Electronic Supplementary Information for

Highly efficient cold-white light emission in a $[Au_2CuCl_2(P\cap N)_2]PF_6$ type salt

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General remarks.

All solvents and other reagents were commercially obtained and used as received. [AuCl(tht)] was prepared according to published procedures.[1] NMR spectra were recorded on an Avance DRX 300 (300 MHz) spectrometer, and ^1H shifts are reported in ppm relative to $SiMe_4$, with the residual signal of the deuterated solvent as internal reference. Single-crystal structure analysis was carried out on a Rigaku XtaLAB mini II and Bruker Smart X2S diffractometer with graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å). The structures were solved by direct methods (SHELXS-97) and refined by full-matrix least-squares on F^2 (SHELXL-97).[2,3] The H atoms were calculated geometrically, and a riding model was applied in the refinement process. CCDC 1524169 – 1524169 contain the supplementary crystallographic data for **1** and **2**. These data can be obtained free of charge from *The Cambridge Crystallographic Data Centre* at https://summary.ccdc.cam.ac.uk/structure-summary-form. Mass spectra were collected on a Finnigan LCQ DecaXPPlus ion trap mass spectrometer with ESI ion source.

Synthesis.

$[AuCl(P\cap N)]$ (**1**): In 25 ml dichloromethane [AuCl(tht)] (0.30 g, 0.94 mmol) and 2-diphenylphoshano-6-methyl-pyridine (0.26 g, 0.94 mmol) was stirred for one hour. The solvent was evaporated to ~2 ml in a stream of nitrogen. The addition of diethyl ether gave complex **1** as white solid. Crystals suitable for single crystal X-ray diffraction were obtained by gas-phase diffusion of diethyl ether into a solution of **1** in dcm. Elemental analysis: calc. for $C_{18}H_{16}NPAuCl$ (509.70 g·mol^{-1}): calcd. C, 42.41, H, 3.16, N, 2.75; found: C, 42.45, H, 3.21, N, 2.85. ^1H NMR (300 MHz, $CDCl_3$): δ = 2.52 (3H, s), 7.22 (1H, d), 7.45 (4H, m), 7.48 (1H, m), 7.52 (1H, m), 7.60 (6H, m) ppm; $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ = 160.5 (d, J_{CP} = 16 Hz), 152.6 (d, J_{CP} = 85 Hz), 136.7 (d, J_{CP} = 11 Hz), 134.6 (d, J_{CP} = 13 Hz), 131.9 (d, J_{CP} = 3 Hz), 129.0 (d, J_{CP} = 34 Hz), 129.0 (d, J_{CP} = 12 Hz), 128.4 (d, J_{CP} = 3 Hz), 125.3 (d, J_{CP} = 2 Hz), 24.6 (s); $^{31}P\{^1H\}$ NMR (121 MHz, $CDCl_3$,): δ = 31.4 (s) ppm. MS (ESI, $CHCl_3$/MeOH) m/z = 474.04 $[(P\cap N)Au]^+$, 532.13 $[(P\cap N)AuCl\cdot Na]^+$, 751.33 $[(P\cap N)_2Au]^+$, 983.07 $[(P\cap N)Au_2Cl]^+$.

$[Au_2CuCl_2(P\cap N)_2]PF_6$ (**2**): 0.20 g (0.39 mmol) of **1** was dissolved in 40 ml dcm. 73 mg (0.20 mmol) of $[Cu(NCMe)_4]PF_6$ was added to the solution and the mixture was stirred for 3 hours under nitrogen. After filtration, the solution was concentrated to ~4 ml. Complex **2** was obtained as white precipitate after addition of diethyl ether. Crystals suitable for single crystal X-ray diffraction were obtained by gas-phase diffusion of diethyl ether into a solution of **2** in dcm. Elemental analysis calc. for $C_{36}H_{32}Cl_2N_2P_3F_6CuAu_2$ (1227.92 g·mol^{-1}): calc. C, 35.21, H, 2.63, N, 2.28; found: C, 35.50, H, 2.34, N, 2.10. ^1H NMR (300 MHz, $CDCl_3$): δ = 2.22 (6H, s), 7.38 (4H, m), 7.59 (16H, m), 7.80 (4H, m), 7.87 (2H, m). $^{31}P\{^1H\}$ NMR (121 MHz, $CDCl_3$): δ = 31.4 (s) ppm. MS (ESI, $CHCl_3$/MeOH): m/z = 506.07 $[(P\cap N)Au\text{-}Cl]^+$, 751.33 $[(P\cap N)_2Au]^+$, 983.07 $[(P\cap N)Au_2Cl]^+$.

Compound **2** is not very well soluble in non-coordinating solvents. Thus, no analyzable ^{13}C NMR spectrum could be obtained in solvents like $CDCl_3$. In coordinating solvents like acetonitrile it is questionable if the cluster is retained in solution.

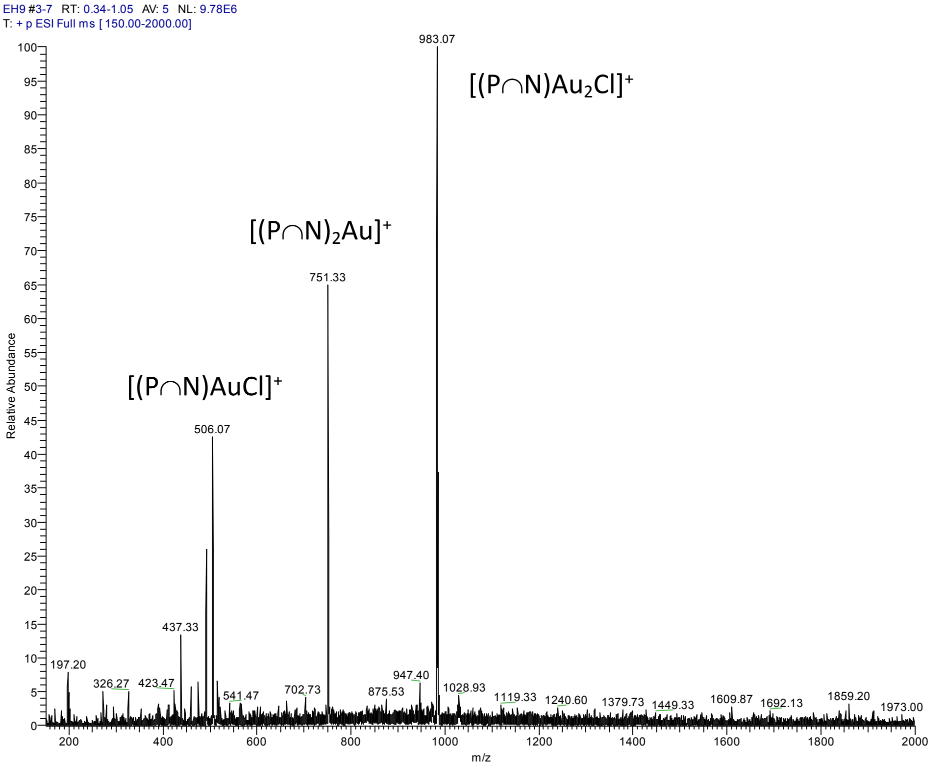


Figure S1. ESI mass spectrum of compound **2** in $CHCl_3$/MeOH.

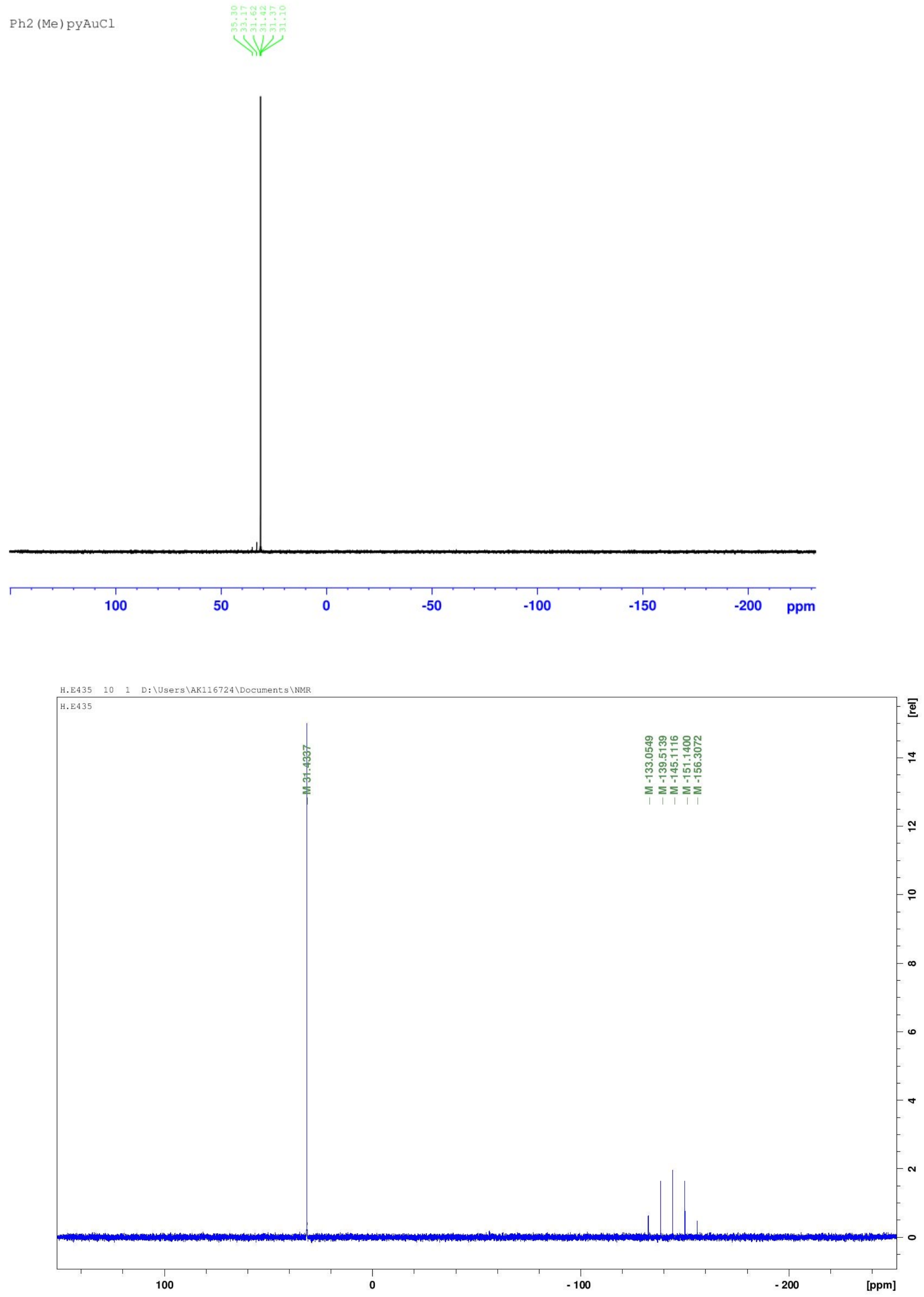
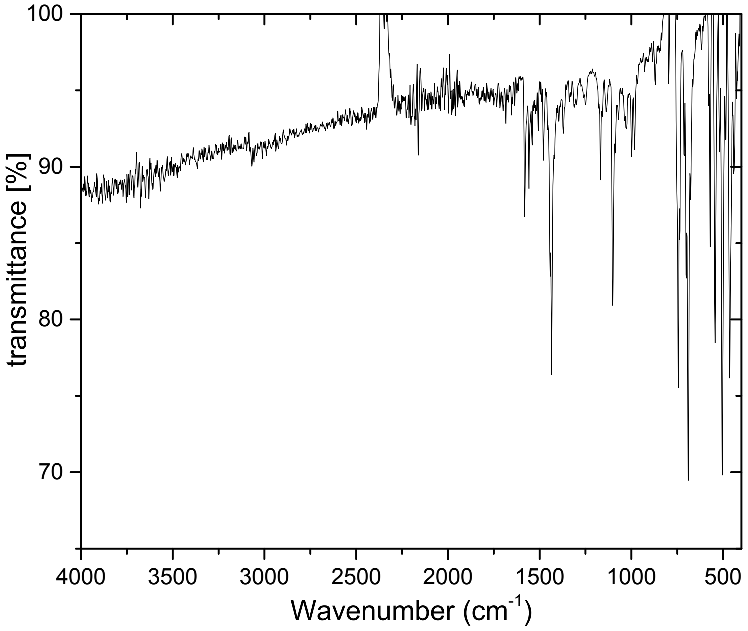


Figure S2. $^{31}P\{^1H\}$ NMR spectrum of compounds **1** (top) and **2** (bottom) in $CDCl_3$.



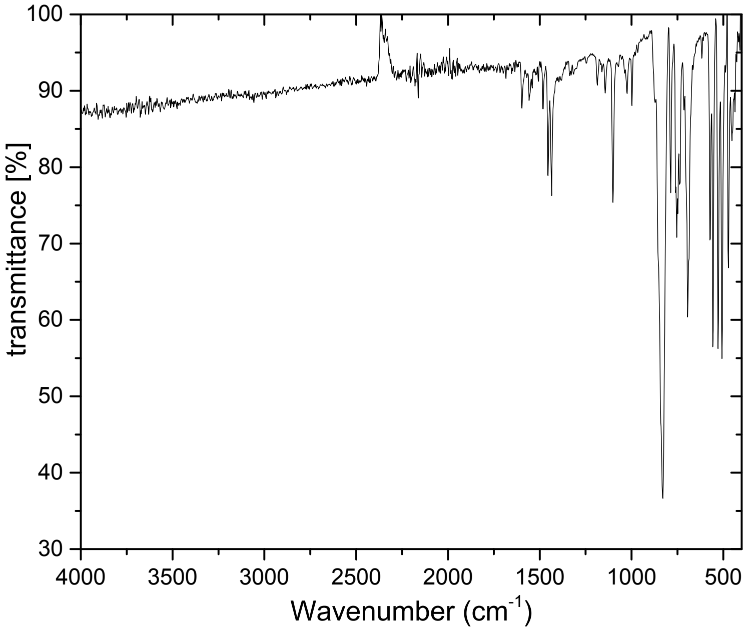


Figure S3. IR spectrum (ATR) of compound **1** (top) and **2** (bottom).

Table S1. Crystal data and data collection and structure refinement details for **1** and **2**.

	1	**2**
Empirical formula	$C_{18}H_{16}ClNPAu$	$C_{36}H_{32}Cl_2N_2P_3F_6CuAu_2$
M_r, g mol^{-1}	509.70	1227.92
Size, mm^3	0.60 × 0.15 × 0.15	0.06 × 0.04 × 0.02
Crystal system	orthorhombic	triclinic
Space group	$P2_12_12_1$	P-1
a, Å	11.438(3)	10.4810(2)
b, Å	12.047(3)	14.0777(3)
c, Å	12.858(3)	14.7299(3)
α, deg	90	86.0014(17)°
β, deg	90	72.374(2)°
γ, deg	90	68.873(2)°
V, Å^3	1771.7(7)	1930.22(7)
$\rho_{\text{calcd.}}$, Mg.m^{-3}	1.911	2.113
Z	4	2
μ(MoK_α), mm^{-1}	8.54	8.45
T, K	300	150
Θ range, deg	2.3-23.2	2.1-29.4
Measured reflections	9414	17722
Independent reflections	2519	8908
Reflections with $I > 2\sigma(I)$)	2153	7478
Absorption correction	multi-scan	multi-scan
$T_{\text{min}}/T_{\text{max}}$	0.11/0.36	0.713/1.00
Restraints/refined param.	0	0
$R1$ ($I \geq 2\sigma(I)$)	0.037	0.027
w$R2$	0.080	0.059
$\Delta\rho_{\text{fin}}$ (max/min), e Å^{-3}	0.75/-0.59	-0.98/1.57
CCDC no.	1524169	1524170

Table S2. Bond lengths [Å] and angles [deg] for **1** and **2**.

	1	**2**
Au–P	2.237(3)	2.232(1)/2.231(1)
Au–Cl	2.282(3)	2.288(1)/2.284(1)
Au1–Au2		3.3079(2)
Au-Cu		2.8087(5)/2.8374(5)
Cu-N		1.933(3)
		1.933(3)
P–Au–Cl	179.4(1)	177.15(4)/177.47(4)
Au–Cu–Au		71.73(1)
Cu–Au–Au		54.54(1)/53.73(1)
N–Cu–N		175.1(1)

Photophysical studies.

All measurements were performed under argon and rigorous exclusion of air to prevent luminescence quenching by molecular oxygen. For solid state measurements, single-crystalline bulk material has been used, which, prior to the photophysical studies, was analyzed by multiple unit cell determinations to ensure the absence of polymorphs. UV-visible absorption spectra were obtained on an Agilent 1100 Series Diode Array spectrophotometer using standard 1 cm path length quartz cells. Excitation and emission spectra were recorded on an Edinburgh Instrument FLSP920 spectrometer, equipped with a 450 W Xenon arc lamp, double monochromators for the excitation and emission pathways, and a red-sensitive photomultiplier (PMT-R928) as detector. The excitation and emission spectra were corrected using the standard corrections supplied by the manufacturer for the spectral power of the excitation source and the sensitivity of the detector. The quantum yields were measured by use of an integrating sphere with an Edinburgh Instrument FLSP920 spectrometer. The luminescence lifetimes were measured using a µF900 pulsed 60 W Xenon microsecond flashlamp, with a repetition rate of 100 Hz, and a multichannel scaling module, or with a TCSPC module using a nanoLED pulsed laser diode. The emission was collected at right angles to the excitation source with the emission wavelength selected using a double grated monochromator and detected by a R928-P PMT. Low temperature measurements were performed in an Oxford Optistat cryostat.

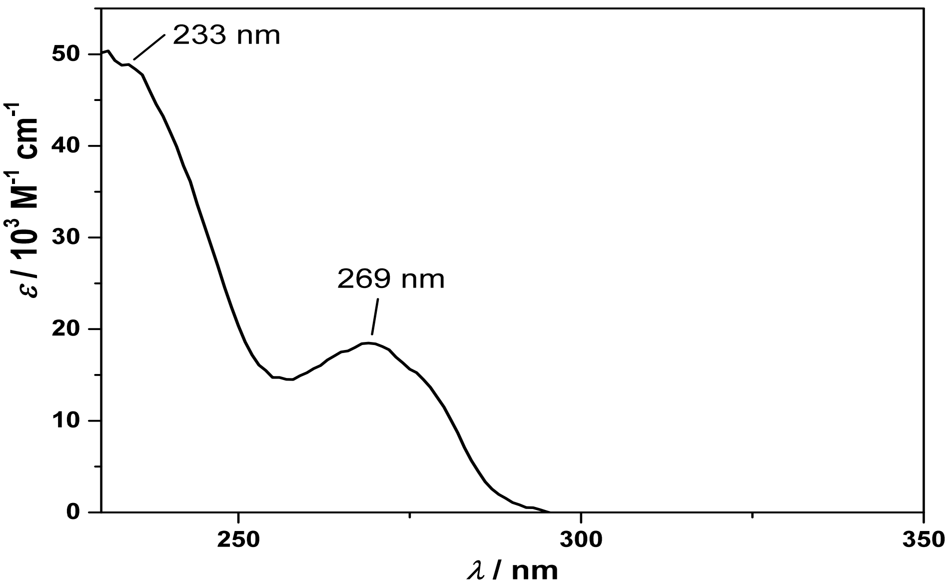


Figure S4. Absorption spectrum of **1** in dichloromethane at room temperature.

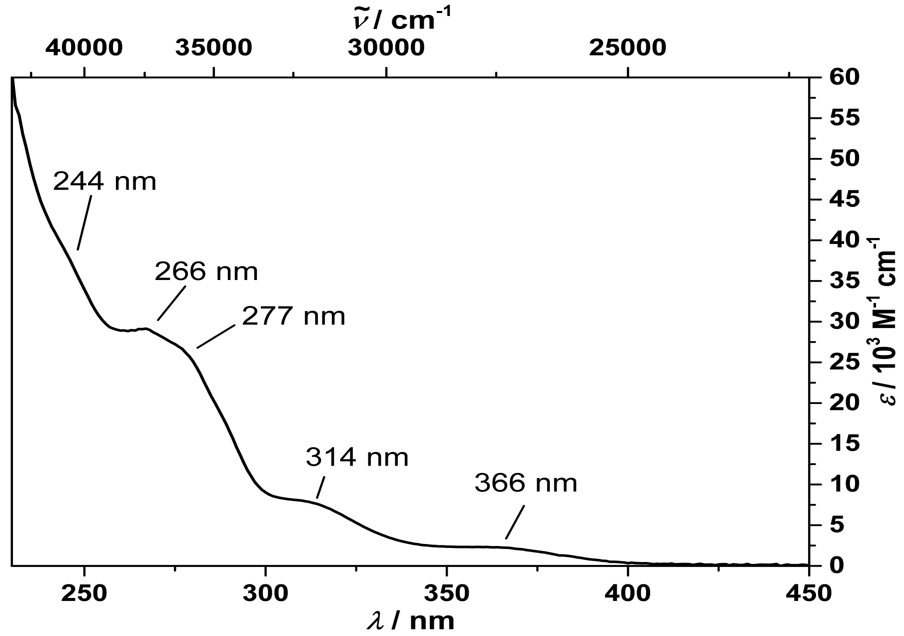
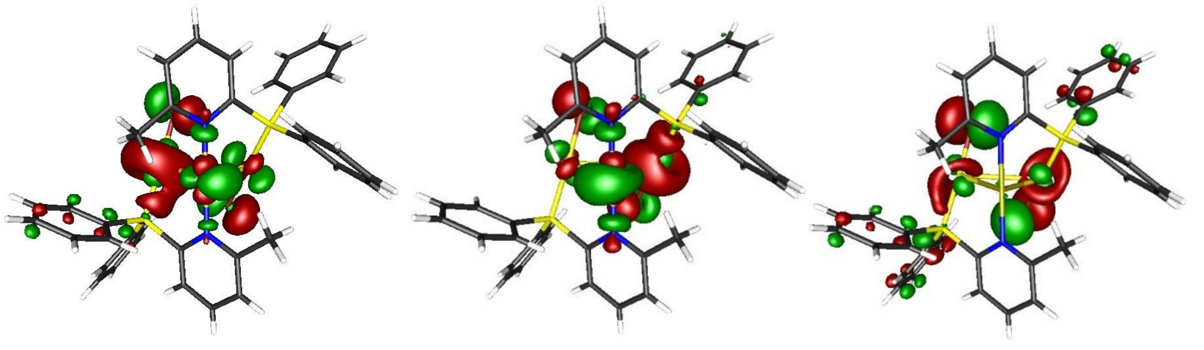


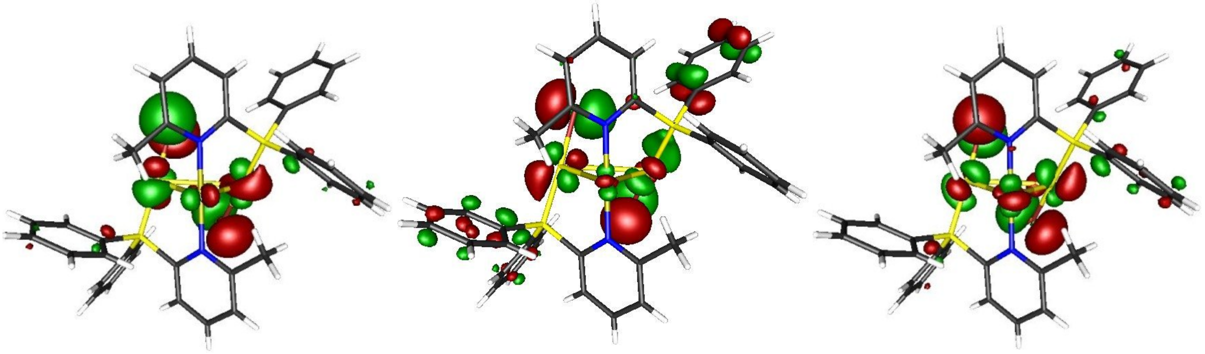
Figure S5. Absorption spectrum of **2** in dichloromethane at room temperature.

Computational studies

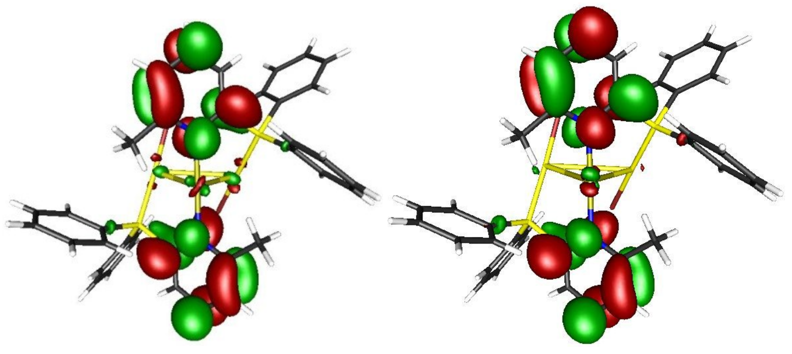
TD-DFT Calculations. Calculations (gas-phase) were performed with the ORCA 3.0.2 program suite.[4] Geometry optimisations were carried out with the PBE0[5] functional as implemented in ORCA. The def2-TZVP[6] basis set was used for all atoms together with the auxiliary basis set def2-TZVP/J in order to accelerate the computations within the framework of RI approximation. Relativistic effects of the Cu^{I} complexes were accounted for by employing the ZORA[7] method, and van der Waals interactions have been considered by an empirical dispersion correction (Grimme-D3BJ).[8] TD-DFT calculations for the first 100 singlet and triplet excited states were performed with the same functional. Representations of molecular orbitals were produced with orca_plot as provided by ORCA 3.0.2 and with gOpenMol 3.00.[9]



HOMO **HOMO-1** **HOMO-2**



HOMO-3 **HOMO-4** **HOMO-5**

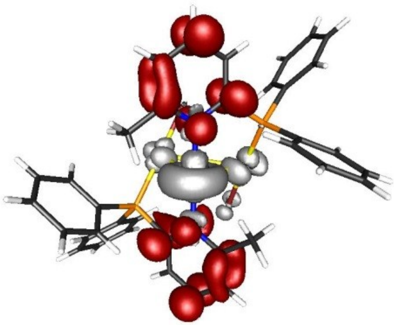


LUMO **LUMO+1**

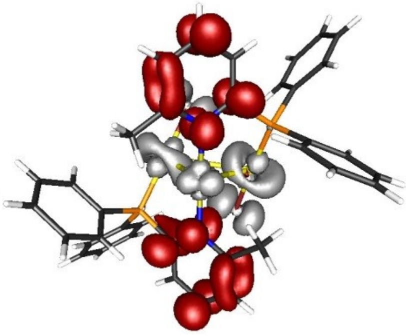
Figure S6. Selected molecular frontier orbitals of the trinuclear cation of **2**.

Table S3. Cartesian coordinates of the optimized geometry of the ground state S_0 of the cation in **2**.

C	0.086220	4.608590	-3.964250
C	0.734670	3.398490	-4.014520
C	-0.092350	5.231630	-2.752200
C	1.200330	2.799760	-2.856940
C	-0.748920	-4.679940	-2.363120
C	-2.022820	1.370250	-2.432160
C	0.226970	-5.548820	-1.916120
C	0.355030	4.648860	-1.579850
C	2.000150	-2.257950	-1.680990
C	1.018710	3.414830	-1.622240
C	-1.293660	-3.751310	-1.496930
C	-4.090190	0.341220	-1.463270
C	-2.709510	0.389950	-1.546080
C	4.053580	-0.870490	-1.305730
C	2.664050	-0.980300	-1.302380
C	4.658320	0.287100	-0.903230
C	0.651920	-5.507650	-0.621190
C	-4.701050	-0.590550	-0.658120
C	3.861980	1.342220	-0.503150
C	2.498120	1.211730	-0.518940
C	-0.851000	-3.684730	-0.180570
C	-3.918190	-1.462690	0.080890
C	-2.552940	-1.346370	-0.007380
C	3.230010	4.672360	0.290420
C	0.138940	-4.571350	0.248030
C	4.062810	5.485870	1.064910
C	2.406620	3.733050	0.910780
C	-2.881900	-4.548320	2.058760
C	4.059710	5.346570	2.436530
C	-2.461910	-3.232240	2.194890
C	2.388700	3.638340	2.296630
C	-3.703560	-5.120580	3.020550
C	3.209020	4.452220	3.057290
C	-2.855400	-2.500550	3.305750
C	-4.105160	-4.387770	4.107600
C	-3.679960	-3.077120	4.258020
H	-0.236100	5.010860	-4.762250
H	0.865090	2.969590	-4.851510
H	-1.045190	-4.721030	-3.264860
H	-2.599900	1.579780	-3.195970
H	-0.529320	6.074580	-2.719870
H	1.647900	1.962630	-2.905740
H	0.606040	-6.180630	-2.516410
H	-1.182100	0.984300	-2.755530
H	2.498750	-2.681350	-2.410360
H	-4.617440	0.951930	-1.964950
H	1.083540	-2.075140	-1.975400
H	-1.834060	2.190040	-1.929970
H	-1.970500	-3.157870	-1.801190
H	4.583990	-1.606480	-1.589040
H	5.605800	0.364840	-0.899530
H	1.980880	-2.858260	-0.906250
H	0.213200	5.083660	-0.746910
H	3.225240	4.759130	-0.654590
H	-5.648970	-0.635840	-0.607230
H	1.304910	-6.126330	-0.316100
H	4.259020	2.156540	-0.215730
H	4.625200	6.130090	0.648810
H	-4.316520	-2.124720	0.634640
H	0.459410	-4.528780	1.140980
H	-2.606040	-5.057840	1.305950
H	4.650480	5.872860	2.961070
H	-3.988120	-6.021870	2.924560
H	1.811760	3.014850	2.722320
H	-2.559260	-1.605360	3.414470
H	3.188590	4.396470	4.005320
H	-4.675400	-4.779050	4.757970
H	-3.955210	-2.573270	5.014430
Au	-0.461730	1.936470	1.017630
Au	0.216020	-1.186990	1.870340
Cl	-2.363300	1.371960	2.158660
Cl	1.874830	0.015310	2.879640
Cu	-0.022800	-0.182860	-0.772600
N	1.892040	0.054740	-0.895150
N	-1.937130	-0.443660	-0.813530
P	1.382350	2.590320	-0.055940
P	-1.417650	-2.409560	0.969300



$S_0 \rightarrow S_1$



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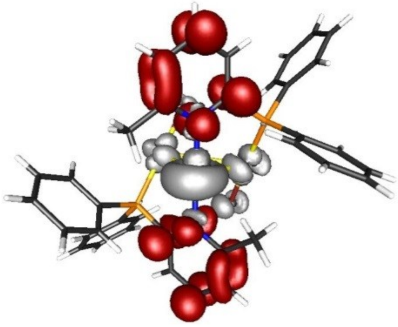
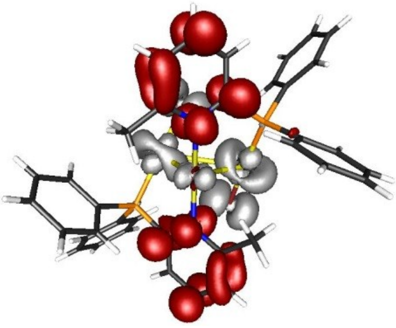
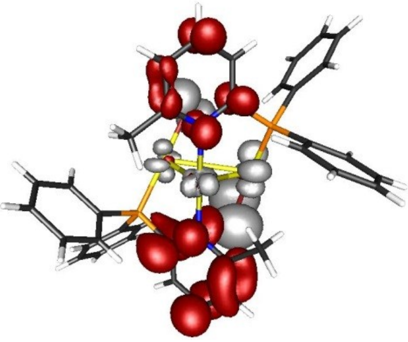


$S_0 \rightarrow S_3$



$S_0 \rightarrow S_4$



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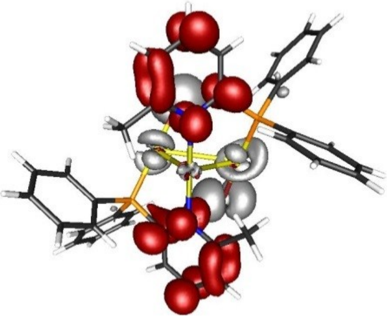
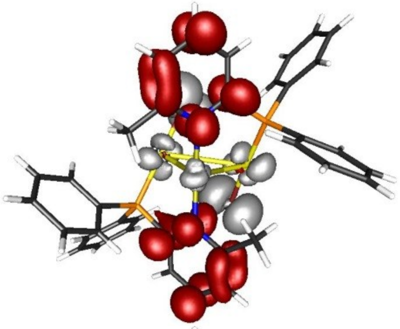
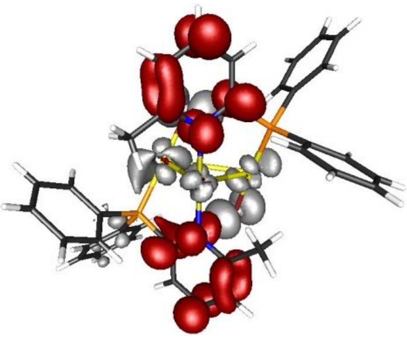
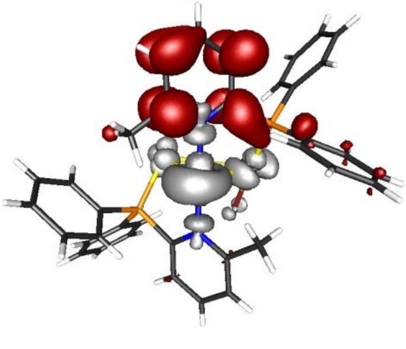


$S_0 \rightarrow S_6$





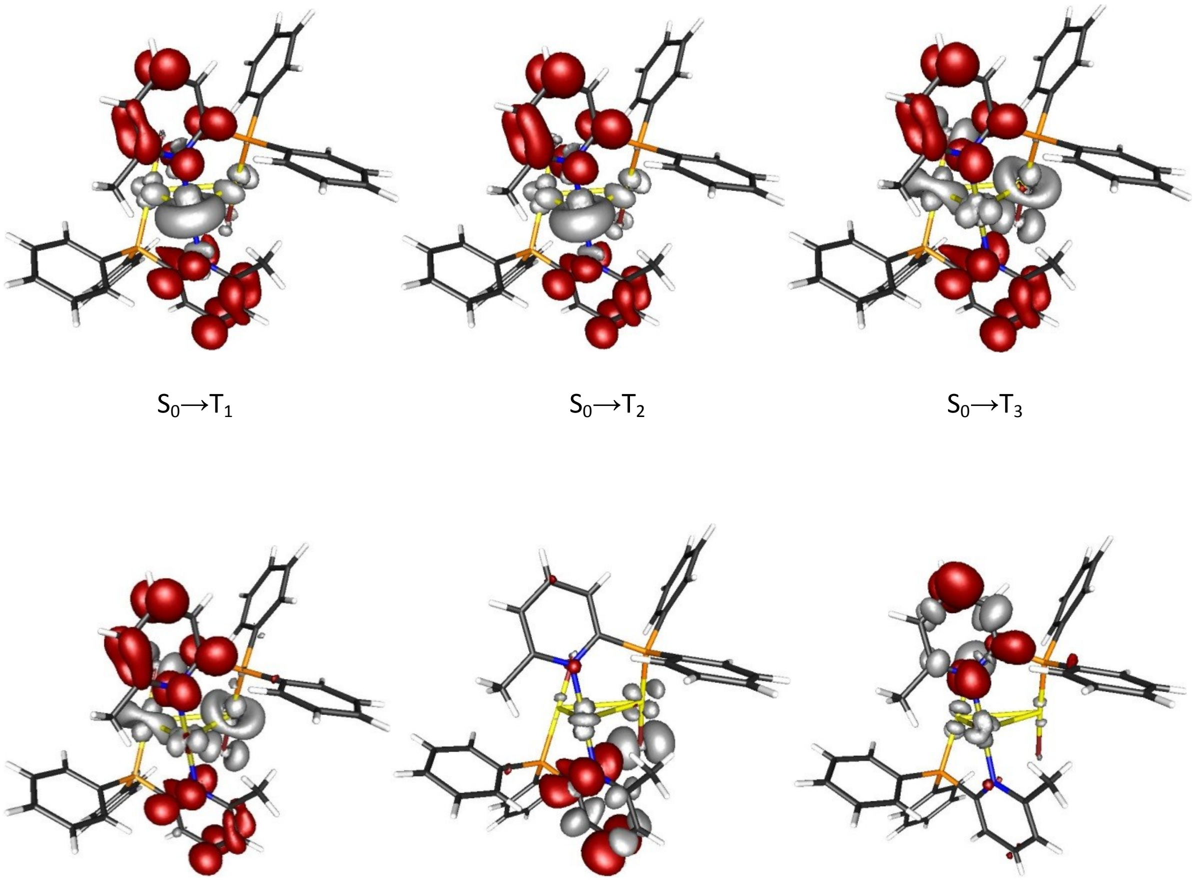


$S_0 \rightarrow S_7$

$S_0 \rightarrow S_8$

$S_0 \rightarrow S_9$

Figure S7. Transition difference plots for the first nine singlet FC transitions from the optimized geometry of the ground state S_0 of the trinuclear cation of **2**.



$S_0 \rightarrow T_1$ $S_0 \rightarrow T_2$ $S_0 \rightarrow T_3$

$S_0 \rightarrow T_4$ $S_0 \rightarrow T_5$ $S_0 \rightarrow T_6$

Figure S8. Transition difference plots for the first six triplet FC transitions from the optimized geometry of the ground state S_0 of the trinuclear cation of **2**.

CAS/NEVPT2/SOC Calculations. The calculations have been performed using the ORCA program (Version 3.0.3).[10] The structure of the complex cation of **2** has been optimized at RI-PBE0-D3/def2-TZVP level of theory (see above). The starting orbitals were taken from natural MP2 orbitals obtained from a single point run using RI-SCS-MP2 level of theory with relaxed density (keywords "*%mp2 density relaxed NatOrbs true end*") but using def2-SVP basis sets for the lighter elements and the SVP-ZORA basis set for Cu[11] and Au[12] and the zero-order relativity approximation (ZORA) as it is implemented in ORCA was used.[13] For the SCF step of the final geometry, convergence criteria were set to "*VERYTIGHTSCF SlowConv*", also the "*RIJCOSX*" approximation was used[14] and "*D3*" was unset in the final SCF step.

The basic idea for the setup of the CA space (CAS) was to possibly emulate the higher states with single determinant configurations as they were suggested by the TD-DFT calculations. They have shown that the lowest singlet and triplet excitations are composed of mainly one virtual excitation from the ground state reference. An optical inspection of the difference density and the KS orbitals engaged, suggested that mainly virtual excitations from d_{z2} type orbitals at Au and Cu (oriented into ligand-metal-ligand directions as a “local” z-axis) into the LUMO and LUMO+1, which are almost pure π*-type orbitals from the two pyridine moieties bound to Cu. Consequently we have used an orbital localization procedure (Pipek-Mezey, keyword “*LocMet PM*”) onto the relaxed natural MP2 orbitals to be able to select the aforementioned metal d-orbitals as active occupied orbitals. Also in the SCS-MP2 natural orbitals the LUMO and LUMO+1 were of the desired π*-pyridine orbitals. In this way a CAS of 5 electrons in 6 orbitals (CAS(5|6)) resulted. For efficiency and also to avoid incorrect higher excitations we have decided to only calculate the lowest 4 singlets and 4 triplets and to carry out the CAS-SCF as a state averaged CAS over these evenly weighted 8 states. During this CAS run it turned that the two Au d_{z2} type orbitals rotate into a set of positive linear combination and a negative linear combination (irrep *a* and *b*, note that the cation of **2** is of C_2 symmetry to good approximation) and that the positive (*a* type combination) is not active in this CAS space. At the same time also the π*-pyridine orbitals rotated analogous *a* and *b* combinations. Therefore we have removed the *a* type Au d_{z2} orbital from the CAS to arrive at CAS(4|4) with an active space of [$b^2a^2a^0b^0$] (the Cu d_{z2} orbital formally transforms also like *a*).[15] With these settings it was possible to achieve *a* set orbitals which were describing the 8 target states as desired as mostly composed of single configurations. It was not possible to achieve convergence to standard criteria. The final orbitals and CAS states were taken from an intermediate step with *E(CAS)=-44035.864526453 Eh DE = -0.002669388; ||g|| = 0.063307555 Max(G)= 0.031572668 Rot=254,208*.

Though these values indicate no numerically stable convergence we decided to use these states anyway for further computing since they seem to model closely the states predicted from the TD-DFT calculation and our primary goal for this calculation was to get an idea about the principal possibilities and size of the spin-orbit-coupling between these states. In detail the states are composed like:

```
BLOCK 1 MULT= 3 NROOTS= 4
ROOT   0:     E=  -44035.8982280560 Eh
              0.98549 [     0]: 2110
              0.01350 [     1]: 2101
ROOT   1:     E=  -44035.8796042393 Eh  0.507 eV   4087.5 cm**-1
              0.98431 [     1]: 2101
              0.01363 [     0]: 2110
ROOT   2:     E=  -44035.7966702081 Eh  2.764 eV  22289.4 cm**-1
              0.99894 [     3]: 1210
ROOT   3:     E=  -44035.7782121412 Eh  3.266 eV  26340.4 cm**-1
              0.99804 [     4]: 1201

BLOCK 2 MULT= 1 NROOTS= 4
ROOT   0:     E=  -44035.9818550428 Eh
              0.99426 [     0]: 2200
              0.00452 [     1]: 2110
ROOT   1:     E=  -44035.8908492940 Eh  2.476 eV  19973.5 cm**-1
              0.95789 [     1]: 2110
              0.03430 [     2]: 2101
              0.00382 [     0]: 2200
              0.00272 [     3]: 2020
ROOT   2:     E=  -44035.8758659500 Eh  2.884 eV  23261.9 cm**-1
              0.96373 [     2]: 2101
              0.03356 [     1]: 2110
ROOT   3:     E=  -44035.7905710136 Eh  5.205 eV  41982.0 cm**-1
              0.99715 [     6]: 1210
```

Hereby the occupations (like: 2110, …) refer to the active orbitals in the order as was outlined above: [(Au d_{z2} *b*)(Cu d_{z2} *a*)(py-π* *a*)(py- π* *b*)]. We again note, that all states are as desired composed mainly of one configuration in close analogy to the TD-DFT results. The energetic ordering of these states is as maybe naively expected (from to the relatively small size of the exchange contributions) …T, S, T, S … with each pair of T (triplet) and S (singlet) belonging to the same configuration. The sequence of configurations at the CAS level is: ground state reference = [], [Cu d_{z2} *a* → py- π* *a*], [Cu d_{z2} *a* → py- π* *b*], [Au d_{z2} *a* → py- π* *a*], [Au d_{z2} *a* → py- π* *b*]. According to expectation, the calculated vertical $S_0 \rightarrow S_n$ transition energies from pure CASSCF, neglecting dynamical correlation, are not in good agreement with the experimental absorption spectra: exp. absorption bands 366, 314 and 269 nm, vs. calc.: 501, 430, 238 nm.

In the next step the perturbation correction for correlation NEVPTn[16] in form of ORCAs SC-NEVPT24[4] was applied. According to expectation the NEVPT2 corrections caused a significant change of the energies of the states and also a reordering:

```
STATE ROOT MULT  DE/a.u.     DE/eV   DE/cm**-1
  1:    3    1   0.127719   3.475   28031.1
  2:    2    3   0.128260   3.490   28149.8
  3:    3    3   0.146594   3.989   32173.6
  4:    0    3   0.154429   4.202   33893.1
  5:    1    1   0.155091   4.220   34038.6
  6:    1    3   0.169331   4.608   37164.0
  7:    2    1   0.170579   4.642   37437.8
```

So in the above used nomenclature the sequence of states after NEVPT2 is now:

S-[], S-[Au d_{z2} *a* → py-π* *b*], T-[Au d_{z2} *a* → py- π* *a*], T-[Au d_{z2} *a* → py- π* *b*], T-[], S-[Cu d_{z2} *a* → py- π* a], T-[Cu d_{z2} *a* → py- π* *a*], S-[Au d_{z2} *a* → py- π* *a*]. We note, that now the vertical $S_0 \rightarrow S_n$ transition energies (357, 294 and 267 nm) are in surprisingly good agreement with the experimental observed absorption bands (see above), which confirms this model of the excited electronic states. Finally the spin-orbit coupling (SOC) between the NEVPT2 corrected states were calculated (keywords "*%casscf*" used was "*rel dosoc true*").[17]

In part large SOC matrix elements were found:

```
QDPT WITH    PT2 DIAGONAL ENERGIES
---------------------------------
--------------------------------------------------------------------------
                        CALCULATED REDUCED SOC MATRIX ELEMENTS
--------------------------------------------------------------------------
        Block                Root          <I|Lx S |J> <I|Ly S |J> <I|Lz S |J>
 I(Mult)     J(Mult)       I         J          cm-1        cm-1        cm-1
--------------------------------------------------------------------------
 0( 3)       0( 3)         0         0          0.00        0.00        0.00
 0( 3)       0( 3)         1         0        107.80      -78.36       33.89
 0( 3)       0( 3)         1         1          0.00       -0.00        0.00
 0( 3)       0( 3)         2         0       -450.69       89.27     -118.00
 0( 3)       0( 3)         2         1         55.85      -10.51       15.68
 0( 3)       0( 3)         2         2         -0.00        0.00       -0.00
 0( 3)       0( 3)         3         0        -56.48       11.12      -16.64
 0( 3)       0( 3)         3         1       -446.40       86.51     -116.75
 0( 3)       0( 3)         3         2        103.62      -65.43       31.07
 0( 3)       0( 3)         3         3          0.00        0.00       -0.00
 0( 3)       1( 1)         0         0        -18.82        2.15      -20.50
 0( 3)       1( 1)         0         1         -2.24        3.23        0.91
```

```
 0( 3)       1( 1)       0        2       -76.13       55.11      -24.86
 0( 3)       1( 1)       0        3      -321.56       62.44      -84.42
 0( 3)       1( 1)       1        0       -72.96      -79.38       -8.99
 0( 3)       1( 1)       1        1        95.08      -48.91       27.58
 0( 3)       1( 1)       1        2       -11.99        0.02       -2.46
 0( 3)       1( 1)       1        3        28.41       -5.50        7.65
 0( 3)       1( 1)       2        0      -297.67      192.09     -136.08
 0( 3)       1( 1)       2        1       321.48      -66.72       86.65
 0( 3)       1( 1)       2        2       -68.46       16.76      -19.08
 0( 3)       1( 1)       2        3         0.82       -0.71        1.66
 0( 3)       1( 1)       3        0        26.85       -2.69      168.76
 0( 3)       1( 1)       3        1        60.53      -11.93       11.57
 0( 3)       1( 1)       3        2       317.33      -63.76       87.40
 0( 3)       1( 1)       3        3        72.46      -46.32       20.52
-----------------------------------------------------------------------------
```

The finally resulting vertical absorption spectra is:

```
-------------------------------------------------------------------------------------------
                    SOC CORRECTED ABSORPTION SPECTRUM
-------------------------------------------------------------------------------------------
  States    Energy    Wavelength   fosc          T2         |TX|        |TY|       |TZ|
            (cm-1)      (nm)                   (D**2)       (D)         (D)        (D)
-------------------------------------------------------------------------------------------
  0    1    28023.5    356.8   0.044724433   3.38903   0.43150   1.76600   0.28994
  0    2    28142.2    355.3   0.000020878   0.00158   0.03521   0.01653   0.00789
  0    3    28142.2    355.3   0.000018755   0.00142   0.02622   0.00352   0.02674
  0    4    28145.5    355.3   0.000081711   0.00616   0.00476   0.03717   0.06900
  0    5    32166.1    310.9   0.000142268   0.00939   0.08606   0.02176   0.03890
  0    6    32166.3    310.9   0.000009332   0.00062   0.00451   0.01737   0.01714
  0    7    32166.7    310.9   0.000012764   0.00084   0.02708   0.00862   0.00593
  0    8    33904.7    294.9   0.000095137   0.00596   0.03121   0.07005   0.00883
  0    9    33905.2    294.9   0.000016098   0.00101   0.01858   0.00272   0.02560
  0   10    33905.2    294.9   0.000004598   0.00029   0.01436   0.00167   0.00889
  0   11    34050.7    293.7   0.061890836   3.85970   0.41891   0.36393   1.88461
  0   12    37169.0    269.0   0.000055389   0.00316   0.01026   0.03223   0.04495
  0   13    37179.7    269.0   0.000004120   0.00024   0.00585   0.00684   0.01242
  0   14    37179.7    269.0   0.000001106   0.00006   0.00580   0.00521   0.00151
  0   15    37453.5    267.0   0.026875230   1.52375   0.52628   1.11639   0.02085
  1    2      118.7  84261.3    0.000000000    0.00020   0.01418   0.00192   0.00040
  1    3      118.7  84225.3    0.000000000    0.00005   0.00684   0.00061   0.00045
  1    4      122.0  81981.2    0.000000000    0.02672   0.16342   0.00024   0.00343
  1    5     4142.6   2413.9   0.000000000   0.00568   0.07073   0.02599   0.00070
  1    6     4142.8   2413.8   0.000000000   0.00040   0.01894   0.00615   0.00121
  1    7     4143.2   2413.6   0.000000000   0.01267   0.11095   0.01875   0.00367
  1    8     5881.2   1700.3   0.000000000   0.00091   0.02996   0.00159   0.00297
  1    9     5881.7   1700.2   0.000000000   0.00055   0.00156   0.02299   0.00389
  1   10     5881.7   1700.2   0.000000000   0.00006   0.00093   0.00717   0.00185
  1   11     6027.2   1659.1   0.000000000   2.27856   0.46643   1.41175   0.26069
  1   12     9145.6   1093.4   0.000000000   0.23794   0.48411   0.05565   0.02189
  1   13     9156.2   1092.2   0.000000000   0.00002   0.00381   0.00173   0.00022
  1   14     9156.2   1092.2   0.000000000   0.00001   0.00289   0.00252   0.00044
  1   15     9430.0   1060.4   0.000000000   0.07587   0.05632   0.26232   0.06231
  2    3        0.1   197538863.0    0.000000000    0.00000    0.00033    0.00003    0.00002
  2    4        3.3   3029684.7    0.000000000    0.00000    0.00131    0.00024    0.00007
  2    5     4023.9   2485.1   0.000000000   7.23261   2.67574   0.25693   0.08382
  2    6     4024.1   2485.0   0.000000000  30.16248   5.46368   0.53006   0.17245
  2    7     4024.5   2484.8   0.000000000  96.28769   9.76453   0.92228   0.30187
  2    8     5762.5   1735.3   0.000000000   0.01848   0.02855   0.13078   0.02370
  2    9     5763.0   1735.2   0.000000000   2.12436   0.29548   1.40505   0.25079
  2   10     5763.0   1735.2   0.000000000   0.11962   0.28003   0.20057   0.03132
  2   11     5908.5   1692.5   0.000000000   0.00157   0.02773   0.02754   0.00613
  2   12     9026.9   1107.8   0.000000000   0.00104   0.00712   0.02890   0.01231
  2   13     9037.5   1106.5   0.000000000   0.00809   0.01519   0.08355   0.02971
  2   14     9037.5   1106.5   0.000000000   0.06084   0.06665   0.22417   0.07839
  2   15     9311.3   1074.0   0.000000000   0.00010   0.00970   0.00284   0.00077
```

With these results as is outline in the main text one can estimate also the lifetimes of the triplet states using the Strickler-Berg estimation. The resulting values again were in surprisingly good agreement with the experimental values.

In conclusion: Using a simplistic model electronic structure it was possible to derive estimates for the size of SOC and ZFS as well as lifetimes of states. The results are in surprising agreement with experiments but may be largely based on error cancellation. Apart from numerical accuracy it is very likely that the nature of the configurations (orbital space) is described correctly in this simple model, most of all since this is also in agreement with the independent results from the TD-DFT calculations.

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