Supplementary Material (ESI) for Chemical Communications

Supporting Information

Octanuclear gold(I) alkynyl-diphosphine clusters showing thermochromic luminescence

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Experimental

General comments

$(AuC_2Bu^t)_n$,[1] 1,4-$PR_2C_6H_4PR_2$ (R = Ph, NC_4H_4)[2] were obtained according to literature methods. Complexes $[Au_2(PR_2C_6H_4PR_2)_2]^{2+}$ were prepared similarly to the published analogues.[3] The solution 1D ^1H, ^{31}P NMR and ^1H-^1H COSY spectra were recorded on Bruker Avance 400 and Bruker DPX 300 spectrometers. Mass spectra were determined in the ESI^+ mode at St.-Petersburg State University. Microanalyses were carried out in the analytical laboratory of the University of Eastern Finland.

$[Au_8(C_2Bu^t)_6(PPh_2C_6H_4PPh_2)_2](PF_6)_2$ (1)

$(AuC_2Bu^t)_n$ (50 mg, 0.180 mmol) was suspended in dichloromethane (10 cm^3) and $[Au_2(PPh_2C_6H_4PPh_2)_2](PF_6)_2$ (48 mg, 0.03 mmol). The suspension was stirred for 1.5 h in the absence of light. The resulting transparent pale-yellow solution was filtered, evaporated and recrystallized by slow evaporation of its solution in CH_2Cl_2/acetone/methanol/EtOH mixture at room temperature using minimum amount of CH_2Cl_2. Bright yellow block crystals were washed with diethyl ether and vacuum dried (83 mg, 85 %). Anal. Calc. for $Au_8C_{96}H_{102}F_{12}P_6$: C, 35.53; H, 3.17. Found C, 35.50; H 3.45.

$[Au_8(C_2Bu^t)_6\{P(NC_4H_4)_2C_6H_4P(NC_4H_4)_2\}_2](PF_6)_2$ (2)

Prepared analogously to **1** using $[Au_2(P(NC_4H_4)_2C_6H_4P(NC_4H_4)_2)_2](PF_6)_2$. Recrystallized by gas-phase diffusion of diethyl ether into CH_2Cl_2/MeOH solution of **2** at +5 ^oC. Yellow-greenish

crystalline material (84%). ES MS (*m/z*): $[Au_8(C_2Bu^t)_6(P(NC_4H_4)_2C_6H_4P(NC_4H_4)_2)_2]^{2+}$ 1433.7 (calcd 1433.7). $^{31}P\{^1H\}$ NMR (acetone-d_6, 25°C; δ): 79.8 (s, 4P), -144.8 (sept, $2PF_6$). ^1H NMR (acetone-d_6, 25°C; δ): **diphosphine**: **P-C$_6$H$_4$-P** 7.59 (m AA′ XX′, 8H, ^3J (H–H) 6.5, ^3J (P-H) 13, ^4J(P-H) 4 Hz), 7.42 (m, 16H, P-NC$_4$H$_4$), 6.61 (m, 16H, P-NC$_4$H$_4$), **alkynyl-Bu^t:** 1.63 (s, 18H), 1.32 (s, 36H). Anal. Calc. for $Au_8C_{80}H_{94}F_{12}N_8P_6$: C, 30.43; H; 3.00, N, 3.55. Found C, 30.11; H 3.30; N, 3.44.

$[Au_8(C_2Bu^t)_6(PPh_2C_2PPh_2)_2](ClO_4)_2$ (3)

Prepared analogously to **1** using $[Au_2(PPh_2C_2PPh_2)_2](ClO_4)_2$. Recrystallized by gas-phase diffusion of diethyl ether into acetone-CH_2Cl_2 solution of **3** at +5 °C. Yellow crystalline material (87%). ES MS (*m/z*): $[Au_8(C_2Bu^t)_6(PPh_2C_2PPh_2)_2]^{2+}$ 1425.7 (calcd 1425.7). $^{31}P\{^1H\}$ NMR (acetone-d_6, 25°C; δ): 25.4 ($2P_1$, m, ^3J(P-P) 7.1Hz), 29.0 ($2P_2$, m, ^3J(P-P) 7.1Hz). ^1H NMR (acetone-d_6, 25°C; δ): **diphosphine**: **P$_1$Ph**: *ortho*-H(Ph_1) 8.19 (dd, 4H, J (H–H) ca 7, J (P-H) 14.5Hz), *ortho*-H(Ph_2) 8.15 (dd, 4H, J (H–H) ca 7, J (P-H) 14.5 Hz) , **P$_2$Ph**: *ortho*-H(Ph_1) 8.06 (dd, 4H, J (H–H) ca 7.5, J (P-H) ca 15 Hz), *ortho*-H(Ph_2) 8.04 (dd, 4H, J (H–H) ca 7.5, J (P-H) 15 Hz), 7.65-7.85, 24H, unresolved multiplet of meta- and para-phenyl protons at P_1 and P_2; **alkynyl-Bu^t**: 1.51 (s, 18H), 0.93 (s, 18H), 0.88 (s, 18H). Anal. Calc. for $Au_8C_{88}H_{94}Cl_2O_8P_4$: C, 34.65; H, 3.11. Found C, 34.47; H 3.46.

X-ray structure determination.

The crystal of **1**, **1**(296), **2**, and **3** were immersed in cryo-oil, mounted in a Nylon loop, and measured at a temperature of 100 K or at 296 K. The X-ray diffraction data were collected on a Bruker Kappa Apex II, Bruker AXS Smart ApexII, or Bruker Kappa Apex II Duo diffractometer using Mo Kα radiation (λ = 0.710 73 Å). The *APEX2*[4]program package was used for cell refinements and data reductions. The structure was solved by direct methods using the *SHELXS-97*[5] program with the *WinGX*[6] graphical user interface. A numerical absorption correction (*SADABS*)[7] was applied to the data. Structural refinements were carried out using *SHELXL-97*.[5] In **1** some residual electron density was unresolved after refinement of the Au molecule and the anion. Furthermore, the crystal contained solvent accessible voids. Since, the remaining residual density could not be unambiguously identified and it was equated to 1 molecule of methanol per molecule of the Au complex and taken into account using the SQUEEZE routine in PLATON.[8] In **1** the carbon atoms C18 and C16 were disordered over two sites with equal occupancies. The carbon-carbon distances in the disordered units were restrained to be similar. The carbon atoms C18A, C18B as well as C7 were restrained with effective standard deviation 0.01 so that their U_{ij} components approximate to isotropic behavior. The crystal of **1**(296) also contained solvent

accessible voids but there was no considerable residual electron density. The potential solvent accessible volume per cell was 372.5 $Å^3$, with a total electron count of 52. The SQUEEZE routine was not able to handle the voids satisfactorily and the contribution of the possible solvent was not taken into account. It is likely, that some solvent has been lost. The carbon atoms C18 and C16 in **1**(296) were disordered over two sites with equal occupancies. The carbon-carbon distances in the disordered units were restrained to be similar. The carbon atoms C18A, C18B as well as C37 were restrained so that their U_{ij} components approximate to isotropic behavior. In **2** one of the CH_2Cl_2 and one of the Et_2O solvent molecules were partially lost and therefore refined with occupancies 0.5. Furthermore, the carbon atom of the partially lost CH_2Cl_2 was disordered over two sites with equal occupancies. Some methyl carbons of the t-butyl moieties were slightly disordered. No satisfactory disorder model was found for these carbons, which led to relatively large displacement parameters. Some of the Au atoms were accompanied by relatively large residual electron densities due to the absorption despite the analytical absorption correction. In **3** one of the ClO_4^- anions was disordered over two sites with equal occupancies. Another ClO_4^- anion was refined with occupancy of 0.5 to compensate the charge of the Au molecule. The carbon atoms C_{55}, C_{56}, C_{57}, C_{58}, C_{67}, C_{68}, C_{69}, and C_{70} were restrained with effective standard deviation 0.01 so that its U_{ij} components approximate to isotropic behavior. The hydrogen atoms were positioned geometrically and were also constrained to ride on their parent atoms, with C-H = 0.93-0.99 Å, and U_{iso} = 1.2-1.5 U_{eq}(parent atom). The crystallographic details are summarized in Table S1**.**

Photophysical measurements.

Steady-state absorption and emission measurements both in solution and in the solid state were recorded on a Hitachi (U-3310) spectrophotometer and an Edinburgh (FS920) fluorometer, respectively. Both the wavelength-dependent excitation and emission response of the fluorometer have been calibrated. To determine the photoluminescence quantum yield in solution, the samples were degassed by three freeze-pump-thaw cycles. Coumarin 480 and 4-(Dicyanomethylene)-2-methyl-6-(paradimethylaminostyryl)-4H-pyran (DCM, Exciton) with a quantum yield of ~0.87 (λ_{max} = 480 nm) and ~ 0.4 (λ_{max} = 615 nm), respectively, in methanol served as the standard for measuring the quantum yield. Solid state quantum yields were determined with a calibrated integrating sphere system. The uncertainty of the quantum yield measurement was in the range of < 2% (an average of three replica). Lifetime studies were performed with an Edinburgh FL 900 photon-counting system using a hydrogen-filled lamp as the excitation source. The emission decays were fitted by the sum of exponential functions with a temporal resolution of ~300 ps by the deconvolution of instrument response function. The crystal was examined by a Zeiss LSM710

Inverted Confocal Spectral Microscope equipped with a X20 (NA 0.8) objective and a 405 nm diode laser were employed as the excitation sources.

Computational details. The geometries of the studied complexes **1–3** and several dissociated forms of **1** were optimized using the BP86 density functional method.[9] The gold atoms were described by a triple-valence-zeta quality basis set with polarization functions (def2-TZVP).[10] Scalar relativistic effects were taken into account by employing a 60-electron relativistic effective core potential.[11] A split-valence basis set with polarization functions on non-hydrogen atoms was used for all the other atoms (def2-SV(P)).[10, 12] The multipole-accelerated resolution-of-the-identity technique was used to speed up the calculations.[13] The lowest triplet states of the complexes were studied using spin-unrestricted formalism. The reported computational results were obtained using the following point group symmetries to facilitate comparisons with the experiments: **1** and **2**: C_{2h} (symmetry lowered from ideal D_{2h} due to capping Bu^t substituents) **3**: C_2. Dissociated forms of complex **1** were studied without any symmetry constraints. All electronic structure calculations were carried out with the TURBOMOLE program package (version 6.1).[14]

Table S1. Crystal data and structure refinement for **1-3**.

Identification code	**1**	**1 (296 K)**	**2**	**3**
Empirical formula	$C_{97}H_{106}Au_8F_{12}OP_6$	$C_{96}H_{102}Au_8F_{12}P_6$	$C_{84.5}H_{104}Au_8Cl_5F_{12}N_8O_{0.5}P_6$	$C_{88}H_{94}Au_8Cl_2O_8P_4$
Formula weight	3277.37	3245.33	3406.56	3050.14
Temperature	100(2) K	296(2) K	100(2) K	100(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Orthorhombic	Orthorhombic	Monoclinic	Triclinic
Space group	Pbca	Pbca	$P2_1/n$	$P\bar{1}$
Unit cell dimensions	a = 22.3376 (17) Å α= 90°	a = 22.3988 (12) Å α= 90°	a = 24.3129 (6) Å α= 90°	a = 13.0014 (7) Å α= 106.781 (3)°
	b = 18.7149 (14) Å β= 90°	b = 18.9734 (11) Å β= 90°	b = 16.0611 (4) Å β= 92.2450 (10)°	b = 17.4798 (10) Å β= 95.591 (3)°
	c = 23.4710 (16) Å γ = 90°	c = 23.7764 (13) Å γ = 90°	c = 28.0596 (7) Å γ = 90°	c = 23.2057 (19) Å γ = 111.261 (2)°
Volume	9812.0(12) Å3	10104.5(10) Å^3	10948.6(5) Å^3	4583.2(5) Å^3
Z	4	4	4	2
Density (calc.)	2.219 Mg/m^3	2.133 Mg/m^3	2.067 Mg/m^3	2.210 Mg/m^3
Absorption coefficient	12.079 mm^{-1}	11.727 mm^{-1}	10.948 mm^{-1}	12.931 mm^{-1}
F(000)	6104	6032	6344	2824
Crystal size, mm^3	0.31 x 0.29 x 0.28	0.31 x 0.29 x 0.28	0.23 x 0.14 x 0.06 mm^3	0.22 x 0.16 x 0.08
Theta range for data collection	1.96 to 26.00°.	2.22 to 26.00°.	1.09 to 27.42°.	1.69 to 26.75°.
Index ranges	-27<=h<=27, -16<=k<=23, -24<=l<=28	-13<=h<=27, -22<=k<=11, -28<=l<=16	-31<=h<=31, -17<=k<=20, -33<=l<=36	-16<=h<=16, -22<=k<=22, -28<=l<=29
Reflections collected	34524	29060	91935	62956
Independent reflections	9558 [R(int) = 0.0878]	9632 [R(int) = 0.0333]	24912 [R(int) = 0.0368]	19414 [R(int) = 0.0276]

Completeness to theta	99.2 %	97.0 %	99.8 %	99.4 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Analytical	Numerical
Max. and min. transmission	0.1359 and 0.1175	0.1408 and 0.1219	0.5595 and 0.1883	0.4097 and 0.1666
Refinement method	Full-matrix least-squares on F2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	9558 / 18 / 579	9632 / 25 / 567	24912 / 62 / 1176	19414 / 48 / 1054
Goodness-of-fit on F2	0.879	1.033	1.030	1.027
Final R indices [I>2sigma(I)]	R1 = 0.0404, wR2 = 0.0670	R1 = 0.0369, wR2 = 0.0689	R1 = 0.0430, wR2 = 0.0988	R1 = 0.0344, wR2 = 0.0778
R indices (all data)	R1 = 0.0735, wR2 = 0.0720	R1 = 0.0691, wR2 = 0.0786	R1 = 0.0662, wR2 = 0.1100	R1 = 0.0517, wR2 = 0.0871
Largest diff. peak and hole, e.$Å^{-3}$	1.808 and -1.601	1.579 and -1.012	5.177 and -2.286 e.$Å^{-3}$	2.482 and -1.160

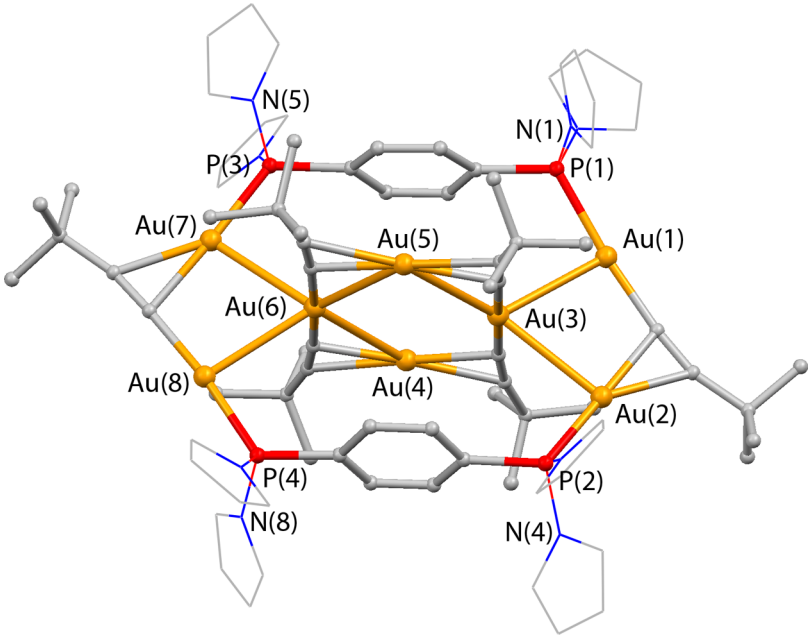

Figure S1. Molecular view of the dication **2**. Selected bond lengths (Å): Au(1)-P(1) 2.245(2), Au(1)-Au(3) 2.9633(4), Au(1)-Au(2) 3.3421(4), Au(2)-P(2) 2.255(2), Au(2)-Au(3) 2.9242(4), Au(3)-Au(5) 3.2198(5), Au(3)-Au(4) 3.2542(4), Au(4)-Au(6) 3.1939(5), Au(5)-Au(6) 3.2116(5), Au(6)-Au(7) 2.8798(4), Au(6)-Au(8) 2.9270(5), Au(7)-P(3) 2.249(2), Au(7)-Au(8) 3.3107(5), Au(8)-P(4) 2.251(2).

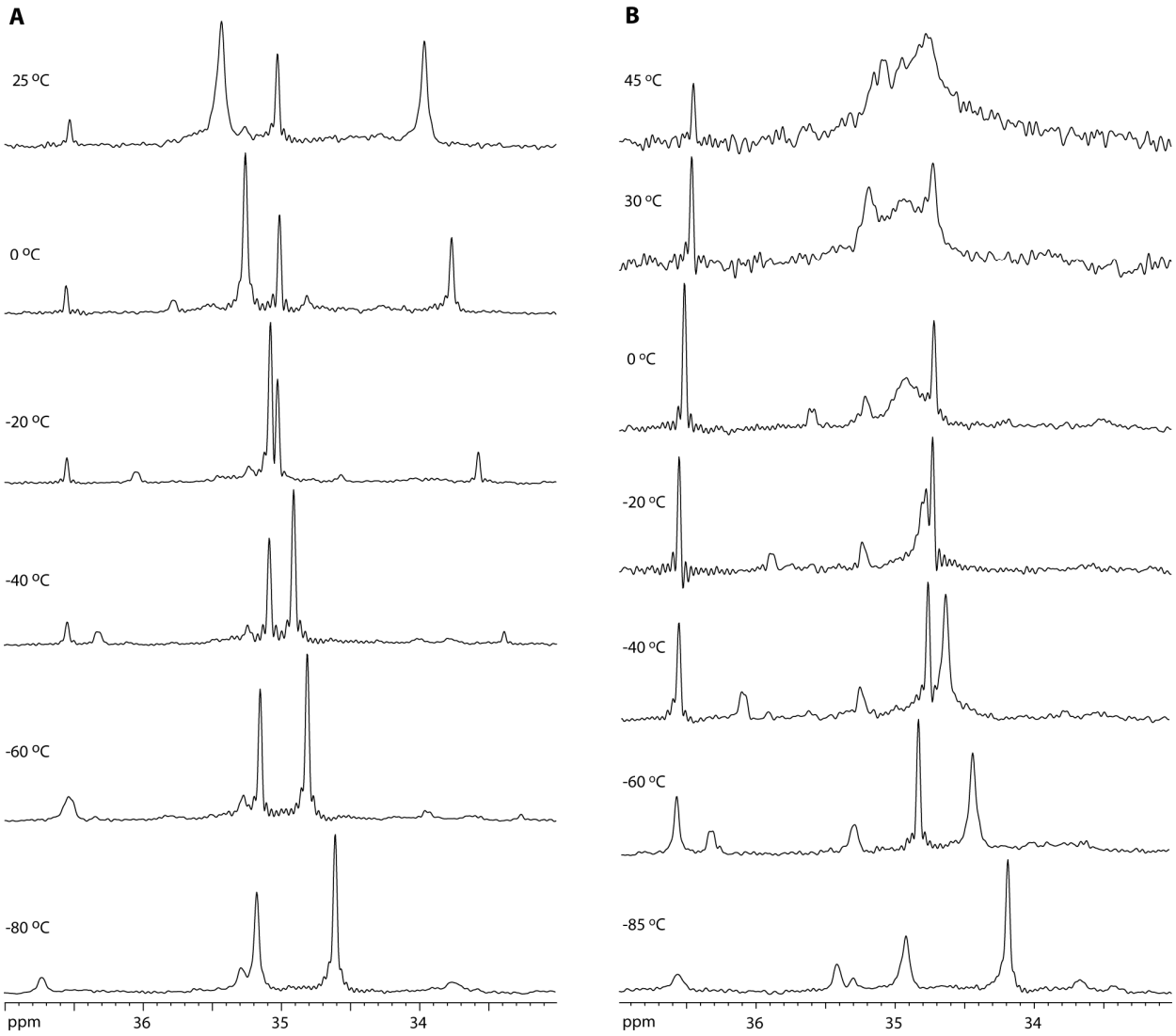

Figure S2. VT ^{31}P NMR spectra of the cluster **1** (**A** – CD_2Cl_2, **B** – acetone-d_6).

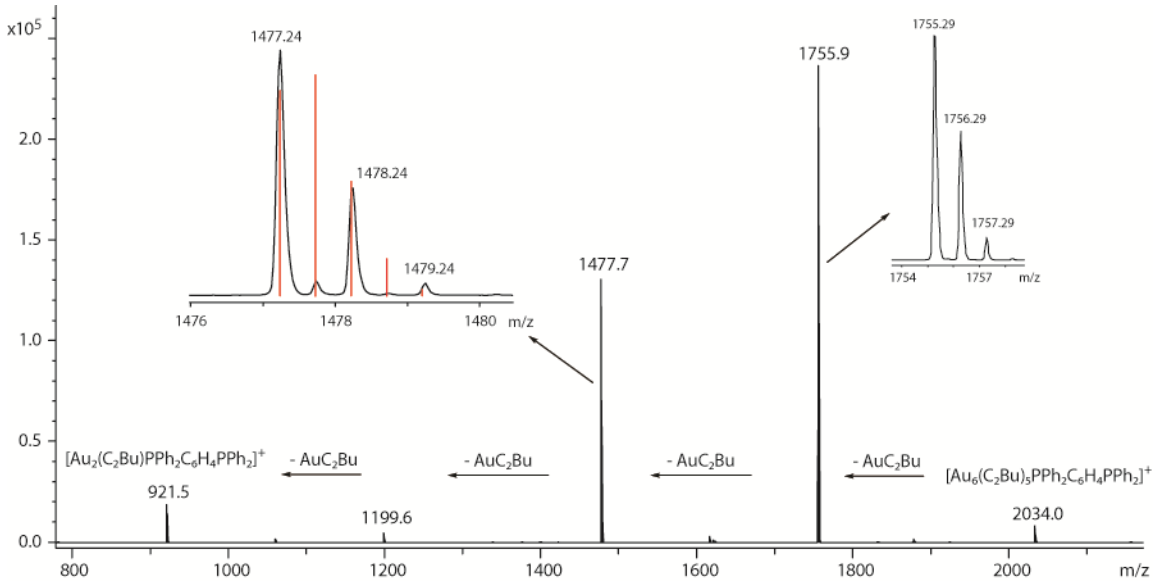

Figure S3. ESI-MS of the cluster **1**. Red – calculated spectrum of $\mathbf{1}^{2+}$ dication.

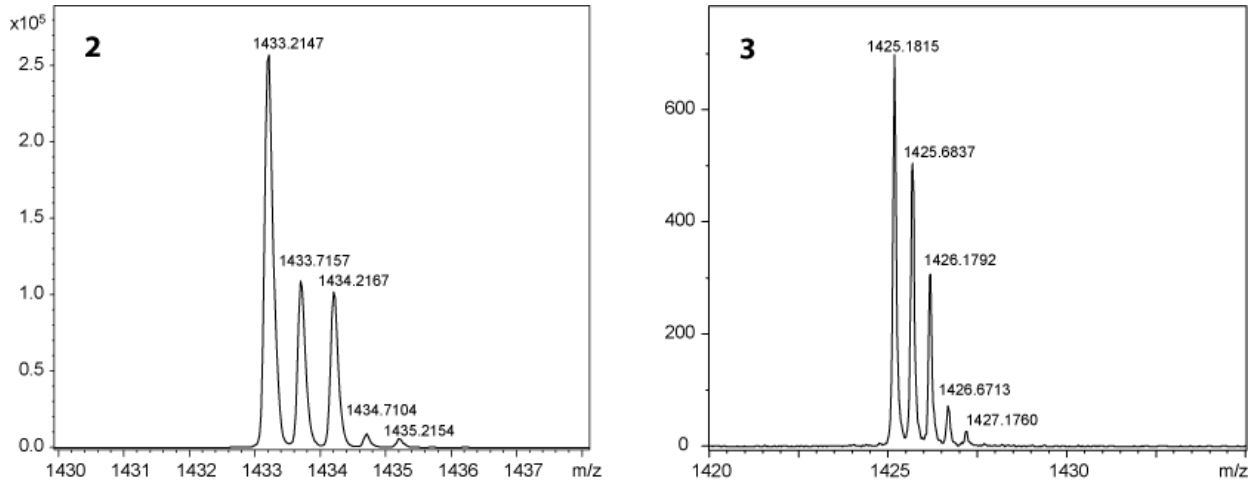

Figure S4. ESI-MS of the clusters **2** and **3**.

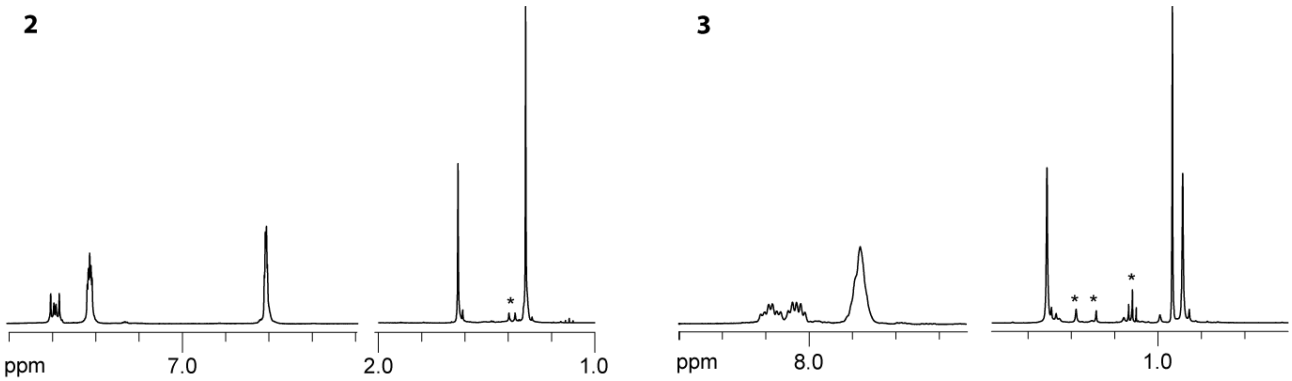

Figure S5. ^{1}H NMR spectra of the clusters **2** and **3**, 400 MHz, 298K, acetone-d_6. The intensity of the low field aromatic region is twice higher than that of the high field part of the spectra. Asterisks denote admixtures.

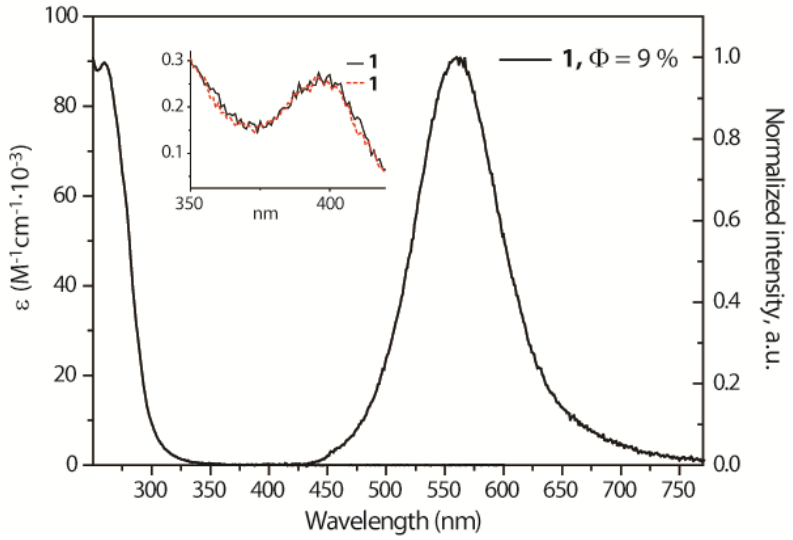

Figure S6. UV/vis absorption and normalized emission spectra of **1** in degassed CH_2Cl_2 at room temperature. Inset: the enlargement of the absorption spectrum of **1** and its excitation spectrum (dashed line) in the region of 350-420 nm.

Computational results

We performed density functional calculations to shed light on the structural characteristics and photophysics of the supramolecular Au(I) complexes **1**–**3**. The geometries of the complexes were optimized at the BP86-DFT level of theory and the general structural motif of the supramolecular complexes **1**–**3** was reproduced well by DFT. For the complex **1**, the Au–Au and π-C≡C-Au contacts holding the outer and inner fragments together, the theoretical values are 2.94–2.97 Å (exp. 2.90–2.91 Å) and 2.22 Å (exp. 2.19 Å). For the complex **2**, the corresponding values are 2.93–3.00 Å (exp. 2.92–2.96) and 2.20 Å (exp. 2.20 Å). The agreement between the theory and experiment remains good for complex **3**, too: 3.02–3.09 Å (exp. 2.95–3.18 Å) and 2.21 Å (2.22 Å).

We also investigated a hypothetical modification of the complex **1**, where the alkynyl Bu^t groups were replaced with phenyl groups, i.e. $[Au_8(C_2Ph)_6(PPh_2C_6H_4PPh_2)_2]^{2+}$. Similar to **1**, the hypothetical Ph-modification was found to be a true local minimum, but its clearly smaller HOMO–LUMO gap (Bu^t: 2.1 eV; Ph: 1.7 eV), suggests it to be kinetically less stable than complex **1**.

The frontier molecular orbitals of the S_0 and T_1 electronic states of the studied complexes **1**–**3** are illustrated in Figures S4–S6. The figures include the S_0 HOMO and HOMO–1, but several other lower energy orbitals were also examined to confirm the nature of the HOMOs. In the case of the complex **1**, the HOMO and LUMO of the S_0 ground state are delocalized over the Au and alkynyl π(C≡C) orbitals, but for complex **2**, the pyrrolyl substituents of diphosphine dominate the HOMOs. For the complex **3**, the frontier orbitals are quite delocalized, but still dominated by contributions from Au atoms and alkynyl orbitals (the C≡C spacer in the diphosphine contributes to the LUMOs, in particular). For all complexes **1**–**3,** the relaxed geometry of the lowest energy triplet state T_1 is similar to the relaxed geometry of the S_0 ground state. For complexes **1** and **3**, the highest singly occupied orbital (HSOMO), occupied by the excited electron, is closely related to the LUMO of the S_0 state, and the lowest singly occupied orbital (LSOMO) is closely related to the HOMO of the S_0 state. However, for complex **2**, the LSOMO is very different from HOMO, being located on the central Au-alkynyl fragment. Therefore, the characteristics of the T_1 states are fairly similar for all three studied complexes: both the T_1 LSOMO and HSOMO are mainly composed of Au and alkynyl π*(C≡C) orbitals.

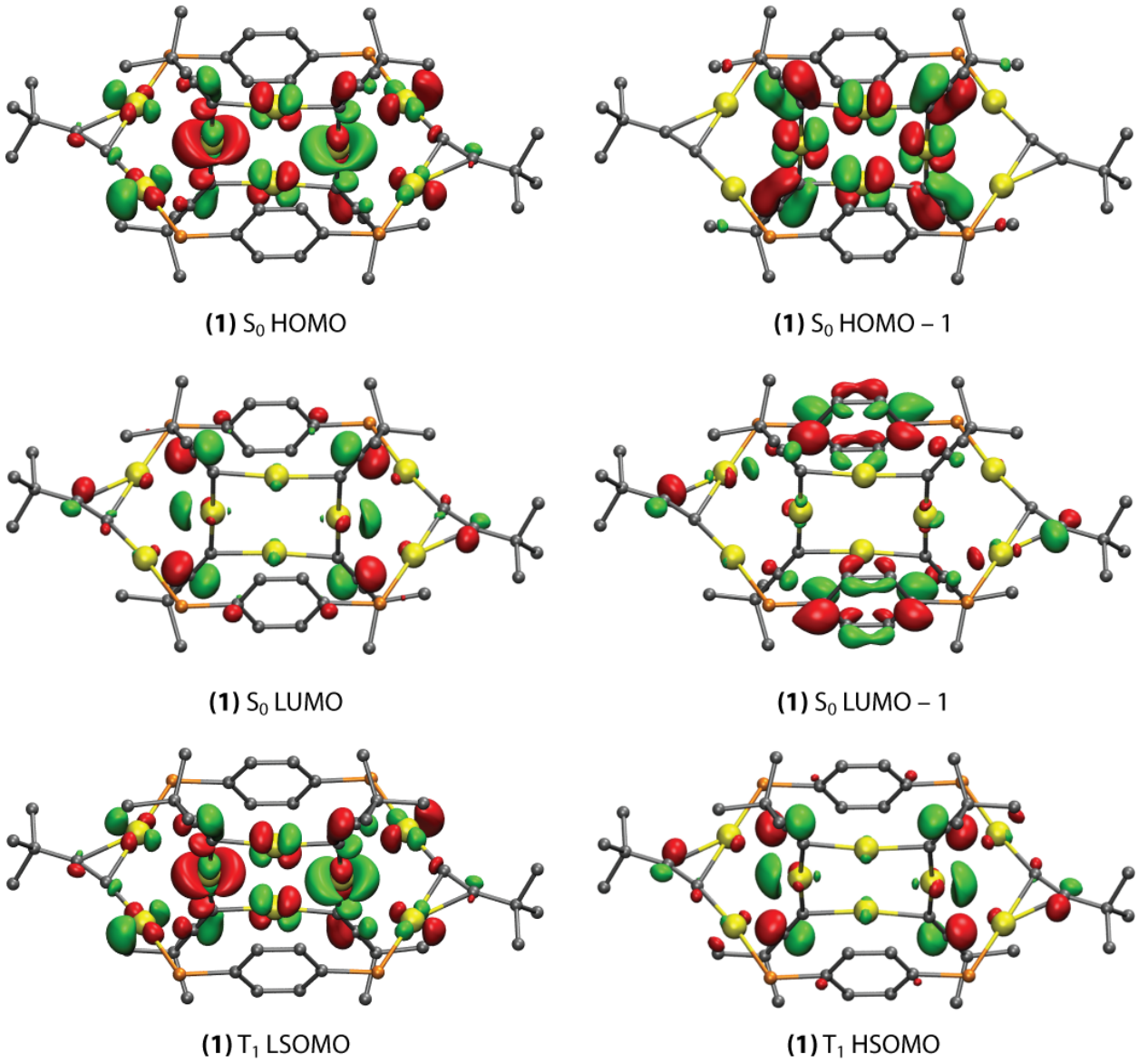

Figure S7. Frontier molecular orbital isodensity plots for complex **1** (isodensity value 0.04 a.u.). Hydrogen atoms and diphosphine-based phenyl rings omitted for clarity.

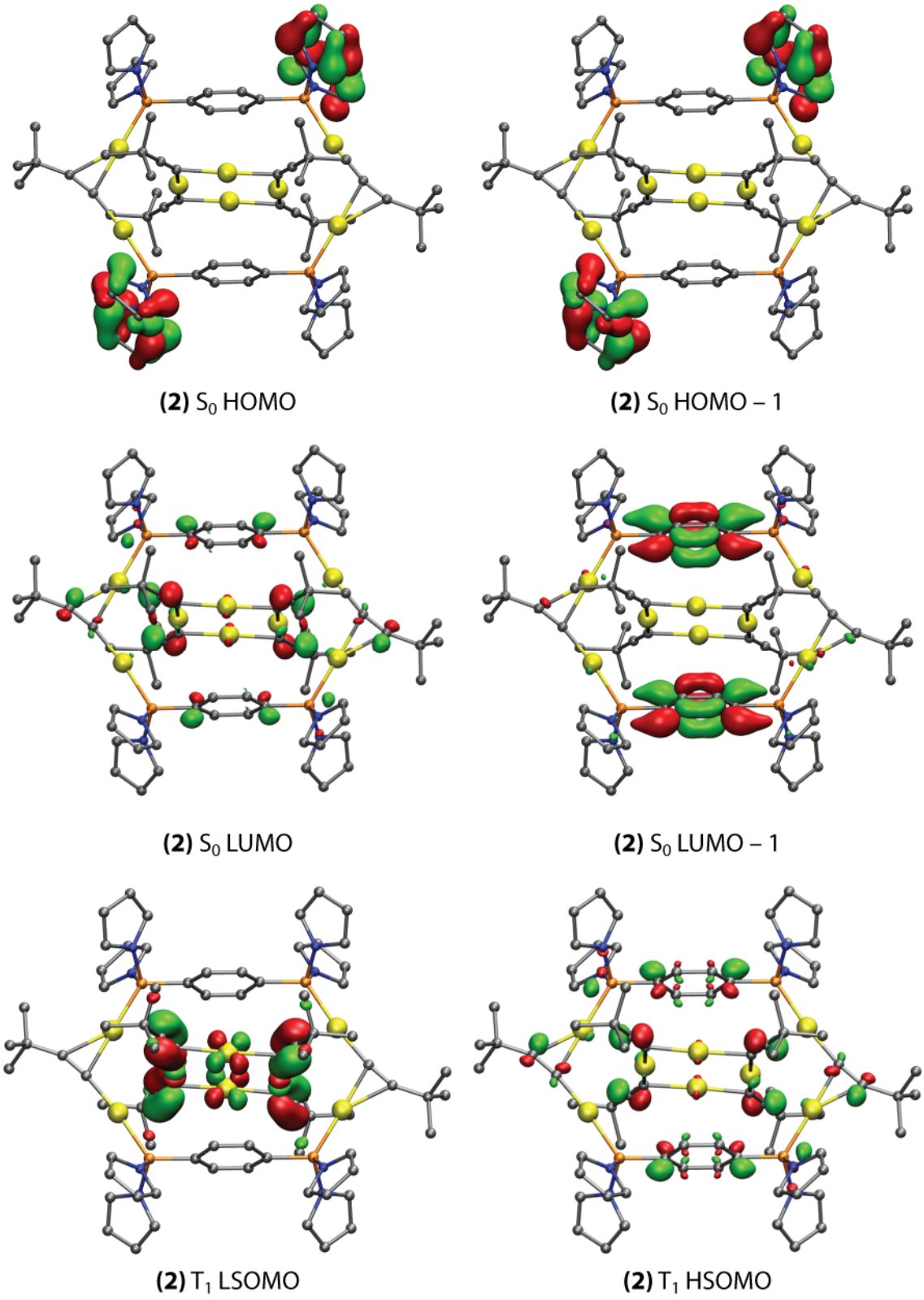

Figure S8. Frontier molecular orbital isodensity plots for complex **2** (isodensity value 0.04 a.u.). Hydrogen atoms omitted for clarity.

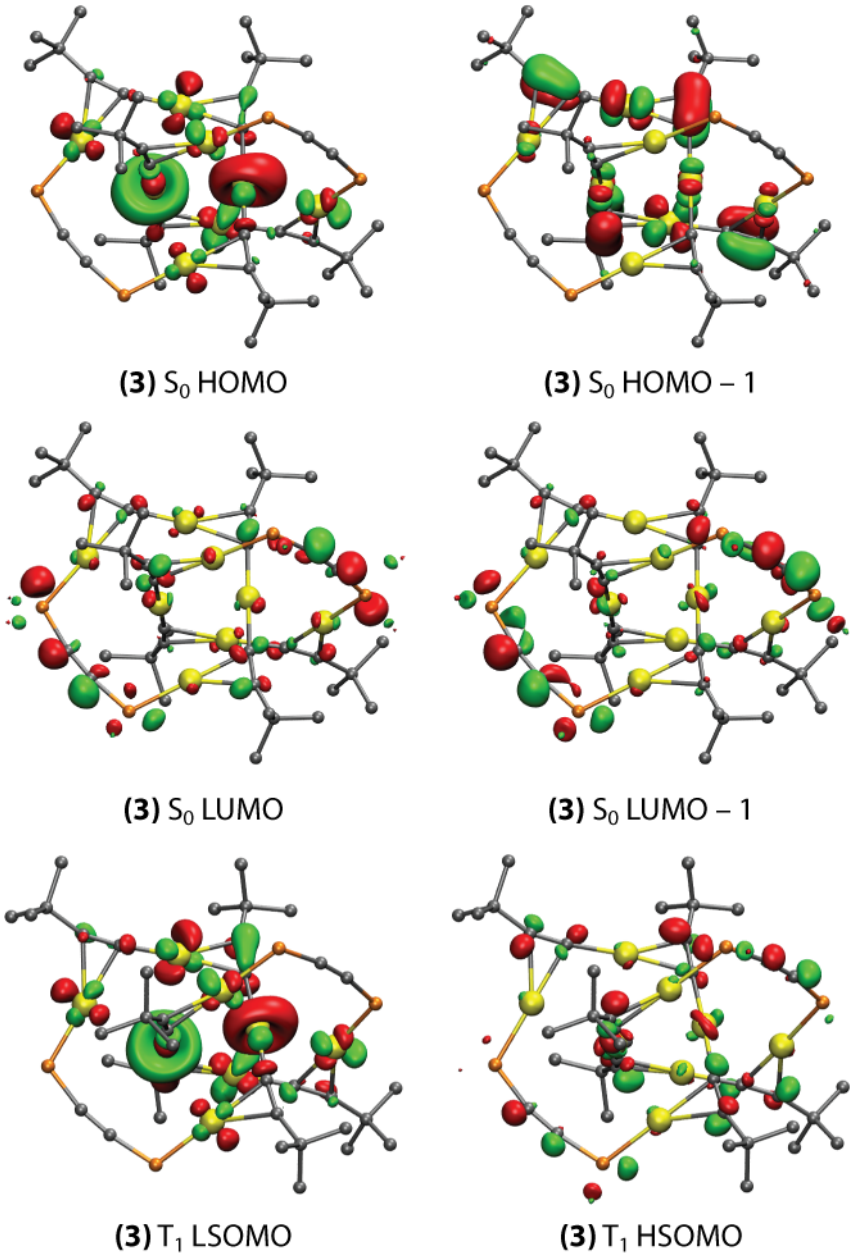

Figure S9. Frontier molecular orbital isodensity plots for complex **3** (isodensity value 0.04 a.u.). Hydrogen atoms and diphosphine-based phenyl rings omitted for clarity.

Table S3. Selected bond lengths [Å] for the complex **1** at 296 K and 100 K.

	100 K	**296 K**
Au(1)-P(2)	2.268(2)	2.274(2)
Au(2)-P(1)	2.285(2)	2.290(2)
Au(1)-Au(2)	3.3075(5)	3.3363(5)
Au(1)-Au(3)	2.8987(5)	2.9034(5)
Au(2)-Au(3)	2.9143(5)	2.9415(5)
Au(3)-Au(4´)	3.0165(6)	3.0767(5)
Au(3)-Au(4)	3.3751(5)	3.3126(5)

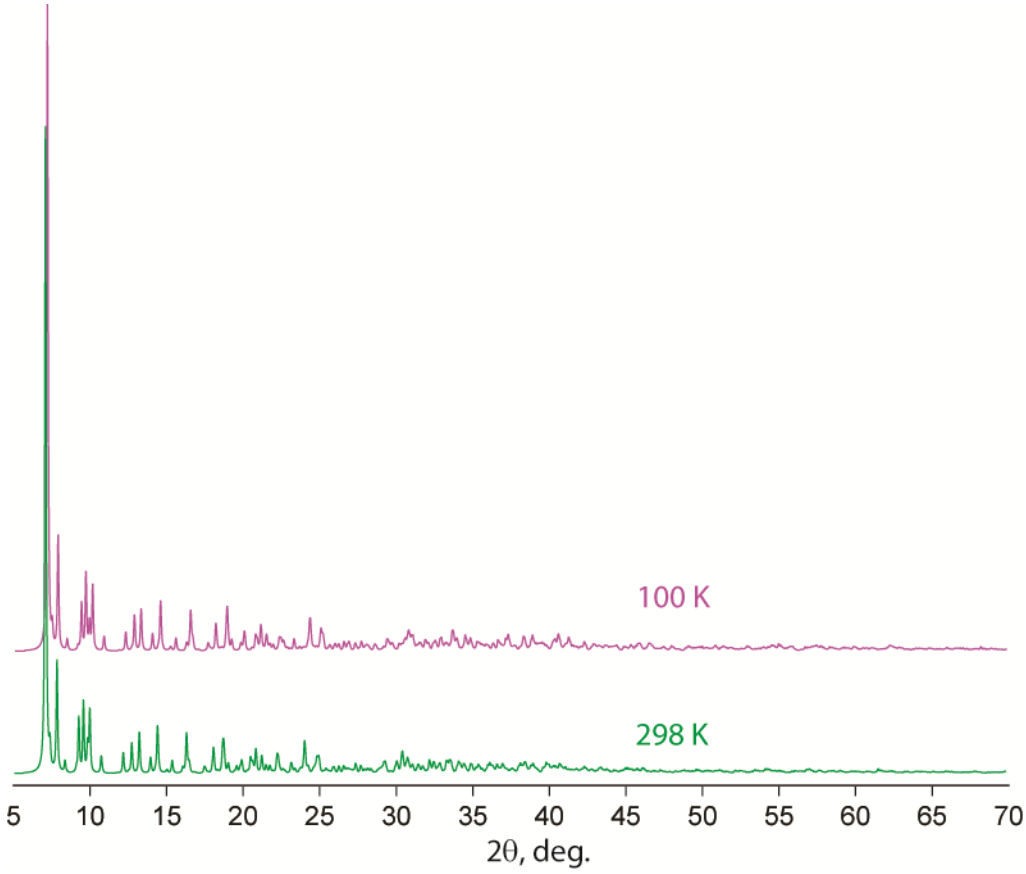

Figure S10. Powder XRD spectra of complex **1** calculated from the single crystal data.

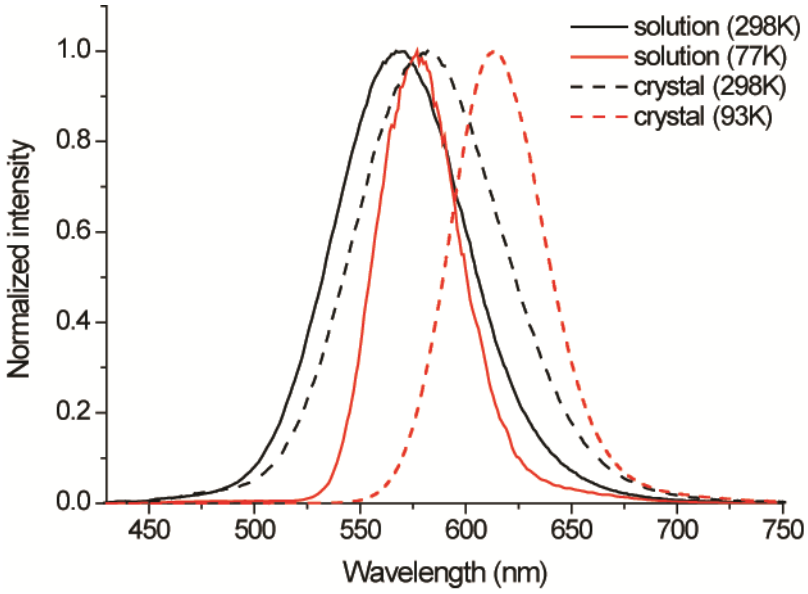

Figure S11. The emission spectra of **2** in solution (CH_2Cl_2) at room temperature and 77K.

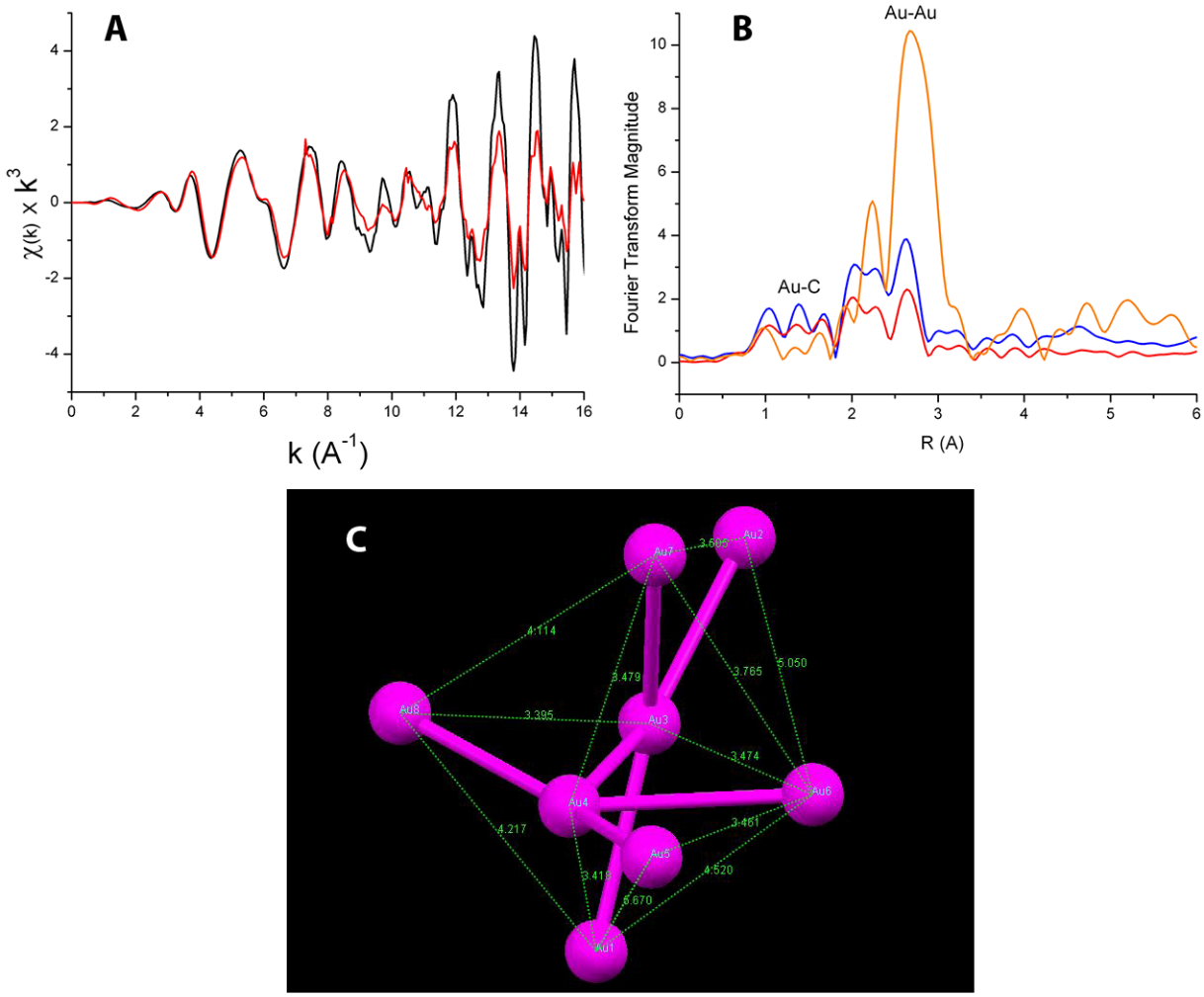

Figure S12. **A:** EXAFS measurements for **3** in terms of k space value in crystalline (red) amorphous (black) form; around 12-15($Å^{-1}$) oscillates stronger in amorphous sample (c.f. the crystal sample). **B:** upon converting (Fourier transform) to RDF plot, (red) crystalline, (blue) amorphous form. For comparison, the data for bulk Au foil is shown in orange color. **C:** only Au atoms are shown to calculate the interatomic distances in Au-complex **3**.

References

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Optimized cartesian coordinates of the studied systems in atomic units (BP86 level of theory).

$[Au_8(C_2Bu^t)_6(PPh_2C_6H_4PPh_2)_2]^{2+}$ (1)

8.37821785014327	2.98478092757604	0.00000000000000	au
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3.88650354159654	-0.43614639152222	0.00000000000000	au
0.00000000000000	0.00000000000000	-3.68508389226148	au
5.93460907766256	-7.51955678470084	0.00000000000000	p
-6.42195165032186	-6.95984055125459	0.00000000000000	p
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10.50608406994831	-0.18983934931042	0.00000000000000	c
2.44587775517480	-7.22188005446969	0.00000000000000	c
1.09197630988700	-7.09466981019845	2.29627837167820	c
-1.56039708347545	-6.98321445279193	2.29575443542562	c
-2.92167426100125	-6.99918030534758	0.00000000000000	c
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5.13350528988174	-0.45309455039351	5.97335690352069	c
3.93431245937664	-0.41729820506087	-3.92833547948226	c
5.13350528988174	-0.45309455039351	-5.97335690352069	c
6.53781604646800	-0.45392001510014	-8.37030974429407	c
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5.81900061109197	-2.81689697161336	-9.95222575289341	c
9.40893398563732	-0.50879692123501	-7.74839162634467	c
6.53781604646800	-0.45392001510014	8.37030974429407	c
5.90253861800964	1.98684233750958	9.87179856548039	c
9.40893398563732	-0.50879692123501	7.74839162634467	c
5.81900061109197	-2.81689697161336	9.95222575289341	c
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0.00000000000000	0.00000000000000	3.68508389226148	au
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4.44362597599555	11.75171468693644	2.33167090923875	h
9.12597194943739	11.85499001246764	6.81250182037735	c
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-8.44935439904369	13.68414537979842	8.64100765628393	h

$[Au_8(C_2Bu^t)_6\{P(NC_4H_4)_2C_6H_4P(NC_4H_4)_2\}_2]^{2+}$ (2)

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0.00000000000000	0.00000000000000	3.73479612161549	au
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$[Au_8(C_2Bu^t)_6(PPh_2C_2PPh_2)_2]^{2+}$ (3)

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