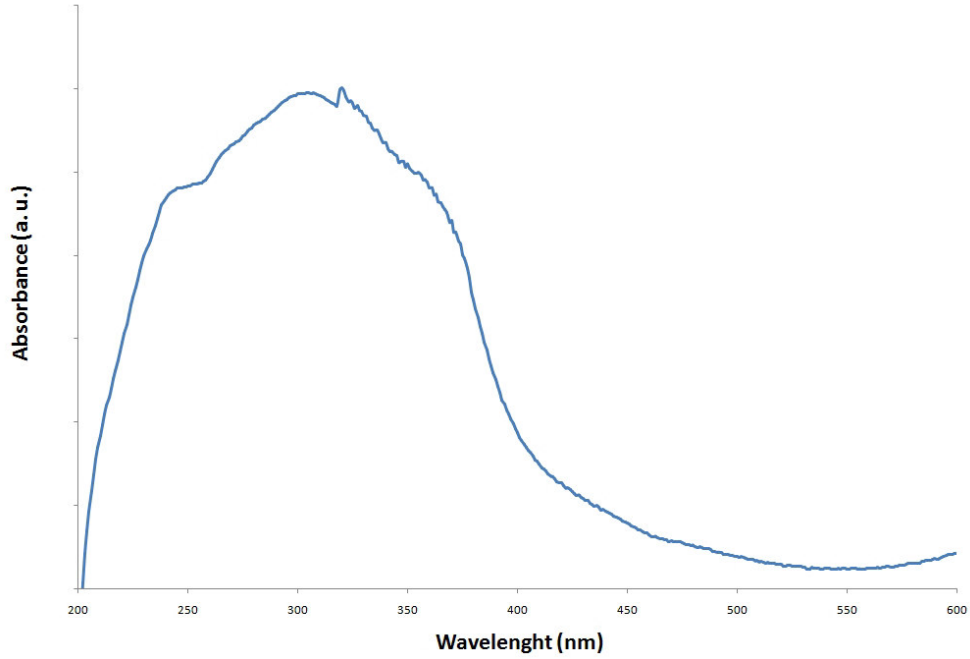


Fig S3. Solid state UV-Vis absorption spectrum of **2**.

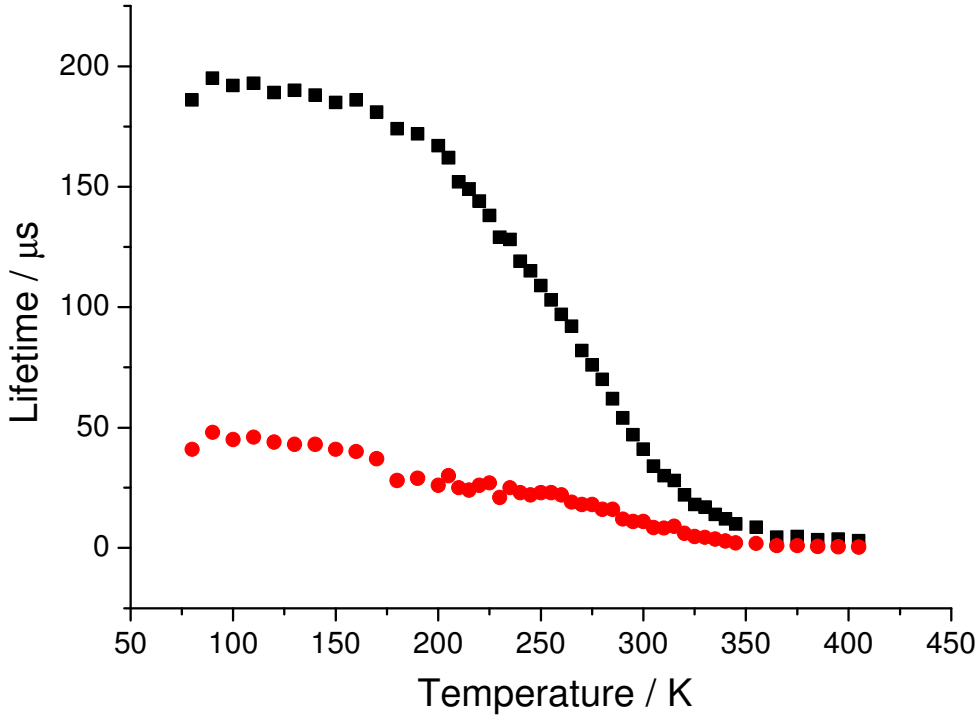
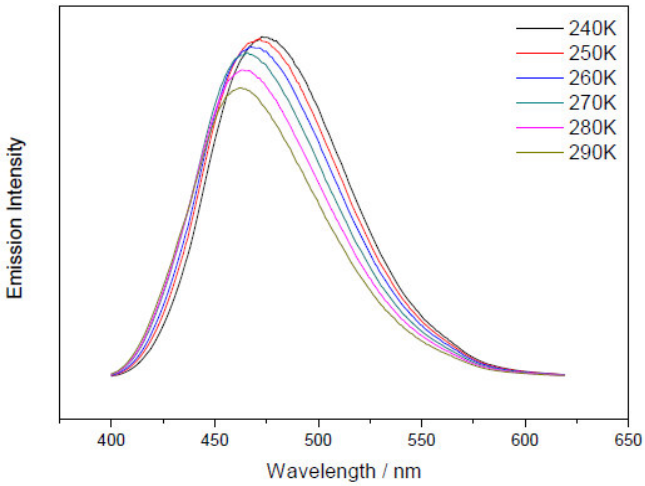
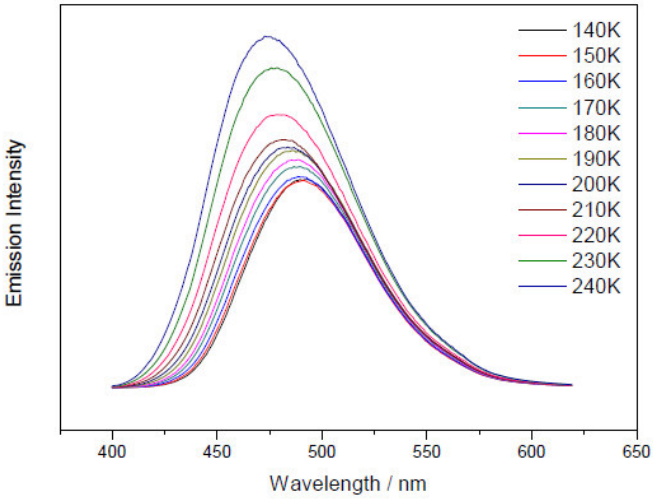


Fig. S4. Temperature-dependence of emission lifetime, τ_1 (■) and τ_2 (●)*, from 80 K to 405 K.

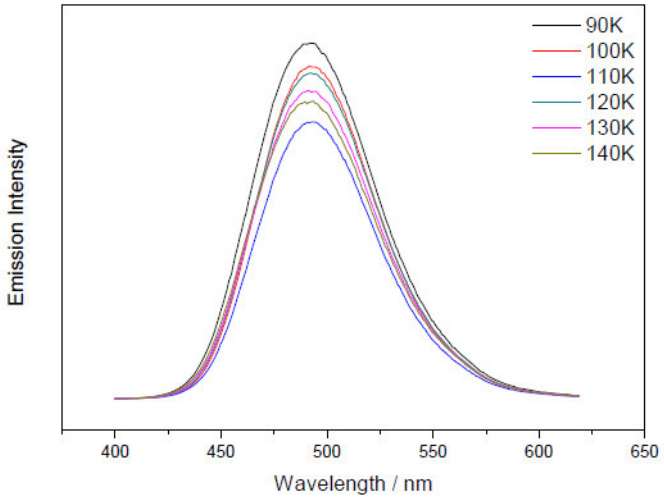
* : The origin of the τ_2 shorter-lived component is not very clear. One possible suggestion may be due to the fact that given the rather small spin-orbit coupling, in addition to direct ISC, vibronic ISC and spin-vibronic ISC may also occur (see Yersin et al., Inorg. Chem, 2016, 2441). The presence of such mechanisms would lead to differences in the radiative decay and hence, emission decay lifetimes that are not taken into account in equation 1."



a)



b)



c)

Fig. S5. Non-normalized solid state emission spectra of 2 at different temperatures: a) from 290 K to 240 K; b) from 240 K to 140 K; c) from 140 K to 90K.

Table S1. Photophysical data for complex **2**

Complex	Medium (T / K)	Absorption λ_{abs} / nm (ε / dm^3 mol^{-1} cm^{-1})	Emission λ_{em} / nm (τ_o / μs)[a]	ϕ_{lum}
2	Dichloromethane (298)	303 sh (12270)	506 (104)	0.43[b]
	Solid (298)	–[b]	457 (41)	0.72[c]
	Solid (80)	–[b]	486 (186)	–[d]

[a] Long-lived component listed
[b] The relative luminescence quantum yield measured at room temperature using quinine sulphate in 1N sulphuric acid (ϕ_{lum} = 0.546, λ_{ex} = 365 nm) as the reference
[c] The luminescence quantum yield in solid state measured at room temperature using Hamamatsu C9920-03G Absolute PLQY Measurement System
[d] Not determined

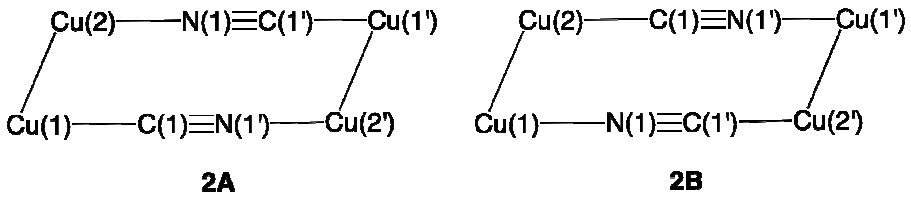
II. X-ray Crystallographic Study.

Single crystals of **2** suitable for X-ray crystal analyses were obtained by slow diffusion of vapors of pentane into dichloromethane solutions. Single crystal data collection was performed at 100 K, 150 K, 200 K or 250 K with an APEX II 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.[2] Structure determinations were performed by direct methods with the solving program SIR97,[3] that revealed all the non-hydrogen atoms. SHELXL program[4] 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 (100 K , 150 K, 200 K or 250 K) as quickly as possible on the diffractometer goniometer and X-ray data collection was performed at low temperature (100 K, 150 K, 200 K or 250 K). Note that at 250 K, the cooling of the crystal was sufficient all along the time of the data collection to allow a stabilization of the single crystal in the oil without its collapse, due to included solvent evaporation. Temperature-dependant measurements were performed on the same single crystal applying the same measurement strategy for each measurement. No phase transition was observed during this cooling process.

The included dichloromethane solvent molecules were found to be highly disordered and the modelling of the disorder of these solvent molecules was not possible leading to rather high anisotropic displacement parameters for some of their atoms. A modelling of these disorders was not possible and we have proceeded to a 'squeeze' treatment[5] in order to remove the scattering contribution of these molecules which cannot be satisfactorily modelled. 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 leading to,

due to crystallography symmetry, two refined conformations **2A** and **2B** (see Scheme S1 and Fig. S5) 'overlapping' in the X-ray crystal structure of the metallacycle **2**.



2A **2B**

Scheme S1. Schematic views of the conformations **2A** and **2B** modelled in the X-ray crystal structure of the derivative **2**.

The relative occupancies of **2A** conformation versus **2B** conformation were found to be 0.71888/0.28112, 0.74124/0.25876, 0.73426/0.26574 and 0.74249./0.25751 at 100 K, 150 K, 200 K and 250 K respectively. This suggests that the conformer **2A** is dominant in the solid state, which is supported by the data collected from the theoretical calculations (relative energy of the ground states of the three different possible conformers) and the agreement between the observed photophysical measurements and the theoretical calculations conducted considering the geometry of the conformation **2A** (*vide infra*). These observations have guided us to choose the conformer **2A** as model for the sake of the clarity of the description of the results in this communication. Nevertheless, the conformer **2B** was also considered in the theoretical calculations performed (*vide infra*), revealing similar behaviours but a somewhat lower degree of agreement between the energy values calculated and those deduced from the experimental photophysical measurements.

Table S2 and S3 give the crystallographic data at 100 K, 150 K, 200 K and 250 K for the derivative **2** after this 'squeeze' treatment and before 'squeeze' treatment, respectively.

Atomic scattering factors for all atoms were taken from International Tables for X-ray Crystallography.[6] CCDC reference numbers 1465319, 1465320, 1465321 and 1465322 contain the supplementary crystallographic data for derivatives **2** at 100 K, 150 K, 200 K and 250 K respectively. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre.

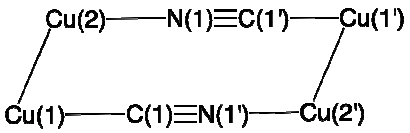
Table S2. Crystal data and structure refinement for **2A** at 100 K, 150 K, 200 K and 250 K.

	2 . $2PF_6$	**2** . $2PF_6$	**2** . $2PF_6$	**2** . $2PF_6$
Molecular formula	$C_{102}H_{88}Cu_4F_{12}N_2P_{10}$	$C_{102}H_{88}Cu_4F_{12}N_2P_{10}$	$C_{102}H_{88}Cu_4F_{12}N_2P_{10}$	$C_{102}H_{88}Cu_4F_{12}N_2P_{10}$
CCDC number	1465319	1465320	1465321	1465322
Molecular weight	2133.60	2133.60	2133.60	2133.60
a (Å)	13.8020(17)	13.869(4)	13.935(3)	14.023(3)
b (Å)	20.7715(13)	20.739(7)	20.745(5)	20.778(5)
c (Å)	18.8547(11)	18.963(6)	19.086(4)	19.191(4)
α (°)	90	90	90	90
β (°)	100.480(2)	100.223(2)	100.550(5)	100.733(9)
γ (°)	90	90	90	90
V (Å^3)	5315.3(8)	5368(3)	5424(2)	5494(2)
Z	2	2	2	2
Dc (g cm^{-3})	1.333	1.320	1.306	1.290
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	P21/n	P21/n	P21/n	P21/n
Temperature (K)	100(2)	150(2)	200(2)	250(2)
Wavelength Mo-$K\alpha$ (Å)	0.71069	0.71069	0.71069	0.71069
Crystal size (mm)	0.22 * 0.14 * 0.11	0.22 * 0.14 * 0.11	0.22 * 0.14 * 0.11	0.22 * 0.14 * 0.11
μ (mm^{-1})	1.005	0.995	0.985	0.972
F(000)	2176	2176	2176	2176
θ limit (°)	1.47 –26.37	1.47 –26.39	1.46 –26.43	1.46 – 26.43
Index ranges hkl	$-15 \le h \le 17$, $-25 \le k \le 25$, $-23 \le l \le 23$	$-17 \le h \le 15$, $-25 \le k \le 25$, $-23 \le l \le 23$	$-17 \le h \le 15$, $-25 \le k \le 25$, $-23 \le l \le 23$	$-17 \le h \le 16$, $-26 \le k \le 25$, $-23 \le l \le 23$
Reflections collected	35647	36042	36513	36667
Independant reflections	10842	10973	11128	11250
Reflections [$I>2\sigma(I)$]	8729	8283	7939	7341
Data/restraints/parameters	10842 / 0 / 574	10973/ 0 / 574	11128/ 0 / 574	11250/ 0 /574
Goodness-of-fit on F^2	1.113	1.150	1.042	0.977
Final R indices [$I>2\sigma(I)$]	$R1$= 0.0566	$R1$= 0.0589	$R1$= 0.0561	$R1$= 0.0561
	$wR2$= 0.1677	$wR2$= 0.1689	$wR2$= 0.1587	$wR2$= 0.1514
R indices (all data)	$R1$= 0.0671	$R1$= 0.0738	$R1$= 0.0755	$R1$= 0.0834
	$wR2$= 0.1753	$wR2$= 0.1777	$wR2$= 0.1701	$wR2$= 0.1646
Largest diff peak and hole (e Å^{-3})	2.175 and -0.884	1.762 and -1.050	1.327 and -0.679	0.854 and -0.567

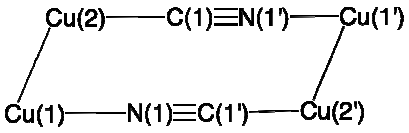
Table S3. Crystal data and structure refinement for **2B** at 100 K, 150 K, 200 K and 250 K before the 'squeeze' treatment.

	2 . $2PF_6$.$4CH_2Cl_2$	**2** . $2PF_6$.$4CH_2Cl_2$	**2** . $2PF_6$.$4CH_2Cl_2$	**2** . $2PF_6$.$4CH_2Cl_2$
Molecular formula	$C_{106}H_{92}Cu_4Cl_8F_{12}N_2P_{10}$	$C_{106}H_{92}Cu_4Cl_8F_{12}N_2P_{10}$	$C_{106}H_{92}Cu_4Cl_8F_{12}N_2P_{10}$	$C_{106}H_{92}Cu_4Cl_8F_{12}N_2P_{10}$
Molecular weight	2469.28	2469.28	2469.28	2469.28
a (Å)	13.8020(17)	13.869(4)	13.935(3)	14.023(3)
b (Å)	20.7715(13)	20.739(7)	20.745(5)	20.778(5)
c (Å)	18.8547(11)	18.963(6)	19.086(4)	19.191(4)
α (°)	90	90	90	90
β (°)	100.480(2)	100.223(2)	100.550(5)	100.733(9)
γ(°)	90	90	90	90
V (Å^3)	5315.3(8)	5368(3)	5424(2)	5494(2)
Z	2	2	2	2
*D*c (g cm^{-3})	1.543	1.528	1.512	1.483
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	P21/n	P21/n	P21/n	P21/n
Temperature (K)	100(2)	150(2)	200(2)	250(2)
Wavelength Mo-*K*α (Å)	0.71069	0.71069	0.71069	0.71069
Crystal size (mm)	0.22 * 0.14 * 0.11	0.22 * 0.14 * 0.11	0.22 * 0.14 * 0.11	0.22 * 0.14 * 0.11
μ (mm^{-1})	1.211	1.199	1.186	1.171
F(000)	2504	2504	2504	2504
θ limit (°)	1.47 –26.37	1.47 –26.39	1.46 –26.43	1.46 – 26.43
Index ranges *hkl*	-15 ≤ *h* ≤ 17,	-17 ≤ *h* ≤ 15,	-17 ≤ *h* ≤ 15,	-17 ≤ *h* ≤ 16,
	-25≤ *k* ≤ 25,	-25≤ *k* ≤ 25,	-25≤ *k* ≤ 25,	-26≤ *k* ≤ 25,
	-23 ≤ *l* ≤ 23	-23 ≤ *l* ≤ 23	-23 ≤ *l* ≤ 23	-23 ≤ *l* ≤ 23
Reflections collected	35647	36042	36513	36667
Independant reflections	10842	10973	11128	11250
Reflections [$I>2\sigma(I)$]	8829	8309	7943	7290
Data/restraints/parameters	10842 / 0 / 641	10973/ 0 / 641	11128/ 0 / 641	11250/ 0 /641
Goodness-of-fit on F^2	1.070	1.089	1.042	1.048
Final *R* indices [$I>2\sigma(I)$]	*R*1= 0.0649	*R*1= 0.0659	*R*1= 0.0622	*R*1= 0.0637
	*wR*2= 0.1817	*wR*2= 0.1771	*wR*2= 0.1682	*wR*2= 0.1724
R indices (all data)	*R*1= 0.0811	*R*1= 0.0899	*R*1= 0.0923	*R*1= 0.1053
	*wR*2= 0.2005	*wR*2= 0.2045	*wR*2= 0.2003	*wR*2= 0.2118
Largest diff peak and hole (e Å^{-3})	2.392 and -1.911	2.152 and -0.956	1.509 and -0.712	1.109 and -0.679

Table S4. Selected bond lengths [Å] and angles [°] observed at 100 K, 150 K, 200 K and 250 K in the X-ray crystal structure of the metallacycle for the isomers a) **2A** and b) **2B**.



2A



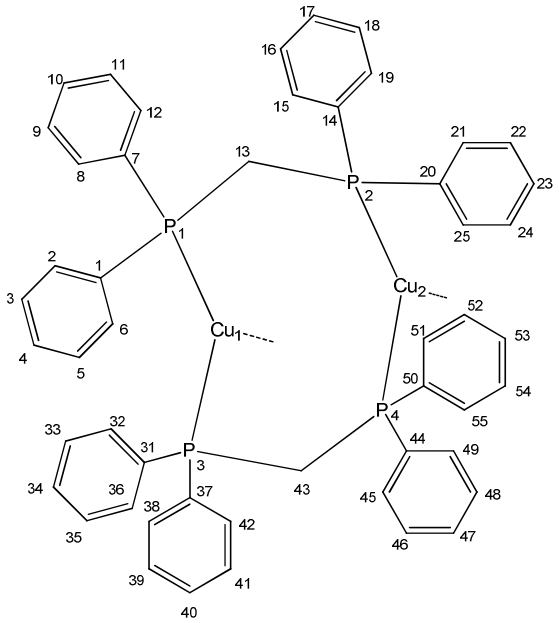
2B

a)

T	Cu–P	Cu–N	Cu–C	Cu···Cu	C≡N	Cu(1)-Cu(2')	Cu(1)-Cu(1')	Cu(2)-Cu(2')	C-Cu(1)-Cu(2)	N-Cu(2)-Cu(1)	C-Cu-Cu-N
100K	2.2429(10) 2.2642(10) 2.2565(10) 2.2590(10)	1.949(11)	1.962(13)	2.8669(6)	1.141(17)	5.010	6.597	4.272	64.1(4)	131.0(3)	5.99
150K	2.2472(12) 2.2612(12) 2.2621(12) 2.2590(12)	1.971(11)	1.941(9)	2.8655(8)	1.139(14)	5.007	6.983	4.219	62.9(3)	132.1(3)	1.92
200K	2.2507(11) 2.2621(11) 2.2587(11) 2.2679(11)	1.969(10)	1.947(9)	2.8662(7)	1.119(12)	5.001	6.957	4.247	62.8(3)	130.2(3)	2.34
250K	2.2511(11) 2.2590(11) 2.2586(11) 2.2674(12)	1.981(13)	1.910(14)	2.8668(7)	1.13(2)	4.992	6.927	4.278	63.5(5)	128.5(4)	0.96

b)

T	Cu–P	Cu–N	Cu–C	Cu···Cu	C≡N	Cu(1)-Cu(2')	Cu(1)-Cu(1')	Cu(2)-Cu(2')	C-Cu(2)-Cu(1)	N-Cu(1)-Cu(2)	C-Cu-Cu-N
100K	2.2429(10) 2.2642(10) 2.2565(10) 2.2590(10)	1.92(2)	2.00(3)	2.8669(6)	1.14(4)	5.010	6.597	4.272	129.9(9)	67.9(7)	9.46
150K	2.2472(12) 2.2612(12) 2.2621(12) 2.2590(12)	1.956(17)	1.96(4)	2.8655(8)	1.17(4)	5.007	6.983	4.219	131.4(10)	69.2(6)	12.61
200K	.2507(11) 2.2621(11) 2.2587(11) 2.2679(11	1.932(17)	1.96(3)	2.8662(7)	1.21(3)	5.001	6.957	4.247	134.0(9)	70.2(7)	11.01
250K	2.2511(11) 2.2590(11) 2.2586(11) 2.2674(12)	2.03(3)	1.89(4)	2.8668(7)	1.19(6)	4.992	6.927	4.278	135.7(11)	69.8(8)	9.46



Scheme S2. Labelling scheme adopted for the atoms of the [Cu_2dppm_2] fragments in the X-ray crystal structure of the derivative **2**.

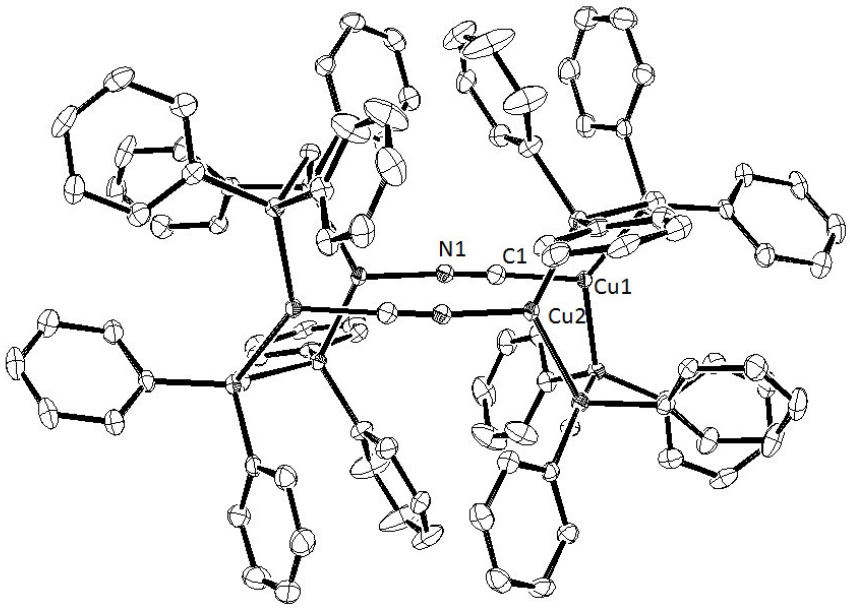


Fig. S6a. Molecular structure of the cationic part of complex **2** (conformer **2A**, thermal ellipsoids 50% probability; measurement performed at 100K). Hydrogen atoms have been omitted for clarity.

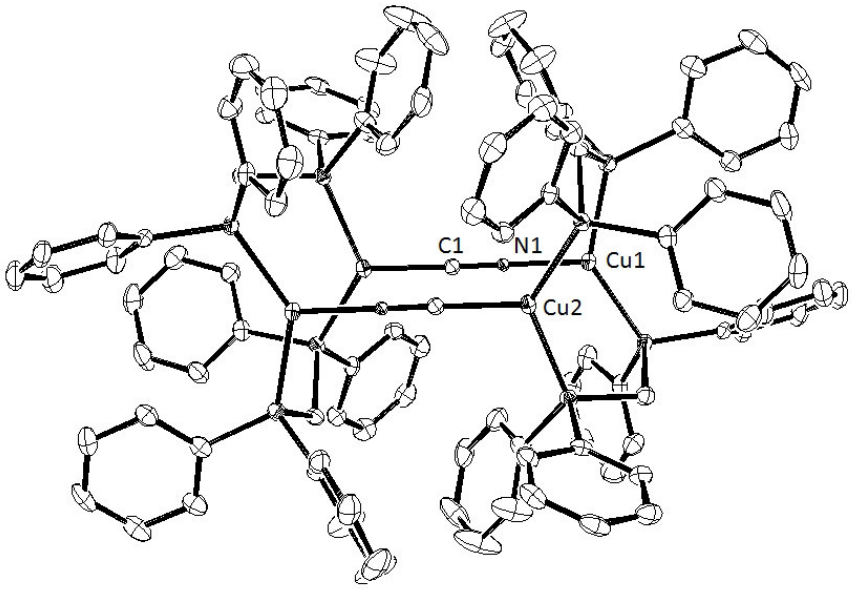


Fig. S6b. Molecular structure of the cationic part of complex **2** (conformer **2B**, thermal ellipsoids 50% probability; measurement performed at 100K). Hydrogen atoms have been omitted for clarity.

References for the supporting information, X-ray crystallographic study section.

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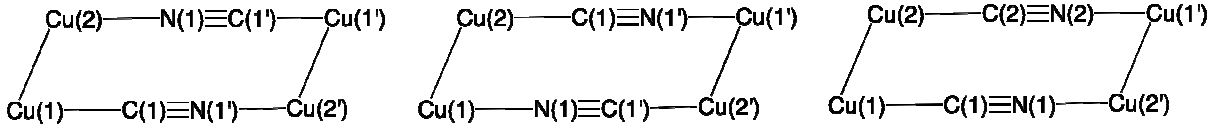
III. Theoretical Study.

Computational details.

DFT calculations were carried out mainly with the Gaussian 09 program.[1] The different isomers of **2** (see Scheme 3) were fully optimized imposing a C_i symmetry for **2A** and **2B** and without any symmetry constraint for the excited states and for the isomer **2C** using PBE0[2] functional and SVP[3] atomic basis set. Harmonic vibrational frequency calculations were not realisable because of the size of the systems (204 atoms, 2136 basis functions). Tighter criteria of energy convergence were applied to ensure high quality of calculations (10^{-10} u.a.). Their Cartesian coordinates and their relative energies are given in Table S6 and S7 respectively. **2A** is the most stable arrangement but the energy differences being moderate, we have reported all data obtained for the less stable arrangement **2B** for comparison purpose, **2C** having an intermediate behaviour. The iso-surface representations were done using the GaussView 5.0 program.[4] The ground (S_0) and excited-state (S_1 an T1) structures were optimized using analytic DFT and TD-DFT gradients respectively. Their xyz Cartesian coordinates are given in Table S5. DFT 2-component spin-orbit coupling calculations were performed with the ADF2014.07 package on the previously optimized S_1 and T_1 structures. For these calculations the same hybrid functional PBE0 was used, with an all-electron triple-zeta Slater basis set with two additional polarization function.[5] 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.[6]



2A **2B** **2C**

Scheme S3.

Table S5. Cartesian coordinates of **2A** and **2B** for their S_0, S_1 and T_1 states.

204
2A S_0

Cu	3.307092	0.093718	-1.230975
C	1.391051	0.094597	-1.450318
N	0.233980	0.128841	-1.497419
Cu	-1.708352	0.194709	-1.192068
Cu	-3.307090	-0.093706	1.230976
C	-1.391051	-0.094576	1.450330
N	-0.233980	-0.128816	1.497439
Cu	1.708366	-0.194708	1.192076
P	4.474646	-1.816572	-0.979326
P	3.985411	2.239665	-0.982945
P	-3.012069	-1.516355	-1.884433
P	-2.456046	2.328823	-1.269820
P	-3.985414	-2.239654	0.982974
P	-4.474674	1.816564	0.979317
P	2.456052	-2.328826	1.269808
P	3.012093	1.516345	1.884446
C	4.195986	-2.523752	0.698013
C	-3.383311	-2.839478	-0.655933
C	-4.195984	2.523746	-0.698037
C	3.383333	2.839475	0.655953
H	4.805254	-1.926777	1.396492
H	4.542165	-3.568075	0.739723
C	-4.641005	-1.015577	-2.569209
C	-5.857095	-1.619157	-2.230852

C	-7.043414	-1.205093	-2.840490
C	-7.027515	-0.191247	-3.795267
C	-5.817143	0.412879	-4.141880
C	-4.633586	0.005621	-3.532387
C	-2.314384	-2.435408	-3.311563
C	-2.938651	-3.579829	-3.829397
C	-2.421800	-4.209859	-4.957898
C	-1.292713	-3.690215	-5.594957
C	-0.677276	-2.546086	-5.093239
C	-1.178601	-1.924388	-3.949065
C	-5.741853	-2.744443	1.046060
C	-6.706538	-1.805960	1.422081
C	-8.050192	-2.174798	1.509961
C	-8.434698	-3.480936	1.218063
C	-7.474827	-4.426112	0.845781
C	-6.133928	-4.063403	0.766368
C	-3.224973	-3.384721	2.201311
C	-3.967120	-3.759788	3.331257
C	-3.399707	-4.570540	4.311809
C	-2.086887	-5.018945	4.177383
C	-1.339409	-4.638650	3.064400
C	-1.897713	-3.816067	2.086826
C	-2.522225	2.856407	-3.024100
C	-1.420107	2.527413	-3.827900
C	-1.395661	2.888487	-5.173538
C	-2.473421	3.573036	-5.734834
C	-3.574282	3.900327	-4.944063
C	-3.600588	3.545667	-3.595281
C	-1.593585	3.717305	-0.436021
C	-0.794504	3.460260	0.684535
C	-0.196014	4.515515	1.375270
C	-0.372421	5.827628	0.939253
C	-1.153678	6.088350	-0.187001
C	-1.765254	5.039547	-0.869600
C	-3.994162	3.135085	2.150725
C	-3.220068	2.798924	3.266194
C	-2.899614	3.768290	4.216582
C	-3.337662	5.079741	4.051043
C	-4.104080	5.424112	2.936042
C	-4.437598	4.456004	1.994266
C	-6.310794	1.838767	1.089706
C	-6.935395	2.188235	2.295320
C	-8.324664	2.152839	2.406860
C	-9.107450	1.771809	1.318070
C	-8.492624	1.409589	0.120071
C	-7.103959	1.433017	0.007004
C	4.641027	1.015555	2.569219
C	5.857122	1.619123	2.230858
C	7.043439	1.205046	2.840493
C	7.027532	0.191200	3.795270
C	5.817155	-0.412914	4.141887
C	4.633600	-0.005643	3.532398
C	2.314410	2.435400	3.311576
C	2.938712	3.579789	3.829440
C	2.421854	4.209830	4.957931
C	1.292722	3.690233	5.594948
C	0.677248	2.546137	5.093199
C	1.178584	1.924426	3.949036
C	5.741853	2.744445	-1.046050
C	6.706528	1.805959	-1.422087
C	8.050183	2.174790	-1.509981
C	8.434699	3.480926	-1.218084
C	7.474837	4.426105	-0.845786
C	6.133937	4.063402	-0.766358
C	3.224969	3.384735	-2.201281
C	3.967112	3.759790	-3.331233
C	3.399699	4.570541	-4.311787
C	2.086882	5.018954	-4.177356
C	1.339408	4.638669	-3.064368
C	1.897712	3.816089	-2.086791
C	2.522251	-2.856399	3.024090
C	1.420154	-2.527379	3.827907
C	1.395725	-2.888441	5.173548
C	2.473483	-3.573004	5.734831
C	3.574324	-3.900320	4.944044
C	3.600614	-3.545672	3.595258
C	1.593570	-3.717311	0.436035
C	0.794455	-3.460271	-0.684497
C	0.195931	-4.515528	-1.375200
C	0.372339	-5.827638	-0.939173
C	1.153630	-6.088355	0.187059
C	1.765238	-5.039550	0.869626
C	3.994131	-3.135085	-2.150741
C	3.220053	-2.798916	-3.266218
C	2.899617	-3.768273	-4.216621
C	3.337664	-5.079725	-4.051088
C	4.104065	-5.424105	-2.936078
C	4.437567	-4.456005	-1.994288
C	6.310766	-1.838775	-1.089745
C	6.935347	-2.188225	-2.295374
C	8.324614	-2.152829	-2.406937
C	9.107419	-1.771818	-1.318153
C	8.492613	-1.409617	-0.120138
C	7.103950	-1.433044	-0.007049
H	-5.905345	-2.415536	-1.487139
H	-7.983817	-1.688461	-2.565481
H	-7.955806	0.123880	-4.277666
H	-5.791095	1.201823	-4.897180
H	-3.692026	0.480522	-3.822980
H	-3.846370	-3.975918	-3.366232
H	-2.913239	-5.100988	-5.355325
H	-0.901650	-4.176468	-6.491909
H	0.195580	-2.125757	-5.598434
H	-0.685249	-1.035743	-3.548481
H	-2.414600	-3.339157	-0.491493
H	-4.062845	-3.602314	-1.066193
H	-6.407836	-0.778702	1.640986
H	-8.794339	-1.432089	1.805627
H	-9.485971	-3.770803	1.286364
H	-7.774355	-5.453978	0.628019
H	-5.387985	-4.819373	0.503597
H	-5.002940	-3.431077	3.443371
H	-3.994474	-4.861676	5.180801
H	-1.646900	-5.666518	4.939347
H	-0.309131	-4.980995	2.949041
H	-1.277331	-3.522920	1.236205
H	-4.419782	4.439232	-5.378456
H	-2.456862	3.851370	-6.791154
H	-0.529323	2.630979	-5.787253
H	-0.572484	1.987722	-3.395781
H	-0.642832	2.433159	1.023372
H	0.405740	4.306424	2.263075
H	0.099264	6.652164	1.479134
H	-1.289548	7.115128	-0.534938
H	-2.374942	5.254160	-1.751534
H	-4.542163	3.568068	-0.739746
H	-4.805250	1.926771	-1.396519
H	-2.864826	1.771702	3.390307
H	-2.303419	3.497870	5.090283
H	-3.086524	5.838963	4.795489
H	-4.453098	6.451147	2.806736
H	-5.065350	4.733500	1.143193
H	-6.337567	2.505632	3.152979
H	-8.797205	2.436962	3.350036
H	-10.196660	1.759368	1.402659
H	-9.096660	1.104124	-0.737543
H	-6.653636	1.119459	-0.938133
H	-4.475924	3.809795	-2.997745
H	5.905378	2.415501	1.487146
H	7.983846	1.688405	2.565482
H	7.955822	-0.123937	4.277666
H	5.791102	-1.201857	4.897187
H	3.692037	-0.480533	3.822994
H	3.846464	3.975842	3.366308
H	2.913320	5.100933	5.355383
H	0.901651	4.176496	6.491891
H	-0.195645	2.125844	5.598359
H	0.685202	1.035808	3.548426
H	2.414621	3.339159	0.491530
H	4.062870	3.602306	1.066219
H	6.407818	0.778703	-1.640993
H	8.794322	1.432079	-1.805660

H	9.485972	3.770788	-1.286396
H	7.774372	5.453968	-0.628024
H	5.388001	4.819375	-0.503575
H	5.002929	3.431072	-3.443351
H	3.994463	4.861668	-5.180783
H	1.646895	5.666524	-4.939321
H	0.309133	4.981020	-2.949005
H	1.277333	3.522951	-1.236166
H	4.419823	-4.439236	5.378427
H	2.456938	-3.851328	6.791154
H	0.529402	-2.630912	5.787277
H	0.572532	-1.987677	3.395798
H	0.642777	-2.433172	-1.023338
H	-0.405853	-4.306441	-2.262986
H	-0.099373	-6.652175	-1.479029
H	1.289500	-7.115130	0.535005
H	2.374948	-5.254157	1.751546
H	2.864813	-1.771693	-3.390329
H	2.303437	-3.497846	-5.090330
H	3.086541	-5.838940	-4.795545
H	4.453085	-6.451140	-2.806776
H	5.065310	-4.733507	-1.143211
H	6.337504	-2.505607	-3.153028
H	8.797139	-2.436938	-3.350125
H	10.196627	-1.759378	-1.402760
H	9.096663	-1.104167	0.737471
H	6.653643	-1.119502	0.938101
H	4.475934	-3.809820	2.997709

204

2B S_0

Cu	-1.672901	0.293096	-1.117845
Cu	-3.404661	-0.108705	1.120919
P	-3.037041	-1.465181	-1.869956
P	-3.974421	-2.334080	0.940386
P	-2.556976	2.455512	-1.182660
P	-4.600807	1.835783	1.036499
C	0.282559	0.205625	-1.429661
N	1.450819	0.124759	-1.407561
C	-4.705330	-1.016212	-2.486885
C	-5.859148	-1.779459	-2.277137
H	-5.834471	-2.681672	-1.664588
C	-7.072543	-1.392811	-2.849231
H	-7.964867	-1.998200	-2.673894
C	-7.144725	-0.249687	-3.642447
H	-8.093923	0.043839	-4.097070
C	-5.995890	0.512116	-3.864637
H	-6.037959	1.402477	-4.496682
C	-4.786169	0.132786	-3.288628
H	-3.889752	0.729373	-3.482289
C	-2.334940	-2.284922	-3.359017
C	-2.909093	-3.444730	-3.899668
H	-3.781478	-3.905357	-3.428503
C	-2.388481	-4.011164	-5.059834
H	-2.842494	-4.914520	-5.473894
C	-1.303121	-3.414424	-5.704904
H	-0.907638	-3.852626	-6.624410
C	-0.738057	-2.253835	-5.181788
H	0.099908	-1.772364	-5.691764
C	-1.246653	-1.694075	-4.009216
H	-0.797558	-0.788275	-3.595787
C	-3.284797	-2.874334	-0.697871
H	-2.272459	-3.274134	-0.528502
H	-3.882495	-3.689479	-1.134091
C	-5.712168	-2.892920	0.944238
C	-6.718556	-1.967126	1.232350
H	-6.455925	-0.924925	1.426482
C	-8.054817	-2.369021	1.263320
H	-8.832832	-1.637237	1.491979
C	-8.388974	-3.695609	1.001929
H	-9.434527	-4.012062	1.026677
C	-7.386804	-4.627460	0.717354
H	-7.648435	-5.670381	0.523594
C	-6.052927	-4.231669	0.695076
H	-5.273091	-4.973824	0.500023
C	-3.200386	-3.458078	2.165991
C	-3.934733	-3.791530	3.314538
H	-4.963120	-3.440351	3.430520
C	-3.371514	-4.589396	4.307242
H	-3.960743	-4.848105	5.190145
C	-2.069103	-5.066616	4.167458
H	-1.632078	-5.704687	4.939098
C	-1.329580	-4.728888	3.035917
H	-0.308600	-5.096639	2.915359
C	-1.884144	-3.919978	2.044428
H	-1.269250	-3.665561	1.177645
C	-2.636023	3.039823	-2.917795
C	-3.696516	4.170829	-4.784002
H	-4.537012	4.742074	-5.185412
C	-2.616191	3.847297	-5.603946
H	-2.611236	4.160348	-6.650608
C	-1.544667	3.121446	-5.084516
H	-0.694485	2.865968	-5.721227
C	-1.555686	2.714840	-3.751879
H	-0.713889	2.141959	-3.352736
C	-1.659629	3.792884	-0.306073
C	-0.919476	3.471861	0.838923
H	-0.850741	2.433167	1.169535
C	-0.280225	4.476942	1.566121
H	0.276872	4.218271	2.470107
C	-0.357660	5.802966	1.142201
H	0.145781	6.589538	1.709459
C	-1.080076	6.126552	-0.006757
H	-1.138635	7.164341	-0.343504
C	-1.732384	5.127877	-0.726873
H	-2.296543	5.391234	-1.625704
C	-4.296497	2.657979	-0.590921
H	-4.607809	3.713734	-0.563478
H	-4.926998	2.128271	-1.323337
C	-4.109957	3.055038	2.301831
C	-3.305789	2.629978	3.365104
H	-2.955298	1.594306	3.399861
C	-2.942342	3.523630	4.372198
H	-2.319676	3.183586	5.202223
C	-3.368737	4.848300	4.315891
H	-3.083940	5.549332	5.104037
C	-4.165286	5.281292	3.254128
H	-4.503819	6.319028	3.210852
C	-4.540243	4.388857	2.254604
H	-5.187158	4.735122	1.443918
C	-6.433689	1.822859	1.122485
C	-7.096792	2.186247	2.302336
H	-6.529145	2.537819	3.166874
C	-8.487417	2.115810	2.378737
H	-8.992023	2.409618	3.302094
C	-9.230644	1.685061	1.281268
H	-10.320890	1.644043	1.339225
C	-8.575861	1.307672	0.108690
H	-9.149147	0.962435	-0.754919
C	-7.186248	1.365416	0.030368
H	-6.700228	1.038100	-0.893203
C	-3.707915	3.772162	-3.447403
H	-4.565083	4.038784	-2.825250
Cu	1.672897	-0.292958	1.117845
Cu	3.404636	0.108742	-1.121029
P	3.037154	1.465253	1.869882
P	3.974652	2.334028	-0.940486
P	2.556869	-2.455400	1.182794
P	4.600602	-1.835864	-1.036537
C	-0.282574	-0.205422	1.429500
N	-1.450825	-0.124453	1.407396
C	4.705396	1.016176	2.486857
C	5.859272	1.779344	2.277139
H	5.834671	2.681567	1.664604
C	7.072626	1.392607	2.849260
H	7.964996	1.997937	2.673952
C	7.144710	0.249471	3.642470
H	8.093877	-0.044122	4.097113
C	5.995816	-0.512252	3.864628
H	6.037807	-1.402620	4.496668
C	4.786134	-0.132830	3.288597
H	3.889672	-0.729357	3.482232
C	2.335098	2.285105	3.358902

C	2.909377	3.444851	3.899551
H	3.781841	3.905354	3.428409
C	2.388791	4.011376	5.059684
H	2.842902	4.914683	5.473744
C	1.303335	3.414782	5.704728
H	0.907874	3.853052	6.624211
C	0.738150	2.254249	5.181619
H	-0.099886	1.772887	5.691580
C	1.246720	1.694401	4.009077
H	0.797540	0.788637	3.595663
C	3.285037	2.874354	0.697753
H	2.272727	3.274213	0.528358
H	3.882779	3.689472	1.133964
C	5.712463	2.892667	-0.944309
C	6.718760	1.966735	-1.232292
H	6.456022	0.924548	-1.426353
C	8.055069	2.368474	-1.263216
H	8.833012	1.636581	-1.491775
C	8.389364	3.695043	-1.001910
H	9.434955	4.011374	-1.026623
C	7.387285	4.627032	-0.717462
H	7.649026	5.669937	-0.523766
C	6.053362	4.231396	-0.695229
H	5.273601	4.973654	-0.500270
C	3.200782	3.458074	-2.166151
C	3.935204	3.791356	-3.314699
H	4.963547	3.440032	-3.430630
C	3.372121	4.589229	-4.307473
H	3.961407	4.847804	-5.190377
C	2.069766	5.066622	-4.167762
H	1.632843	5.704691	-4.939461
C	1.330166	4.729061	-3.036221
H	0.309227	5.096943	-2.915725
C	1.884597	3.920152	-2.044656
H	1.269642	3.665869	-1.177878
C	2.636033	-3.039560	2.917974
C	3.696614	-4.170474	4.784186
H	4.537102	-4.741748	5.185568
C	2.616393	-3.846777	5.604203
H	2.611513	-4.159727	6.650895
C	1.544879	-3.120885	5.084808
H	0.694780	-2.865275	5.721577
C	1.555805	-2.714406	3.752132
H	0.714017	-2.141490	3.353016
C	1.659342	-3.792794	0.306418
C	0.918995	-3.471813	-0.838461
H	0.850232	-2.433135	-1.169118
C	0.279555	-4.476913	-1.565469
H	-0.277707	-4.218275	-2.469363
C	0.357006	-5.802911	-1.141474
H	-0.146583	-6.589496	-1.708583
C	1.079609	-6.126453	0.007379
H	1.138168	-7.164219	0.344195
C	1.732094	-5.127760	0.727309
H	2.296380	-5.391080	1.626070
C	4.296327	-2.658002	0.590926
H	4.607555	-3.713781	0.563473
H	4.926912	-2.128330	1.323296
C	4.109595	-3.055136	-2.301797
C	3.305174	-2.630139	-3.364902
H	2.954597	-1.594494	-3.399588
C	2.941575	-3.523826	-4.371911
H	2.318696	-3.183834	-5.201799
C	3.368081	-4.848462	-4.315687
H	3.083166	-5.549521	-5.103768
C	4.164893	-5.281390	-3.254094
H	4.503516	-6.319100	-3.210888
C	4.539996	-4.388922	-2.254655
H	5.187119	-4.735126	-1.444107
C	6.433481	-1.823078	-1.122643
C	7.096439	-2.186332	-2.302618
H	6.528679	-2.537742	-3.167148
C	8.487059	-2.115974	-2.379158
H	8.991548	-2.409682	-3.302611
C	9.230431	-1.685425	-1.281707
H	10.320673	-1.644466	-1.339773
C	8.575795	-1.308158	-0.109010
H	9.149194	-0.963074	0.754586
C	7.186185	-1.365831	-0.030545
H	6.700289	-1.038606	0.893122
C	3.707918	-3.771931	3.447548
H	4.565008	-4.038678	2.825341

204

2A T_1

Cu	-2.974333	-0.121830	-1.067981
C	-1.200014	-0.534319	-1.724777
N	-0.031255	-0.598138	-1.798329
Cu	1.854022	-0.426016	-1.138411
Cu	3.199420	0.278711	1.038001
C	1.218643	0.241509	1.008531
N	0.074660	0.333822	1.246707
Cu	-1.891289	0.401407	1.220184
P	-4.721120	1.441827	-1.082211
P	-3.697447	-2.331131	-0.872587
P	3.128934	1.334183	-2.013156
P	2.798743	-2.555502	-0.993281
P	3.821383	2.503563	0.778114
P	4.604033	-1.546025	1.273091
P	-2.863380	2.460520	1.162673
P	-3.112533	-1.352231	2.042506
C	-4.585583	2.405695	0.481182
C	3.232920	2.850168	-0.950673
C	4.496811	-2.559760	-0.268460
C	-3.245737	-2.786589	0.863237
H	-5.189852	1.864146	1.228251
H	-5.033277	3.402926	0.348955
C	4.849175	0.911604	-2.485696
C	5.962044	1.728251	-2.255829
C	7.223745	1.346368	-2.716400
C	7.385895	0.152826	-3.416477
C	6.279754	-0.665406	-3.655428
C	5.021929	-0.290327	-3.190436
C	2.484411	2.036492	-3.586099
C	3.209849	3.008694	-4.290551
C	2.712355	3.530896	-5.480790
C	1.491884	3.078648	-5.986305
C	0.773422	2.105012	-5.296882
C	1.264180	1.583191	-4.098643
C	5.535670	3.131982	0.832226
C	6.541483	2.328370	1.375577
C	7.853280	2.799989	1.454794
C	8.166286	4.073466	0.986938
C	7.164743	4.885338	0.447624
C	5.854856	4.421486	0.376712
C	2.927462	3.719671	1.821657
C	3.606227	4.383983	2.853559
C	2.926337	5.262800	3.694615
C	1.563919	5.492392	3.514884
C	0.880125	4.824148	2.500263
C	1.551096	3.931249	1.666988
C	3.034121	-3.337818	-2.631745
C	2.067343	-3.064870	-3.611668
C	2.179064	-3.620023	-4.885228
C	3.261376	-4.441369	-5.199472
C	4.232718	-4.708517	-4.235201
C	4.121171	-4.161584	-2.957203
C	1.927175	-3.823411	0.008854
C	1.076191	-3.398929	1.037508
C	0.454679	-4.333818	1.866850
C	0.660848	-5.697072	1.660680
C	1.493496	-6.126864	0.627043
C	2.127288	-5.195953	-0.193582
C	4.134760	-2.668685	2.634156
C	3.258446	-2.199431	3.618271
C	2.921084	-3.009570	4.702071
C	3.443212	-4.296903	4.800559
C	4.311642	-4.774958	3.817640
C	4.662826	-3.962897	2.743661
C	6.420977	-1.371573	1.477397
C	7.016078	-1.530591	2.736375
C	8.390310	-1.353078	2.893747
C	9.185518	-1.018211	1.799089

C	8.597043	-0.841199	0.546943
C	7.223194	-1.005494	0.386668
C	-4.829374	-0.985756	2.576067
C	-5.934622	-1.810549	2.339529
C	-7.186134	-1.484612	2.864997
C	-7.347074	-0.333736	3.634077
C	-6.250370	0.495684	3.875987
C	-5.001817	0.172622	3.350090
C	-2.440755	-2.186916	3.540075
C	-3.034929	-3.319086	4.115328
C	-2.519138	-3.862458	5.288896
C	-1.417947	-3.269167	5.909870
C	-0.829575	-2.137975	5.348694
C	-1.332888	-1.601651	4.163115
C	-5.454442	-2.722374	-1.144169
C	-6.193887	-1.944019	-2.039764
C	-7.500137	-2.302511	-2.372180
C	-8.074134	-3.440533	-1.811440
C	-7.336866	-4.231279	-0.927325
C	-6.030598	-3.880989	-0.599684
C	-2.843510	-3.544264	-1.932629
C	-3.518694	-4.105037	-3.029185
C	-2.873722	-5.019692	-3.857250
C	-1.553411	-5.386175	-3.602650
C	-0.874389	-4.823728	-2.521680
C	-1.507127	-3.898586	-1.696729
C	-3.106809	3.319657	2.769009
C	-2.089626	3.152599	3.721223
C	-2.183322	3.757032	4.972675
C	-3.304921	4.520122	5.297803
C	-4.328347	4.680354	4.364788
C	-4.230945	4.087038	3.105762
C	-2.024658	3.705404	0.107922
C	-1.180040	3.255503	-0.915789
C	-0.579754	4.167599	-1.783818
C	-0.797024	5.535534	-1.619250
C	-1.617735	5.991401	-0.587603
C	-2.233278	5.081677	0.270620
C	-4.194975	2.539810	-2.441286
C	-3.609753	1.949960	-3.570524
C	-3.251260	2.731752	-4.667293
C	-3.464963	4.108167	-4.640322
C	-4.041332	4.702800	-3.516589
C	-4.409074	3.924754	-2.422897
C	-6.534751	1.281916	-1.263964
C	-7.177751	1.653762	-2.452936
C	-8.558274	1.503498	-2.577471
C	-9.307174	0.980329	-1.523780
C	-8.669042	0.597532	-0.343767
C	-7.290513	0.739638	-0.213417
H	5.865953	2.668874	-1.712359
H	8.082471	1.994794	-2.527569
H	8.372695	-0.138185	-3.784471
H	6.393995	-1.598353	-4.212594
H	4.160554	-0.933663	-3.393177
H	4.181450	3.349255	-3.921832
H	3.285422	4.285601	-6.024511
H	1.108988	3.481522	-6.927090
H	-0.175263	1.738850	-5.695944
H	0.699503	0.816851	-3.562789
H	2.191476	3.202977	-0.877720
H	3.809948	3.654522	-1.433317
H	6.302521	1.324954	1.733753
H	8.629566	2.161709	1.882272
H	9.192808	4.442826	1.048015
H	7.406190	5.889672	0.091642
H	5.075032	5.077598	-0.020825
H	4.677153	4.226707	2.998776
H	3.471530	5.778219	4.488827
H	1.034225	6.192778	4.164902
H	-0.187468	4.996144	2.350479
H	0.982659	3.404906	0.896581
H	5.084199	-5.348777	-4.477951
H	3.352889	-4.869500	-6.200473
H	1.420036	-3.400149	-5.639659
H	1.226286	-2.405812	-3.376071
H	0.903272	-2.331842	1.196227
H	-0.188167	-3.990579	2.681712
H	0.172040	-6.429132	2.307989
H	1.652949	-7.194749	0.459440
H	2.776789	-5.544345	-1.001141
H	4.884891	-3.575328	-0.095795
H	5.140562	-2.064425	-1.013268
H	2.836399	-1.193406	3.533997
H	2.245198	-2.633704	5.472347
H	3.177835	-4.932161	5.648935
H	4.726111	-5.782719	3.895189
H	5.368667	-4.338304	1.997836
H	6.408877	-1.808764	3.600811
H	8.841961	-1.489913	3.879098
H	10.264276	-0.895631	1.921602
H	9.209845	-0.569746	-0.315832
H	6.789028	-0.833986	-0.601913
H	4.895355	-4.383028	-2.218987
H	-5.840661	-2.715406	1.738711
H	-8.038481	-2.140608	2.672426
H	-8.325672	-0.084471	4.051110
H	-6.364251	1.396902	4.483082
H	-4.145145	0.823104	3.551927
H	-3.920772	-3.773003	3.662456
H	-2.989151	-4.743124	5.733040
H	-1.027725	-3.686724	6.841140
H	0.019295	-1.659060	5.842327
H	-0.871123	-0.716080	3.716086
H	-2.218677	-3.183763	0.813194
H	-3.879725	-3.607131	1.236268
H	-5.743796	-1.057327	-2.490761
H	-8.068509	-1.683134	-3.069137
H	-9.097543	-3.722018	-2.070274
H	-7.777718	-5.136197	-0.502675
H	-5.455606	-4.536453	0.059676
H	-4.558127	-3.841568	-3.233310
H	-3.413628	-5.455413	-4.700966
H	-1.051590	-6.111940	-4.246787
H	0.160184	-5.103227	-2.314814
H	-0.940027	-3.458825	-0.873524
H	-5.209780	5.275367	4.615861
H	-3.384797	4.986333	6.282604
H	-1.380191	3.623132	5.701171
H	-1.218718	2.536182	3.477163
H	-0.992973	2.183460	-1.030634
H	0.058717	3.805060	-2.593728
H	-0.321322	6.250386	-2.294994
H	-1.780211	7.063028	-0.448906
H	-2.872600	5.449215	1.077988
H	-3.438700	0.868362	-3.594547
H	-2.808139	2.261066	-5.547706
H	-3.185726	4.722734	-5.499357
H	-4.211932	5.781436	-3.494490
H	-4.869375	4.407882	-1.558663
H	-6.605602	2.078475	-3.281064
H	-9.052494	1.811363	-3.502010
H	-10.390162	0.874453	-1.621171
H	-9.247620	0.183601	0.485257
H	-6.812939	0.417923	0.715742
H	-5.045492	4.232288	2.392730

204

2B T_1

Cu	-2.909600	0.135974	1.043984
N	-1.181421	0.511691	1.897887
C	-0.009154	0.540943	1.867575
Cu	1.871666	0.439486	1.297766
Cu	3.203551	-0.272772	-1.062403
N	1.225324	-0.235375	-1.059463
C	0.063625	-0.315670	-1.218280
Cu	-1.876218	-0.427619	-1.262278
P	-4.718244	-1.372729	1.118630
P	-3.738184	2.315576	0.848357
P	3.222385	-1.323307	2.048010
P	2.850801	2.540713	1.002084
P	3.804906	-2.491825	-0.773671
P	4.573386	1.550640	-1.330636

P	-2.903880	-2.456485	-1.136733
P	-3.168506	1.291818	-2.064950
C	-4.615502	-2.365184	-0.426407
C	3.290372	-2.836493	0.978298
C	4.522026	2.556762	0.217908
C	-3.304277	2.740971	-0.897748
H	-5.231458	-1.836748	-1.173147
H	-5.068366	-3.355151	-0.259810
C	4.957249	-0.877866	2.437452
C	6.069003	-1.676507	2.146654
C	7.346459	-1.280898	2.548576
C	7.526274	-0.091407	3.250933
C	6.421954	0.709295	3.550371
C	5.148085	0.320715	3.143484
C	2.665870	-2.053395	3.643350
C	3.495188	-2.928802	4.360092
C	3.055449	-3.495035	5.553165
C	1.787397	-3.187071	6.048768
C	0.963483	-2.310510	5.347008
C	1.398937	-1.742340	4.148845
C	5.518896	-3.111070	-0.898253
C	6.494042	-2.308271	-1.495754
C	7.802727	-2.775142	-1.632905
C	8.143366	-4.043165	-1.169385
C	7.172210	-4.854288	-0.576102
C	5.865096	-4.395211	-0.447311
C	2.880251	-3.717942	-1.777668
C	3.522877	-4.379436	-2.834314
C	2.816271	-5.262302	-3.648576
C	1.462543	-5.497930	-3.417991
C	0.814155	-4.832165	-2.378856
C	1.511865	-3.935780	-1.571616
C	3.135658	3.354001	2.618787
C	2.189660	3.122722	3.629243
C	2.341448	3.705829	4.885835
C	3.444276	4.516134	5.153493
C	4.394840	4.743597	4.158947
C	4.243077	4.167673	2.897854
C	1.936439	3.785043	0.010064
C	1.083527	3.335205	-1.005864
C	0.431926	4.251955	-1.832309
C	0.611468	5.620523	-1.636289
C	1.448449	6.074396	-0.616401
C	2.112070	5.162329	0.201736
C	4.067018	2.676857	-2.675451
C	3.150248	2.214164	-3.625195
C	2.782276	3.024900	-4.698590
C	3.316032	4.305428	-4.820927
C	4.225906	4.776437	-3.872598
C	4.606440	3.964015	-2.808928
C	6.381044	1.368839	-1.601235
C	6.919107	1.493056	-2.889769
C	8.284688	1.310286	-3.104602
C	9.128974	1.004589	-2.038399
C	8.597473	0.861937	-0.756924
C	7.232124	1.031881	-0.538854
C	-4.889488	0.914901	-2.582162
C	-5.996037	1.737964	-2.345340
C	-7.250138	1.403381	-2.858963
C	-7.412682	0.245220	-3.616722
C	-6.314792	-0.582301	-3.859323
C	-5.063619	-0.250404	-3.345180
C	-2.520135	2.124212	-3.575407
C	-3.107738	3.270887	-4.128389
C	-2.611604	3.813192	-5.310925
C	-1.537262	3.204964	-5.963561
C	-0.956257	2.058849	-5.425404
C	-1.439937	1.523721	-4.231201
C	-5.489961	2.715357	1.137918
C	-6.201380	1.984015	2.094549
C	-7.496869	2.359550	2.448530
C	-8.090695	3.465888	1.846269
C	-7.382390	4.209435	0.900204
C	-6.085236	3.843795	0.552946
C	-2.867253	3.530178	1.891468
C	-3.536178	4.133832	2.968986
C	-2.872324	5.046699	3.783872
C	-1.538878	5.367177	3.535886
C	-0.866432	4.761709	2.474295
C	-1.518459	3.838611	1.662302
C	-3.196131	-3.362753	-2.711743
C	-2.188732	-3.252168	-3.681967
C	-2.313105	-3.895543	-4.911090
C	-3.457137	-4.641070	-5.196487
C	-4.471571	-4.744900	-4.245804
C	-4.342738	-4.113252	-3.008238
C	-2.077874	-3.697961	-0.064765
C	-1.219026	-3.247018	0.946201
C	-0.623776	-4.155505	1.821052
C	-0.863473	-5.522386	1.679297
C	-1.702537	-5.979825	0.663511
C	-2.310597	-5.072951	-0.203539
C	-4.156820	-2.422364	2.498720
C	-3.544501	-1.797914	3.594586
C	-3.168125	-2.545164	4.709169
C	-3.390792	-3.920578	4.733078
C	-3.994139	-4.549004	3.642609
C	-4.379141	-3.805934	2.530610
C	-6.527271	-1.215063	1.339151
C	-7.139387	-1.544894	2.557569
C	-8.516274	-1.392964	2.711606
C	-9.293362	-0.906591	1.660244
C	-8.686364	-0.563099	0.451915
C	-7.311712	-0.708339	0.290948
H	5.959949	-2.614741	1.601679
H	8.203373	-1.915989	2.312223
H	8.525609	0.210103	3.573925
H	6.550473	1.638846	4.110089
H	4.289733	0.951068	3.394700
H	4.500118	-3.159832	3.996472
H	3.710040	-4.173437	6.105334
H	1.448408	-3.625911	6.990229
H	-0.025084	-2.056678	5.736174
H	0.752840	-1.047174	3.608019
H	2.248723	-3.195208	0.949956
H	3.890496	-3.635426	1.441780
H	6.232784	-1.309686	-1.851601
H	8.554796	-2.137509	-2.102477
H	9.167476	-4.408862	-1.276011
H	7.434681	-5.854430	-0.223230
H	5.108056	-5.051103	-0.007643
H	4.586603	-4.216539	-3.020222
H	3.333885	-5.775975	-4.462154
H	0.911919	-6.201046	-4.047368
H	-0.246221	-5.008461	-2.188831
H	0.970606	-3.412517	-0.780144
H	5.261963	5.375892	4.364290
H	3.567493	4.967060	6.140966
H	1.597549	3.516728	5.663303
H	1.331098	2.474207	3.432171
H	0.938373	2.263005	-1.157557
H	-0.212018	3.890698	-2.638719
H	0.099428	6.338235	-2.281716
H	1.588046	7.146430	-0.457956
H	2.765658	5.528526	0.998093
H	4.897539	3.575631	0.037056
H	5.193207	2.059714	0.936572
H	2.717819	1.214696	-3.519692
H	2.071402	2.655584	-5.440116
H	3.026907	4.941233	-5.661116
H	4.649242	5.778846	-3.969446
H	5.343474	4.332902	-2.090407
H	6.273799	1.748788	-3.733369
H	8.690981	1.420343	-4.112788
H	10.201166	0.877943	-2.206030
H	9.248888	0.613595	0.084252
H	6.844295	0.887805	0.472897
H	5.002041	4.359241	2.135980
H	-5.901067	2.648513	-1.753632
H	-8.103319	2.058249	-2.666203
H	-8.393402	-0.011037	-4.024408
H	-6.429526	-1.489437	-4.457340

H	-4.206479	-0.900175	-3.546874
H	-3.973735	3.738184	-3.651500
H	-3.076614	4.705349	-5.737036
H	-1.162916	3.622378	-6.901406
H	-0.129574	1.567230	-5.944017
H	-0.987459	0.624108	-3.802738
H	-2.279537	3.145875	-0.859633
H	-3.945012	3.552732	-1.277878
H	-5.738571	1.120869	2.577177
H	-8.042012	1.778379	3.195092
H	-9.106469	3.759619	2.120996
H	-7.837691	5.090537	0.442096
H	-5.532160	4.466009	-0.155355
H	-4.584921	3.906524	3.167753
H	-3.407430	5.516977	4.611939
H	-1.021613	6.090855	4.170120
H	0.177978	5.005843	2.272762
H	-0.959052	3.365490	0.852760
H	-5.370542	-5.325810	-4.465931
H	-3.561557	-5.137615	-6.164023
H	-1.516711	-3.805684	-5.653660
H	-1.301969	-2.646925	-3.468485
H	-1.025568	-2.174925	1.048861
H	0.027262	-3.791756	2.620310
H	-0.391984	-6.234576	2.360794
H	-1.884369	-7.050515	0.542697
H	-2.961896	-5.442777	-1.000110
H	-3.364356	-0.718081	3.582980
H	-2.705361	-2.046931	5.564099
H	-3.097905	-4.507591	5.606729
H	-4.172351	-5.626445	3.660718
H	-4.860233	-4.314024	1.692400
H	-6.545497	-1.940414	3.384823
H	-8.986343	-1.670881	3.658009
H	-10.373707	-0.798930	1.781818
H	-9.286955	-0.178479	-0.375581
H	-6.859450	-0.418409	-0.660932
H	-5.150992	-4.215409	-2.280477

204

2A S_1

Cu	1.797385	0.388267	1.240849
Cu	3.247792	-0.016609	-0.924456
P	3.167269	-1.344696	2.021256
P	3.993052	-2.216396	-0.838677
P	2.607043	2.579700	1.312710
P	4.553479	1.896016	-0.957046
N	-0.105234	0.402075	1.863907
C	-1.267303	0.299899	1.735735
C	4.844462	-0.858098	2.580817
C	6.012970	-1.580049	2.312638
H	5.991427	-2.472172	1.685312
C	7.235915	-1.163519	2.842636
H	8.138777	-1.738663	2.624214
C	7.304269	-0.028581	3.647748
H	8.261239	0.289321	4.068465
C	6.142706	0.696350	3.922403
H	6.183981	1.582751	4.559959
C	4.922910	0.286160	3.390518
H	4.016787	0.854230	3.621606
C	2.526792	-2.208439	3.512575
C	3.288505	-3.192711	4.159949
H	4.286553	-3.450296	3.794566
C	2.791747	-3.833896	5.290880
H	3.392885	-4.597199	5.790518
C	1.535295	-3.490870	5.794235
H	1.152501	-3.988229	6.688667
C	0.779943	-2.506339	5.162044
H	-0.197972	-2.225757	5.560212
C	1.270344	-1.864771	4.023360
H	0.676539	-1.090534	3.531737
C	3.404653	-2.754949	0.841206
H	2.395947	-3.180278	0.716227
H	4.035834	-3.551410	1.265630
C	5.744374	-2.731361	-0.915208
C	6.705630	-1.815912	-1.351305
H	6.407992	-0.798020	-1.610749
C	8.045918	-2.194615	-1.447712
H	8.787178	-1.469213	-1.789987
C	8.431271	-3.487890	-1.104477
H	9.479975	-3.785343	-1.179675
C	7.474985	-4.410690	-0.671845
H	7.774371	-5.429115	-0.413169
C	6.137257	-4.038095	-0.583203
H	5.393779	-4.777130	-0.270422
C	3.191045	-3.388958	-2.000074
C	3.921298	-3.909731	-3.078254
H	4.979600	-3.666507	-3.195290
C	3.310335	-4.755703	-4.001861
H	3.895296	-5.159287	-4.831678
C	1.966892	-5.096423	-3.858820
H	1.492377	-5.773124	-4.573392
C	1.231268	-4.570311	-2.797914
H	0.177995	-4.830670	-2.676045
C	1.831963	-3.708357	-1.882228
H	1.222351	-3.291295	-1.077091
C	2.731306	3.231172	3.020001
C	3.776794	4.534507	4.779424
H	4.571346	5.208599	5.108332
C	2.799061	4.113694	5.680559
H	2.828859	4.455641	6.717806
C	1.790387	3.249059	5.256808
H	1.027924	2.908968	5.961528
C	1.758401	2.803475	3.936538
H	0.977174	2.108858	3.613602
C	1.694122	3.875411	0.383169
C	0.943753	3.496010	-0.738055
H	0.867459	2.441166	-1.012378
C	0.299081	4.461313	-1.513194
H	-0.263417	4.154625	-2.398916
C	0.383281	5.808605	-1.164614
H	-0.122406	6.564193	-1.770626
C	1.116756	6.191877	-0.041605
H	1.181717	7.246388	0.237239
C	1.772390	5.232022	0.727311
H	2.342983	5.545547	1.605746
C	4.324690	2.764472	0.658665
H	4.645170	3.815561	0.595374
H	4.979269	2.248384	1.379795
C	4.066992	3.088691	-2.250682
C	3.375025	2.607226	-3.367857
H	3.085929	1.552803	-3.414260
C	3.058091	3.463981	-4.421553
H	2.535917	3.077431	-5.299017
C	3.410078	4.810086	-4.356636
H	3.160348	5.481991	-5.181175
C	4.089585	5.299836	-3.240073
H	4.370330	6.354278	-3.188353
C	4.425065	4.442771	-2.196218
H	4.984380	4.836413	-1.343728
C	6.384987	1.858860	-1.096574
C	7.021633	2.213525	-2.293506
H	6.435601	2.560591	-3.147381
C	8.410447	2.142716	-2.400490
H	8.894038	2.430586	-3.336908
C	9.178241	1.721422	-1.316397
H	10.267036	1.681062	-1.397914
C	8.549569	1.352655	-0.127016
H	9.141382	1.013231	0.726268
C	7.162249	1.410071	-0.018592
H	6.697112	1.089353	0.917558
C	3.744628	4.097462	3.455482
H	4.523027	4.436686	2.768013
Cu	-1.812915	-0.414811	-1.312526
Cu	-3.011377	-0.094267	0.979942
P	-3.085741	1.307762	-2.097679
P	-3.861280	2.080625	0.833817
P	-2.678982	-2.522309	-1.401550
P	-4.658230	-1.747634	0.838603
N	0.138497	-0.235686	-1.252328
C	1.265440	-0.095133	-0.955593
C	-4.752766	0.896346	-2.744155
C	-5.901981	1.671921	-2.555191

H	-5.877750	2.564051	-1.929384
C	-7.106279	1.313542	-3.162793
H	-7.994084	1.930963	-3.006216
C	-7.175524	0.178705	-3.968916
H	-8.117434	-0.096470	-4.449312
C	-6.033934	-0.599584	-4.167221
H	-6.075045	-1.486443	-4.804056
C	-4.832426	-0.243594	-3.559121
H	-3.939061	-0.852431	-3.728171
C	-2.375735	2.277529	-3.492514
C	-3.016752	3.388986	-4.058050
H	-3.970499	3.744436	-3.658046
C	-2.458462	4.035812	-5.157467
H	-2.965368	4.898500	-5.596314
C	-1.264545	3.569465	-5.711789
H	-0.838679	4.068886	-6.585333
C	-0.628049	2.460222	-5.159334
H	0.296399	2.081792	-5.601072
C	-1.177531	1.817698	-4.049877
H	-0.682034	0.946189	-3.611311
C	-3.348939	2.659279	-0.840609
H	-2.343721	3.092134	-0.707245
H	-3.994562	3.480601	-1.192406
C	-5.646655	2.330492	1.060876
C	-6.330776	1.496505	1.952141
H	-5.816902	0.645701	2.404824
C	-7.661376	1.756196	2.276635
H	-8.185693	1.097407	2.971664
C	-8.316754	2.846328	1.708978
H	-9.360056	3.049739	1.961338
C	-7.637443	3.688435	0.826492
H	-8.143671	4.555890	0.396727
C	-6.305755	3.439196	0.507884
H	-5.778910	4.136820	-0.148029
C	-3.120873	3.243413	2.020378
C	-3.889894	3.741396	3.086231
H	-4.937177	3.455114	3.194603
C	-3.327046	4.624153	4.003092
H	-3.937823	5.013044	4.820840
C	-1.996648	5.017759	3.870261
H	-1.557644	5.716032	4.586630
C	-1.225248	4.517420	2.820325
H	-0.182408	4.818880	2.710518
C	-1.775083	3.625386	1.906012
H	-1.139083	3.230464	1.110642
C	-2.830470	-3.289306	-3.065501
C	-3.942140	-4.595615	-4.782765
H	-4.789577	-5.208161	-5.100061
C	-2.896023	-4.338465	-5.667539
H	-2.924239	-4.745641	-6.680919
C	-1.817924	-3.553731	-5.257286
H	-0.997482	-3.343635	-5.947485
C	-1.790180	-3.024192	-3.969286
H	-0.954601	-2.389204	-3.658389
C	-1.801866	-3.787486	-0.405155
C	-0.986406	-3.360462	0.651041
H	-0.844685	-2.289912	0.826473
C	-0.349068	-4.294568	1.468545
H	0.268988	-3.952172	2.302573
C	-0.503629	-5.658702	1.223389
H	0.000262	-6.389724	1.860210
C	-1.299082	-6.089898	0.161476
H	-1.414043	-7.157851	-0.039011
C	-1.949602	-5.160301	-0.647602
H	-2.567258	-5.508535	-1.479992
C	-4.419369	-2.612414	-0.772163
H	-4.799210	-3.643757	-0.710984
H	-5.036526	-2.069601	-1.506993
C	-4.199644	-2.932683	2.149908
C	-3.601393	-2.432870	3.314191
H	-3.367051	-1.365792	3.390270
C	-3.306031	-3.286803	4.375694
H	-2.847783	-2.886687	5.282924
C	-3.599248	-4.645176	4.279196
H	-3.370610	-5.315522	5.111044
C	-4.190557	-5.150802	3.120055
H	-4.424214	-6.215149	3.043967
C	-4.491570	-4.301068	2.059652
H	-4.967421	-4.713767	1.167119
C	-6.481681	-1.625531	0.926458
C	-7.180576	-2.070442	2.057566
H	-6.644220	-2.524051	2.894253
C	-8.568938	-1.956820	2.112216
H	-9.105251	-2.322439	2.991181
C	-9.271415	-1.396526	1.045766
H	-10.360437	-1.319688	1.086954
C	-8.578587	-0.938990	-0.075240
H	-9.120469	-0.495198	-0.913509
C	-7.191909	-1.045021	-0.135557
H	-6.673381	-0.665634	-1.020101
C	-3.910412	-4.077866	-3.487516
H	-4.741274	-4.298405	-2.814082

204

2B S_1

Cu	-1.772642	0.382525	-1.404134
Cu	-2.970976	0.026969	0.906806
P	-3.078459	-1.330782	-2.166608
P	-3.896398	-2.111948	0.761221
P	-2.722813	2.449360	-1.477542
P	-4.677366	1.640187	0.777768
C	0.143914	0.194820	-1.206785
N	1.284773	0.068389	-0.944472
C	-4.737228	-0.924067	-2.841586
C	-5.898330	-1.676609	-2.632941
H	-5.890096	-2.548812	-1.979595
C	-7.095383	-1.320590	-3.256414
H	-7.992274	-1.920456	-3.083945
C	-7.145644	-0.211408	-4.098596
H	-8.081775	0.061637	-4.591317
C	-5.992215	0.543784	-4.316501
H	-6.017930	1.411129	-4.980368
C	-4.798346	0.190731	-3.692071
H	-3.897051	0.783514	-3.874145
C	-2.354756	-2.313940	-3.547385
C	-2.969099	-3.456887	-4.078835
H	-3.905615	-3.832749	-3.657426
C	-2.407261	-4.110904	-5.172256
H	-2.893821	-4.998374	-5.583852
C	-1.237308	-3.620599	-5.756253
H	-0.810176	-4.125631	-6.626000
C	-0.627576	-2.479883	-5.238629
H	0.276039	-2.080332	-5.705499
C	-1.180125	-1.831329	-4.134115
H	-0.710108	-0.932171	-3.723458
C	-3.372972	-2.683260	-0.911377
H	-2.374306	-3.126991	-0.766057
H	-4.021117	-3.496757	-1.275806
C	-5.678397	-2.379792	0.989100
C	-6.359091	-1.575733	1.910495
H	-5.846168	-0.735438	2.383344
C	-7.685164	-1.851004	2.239915
H	-8.205710	-1.215484	2.959084
C	-8.341437	-2.926634	1.645901
H	-9.381751	-3.141637	1.900948
C	-7.666173	-3.739398	0.733574
H	-8.172313	-4.596163	0.282823
C	-6.337978	-3.475351	0.411649
H	-5.814499	-4.152578	-0.267667
C	-3.144845	-3.257811	1.957718
C	-3.916622	-3.797328	3.001060
H	-4.978230	-3.560232	3.085436
C	-3.336775	-4.660225	3.926218
H	-3.949505	-5.083096	4.725439
C	-1.986447	-4.990603	3.825450
H	-1.533889	-5.672802	4.548857
C	-1.212869	-4.448183	2.798483
H	-0.154915	-4.700857	2.712863
C	-1.780595	-3.576625	1.875322
H	-1.146217	-3.148109	1.096711
C	-2.912438	3.232704	-3.133743
C	-4.075717	4.518745	-4.832336
H	-4.946160	5.103402	-5.139923

C	-3.023816	4.310703	-5.723074
H	-3.069995	4.728664	-6.731405
C	-1.916489	3.561326	-5.324671
H	-1.090568	3.389795	-6.019063
C	-1.866056	3.017590	-4.043254
H	-1.008269	2.408094	-3.741512
C	-1.897931	3.750251	-0.478952
C	-1.098554	3.361104	0.603672
H	-0.941593	2.296596	0.802244
C	-0.510378	4.322993	1.425144
H	0.096776	4.009726	2.278323
C	-0.699426	5.679390	1.160429
H	-0.233616	6.432312	1.800770
C	-1.479975	6.073740	0.073867
H	-1.621601	7.135299	-0.143210
C	-2.079917	5.115167	-0.741333
H	-2.685045	5.435331	-1.593866
C	-4.464988	2.489736	-0.839123
H	-4.880150	3.508154	-0.784954
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C	-4.169766	2.797782	2.092470
C	-3.651437	2.257536	3.277659
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C	-3.501862	4.468397	4.233891
H	-3.247114	5.123355	5.070435
C	-4.007235	5.013331	3.052352
H	-4.146714	6.092923	2.962704
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H	-4.749660	4.629347	1.075399
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C	-8.555124	1.882855	2.140218
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H	-10.374906	1.264025	1.153968
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H	-9.188104	0.434193	-0.876229
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H	-6.742126	0.580311	-1.036136
C	-4.021050	3.986720	-3.543454
H	-4.857986	4.169030	-2.866154
Cu	1.772032	-0.347670	1.435482
Cu	3.264894	0.014783	-0.880735
P	3.171828	1.417957	2.082662
P	3.938080	2.232023	-0.814624
P	2.681667	-2.505058	1.438803
P	4.576360	-1.870536	-0.881027
C	-0.129063	-0.325232	1.945567
N	-1.298984	-0.257833	1.893302
C	4.862480	0.942187	2.609506
C	6.024561	1.650312	2.282695
H	5.986728	2.520566	1.625928
C	7.261430	1.249981	2.792564
H	8.158480	1.814868	2.528267
C	7.350472	0.144909	3.636080
H	8.318155	-0.159805	4.041811
C	6.195742	-0.566719	3.968793
H	6.253168	-1.429654	4.636588
C	4.961968	-0.172522	3.457231
H	4.062544	-0.730464	3.734896
C	2.581235	2.340417	3.562119
C	3.422925	3.245714	4.225287
H	4.453797	3.388534	3.890097
C	2.961700	3.954452	5.330809
H	3.626255	4.654768	5.842200
C	1.658281	3.761647	5.791783
H	1.301409	4.312813	6.665109
C	0.820931	2.856807	5.143774
H	-0.196508	2.693962	5.506540
C	1.278581	2.145092	4.033731
H	0.621852	1.427993	3.535922
C	3.378441	2.800263	0.864057
H	2.366301	3.221050	0.752829
H	4.014733	3.605208	1.264654
C	5.680270	2.768427	-0.940975
C	6.644468	1.857121	-1.379050
H	6.355042	0.829932	-1.609079
C	7.976403	2.252612	-1.515384
H	8.719906	1.530167	-1.858926
C	8.350190	3.558757	-1.210154
H	9.392343	3.869515	-1.316285
C	7.390431	4.477479	-0.776551
H	7.680572	5.505783	-0.548217
C	6.060693	4.088137	-0.648607
H	5.313458	4.823376	-0.335841
C	3.105641	3.368973	-1.989753
C	3.803661	3.821088	-3.119558
H	4.851801	3.549704	-3.264119
C	3.175202	4.635073	-4.059506
H	3.736035	4.985857	-4.929049
C	1.845149	5.011712	-3.882983
H	1.356879	5.663545	-4.611274
C	1.141274	4.554157	-2.770363
H	0.099162	4.843104	-2.620381
C	1.759838	3.724794	-1.836227
H	1.173498	3.365410	-0.987779
C	2.829663	-3.150374	3.148059
C	3.935714	-4.406408	4.905981
H	4.764738	-5.037985	5.234165
C	2.930832	-4.049119	5.804091
H	2.972990	-4.397485	6.838733
C	1.877792	-3.239403	5.379707
H	1.092810	-2.947923	6.081453
C	1.829153	-2.786583	4.062598
H	1.010782	-2.135418	3.742347
C	1.778267	-3.818191	0.527035
C	1.020022	-3.454253	-0.593298
H	0.940451	-2.402199	-0.877064
C	0.380257	-4.431990	-1.356654
H	-0.189688	-4.138414	-2.242420
C	0.479155	-5.775341	-0.997349
H	-0.022729	-6.540889	-1.593956
C	1.223826	-6.142857	0.123873
H	1.301337	-7.194606	0.409710
C	1.873875	-5.170866	0.881858
H	2.452968	-5.470802	1.759540
C	4.394594	-2.678553	0.770785
H	4.732840	-3.725591	0.740386
H	5.045000	-2.121501	1.464105
C	4.105349	-3.133737	-2.112588
C	3.286319	-2.755461	-3.181836
H	2.896087	-1.734502	-3.231586
C	2.962289	-3.675968	-4.178207
H	2.328172	-3.372591	-5.013452
C	3.441816	-4.981497	-4.104675
H	3.187369	-5.703071	-4.884618
C	4.252548	-5.368263	-3.035985
H	4.633176	-6.390645	-2.978792
C	4.589593	-4.447852	-2.048474
H	5.251216	-4.755927	-1.234411
C	6.402984	-1.789010	-1.061462
C	7.005624	-2.089684	-2.291014
H	6.397460	-2.421112	-3.135775
C	8.387898	-1.986739	-2.442796
H	8.844316	-2.233812	-3.404186
C	9.184529	-1.585818	-1.371547
H	10.268950	-1.521020	-1.488093
C	8.589903	-1.269246	-0.150459
H	9.204136	-0.946167	0.693281
C	7.208270	-1.359518	0.003273
H	6.772084	-1.079945	0.965829
C	3.886831	-3.961672	3.585040
H	4.686871	-4.253501	2.901380

Table S6. Relative energies of the isomer **2A**, **2B** and **2C** (in eV) and calculated emission energies for **2A** and **2B**.

State	**2A**-S_0	**2B**-S_0	**2C**-S_0	**2A**-T_1	**2B**-T_1	**2A**-S_1	**2B**-S_1
Relative Energy	0.000	0.087	0.040	2.910	3.023	3.118	3.217
$E_{emission}$ (eV)				2.388	2.250	2.704	2.555
$E_{emission}$ (nm)				519	551	458	485

Table S7. Main characteristics of the first Franck Condon singlet and triplet excited states of S_0 together with the iso-contour plots of the frontier molecular orbitals (± 0.035 [e/bohr^3]$^{1/2}$)*

Franck-Condon (FC) excited state	λ_{abs} in eV	λ_{abs} in nm	Oscillator strength	Nature of the excitation
T_1-FC	3.424	362	0.00	44 % HOMO to LUMO 15% HOMO-2 to LUMO
S_1-FC	4.097	303	0.00	70 % HOMO-1 to LUMO 11 % HOMO to LUMO+1
S_2-FC	4.216	294	0.00	47% HOMO-2 to LUMO 24% HOMO to LUMO+1 5% HOMO-3 to LUMO

* The experimental solid-state absorption spectrum in Fig S3 shows a low intensity band around 400-450 nm. This is not obtained from the isolated complex **2** as far as the calculations given here are valid. The presence of solvent, counterions as well as phonon arising from the crystal can explain this slight discrepancy.

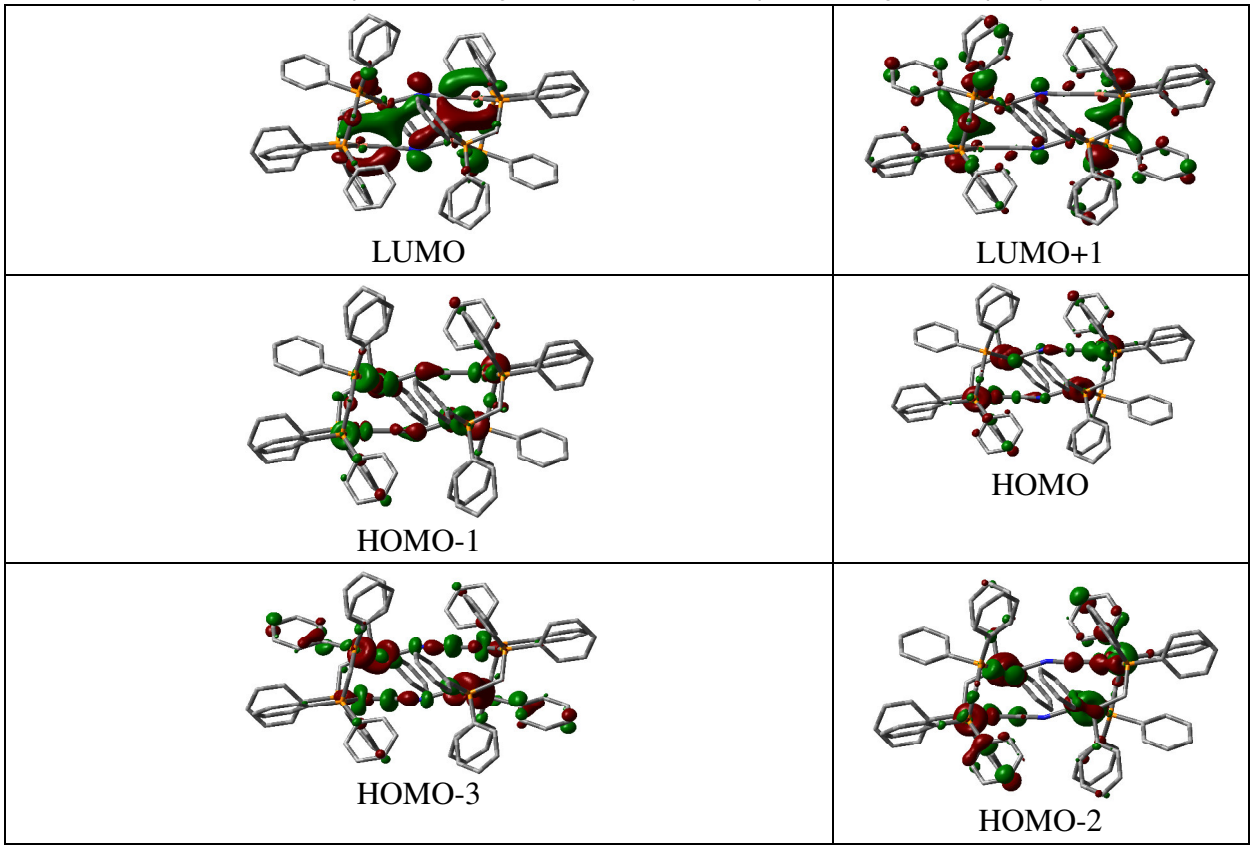
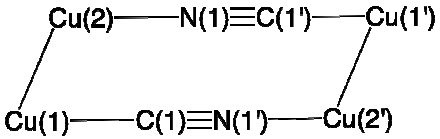
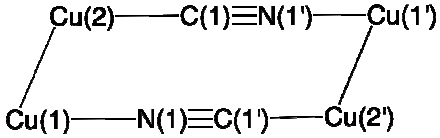


Table S8. Selected metric data for the X-ray crystal structure of **2** a) isomer **2A** and b) isomer **2B**, measured at 100 K and the computed geometry of the S_0, T_1 and S_1 states of **2**. Distances in [Å] and angles in [°]. *The experimental X-ray crystal structure and calculated ground state of **2** are centrosymmetric; calculated excited state geometries were not constrained to be centrosymmetric.*



2A



2B

a)

	Cu(1)-Cu(2) Cu(1')-Cu(2')	Cu(1)-Cu(2') Cu(1')-Cu(2)	Cu(1)-Cu(1') Cu(2)-Cu(2')	Cu(1)-C(1) Cu(1')-C(1')	Cu(2)-C(1) Cu(2')-C(1')	Cu(2)-N(1) Cu(2')-N(1')	C(1)-N(1') C(1')-N(1)	C(1)-Cu(1)-Cu(2) N(1)-Cu(2)-Cu(1)	C(1')-Cu(1')-Cu(2') N(1')-Cu(2')-Cu(1')
X-ray	2.8669(6)	5.010	6.957	1.962(13)	2.676(6)	1.949(11)	1.141(17)	64.1(4)	-
100K	-	-	4.272	-	-	-	-	131.0(3)	-
2A-S_0	2.917	5.017	7.060	1.929	2.677	1.967	1.159	63.26	-
	-	-	-	-	-	-	-	131.81	-
2A-T_1	2.585	4.838	6.535	1.936	3.166	1.967	1.173	87.68	58.40
	2.654	5.095	4.503	1.981	2.336	2.005	1.172	115.07	140.30
2A-S_1	2.607	4.840	6.543	1.941	3.178	1.961	1.174	87.38	57.96
	2.607	5.091	4.494	1.984	2.311	2.022	1.174	114.80	141.18

b)

	Cu(1)-Cu(2) Cu(1')-Cu(2')	Cu(1)-Cu(2') Cu(1')-Cu(2)	Cu(1)-Cu(1') Cu(2)-Cu(2')	Cu(1)-N(1) Cu(1')-N(1')	Cu(2)-N(1) Cu(2')-N(1')	Cu(2)-C(1) Cu(2')-C(1')	C(1)-N(1') C(1')-N(1)	N(1)-Cu(1)-Cu(2) C(1)-Cu(2)-Cu(1)	N(1')-Cu(1')-Cu(2') C(1')-Cu(2')-Cu(1')
X-ray	2.8669(6)	5.010	6.957	1.92(2)	2.786	2.00(3)	1.14(4)	67.9(7)	-
100K	-	-	4.272	-	-	-	-	129.9(9)	-
2A-S_0	2.859	5.081	7.172	1.975	2.569	1.982	1.171	61.07	-
	-	-	-	-	-	-	-	135.61	-
2A-T_1	2.589	4.798	6.479	1.964	3.369	1.968	1.173	94.46	61.23
	2.779	5.086	4.621	1.979	2.536	1.944	1.175	111.45	135.34
2A-S_1	2.627	4.787	6.487	1.962	3.392	1.968	1.173	94.20	59.58
	2.779	5.078	4.600	1.982	2.465	1.936	1.177	110.41	137.16

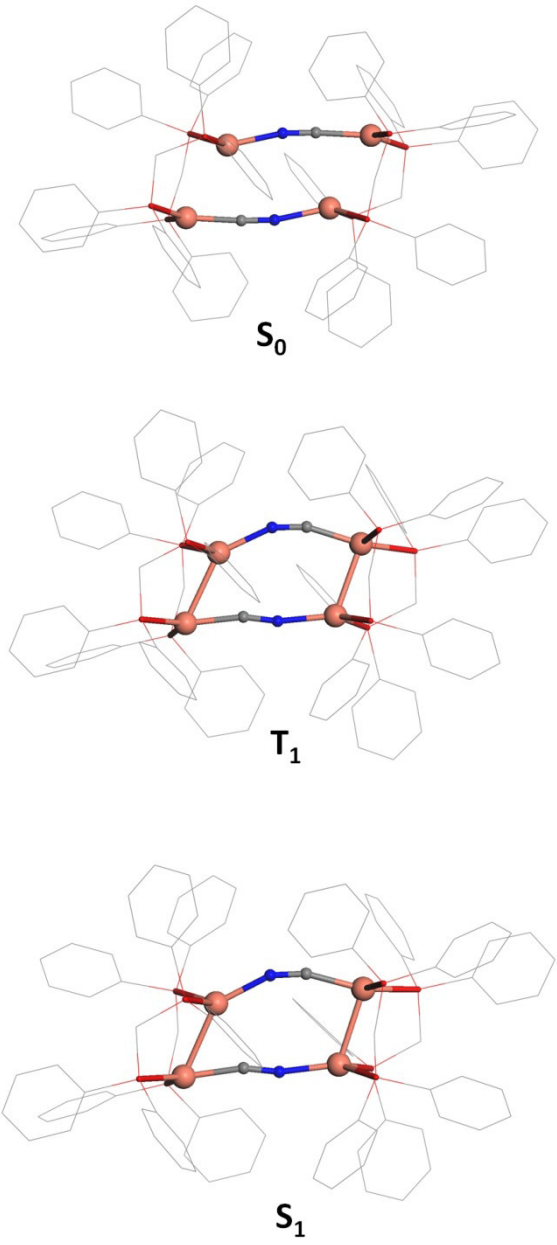


Fig. S7. Views of the computed geometries of the S_0, T_1 and S_1 states of **2** (isomer **2A**).

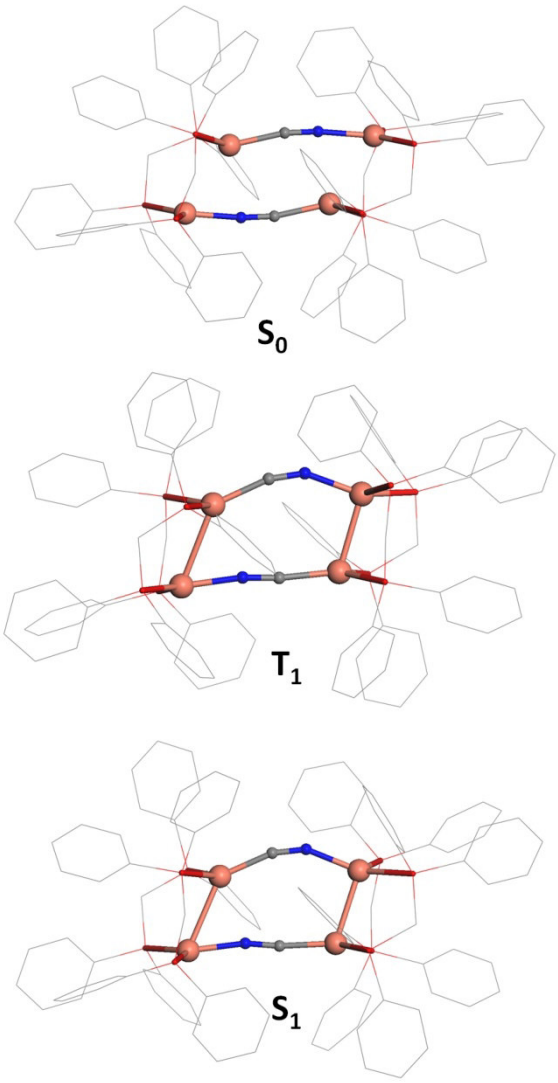


Fig. S8. Views of the computed geometries of the S_0, T_1 and S_1 states of **2** (isomer **2B**)

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