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Supplementary Information

A stimuli responsive Au(I) complex based on aminomethylphosphine template: synthesis, crystalline phases and luminescent properties.

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General comments

All solvents were purified according with the common procedures[1] and were kept under molecular sieves 4Å. The 1,5-bis(p-tolyl)-3,7-bis(pyridine-2-yl)-1,5-diaza-3,7-diphosphacyclooctane (***PNNP***) was synthesized by the published method[2] under argon atmosphere. All manipulations with complex **1** were carried out under normal conditions without inert atmosphere. After manipulations no oxidized compounds were detected. Solution ^{1}H and ^{31}P NMR spectra were recorded on Bruker Avance 400 spectrometer. Mass spectra were recorded on a Bruker micrOTOF 10223 instrument in the ESI^{+} mode. Elemental analyses were carried out with Eurovector Euro-EA3028-HT.

Synthetic procedure for 1 preparation

To a solution of [Au(tht)Cl] (132 mg, 0.4 mmol) in dichloromethane (15 ml) a solution of ***PNNP*** (100 mg, 0.2 mmol) in dichloromethane was added. Reaction mixture was stirred for 0.5 h at room temperature in the absence of light, after that a white precipitate was formed. Precipitate was filtered, washed with dichloromethane 3×10 ml, and recrystallized from the same solvents. Yield: 165 mg (87%).

Anal. calc. for $C_{28}H_{30}N_4P_2Au_2Cl_2$ [949.5]: C 35.42, H 3.19, N 5.90, P 6.53, Au 41.49, Cl 7.47. Found: C 35.41, H 3.05, N 5.6, P 6.62 Au 41.42, Cl 7.34. NMR ^{1}H ($CDCl_3$, room temperature): 8.79 (d, $^{3}J_{HH}$ 4.6 Hz, 2H, H^2); 8.08 (m, $^{3}J_{HH}$ 6.9 Hz, $^{3}J_{HH}$ 7.6 Hz, 2H, H^5); 7.78 (dd, $^{3}J_{HH}$ 7.6 Hz, $^{3}J_{HH}$ 6.1 Hz, 2H, H^4); 7.44 (dd, $^{3}J_{HH}$ 6.1 Hz, $^{3}J_{HH}$ 4.6 Hz, 2H, H^3); 7.09 (d, $^{3}J_{HH}$ 8.5 Hz, 4H, H^6), 6.96 (d, $^{3}J_{HH}$ 8.5 Hz, 4H, H^7); 4.94 (d, $^{2}J_{HH}$ 15.6 Hz, $^{3}J_{PH} \sim 2.0$ Hz, 4H, H^1); 4.59 (d, $^{2}J_{HH}$ 15.6 Hz, 4H, H^1); 2.26 (s, 6H, CH_3). NMR ^{31}P $\{^{1}H\}$ ($CDCl_3$, room temperature): 9.93 ppm.

Photophysical measurements

Absorption spectra were recorded using a Lambda 1050 and Shimadzu UV 1800 spectrophotometers; excitation and emission spectra in solution and solid-state were measured on Fluoromax 3 and Fluorolog 4 spectrofluorimeters. LED (maximum of emission at 265 nm, 340 nm and 390 nm) were used in pulse mode to pump luminescence in lifetime measurements (pulse width 0.9 nm, repetition rate 100 Hz to 10 kHz). The integration sphere was used to measure the solid state emission quantum yield for the complexes **1a-c**.

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1 Wilfred L.F. Armarego and Christina Li Lin Chai, *Purification of Laboratory Chemicals*, 6th Edition, 2009 Elsevier Inc.

2 E.I. Musina, V.V. Khrizanforova, I.D. Strelnik, M.I. Valitov, Y.S. Spiridonova, D.B. Krivolapov, I.A. Litvinov, M.K. Kadirov, P. Lonnecke, E. Hey-Hawkins, Y.H. Budnikova, A.A. Karasik and O.G. Sinyashin, *Chem.-Eur. J.* 2014, **20**, 3169.

Crystalline phases transformation

Recrystallization. The phase **1a** was obtained by the recrystallization of obtained dry powder of **1** from dichloromethane (DCM). The phase **1b** was obtained by the recrystallization of **1a** from acetone. The recrystallization of **1a** or **1b** from the mixture of DCM/acetone gives the phase **1c**. The phase **1b** was also obtained by the recrystallization of **1c** from pure acetone while **1a** resulted due to the recrystallization of **1b−c** from pure DCM.

Vapors treatment. The treatment of the powders of **1a** and **1c** with acetone vapors results in changing the color of emission to that of **1b**. The treatment of **1b** with the vapors of DCM returns the color of emission to that of **1a**.

Crystallographic data for 1a-c

Single crystals of **1** suitable for X-ray analysis were grown from dichloromethane (**1a**), from acetone (**1b**), from acetone/dichloromethane mixture (**1c**). Single crystals of **1c** were also grown after careful recrystallization of **1b** from acetone/dichloromethane mixture.

Crystal structures of **1a**, **1b** and **1c** were determined by the means of single crystal X-ray diffraction analysis. Crystal of **1a** was fixed on a micro mount, placed on Rigaku Oxford Diffraction Supernova Atlas diffractometer and measured at a temperature of 100K using microfocused monochromated Cu$K\alpha$ radiation. Crystals of **1b** and **1c** were fixed on a micro mounts, placed on a Rigaku Oxford Diffraction Excalibur Eos diffractometer and measured at a temperature of 100K using monochromated Mo$K\alpha$ radiation. The unit cell parameters and refinement characteristics for the crystal structures of **1a** – **1c** are given in the Table S1. The unit cell parameters of **1a** were determined and refined by the least-squares techniques on the basis of 25914 reflections with 2θ in the range of 6.23–152.23°. From the systematic absences and statistics of reflection distribution, the space group $P2/c$ was determined. The structure was solved by direct methods and refined to $R_1 = 0.044$ ($wR_2 = 0.109$) for 3895 reflections with $|F_o| \geq 4\sigma F$ using the *SHELXL*-97 program[3] incorporated in the *OLEX2* program package.[4] The unit cell parameters of **1b** were determined and refined by the least-squares techniques on the basis of 13247 reflections with 2θ in the range of 5.99–54.99°. From the systematic absences and statistics of reflection distribution, the space group $P2/c$ was determined. The structure was solved by direct methods and refined to $R_1 = 0.026$ ($wR_2 = 0.047$) for 3217 reflections with $|F_o| \geq 4\sigma F$ using the *SHELXL*-97 program[3] incorporated in the *OLEX2* program package.[4] The unit cell parameters of **1c** were determined and refined by the least-squares techniques on the basis of 10227 reflections with 2θ in the range of 5.66–51.99°. From the systematic absences and statistics of reflection distribution, the space group $C2/m$ was determined. The structure was solved by direct methods and refined to $R_1 = 0.035$ ($wR_2 = 0.082$) for 3325

3 G.M. Sheldrick, *Acta Cryst.*, 2008, A**64**, 112.

4 O.V. Dolomanov, L.J. Bourhis, R.J. Gildea, J.A.K. Howard, H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339.

reflections with $|F_o| \geq 4\sigma F$ using the *SHELXL*-97 program[3] incorporated in the *OLEX2* program package.[4] The final models included coordinates and anisotropic displacement parameters for all non-hydrogen atoms. The carbon-bound H atoms were placed in calculated positions and were included in the refinement in the 'riding' model approximation, with U_{iso}(H) set to 1.5U_{eq}(C) and C–H 0.96 Å for the CH_3 groups, U_{iso}(H) set to 1.2U_{eq}(C) and C–H 0.97 Å for the CH_2 groups, U_{iso}(H) set to 1.2U_{eq}(C) and C–H 0.98 Å for the tertiary CH groups and U_{iso}(H) set to 1.2U_{eq}(C) and C–H 0.93 Å for the CH groups in cyclic fragments. Empirical absorption correction for **1a** and **1b** was applied in CrysAlisPro[5] program complex using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. Analytical numeric absorption correction for **1c** was applied in the CrysAlisPro[5] program using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid.[6] The unit cell of **1a**·3CH_2Cl_2 contains disordered dichloromethane molecules that have been treated as a diffuse contribution to the overall scattering without specific atom positions by SQUEEZE/PLATON.[7] The total approximate amount of solvent molecules in the structural model of **1a** has been calculated taking into account the Electron Count of 283 and a Total Potential Solvent Accessible Void Volume of 589.4 *e*/Å^3. Supplementary crystallographic data for this paper have been deposited at Cambridge Crystallographic Data Centre (CCDC 1030853, 1027244 and 1027245 for **1a**, **1b** and **1c**, respectively) and can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

Computational details

Density functional theory (DFT) calculations were performed with B3LYP hybrid functional.[8] Stuttgart/Dresden effective core potential (MWB60) with the corresponding basis set was used for Au atoms;[9] 6-31G* basis set was chosen for all other atoms. Media effects were considered in the framework of the integral equation formalism for the polarizable continuum model (IEF-PCM)[10] with acetone as solvent. All calculations were carried out using the Gaussian 09 package.[11]

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5 CrysAlisPro, Agilent Technologies, Version 1.171.36.20 (release 27-06-2012).

6 Clark, R.C. and J.S. Reid, *Acta Crystallogr. A*, 1995, **51**, 887.

7 A.L. Spek, *PLATON*, Utrecht University, Utrecht, The Netherlands, 2005.

8 (a) Becke A.D., *J. Chem. Phys.* 1993, **98**, 5648; (b) Lee C.T., Yang W.T., Parr R.G., *Phys. Rev. B* 1988, **37**, 785; (c) Stephens P.J., Devlin F.J., Chabalowski C.F., Frisch M.J., *J. Phys. Chem.* 1994, **98**, 11623.

9 Andrae D., Häußermann U., Dolg M., Stoll H., Preuß H., *Theor. Chim. Acta* 1990, **77**, 123.

10 Scalmani G., Frisch M.J., *J. Chem. Phys.* 2010, **132**, 114110.

11 Frisch M.J., Trucks G.W., Schlegel H.B., Scuseria G.E., Robb M.A., Cheeseman J.R., Scalmani G., Barone V., Mennucci B., Petersson G.A., Nakatsuji H., Caricato M., Li X.,Hratchian H.P., Izmaylov A.F., Bloino J., Zheng G., Sonnenberg J.L., Hada M., Ehara M., Toyota K., Fukuda R., Hasegawa J., Ishida M., Nakajima T., Honda Y., Kitao O., Nakai H., Vreven T., Montgomery J.A., Peralta J.E., Ogliaro F., Bearpark M., Heyd J.J., Brothers E., Kudin K.N., Staroverov V.N., Kobayashi R., Normand J., Raghavachari K., Rendell A., Burant J.C., Iyengar S.S., Tomasi J., Cossi M., Rega N., Millam J.M., Klene M., Knox J.E., Cross J.B., Bakken V., Adamo C., Jaramillo J., Gomperts R., Stratmann R.E., Yazyev O., Austin A.J., Cammi R., Pomelli C., Ochterski J.W., Martin R.L., Morokuma K., Zakrzewski V.G., Voth G.A., Salvador P., Dannenberg J.J.,

Geometry optimizations were performed for free ***PNNP*** ligand and complex **1**, using one or two acetone molecules to model the environment of the complex in **1b** and **1c** phases. However, since the acetone molecules in **1b** and **1c** are not coordinated ligands, full geometry optimizations for these species did not result in structures resembling those obtained from XRD. In order to obtain a more realistic computational representation of structures of the complexes studied in this work, we used constrained geometry optimizations in which Au and P atoms, as well as C and O the atoms constituting the CO group in acetone molecules, were fixed at their crystallographic positions. Such calculations were carried out for the ground singlet states of complex **1** without acetone molecules (model of **1a** phase), with two acetone molecules (**1b**), and with one acetone molecule (**1c**). The excited states of the species under investigation were further studied by time-dependent DFT (TDDFT) calculations.

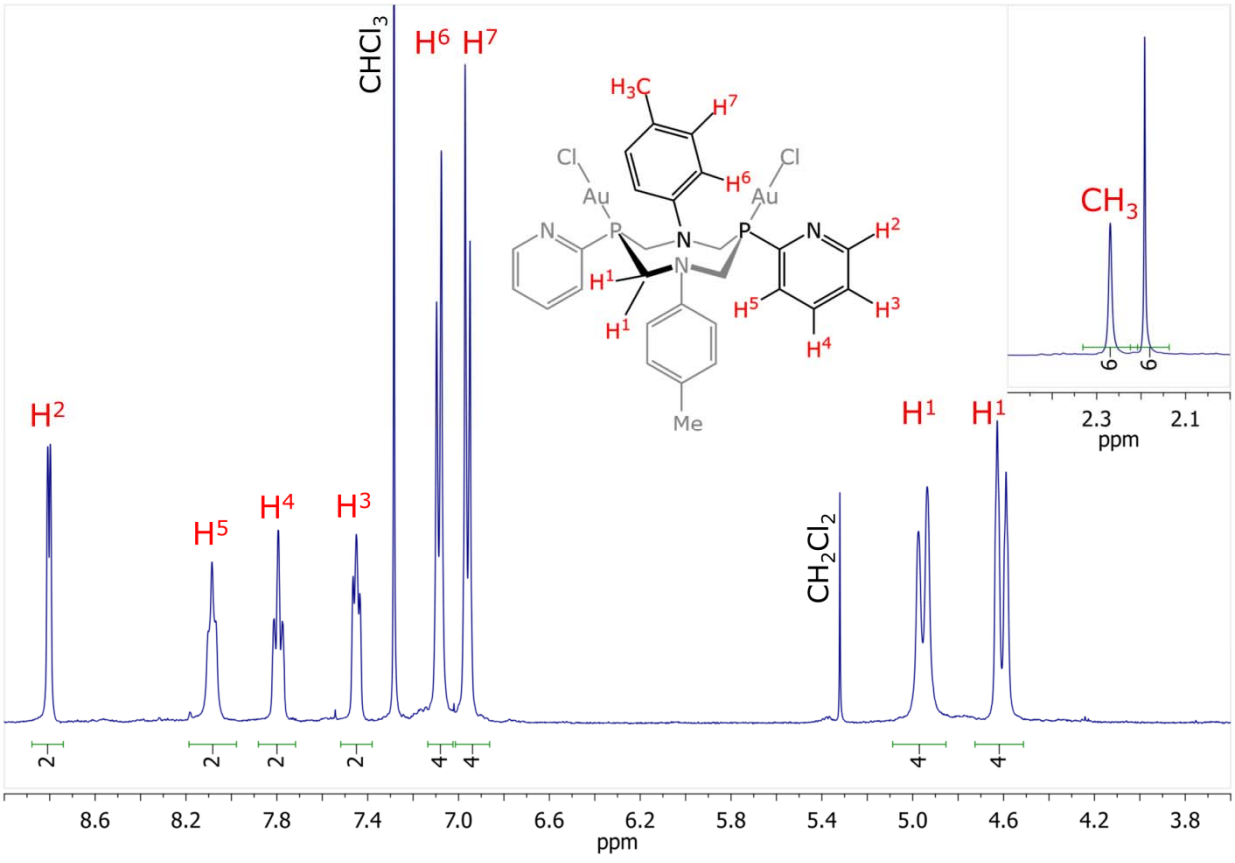

Figure S1. ^{1}H NMR spectra of **1** in $CDCl_3$ solution at room temperature.

Dapprich S., Daniels A.D., Farkas O., Foresman J.B., Ortiz J.V., Cioslowski J., Fox D.J., *Gaussian 09, Revision C.01* 2009.

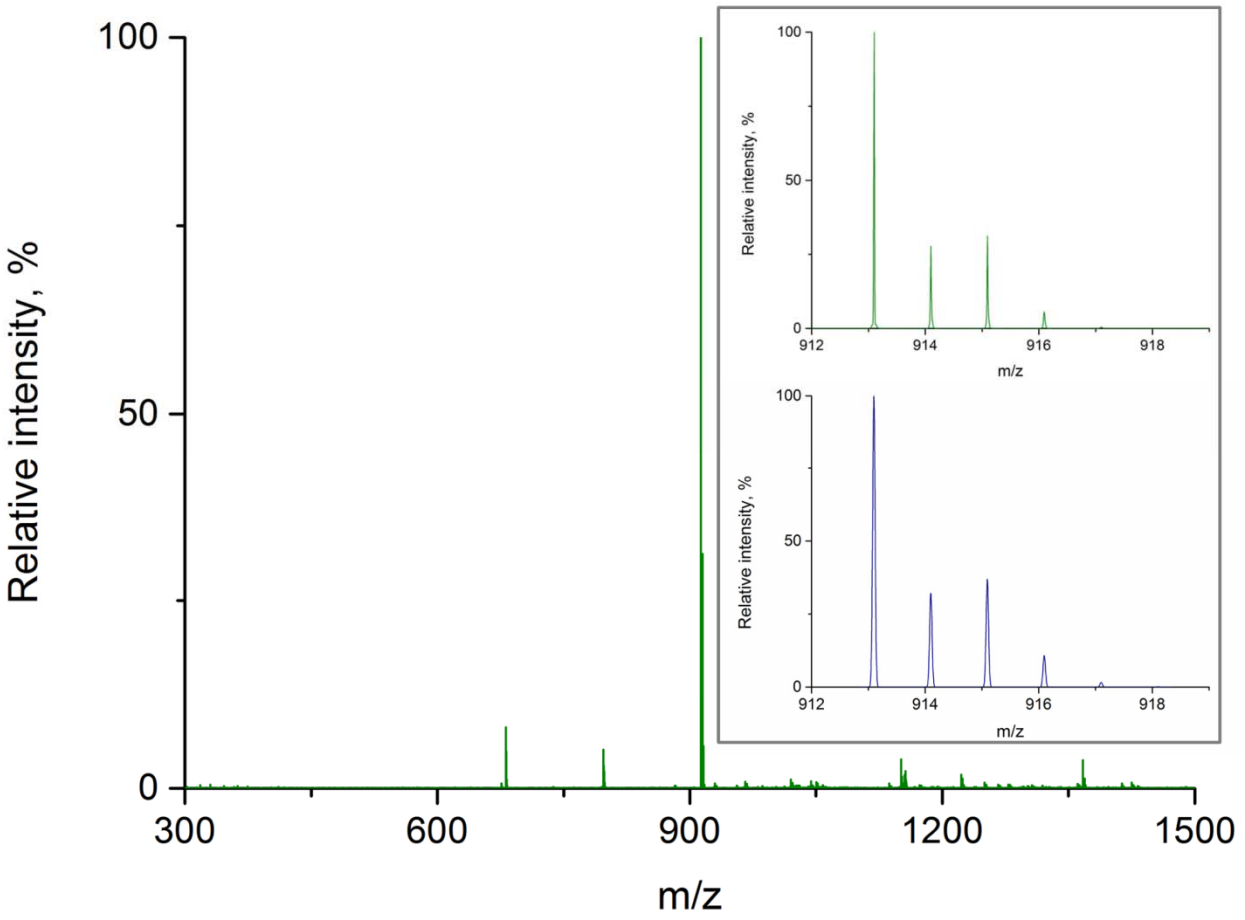

Figure S2. ESI$^+$ MS spectrum of **1** (green − experimental spectrum, navy − simulated signal with *m/z* 913.10 [***PNNP***$Au_2Cl]^+$ = M – Cl^-).

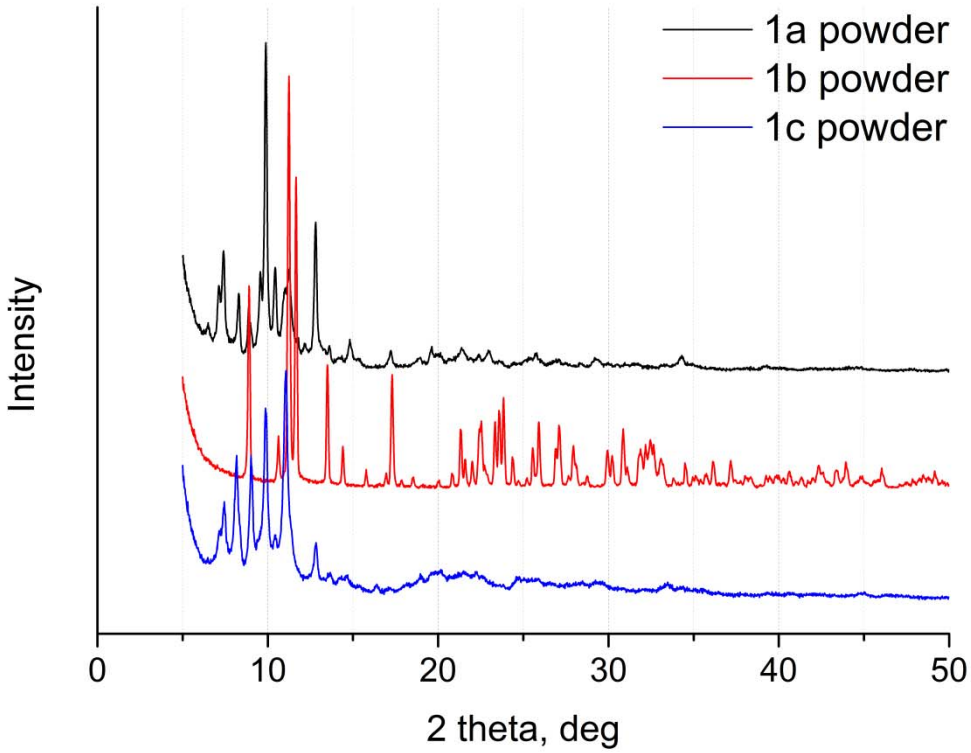

Figure S3. Experimental PXRD patterns for **1a-c**.

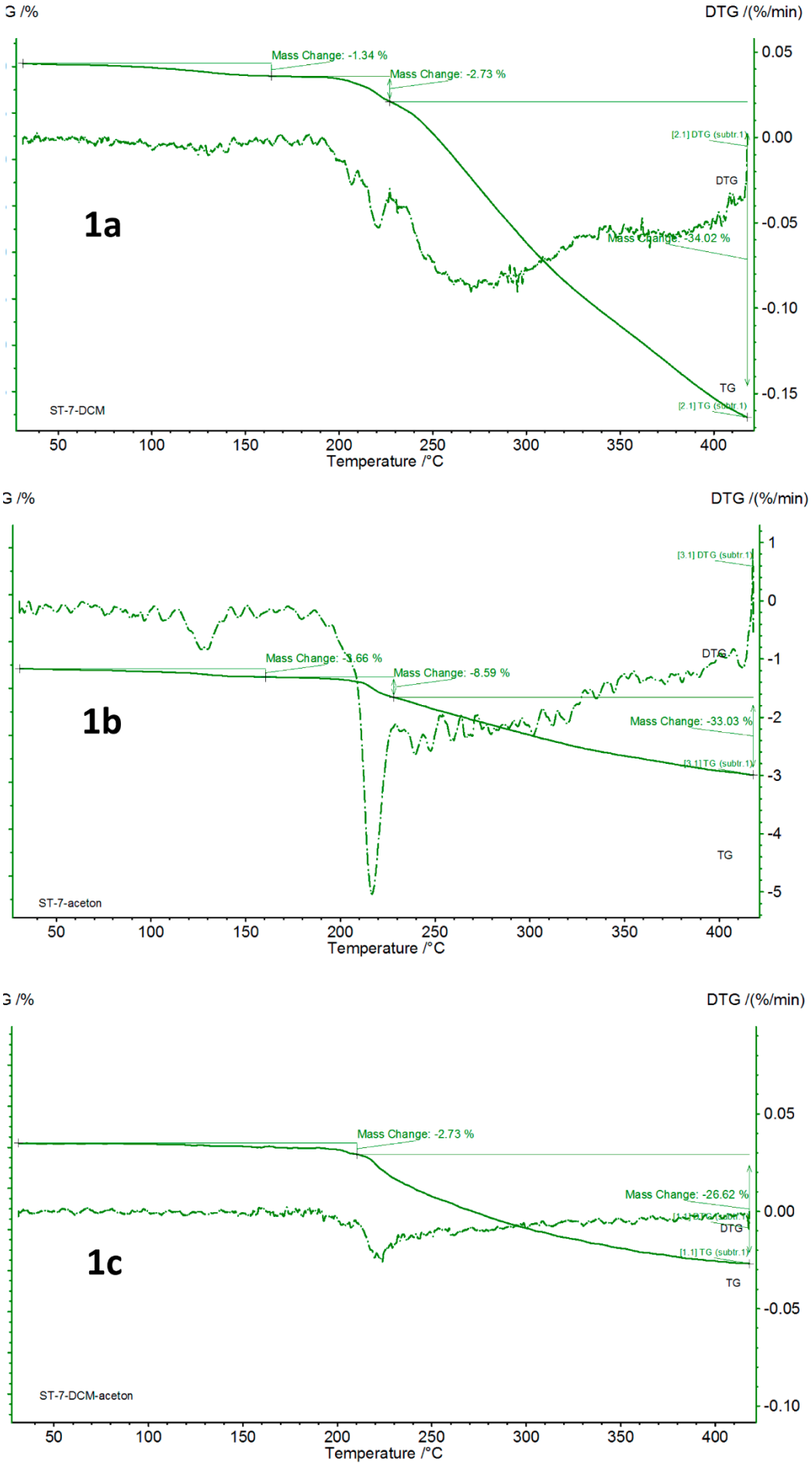

Figure S4. Thermal analysis (TGA and DTG) for **1a-c**.

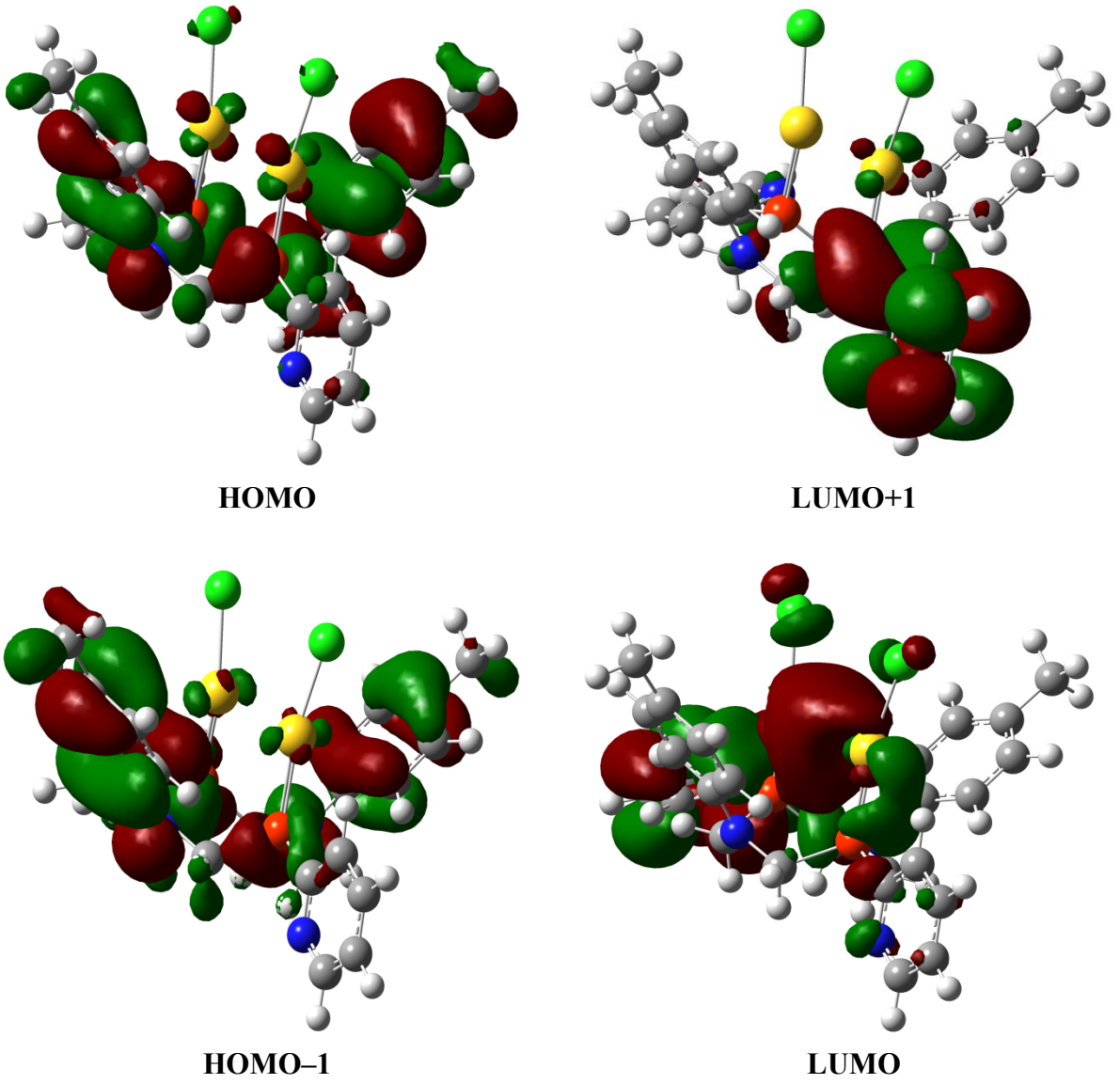

Figure S5. Highest occupied and lowest vacant molecular orbitals for complex **1** without acetone molecules.

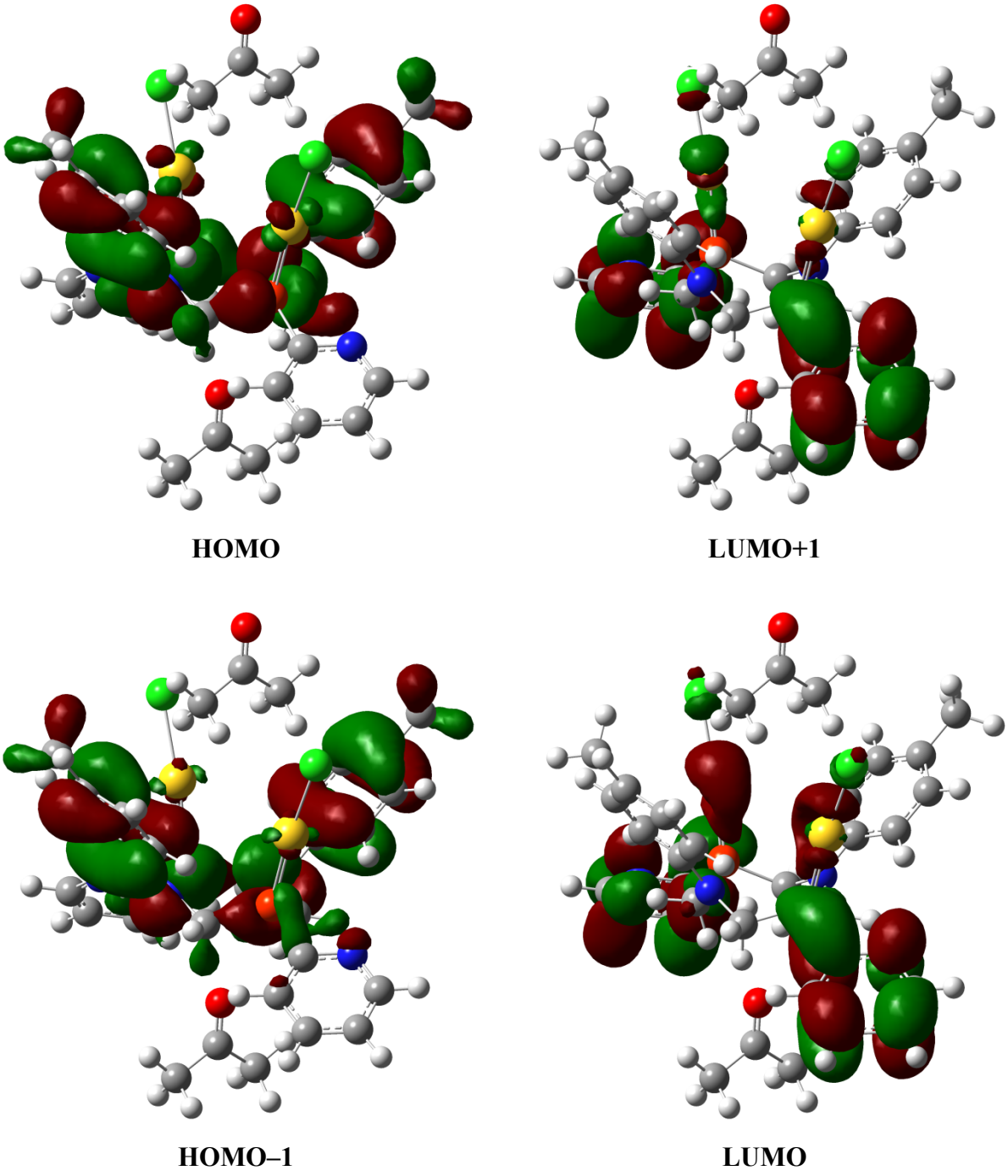

Figure S6. Highest occupied and lowest vacant molecular orbitals for complex **1** with two acetone molecules. Solvent molecules are fixed at their crystallographic positions in **1b** phase.

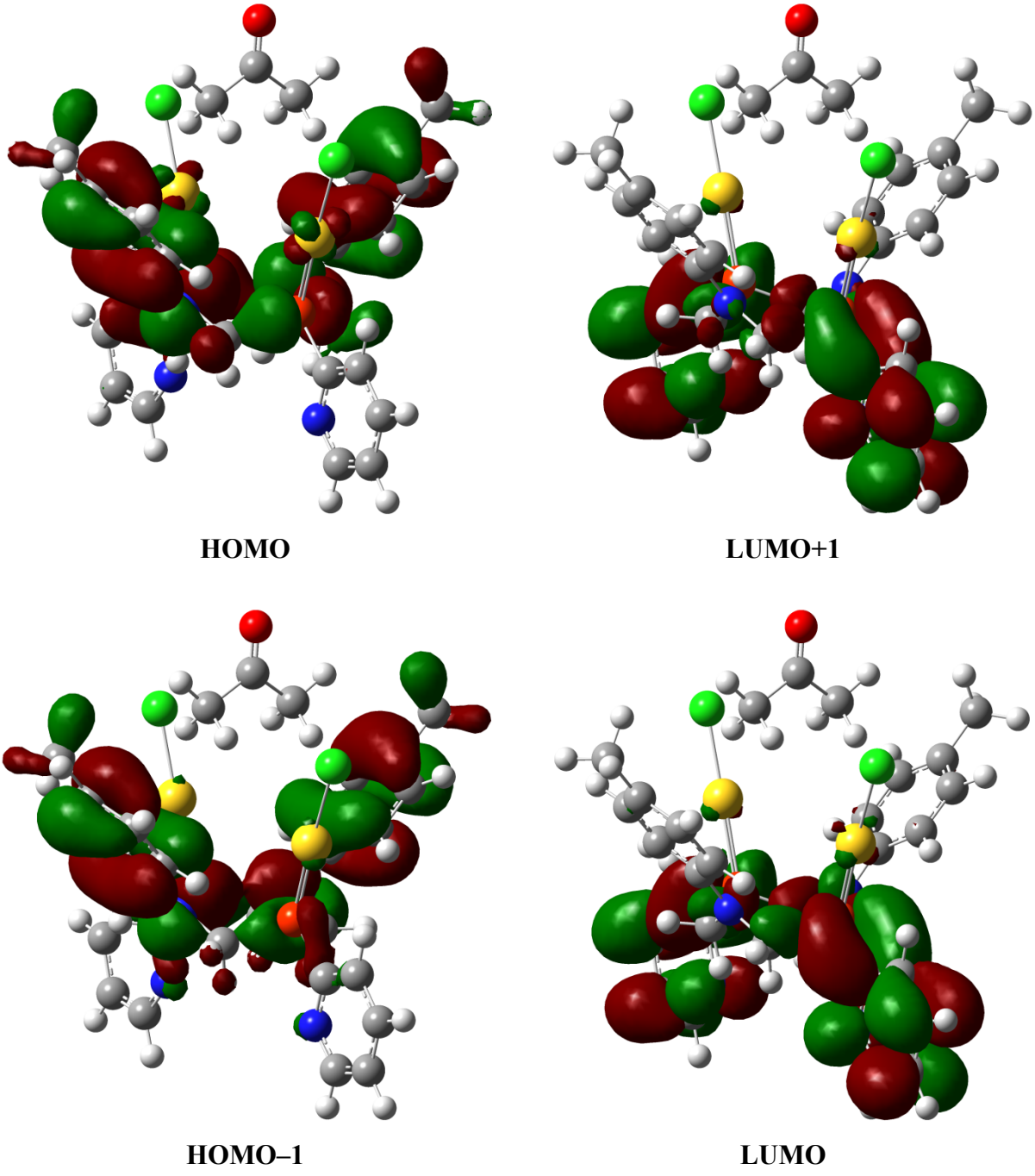

Figure S7. Highest occupied and lowest vacant molecular orbitals for complex **1** with one acetone molecule. Solvent molecule is fixed at its crystallographic position in **1c** phase.

Table S1. Crystallographic data for **1**.

Compound	1a	1b	1c
Formula	$C_{28}H_{30}Au_2Cl_2N_4P_2$, $3(CH_2Cl_2)$*	$C_{28}H_{30}Au_2Cl_2N_4P_2$, C_3H_6O	$C_{28}H_{30}Au_2Cl_2N_4P_2$, $2(C_3H_6O)$
Crystal System	Monoclinic	Monoclinic	Monoclinic
a (Å)	15.3277(5)	8.8698(2)	24.029(4)
b (Å)	8.8720(2)	10.6900(3)	16.9105(16)
c (Å)	14.8008(6)	17.5273(5)	12.0433(18)
α (°)	90	90	90
β (°)	112.309(4)	96.988(3)	124.55(2)
γ (°)	90	90	90
V (Å^3)	1862.06(12)	1649.56(8)	4030.5(13)
Molecular weight	949.33	1007.41	1065.49
Space group	*P*2/*c*	*P*2/*c*	*C*2/*m*
μ (mm^{-1})	16.892	9.174	7.516
Temperature (K)	100(2)	100(2)	100(2)
Z	2	2	4
D_{calc} (g/cm^3)	1.693	2.028	1.756
Crystal size (mm^3)	0.16 × 0.10 × 0.02	0.23 × 0.18 × 0.12	0.20 × 0.19 × 0.11
Radiation	Cu*K*α	Mo*K*α	Mo*K*α
Total reflections	25914	13247	10227
Unique reflections	3895	3693	4098
Angle range 2θ (°)	6.23–152.23	5.99–54.99	5.66–51.99
Reflections with $\|F_o\| \geq 4\sigma_F$	3347	3217	3325
R_{int}	0.0914	0.0372	0.0336
R_σ	0.0487	0.0382	0.0505
R_1 ($\|F_o\| \geq 4\sigma_F$)	0.0444	0.0262	0.0352
wR_2 ($\|F_o\| \geq 4\sigma_F$)	0.1093	0.0472	0.0820
R_1 (all data)	0.0508	0.0342	0.0490
wR_2 (all data)	0.1137	0.0494	0.0879
S	1.052	1.053	1.057
ρ_{min}, ρ_{max}, e/Å^3	–2.653, 2.124	–0.792, 0.750	–1.412, 3.106
CCDC	1030853	1027244	1027245

$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; $w = 1/[\sigma^2(F_o^2)+(aP)^2 + bP]$, where $P = (F_o^2 + 2F_c^2)/3$; $s = \{\Sigma[w(F_o^2 - F_c^2)]/(n - p)\}^{1/2}$ where n is the number of reflections and p is the number of refinement parameters.

* The unit cell of **1a**·3CH_2Cl_2 contains disordered dichloromethane molecules that have been treated as a diffuse contribution to the overall scattering without specific atom positions by SQUEEZE/PLATON. The total approximate amount of solvent molecules in the structural model of **1a** has been calculated taking into account the Electron Count of 283 and a Total Potential Solvent Accessible Void Volume of 589.4 e/Å^3.

Table S2. PXRD data for the crystalline phase **1a**.

Measurement conditions			
X-Ray	30 kV, 10 mA	Scan speed / Duration time	1.0000
Goniometer	–	Step width	0.0202 deg
Attachment	–	Scan axis	2Theta
Filter	–	Scan range	5.0017–84.9923 deg
CBO selection slit	–	Incident slit	–
Diffrected beam mono.	–	Length limiting slit	–
Detector	–	Receiving slit #1	–
Scan mode	STEP	Receiving slit #2	–

Qualitative analysis results				
Phase name	**Formula**	**Figure of merit**	**Phase reg. detail**	**DB card number**
	C31H36Au2Cl2N4OP2	1.606	CIF file	–
Phase name	**Formula**	**Space group**	**Phase reg. detail**	**DB card number**
	C31H36Au2Cl2N4OP2	13: P12/c1, unique – b, cell – 1	CIF file	–

Peak list					
##	**2 theta (deg)**	**d (ang)**	**Phase name**	**Chemical formula**	**Rel. int. I (a.u.)**
1	4.4(3)	19.9(13)	Unknown	Unknown	100.00
2	6.55(3)	13.49(6)	Unknown	Unknown	1.02
3	7.099(9)	12.443(16)	Unknown	Unknown	2.45
4	7.398(7)	11.940(12)	Unknown	Unknown	16.81
5	8.295(7)	10.651(10)	(0,1,0)	C31H36Au2Cl2N4OP2	5.86
6	8.876(7)	9.954(8)	Unknown	Unknown	4.30
7	9.563(8)	9.241(7)	Unknown	Unknown	8.27
8	9.884(3)	8.941(3)	(0,1,1)	C31H36Au2Cl2N4OP2	24.96
9	10.430(5)	8.474(4)	Unknown	Unknown	6.01
10	11.028(13)	8.016(9)	Unknown	Unknown	8.97
11	11.245(6)	7.862(4)	Unknown	Unknown	6.53
12	11.782(11)	7.505(7)	Unknown	Unknown	1.31

13	12.143(15)	7.283(9)	Unknown	Unknown	0.70
14	12.807(3)	6.9067(16)	Unknown	Unknown	10.55
15	13.22(7)	6.69(3)	(1,1,0)	C31H36Au2Cl2N4OP2	1.99
16	13.622(15)	6.495(7)	(1,1,–1)	C31H36Au2Cl2N4OP2	0.57
17	14.31(5)	6.19(2)	(1,1,1)	C31H36Au2Cl2N4OP2	0.35
18	14.820(13)	5.973(5)	Unknown	Unknown	1.75
19	15.32(4)	5.778(16)	(1,0,2)	C31H36Au2Cl2N4OP2	1.87
20	17.224(14)	5.144(4)	(1,1,2)	C31H36Au2Cl2N4OP2	2.36
21	18.956(18)	4.678(4)	(1,1,–3)	C31H36Au2Cl2N4OP2	1.33
22	19.595(15)	4.527(3)	(1,2,0)	C31H36Au2Cl2N4OP2	1.59
23	20.147(11)	4.404(2)	(1,2,–1)	C31H36Au2Cl2N4OP2	1.91
24	20.61(5)	4.305(9)	(1,2,1)	C31H36Au2Cl2N4OP2	1.06
25	21.447(19)	4.140(4)	(1,1,3)	C31H36Au2Cl2N4OP2	3.94
26	22.411(14)	3.964(2)	Unknown	Unknown	0.79
27	23.031(6)	3.8586(10)	(0,2,3)	C31H36Au2Cl2N4OP2	1.97
28	23.643(17)	3.760(3)	(2,0,2)	C31H36Au2Cl2N4OP2	0.40
29	25.812(11)	3.4488(15)	(0,3,0)	C31H36Au2Cl2N4OP2	3.77
30	27.06(3)	3.293(3)	(0,2,4)	C31H36Au2Cl2N4OP2	1.87
31	28.363(14)	3.1442(16)	(2,1,3)	C31H36Au2Cl2N4OP2	0.29
32	29.237(12)	3.0521(13)	(2,2,2)	C31H36Au2Cl2N4OP2	2.46
33	30(3098)	3(2)	(1,2,–3)	C31H36Au2Cl2N4OP2	0.00
34	30.52(3)	2.927(3)	(3,0,0)	C31H36Au2Cl2N4OP2	0.11
35	30.95(6)	2.887(6)	(0,2,5)	C31H36Au2Cl2N4OP2	0.22
36	31.74(4)	2.817(4)	(1,0,–6)	C31H36Au2Cl2N4OP2	0.68
37	33.34(8)	2.685(6)	(2,3,1)	C31H36Au2Cl2N4OP2	0.91
38	34.281(19)	2.6137(14)	(1,0,6)	C31H36Au2Cl2N4OP2	3.16
39	39.19(2)	2.2971(12)	(1,3,5)	C31H36Au2Cl2N4OP2	1.95
40	42.01(17)	2.149(8)	(3,2,–5)	C31H36Au2Cl2N4OP2	0.54
41	44.50(9)	2.034(4)	(0,5,1)	C31H36Au2Cl2N4OP2	3.62

Table S3. PXRD data for the crystalline phase **1b**.

Measurement conditions			
X-Ray	30 kV, 10 mA	Scan speed / Duration time	94.0000
Goniometer	–	Step width	0.0202 deg
Attachment	–	Scan axis	2Theta
Filter		Scan range	5.0017–84.9921 deg
CBO selection slit	–	Incident slit	–
Diffrected beam mono.		Length limiting slit	–
Detector		Receiving slit #1	–
Scan mode	STEP	Receiving slit #2	–

Qualitative analysis results				
Phase name	**Formula**	**Figure of merit**	**Phase reg. detail**	**DB card number**
	C31H36Au2Cl2N4OP2	1.780	CIF file	–
Phase name	**Formula**	**Space group**	**Phase reg. detail**	**DB card number**
	C31H36Au2Cl2N4OP2	13: P12/c1, unique – b, cell – 1	CIF file	–

Peak list

##	2 theta (deg)	d (ang)	Phase name	Chemical formula	Rel. int. I (a.u.)
1	8.9005(18)	9.927(2)	Unknown	Unknown	44.98
2	10.629(6)	8.317(5)	Unknown	Unknown	8.49
3	11.2307(15)	7.8723(11)	Unknown	Unknown	100.00
4	11.6578(15)	7.5848(10)	Unknown	Unknown	63.57
5	13.494(2)	6.5565(11)	(1,0,–2)	C31H36Au2Cl2N4OP2	25.09
6	14.397(5)	6.147(2)	(1,1,1)	C31H36Au2Cl2N4OP2	7.46
7	15.781(7)	5.611(2)	(1,1,–2)	C31H36Au2Cl2N4OP2	2.61
8	16.96(2)	5.223(7)	Unknown	Unknown	2.61
9	17.285(3)	5.1263(8)	(1,1,2)	C31H36Au2Cl2N4OP2	26.71
10	17.85(2)	4.965(7)	Unknown	Unknown	1.21
11	18.498(10)	4.793(2)	Unknown	Unknown	2.54
12	20.02(2)	4.432(5)	(2,0,0)	C31H36Au2Cl2N4OP2	1.21

13	20.807(10)	4.266(2)	Unknown	Unknown	2.66
14	21.314(4)	4.1655(7)	(1,2,−2)	C31H36Au2Cl2N4OP2	13.12
15	21.560(5)	4.1184(10)	(1,0,−4)	C31H36Au2Cl2N4OP2	5.22
16	21.983(6)	4.0401(10)	(0,1,4)	C31H36Au2Cl2N4OP2	5.00
17	22.395(6)	3.9667(10)	Unknown	Unknown	21.72
18	22.543(6)	3.9409(10)	(1,2,2)	C31H36Au2Cl2N4OP2	3.97
19	22.720(11)	3.9108(19)	Unknown	Unknown	4.40
20	23.325(4)	3.8106(7)	Unknown	Unknown	13.61
21	23.568(4)	3.7718(7)	(2,0,2)	C31H36Au2Cl2N4OP2	17.27
22	23.825(3)	3.7318(5)	(1,0,4)	C31H36Au2Cl2N4OP2	17.60
23	24.356(5)	3.6516(8)	Unknown	Unknown	6.23
24	24.658(4)	3.6075(6)	Unknown	Unknown	0.99
25	25.16(4)	3.536(5)	(2,1,2)	C31H36Au2Cl2N4OP2	1.29
26	25.5044(15)	3.4897(2)	(0,3,1)	C31H36Au2Cl2N4OP2	8.28
27	25.893(4)	3.4382(5)	Unknown	Unknown	15.46
28	26.878(4)	3.3144(5)	(0,1,5)	C31H36Au2Cl2N4OP2	7.38
29	27.083(4)	3.2898(5)	(0,3,2)	C31H36Au2Cl2N4OP2	16.48
30	27.655(12)	3.2230(14)	(1,1,−5)	C31H36Au2Cl2N4OP2	2.22
31	27.889(5)	3.1965(5)	Unknown	Unknown	9.89
32	28.080(7)	3.1752(7)	(2,1,3)	C31H36Au2Cl2N4OP2	4.10
33	28.52(4)	3.127(4)	(1,3,−2)	C31H36Au2Cl2N4OP2	1.20
34	28.708(6)	3.1071(7)	Unknown	Unknown	2.35
35	29.918(6)	2.9841(6)	(1,1,5)	C31H36Au2Cl2N4OP2	9.91
36	30.196(6)	2.9574(5)	Unknown	Unknown	6.87
37	30.843(5)	2.8968(4)	(0,0,6)	C31H36Au2Cl2N4OP2	15.41
38	31.097(7)	2.8737(7)	Unknown	Unknown	3.08
39	31.765(15)	2.8147(13)	(2,2,3)	C31H36Au2Cl2N4OP2	6.98
40	31.92(4)	2.801(3)	(0,1,6)	C31H36Au2Cl2N4OP2	6.72
41	32.151(7)	2.7818(6)	(2,3,0)	C31H36Au2Cl2N4OP2	7.80
42	32.413(18)	2.7599(14)	(2,3,−1)	C31H36Au2Cl2N4OP2	19.48
43	32.650(6)	2.7405(5)	(3,1,1)	C31H36Au2Cl2N4OP2	3.99
44	33.102(12)	2.7040(9)	(2,3,1)	C31H36Au2Cl2N4OP2	12.07

45	33.805(13)	2.6494(10)	(0,4,1)	C31H36Au2Cl2N4OP2	1.28
46	34.492(5)	2.5982(4)	Unknown	Unknown	4.52
47	34.939(15)	2.5660(10)	(2,2,4)	C31H36Au2Cl2N4OP2	1.86
48	35.098(17)	2.5547(12)	(0,4,2)	C31H36Au2Cl2N4OP2	2.78
49	35.672(8)	2.5149(6)	(1,4,1)	C31H36Au2Cl2N4OP2	3.18
50	36.126(8)	2.4843(5)	(1,4,−2)	C31H36Au2Cl2N4OP2	5.41
51	37.154(10)	2.4179(6)	(2,3,−4)	C31H36Au2Cl2N4OP2	5.98
52	37.40(3)	2.4025(19)	(3,2,2)	C31H36Au2Cl2N4OP2	1.13
53	38.00(2)	2.3657(13)	Unknown	Unknown	0.79
54	38.349(12)	2.3453(7)	(1,3,5)	C31H36Au2Cl2N4OP2	4.47
55	39.249(13)	2.2936(7)	Unknown	Unknown	1.94
56	39.465(16)	2.2815(9)	(2,4,−1)	C31H36Au2Cl2N4OP2	1.81
57	39.80(4)	2.2629(19)	(1,1,7)	C31H36Au2Cl2N4OP2	4.85
58	40.23(3)	2.2400(14)	(1,4,−4)	C31H36Au2Cl2N4OP2	1.12
59	40.597(15)	2.2205(8)	(3,3,1)	C31H36Au2Cl2N4OP2	3.59
60	41.31(2)	2.1838(11)	(3,2,−5)	C31H36Au2Cl2N4OP2	1.76
61	42.03(2)	2.1480(10)	(4,1,−2)	C31H36Au2Cl2N4OP2	1.77
62	42.302(17)	2.1348(8)	(0,5,0)	C31H36Au2Cl2N4OP2	6.28
63	42.520(12)	2.1244(6)	(0,5,1)	C31H36Au2Cl2N4OP2	3.45
64	43.313(13)	2.0873(6)	(3,3,−4)	C31H36Au2Cl2N4OP2	4.81
65	43.954(15)	2.0583(7)	(1,5,1)	C31H36Au2Cl2N4OP2	6.79
66	44.79(4)	2.0219(18)	(4,1,2)	C31H36Au2Cl2N4OP2	4.00
67	45.579(19)	1.9887(8)	(3,1,−7)	C31H36Au2Cl2N4OP2	0.95
68	46.035(12)	1.9700(5)	(2,4,4)	C31H36Au2Cl2N4OP2	5.95
69	47.553(13)	1.9106(5)	(3,1,6)	C31H36Au2Cl2N4OP2	1.25
70	47.856(11)	1.8992(4)	(2,5,−2)	C31H36Au2Cl2N4OP2	1.64
71	48.16(2)	1.8878(9)	(3,2,−7)	C31H36Au2Cl2N4OP2	3.50
72	48.471(11)	1.8766(4)	(4,0,4)	C31H36Au2Cl2N4OP2	2.49
73	48.722(14)	1.8675(5)	(4,0,−6)	C31H36Au2Cl2N4OP2	3.04
74	49.152(9)	1.8521(3)	(2,4,−6)	C31H36Au2Cl2N4OP2	3.46
75	49.613(6)	1.8360(2)	(2,1,8)	C31H36Au2Cl2N4OP2	1.02
76	50.283(13)	1.8131(4)	(1,1,9)	C31H36Au2Cl2N4OP2	3.39

77	50.85(2)	1.7942(7)	(2,5,3)	C31H36Au2Cl2N4OP2	1.75
78	51.157(13)	1.7841(4)	(2,3,7)	C31H36Au2Cl2N4OP2	0.95
79	51.462(9)	1.7743(3)	(0,6,1)	C31H36Au2Cl2N4OP2	1.82
80	51.998(16)	1.7573(5)	(3,2,−8)	C31H36Au2Cl2N4OP2	0.27
81	52.37(4)	1.7455(12)	(3,4,4)	C31H36Au2Cl2N4OP2	0.50
82	52.880(12)	1.7300(4)	(4,3,3)	C31H36Au2Cl2N4OP2	1.83
83	53.314(16)	1.7169(5)	(0,1,10)	C31H36Au2Cl2N4OP2	0.71
84	53.68(10)	1.706(3)	(5,1,1)	C31H36Au2Cl2N4OP2	2.38
85	54.190(16)	1.6912(5)	(3,1,−9)	C31H36Au2Cl2N4OP2	6.82
86	55.72(9)	1.648(3)	(2,6,0)	C31H36Au2Cl2N4OP2	1.77
87	56.809(15)	1.6193(4)	(1,5,−7)	C31H36Au2Cl2N4OP2	1.55
88	57.66(7)	1.5973(17)	(3,3,7)	C31H36Au2Cl2N4OP2	4.41
89	58.282(19)	1.5818(5)	(5,2,−5)	C31H36Au2Cl2N4OP2	0.43
90	59.25(5)	1.5582(12)	(2,5,−7)	C31H36Au2Cl2N4OP2	2.37
91	60.108(6)	1.53808(14)	(5,3,−4)	C31H36Au2Cl2N4OP2	2.09
92	60.386(9)	1.5317(2)	(2,3,9)	C31H36Au2Cl2N4OP2	1.87
93	60.63(3)	1.5261(7)	(0,7,0)	C31H36Au2Cl2N4OP2	3.71
94	61.75(7)	1.5011(16)	(3,5,5)	C31H36Au2Cl2N4OP2	5.45
95	63.151(18)	1.4711(4)	(5,4,−2)	C31H36Au2Cl2N4OP2	5.97
96	64.154(16)	1.4505(3)	(3,6,3)	C31H36Au2Cl2N4OP2	1.50
97	67.23(6)	1.3914(11)	(5,4,3)	C31H36Au2Cl2N4OP2	1.24

Table S4. PXRD data for the crystalline phase **1c**.

Measurement conditions			
X−Ray	30 kV, 10 mA	Scan speed / Duration time	1.0000
Goniometer	−	Step width	0.0202 deg
Attachment	−	Scan axis	2Theta
Filter	−	Scan range	5.0017 − 84.9923 deg
CBO selection slit	−	Incident slit	−
Diffrected beam mono.	−	Length limiting slit	−
Detector	−	Receiving slit #1	−
Scan mode	STEP	Receiving slit #2	−

Qualitative analysis results				
Phase name	**Formula**	**Figure of merit**	**Phase reg. detail**	**DB card number**
	C34H42Au2Cl2N4O2P2	1.408	CIF file	−
Phase name	**Formula**	**Space group**	**Phase reg. detail**	**DB card number**
	C34H42Au2Cl2N4O2P2	12: C12/m1, unique − b, cell −1	CIF file	−

Peak list					
##	**2 theta (deg)**	**d (ang)**	**Phase name**	**Chemical formula**	**Rel. int. I (a.u.)**
1	6.89(4)	12.82(7)	(1,1,0)	C34H42Au2Cl2N4O2P2	3.60
2	7.16(3)	12.33(5)	Unknown	Unknown	19.52
3	7.444(12)	11.87(2)	Unknown	Unknown	29.58
4	8.194(5)	10.782(7)	(2,0,−1)	C34H42Au2Cl2N4O2P2	48.85
5	9.054(5)	9.759(6)	(0,0,1)	C34H42Au2Cl2N4O2P2	35.08
6	9.59(4)	9.21(4)	Unknown	Unknown	12.84
7	9.86(9)	8.97(8)	Unknown	Unknown	3.40
8	9.907(7)	8.921(6)	Unknown	Unknown	56.14
9	10.46(2)	8.454(19)	(0,2,0)	C34H42Au2Cl2N4O2P2	13.68
10	11.082(4)	7.977(3)	Unknown	Unknown	100.00
11	12.846(14)	6.886(7)	Unknown	Unknown	13.28
12	13.708(14)	6.454(7)	(2,2,−1)	C34H42Au2Cl2N4O2P2	4.85

13	14.64(5)	6.044(19)	(3,1,0)	C34H42Au2Cl2N4O2P2	8.75
14	14.87(9)	5.95(4)	(2,0,−2)	C34H42Au2Cl2N4O2P2	3.95
15	15.39(9)	5.75(3)	Unknown	Unknown	2.56
16	16.393(10)	5.403(3)	(1,3,0)	C34H42Au2Cl2N4O2P2	2.01
17	17.16(6)	5.165(17)	(1,3,−1)	C34H42Au2Cl2N4O2P2	1.27
18	18.10(7)	4.896(19)	(0,0,2)	C34H42Au2Cl2N4O2P2	2.81
19	18.98(4)	4.672(9)	(2,2,1)	C34H42Au2Cl2N4O2P2	3.74
20	19.54(6)	4.540(14)	(3,3,−1)	C34H42Au2Cl2N4O2P2	2.14
21	20.16(6)	4.400(13)	(1,3,1)	C34H42Au2Cl2N4O2P2	4.83
22	21.57(6)	4.116(12)	(0,4,0)	C34H42Au2Cl2N4O2P2	5.92
23	22.274(15)	3.988(3)	Unknown	Unknown	1.66
24	22.68(9)	3.917(15)	(4,0,−3)	C34H42Au2Cl2N4O2P2	4.51
25	24.65(3)	3.608(5)	(2,0,2)	C34H42Au2Cl2N4O2P2	7.68
26	25.44(7)	3.499(10)	(6,0,−3)	C34H42Au2Cl2N4O2P2	7.74
27	25.86(8)	3.443(10)	(2,4,−2)	C34H42Au2Cl2N4O2P2	5.11
28	28.47(8)	3.133(9)	(7,1,−3)	C34H42Au2Cl2N4O2P2	1.70
29	29.36(7)	3.040(7)	(0,2,3)	C34H42Au2Cl2N4O2P2	6.32
30	32.07(5)	2.789(4)	(6,4,−1)	C34H42Au2Cl2N4O2P2	2.36
31	33.478(17)	2.6746(13)	(6,4,−3)	C34H42Au2Cl2N4O2P2	5.32
32	34.45(7)	2.601(5)	(2,2,−4)	C34H42Au2Cl2N4O2P2	4.19
33	35.55(13)	2.523(9)	(3,5,−3)	C34H42Au2Cl2N4O2P2	6.93
34	36.59(17)	2.454(11)	(4,6,−2)	C34H42Au2Cl2N4O2P2	0.87
35	39.32(13)	2.289(7)	(3,5,2)	C34H42Au2Cl2N4O2P2	3.62
36	40.75(10)	2.212(5)	(9,3,−1)	C34H42Au2Cl2N4O2P2	5.06
37	41.83(17)	2.158(8)	(7,3,1)	C34H42Au2Cl2N4O2P2	9.54
38	45.04(2)	2.0114(10)	(5,7,−3)	C34H42Au2Cl2N4O2P2	4.13
39	46.56(5)	1.949(2)	(5,5,2)	C34H42Au2Cl2N4O2P2	5.57

Table S5. Bond lengths for **1a**, Å.

Atom 1	Atom 2	Length
Au1	Au1	3.3134(5)
Au1	Cl1	2.2905(15)
Au1	P1	2.2234(15)
P1	C1	1.841(8)
P1	C6	1.823(7)
P1	C7	1.861(7)
N1	C1	1.465(9)
N1	C7	1.435(10)
N1	C8	1.399(10)
C1	H1A	0.9700*
C1	H1B	0.9700*
N2	C2	1.347(10)
N2	C6	1.337(9)
C2	H2	0.9300*
C2	C3	1.382(12)
C3	H3	0.9300*
C3	C4	1.383(12)
C4	H4	0.9300*
C4	C5	1.413(11)
C5	H5	0.9300*
C5	C6	1.407(10)
C7	N1	1.435(10)
C7	H7A	0.9700*
C7	H7B	0.9700*
C8	C9	1.414(10)
C8	C13	1.401(11)
C9	H9	0.9300*
C9	C10	1.388(13)
C10	H10	0.9300*
C10	C11	1.382(14)
C11	C12	1.365(13)
C11	C14	1.534(13)
C12	H12	0.9300*
C12	C13	1.389(12)
C13	H13	0.9300*
C14	H14A	0.9600*
C14	H14B	0.9600*
C14	H14C	0.9600*

* keep fixed during refinement

Table S6. Angles for **1a**, °.

Atom 1	Atom 2	Atom 3	Angle
Cl1	Au1	Au1	94.38(4)
P1	Au1	Au1	95.72(4)
P1	Au1	Cl1	169.88(6)
C1	P1	Au1	116.7(2)
C1	P1	C7	105.4(4)
C6	P1	Au1	111.5(2)
C6	P1	C1	101.7(3)
C6	P1	C7	102.6(3)
C7	P1	Au1	117.0(2)
C7	N1	C1	116.7(6)
C8	N1	C1	122.4(6)
C8	N1	C7	120.8(6)
P1	C1	H1A	108.6
P1	C1	H1B	108.6
N1	C1	P1	114.5(5)
N1	C1	H1A	108.6
N1	C1	H1B	108.6
H1A	C1	H1B	107.6
C6	N2	C2	117.1(7)
N2	C2	H2	118.0
N2	C2	C3	124.1(7)
C3	C2	H2	118.0
C2	C3	H3	120.6
C2	C3	C4	118.8(7)
C4	C3	H3	120.6
C3	C4	H4	120.6
C3	C4	C5	118.8(7)
C5	C4	H4	120.6
C4	C5	H5	121.2
C6	C5	C4	117.6(7)
C6	C5	H5	121.2
N2	C6	P1	117.1(5)
N2	C6	C5	123.6(7)
C5	C6	P1	119.2(5)
P1	C7	H7A	108.2
P1	C7	H7B	108.2
N1	C7	P1	116.5(5)
N1	C7	H7A	108.2
N1	C7	H7B	108.2
H7A	C7	H7B	107.3
N1	C8	C9	121.3(7)
N1	C8	C13	122.0(7)
C13	C8	C9	116.6(7)
C8	C9	H9	119.2
C10	C9	C8	121.6(8)
C10	C9	H9	119.2
C9	C10	H10	119.3
C11	C10	C9	121.3(8)
C11	C10	H10	119.3
C10	C11	C14	121.2(9)
C12	C11	C10	116.7(8)
C12	C11	C14	122.1(9)
C11	C12	H12	117.8
C11	C12	C13	124.3(9)
C13	C12	H12	117.8
C8	C13	H13	120.3
C12	C13	C8	119.4(7)
C12	C13	H13	120.3
C11	C14	H14A	109.5
C11	C14	H14B	109.5
C11	C14	H14C	109.5
H14A	C14	H14B	109.5
H14A	C14	H14C	109.5
H14B	C14	H14C	109.5

Table S7. Torsions for **1a**, °.

Atom 1	Atom 2	Atom 3	Atom 4	Torsion
Au1	P1	C1	N1	48.6(6)
Au1	P1	C6	N2	-135.2(5)
Au1	P1	C6	C5	47.7(6)
Au1	P1	C7	N1	-26.3(7)
N1	C8	C9	C10	176.6(7)
N1	C8	C13	C12	-175.0(6)
C1	P1	C6	N2	99.7(6)
C1	P1	C6	C5	-77.4(6)
C1	P1	C7	N1	105.3(6)
C1	N1	C8	C9	173.7(6)
C1	N1	C8	C13	-9.6(9)
N2	C2	C3	C4	-0.5(12)
C2	N2	C6	P1	-178.2(5)
C2	N2	C6	C5	-1.3(10)
C2	C3	C4	C5	0.4(11)
C3	C4	C5	C6	-0.7(10)
C4	C5	C6	P1	178.1(5)
C4	C5	C6	N2	1.2(11)
C6	P1	C1	N1	170.1(5)
C6	P1	C7	N1	-148.6(6)
C6	N2	C2	C3	0.9(11)
C7	P1	C1	N1	-83.2(6)
C7	P1	C6	N2	-9.2(6)
C7	P1	C6	C5	173.7(6)
C7	N1	C1	P1	77.9(7)
C7	N1	C8	C9	-3.6(9)
C7	N1	C8	C13	173.0(6)
C8	N1	C1	P1	-99.5(7)
C8	C9	C10	C11	-1.3(12)
C9	C8	C13	C12	1.8(10)
C9	C10	C11	C12	1.2(12)
C9	C10	C11	C14	-178.5(8)
C10	C11	C12	C13	0.5(12)
C11	C12	C13	C8	-2.0(12)
C13	C8	C9	C10	-0.2(11)
C14	C11	C12	C13	-179.8(8)

Table S8. Bond lengths for **1b**, Å.

Atom 1	Atom 2	Length
Au1	P1	2.225(1)
Au1	Cl1	2.289(1)
P1	C1	1.849(4)
P1	C6	1.816(3)
P1	C7	1.862(4)
N1	C8	1.410(5)
N1	C7	1.446(5)
N1	C1	1.456(5)
C8	C13	1.400(5)
C8	C9	1.404(5)
C7	H7A	0.969
C7	H7B	0.971
C7	P1	1.862(4)
C10	H10	0.930
C10	C11	1.395(6)
C10	C9	1.392(6)
N2	C2	1.39(1)
N2	C6	1.397(8)
C14	H14A	0.960
C14	H14B	0.960
C14	H14C	0.960
C14	C11	1.510(6)
C1	H1A	0.970
C1	H1B	0.970
C13	H13	0.929
C13	C12	1.383(6)
C11	C12	1.384(5)
C9	H9	0.930
C12	H12	0.931
C4	H4	0.930
C4	C3	1.35(1)
C4	C5	1.40(1)
C2	H2	0.930
C2	C3	1.38(1)
C3	H3	0.931
C5	H5	0.930
C5	C6	1.353(8)
P1	C1	1.849(4)
P1	C6	1.816(3)
P1	Au1	2.225(1)
N1	C8	1.410(5)
N1	C7	1.446(5)
N1	C1	1.456(5)
C8	C13	1.400(5)
C8	C9	1.404(5)
C7	H7A	0.969
C7	H7B	0.971
C10	H10	0.930
C10	C11	1.395(6)
C10	C9	1.392(6)
N2	C2	1.39(1)
N2	C6	1.397(8)
C14	H14A	0.960
C14	H14B	0.960
C14	H14C	0.960
C14	C11	1.510(6)
C1	H1A	0.970
C1	H1B	0.970
C13	H13	0.929
C13	C12	1.383(6)
C11	C12	1.384(5)
C9	H9	0.930
C12	H12	0.931
C4	H4	0.930
C4	C3	1.35(1)
C4	C5	1.40(1)
C2	H2	0.930
C2	C3	1.38(1)
C3	H3	0.931
C5	H5	0.930
C5	C6	1.353(8)
Au1	Cl1	2.289(1)

Table S9. Angles for **1b**, °.

Atom 1	Atom 2	Atom 3	Angle
P1	Au1	Cl1	175.20(4)
Au1	P1	C1	118.4(1)
Au1	P1	C6	113.3(1)
Au1	P1	C7	114.5(1)
C1	P1	C6	104.4(2)
C1	P1	C7	105.7(2)
C6	P1	C7	98.1(2)
C8	N1	C7	120.7(3)
C8	N1	C1	120.4(3)
C7	N1	C1	117.3(3)
N1	C8	C13	121.8(3)
N1	C8	C9	120.8(3)
C13	C8	C9	117.4(3)
N1	C7	H7A	108.0
N1	C7	H7B	108.0
N1	C7	P1	117.4(3)
H7A	C7	H7B	107.2
H7A	C7	P1	108.0
H7B	C7	P1	108.0
H10	C10	C11	118.9
H10	C10	C9	118.9
C11	C10	C9	122.2(4)
C2	N2	C6	114.0(7)
H14A	C14	H14B	109.5
H14A	C14	H14C	109.5
H14A	C14	C11	109.5
H14B	C14	H14C	109.4
H14B	C14	C11	109.5
H14C	C14	C11	109.5
P1	C1	N1	114.0(3)
P1	C1	H1A	108.7
P1	C1	H1B	108.8
N1	C1	H1A	108.8
N1	C1	H1B	108.8
H1A	C1	H1B	107.6
C8	C13	H13	119.6
C8	C13	C12	120.8(3)
H13	C13	C12	119.6
C10	C11	C14	121.2(4)
C10	C11	C12	116.6(4)
C14	C11	C12	122.3(4)
C8	C9	C10	120.5(3)
C8	C9	H9	119.8
C10	C9	H9	119.7
C13	C12	C11	122.6(4)
C13	C12	H12	118.7
C11	C12	H12	118.8
H4	C4	C3	119.6
H4	C4	C5	119.5
C3	C4	C5	120.9(8)
N2	C2	H2	118.1
N2	C2	C3	123.9(8)
H2	C2	C3	118.0
C4	C3	C2	118.7(8)
C4	C3	H3	120.7
C2	C3	H3	120.6
C4	C5	H5	121.1
C4	C5	C6	117.9(7)
H5	C5	C6	121.0
P1	C6	N2	110.0(4)
P1	C6	C5	125.1(4)

Atom 1	Atom 2	Atom 3	Angle
N2	C6	C5	124.6(5)
C7	P1	C1	105.7(2)
C7	P1	C6	98.1(2)
C7	P1	Au1	114.5(1)
C1	P1	C6	104.4(2)
C1	P1	Au1	118.4(1)
C6	P1	Au1	113.3(1)
C8	N1	C7	120.7(3)
C8	N1	C1	120.4(3)
C7	N1	C1	117.3(3)
N1	C8	C13	121.8(3)
N1	C8	C9	120.8(3)
C13	C8	C9	117.4(3)
P1	C7	N1	117.4(3)
P1	C7	H7A	108.0
P1	C7	H7B	108.0
N1	C7	H7A	108.0
N1	C7	H7B	108.0
H7A	C7	H7B	107.2
H10	C10	C11	118.9
H10	C10	C9	118.9
C11	C10	C9	122.2(4)
C2	N2	C6	114.0(7)
H14A	C14	H14B	109.5
H14A	C14	H14C	109.5
H14A	C14	C11	109.5
H14B	C14	H14C	109.4
H14B	C14	C11	109.5
H14C	C14	C11	109.5
P1	C1	N1	114.0(3)
P1	C1	H1A	108.7
P1	C1	H1B	108.8
N1	C1	H1A	108.8
N1	C1	H1B	108.8
H1A	C1	H1B	107.6
C8	C13	H13	119.6
C8	C13	C12	120.8(3)
H13	C13	C12	119.6
C10	C11	C14	121.2(4)
C10	C11	C12	116.6(4)
C14	C11	C12	122.3(4)
C8	C9	C10	120.5(3)
C8	C9	H9	119.8
C10	C9	H9	119.7
C13	C12	C11	122.6(4)
C13	C12	H12	118.7
C11	C12	H12	118.8
H4	C4	C3	119.6
H4	C4	C5	119.5
C3	C4	C5	120.9(8)
N2	C2	H2	118.1
N2	C2	C3	123.9(8)
H2	C2	C3	118.0
C4	C3	C2	118.7(8)
C4	C3	H3	120.7
C2	C3	H3	120.6
C4	C5	H5	121.1
C4	C5	C6	117.9(7)
H5	C5	C6	121.0
P1	C6	N2	110.0(4)
P1	C6	C5	125.1(4)

Atom 1	Atom 2	Atom 3	Angle
N2	C6	C5	124.6(5)
P1	Au1	Cl1	175.20(4)
H16A	C16	H16B	109.5
H16A	C16	H16C	109.5
H16A	C16	C15	109.4
H16B	C16	H16C	109.6
H16B	C16	C15	109.4
H16C	C16	C15	109.4
C16	C15	O1	121.3
C16	C15	C16	117.4
O1	C15	C16	121.3
C15	C16	H16A	109.4
C15	C16	H16B	109.4
C15	C16	H16C	109.4
H16A	C16	H16B	109.5
H16A	C16	H16C	109.5
H16B	C16	H16C	109.6

Table S10. Torsions for **1b**, °.

Atom 1	Atom 2	Atom 3	Atom 4	Torsion
Cl1	Au1	P1	C1	178.7(5)
Cl1	Au1	P1	C6	55.9(5)
Cl1	Au1	P1	C7	-55.4(5)
Au1	P1	C1	N1	56.0(3)
Au1	P1	C1	H1A	177.5
Au1	P1	C1	H1B	-65.5
C6	P1	C1	N1	-176.9(3)
C6	P1	C1	H1A	-55.3
C6	P1	C1	H1B	61.6
C7	P1	C1	N1	-73.9(3)
C7	P1	C1	H1A	47.6
C7	P1	C1	H1B	164.5
Au1	P1	C6	N2	-29.1(4)
Au1	P1	C6	C5	157.6(5)
C1	P1	C6	N2	-159.3(4)
C1	P1	C6	C5	27.3(5)
C7	P1	C6	N2	92.1(4)
C7	P1	C6	C5	-81.3(5)
Au1	P1	C7	N1	-55.4(3)
Au1	P1	C7	H7A	66.9
Au1	P1	C7	H7B	-177.6
C1	P1	C7	N1	76.8(3)
C1	P1	C7	H7A	-160.9
C1	P1	C7	H7B	-45.4
C6	P1	C7	N1	-175.6(3)
C6	P1	C7	H7A	-53.4
C6	P1	C7	H7B	62.2
C7	N1	C8	C13	173.6(3)
C7	N1	C8	C9	-5.8(5)
C1	N1	C8	C13	8.0(5)
C1	N1	C8	C9	-171.4(3)
C8	N1	C7	H7A	-36.0
C8	N1	C7	H7B	-151.6
C8	N1	C7	P1	86.2(4)
C1	N1	C7	H7A	130.0
C1	N1	C7	H7B	14.5
C1	N1	C7	P1	-107.8(3)
C8	N1	C1	P1	-89.2(4)
C8	N1	C1	H1A	149.3
C8	N1	C1	H1B	32.4
C7	N1	C1	P1	104.7(3)
C7	N1	C1	H1A	-16.8
C7	N1	C1	H1B	-133.7
N1	C8	C13	H13	0.9
N1	C8	C13	C12	-179.3(3)
C9	C8	C13	H13	-179.7
C9	C8	C13	C12	0.2(6)
N1	C8	C9	C10	-180.0(3)
N1	C8	C9	H9	0.0
C13	C8	C9	C10	0.6(6)
C13	C8	C9	H9	-179.4
N1	C7	P1	C1	76.8(3)
N1	C7	P1	C6	-175.6(3)
N1	C7	P1	Au1	-55.4(3)
H7A	C7	P1	C1	-160.9
H7A	C7	P1	C6	-53.4
H7A	C7	P1	Au1	66.9
H7B	C7	P1	C1	-45.4
H7B	C7	P1	C6	62.2
H7B	C7	P1	Au1	-177.6

Atom 1	Atom 2	Atom 3	Atom 4	Torsion
H10	C10	C11	C14	1.2
H10	C10	C11	C12	-179.7
C9	C10	C11	C14	-178.7(4)
C9	C10	C11	C12	0.4(6)
H10	C10	C9	C8	179.2
H10	C10	C9	H9	-0.8
C11	C10	C9	C8	-0.9(6)
C11	C10	C9	H9	179.1
C6	N2	C2	H2	176.8
C6	N2	C2	C3	-3(1)
C2	N2	C6	P1	-171.9(5)
C2	N2	C6	C5	1(1)
H14A	C14	C11	C10	-69.6
H14A	C14	C11	C12	111.3
H14B	C14	C11	C10	170.4
H14B	C14	C11	C12	-8.6
H14C	C14	C11	C10	50.5
H14C	C14	C11	C12	-128.6
C8	C13	C12	C11	-0.7(6)
C8	C13	C12	H12	179.3
H13	C13	C12	C11	179.2
H13	C13	C12	H12	-0.8
C10	C11	C12	C13	0.4(6)
C10	C11	C12	H12	-179.6
C14	C11	C12	C13	179.5(4)
C14	C11	C12	H12	-0.5
H4	C4	C3	C2	-179.3
H4	C4	C3	H3	1
C5	C4	C3	C2	1(1)
C5	C4	C3	H3	-179.2
H4	C4	C5	H5	-2
H4	C4	C5	C6	177.7
C3	C4	C5	H5	177.8
C3	C4	C5	C6	-2(1)
N2	C2	C3	C4	2(1)
N2	C2	C3	H3	-177.9
H2	C2	C3	C4	-177.8
H2	C2	C3	H3	2
C4	C5	C6	P1	173.6(5)
C4	C5	C6	N2	1(1)
H5	C5	C6	P1	-7
H5	C5	C6	N2	-179.0
C7	P1	C1	N1	-73.9(3)
C7	P1	C1	H1A	47.6
C7	P1	C1	H1B	164.5
C6	P1	C1	N1	-176.9(3)
C6	P1	C1	H1A	-55.3
C6	P1	C1	H1B	61.6
Au1	P1	C1	N1	56.0(3)
Au1	P1	C1	H1A	177.5
Au1	P1	C1	H1B	-65.5
C7	P1	C6	N2	92.1(4)
C7	P1	C6	C5	-81.3(5)
C1	P1	C6	N2	-159.3(4)
C1	P1	C6	C5	27.3(5)
Au1	P1	C6	N2	-29.1(4)
Au1	P1	C6	C5	157.6(5)
C7	P1	Au1	Cl1	-55.4(5)
C1	P1	Au1	Cl1	178.7(5)
C6	P1	Au1	Cl1	55.9(5)

Atom 1	Atom 2	Atom 3	Atom 4	Torsion
C7	N1	C8	C13	173.6(3)
C7	N1	C8	C9	-5.8(5)
C1	N1	C8	C13	8.0(5)
C1	N1	C8	C9	-171.4(3)
C8	N1	C7	P1	86.2(4)
C8	N1	C7	H7A	-36.0
C8	N1	C7	H7B	-151.6
C1	N1	C7	P1	-107.8(3)
C1	N1	C7	H7A	130.0
C1	N1	C7	H7B	14.5
C8	N1	C1	P1	-89.2(4)
C8	N1	C1	H1A	149.3
C8	N1	C1	H1B	32.4
C7	N1	C1	P1	104.7(3)
C7	N1	C1	H1A	-16.8
C7	N1	C1	H1B	-133.7
N1	C8	C13	H13	0.9
N1	C8	C13	C12	-179.3(3)
C9	C8	C13	H13	-179.7
C9	C8	C13	C12	0.2(6)
N1	C8	C9	C10	-180.0(3)
N1	C8	C9	H9	0.0
C13	C8	C9	C10	0.6(6)
C13	C8	C9	H9	-179.4
H10	C10	C11	C14	1.2
H10	C10	C11	C12	-179.7
C9	C10	C11	C14	-178.7(4)
C9	C10	C11	C12	0.4(6)
H10	C10	C9	C8	179.2
H10	C10	C9	H9	-0.8
C11	C10	C9	C8	-0.9(6)
C11	C10	C9	H9	179.1
C6	N2	C2	H2	176.8
C6	N2	C2	C3	-3(1)
C2	N2	C6	P1	-171.9(5)
C2	N2	C6	C5	1(1)
H14A	C14	C11	C10	-69.6
H14A	C14	C11	C12	111.3
H14B	C14	C11	C10	170.4
H14B	C14	C11	C12	-8.6
H14C	C14	C11	C10	50.5
H14C	C14	C11	C12	-128.6
C8	C13	C12	C11	-0.7(6)
C8	C13	C12	H12	179.3
H13	C13	C12	C11	179.2
H13	C13	C12	H12	-0.8
C10	C11	C12	C13	0.4(6)
C10	C11	C12	H12	-179.6
C14	C11	C12	C13	179.5(4)
C14	C11	C12	H12	-0.5
H4	C4	C3	C2	-179.3
H4	C4	C3	H3	1
C5	C4	C3	C2	1(1)
C5	C4	C3	H3	-179.2
H4	C4	C5	H5	-2
H4	C4	C5	C6	177.7
C3	C4	C5	H5	177.8
C3	C4	C5	C6	-2(1)
N2	C2	C3	C4	2(1)
N2	C2	C3	H3	-177.9
H2	C2	C3	C4	-177.8
H2	C2	C3	H3	2

Atom 1	Atom 2	Atom 3	Atom 4	Torsion
C4	C5	C6	P1	173.6(5)
C4	C5	C6	N2	1(1)
H5	C5	C6	P1	-7
H5	C5	C6	N2	-179.0
H16A	C16	C15	O1	116.6
H16A	C16	C15	C16	-63.4
H16B	C16	C15	O1	-3.4
H16B	C16	C15	C16	176.6
H16C	C16	C15	O1	-123.5
H16C	C16	C15	C16	56.5
C16	C15	C16	H16A	-63.4
C16	C15	C16	H16B	176.6
C16	C15	C16	H16C	56.5
O1	C15	C16	H16A	116.6
O1	C15	C16	H16B	-3.4
O1	C15	C16	H16C	-123.5

Table S11. Bond lengths for **1c**, Å.

Atom 1	Atom 2	Length
Au1	P1	2.215(1)
Au1	Cl1	2.285(2)
P1	C3	1.815(6)
P1	C1	1.850(8)
P1	C2	1.845(8)
N3	C3	1.349(7)
N3	C7	1.333(7)
N2	C8	1.40
N2	C2	1.447
N2	C2	1.447
N1	C1	1.453
N1	C13	1.41
N1	C1	1.453
C8	C9	1.410
C8	C9	1.410
C14	H14	0.930
C14	C13	1.385
C14	C15	1.41(1)
C3	C4	1.38(1)
C1	H1A	0.969
C1	H1B	0.970
C9	H9	0.930
C9	C10	1.406(9)
C13	C14	1.385
C2	H2A	0.971
C2	H2B	0.970
C15	H15	0.930
C15	C16	1.36
C4	H4	0.930
C4	C5	1.396(9)
C5	H5	0.930
C5	C6	1.38(1)
C7	H7	0.930
C7	C6	1.36(1)
C16	C17	1.49
C16	C15	1.36
C10	H10	0.930
C10	C11	1.39
C6	H6	0.930
C11	C12	1.49
C11	C10	1.39
C12	H12A	0.96
C12	H12B	0.961
C12	H12C	0.96
C12	H12A	0.96
C12	H12B	0.961
C12	H12C	0.96
C17	H17A	0.96
C17	H17B	0.960
C17	H17C	0.96
C17	H17A	0.96
C17	H17B	0.960
C17	H17C	0.96
P1	C3	1.815(6)
P1	C1	1.850(8)
P1	C2	1.845(8)
P1	Au1	2.215(1)
N3	C3	1.349(7)
N3	C7	1.333(7)
C14	H14	0.930
C14	C15	1.41(1)
C3	C4	1.38(1)
C1	H1A	0.969
C1	H1B	0.970
C9	H9	0.930
C9	C10	1.406(9)
C2	H2A	0.971
C2	H2B	0.970
C15	H15	0.930
C4	H4	0.930
C4	C5	1.396(9)
C5	H5	0.930
C5	C6	1.38(1)
C7	H7	0.930
C7	C6	1.36(1)
C10	H10	0.930
C6	H6	0.930
Au1	Cl1	2.285(2)

Table S12. Angles for **1c**, °.

Atom 1	Atom 2	Atom 3	Angle
P1	Au1	Cl1	178.96(7)
Au1	P1	C3	116.5(2)
Au1	P1	C1	116.5(2)
Au1	P1	C2	116.7(2)
C3	P1	C1	99.8(3)
C3	P1	C2	99.7(3)
C1	P1	C2	105.0(3)
C3	N3	C7	117.0(6)
C8	N2	C2	120.1
C8	N2	C2	120.1
C2	N2	C2	117.4
C1	N1	C13	119.5
C1	N1	C1	114.8
C13	N1	C1	119.5
N2	C8	C9	120.7
N2	C8	C9	120.7
C9	C8	C9	118.7
H14	C14	C13	120.6
H14	C14	C15	120.6
C13	C14	C15	118.8
P1	C3	N3	113.4(5)
P1	C3	C4	123.7(6)
N3	C3	C4	122.9(7)
P1	C1	N1	116.1
P1	C1	H1A	108.3
P1	C1	H1B	108.2
N1	C1	H1A	108.3
N1	C1	H1B	108.2
H1A	C1	H1B	107.5
C8	C9	H9	120.3
C8	C9	C10	119.4
H9	C9	C10	120.3
N1	C13	C14	120.6
N1	C13	C14	120.6
C14	C13	C14	118.8
P1	C2	N2	117.1
P1	C2	H2A	108.0
P1	C2	H2B	108.0
N2	C2	H2A	108.1
N2	C2	H2B	108.1
H2A	C2	H2B	107.3
C14	C15	H15	118.1
C14	C15	C16	123.8
H15	C15	C16	118.1
C3	C4	H4	120.5
C3	C4	C5	119.1(7)
H4	C4	C5	120.5
C4	C5	H5	121.2
C4	C5	C6	117.6(8)
H5	C5	C6	121.2
N3	C7	H7	118.1
N3	C7	C6	123.7(7)
H7	C7	C6	118.2
C15	C16	C17	122
C15	C16	C15	115.9
C17	C16	C15	122
C9	C10	H10	118.6
C9	C10	C11	122.7
H10	C10	C11	118.7
C5	C6	C7	119.8(8)
C5	C6	H6	120.2
C7	C6	H6	120.0
C10	C11	C12	121
C10	C11	C10	117
C12	C11	C10	121
C11	C12	H12A	109
C11	C12	H12B	109
C11	C12	H12C	109
C11	C12	H12A	109
C11	C12	H12B	109
C11	C12	H12C	109
H12A	C12	H12B	110
H12A	C12	H12C	109
H12A	C12	H12A	51.1
H12A	C12	H12B	61.4
H12A	C12	H12C	141
H12B	C12	H12C	110
H12B	C12	H12A	61.4
H12B	C12	H12B	141
H12B	C12	H12C	51.1
H12C	C12	H12A	141
H12C	C12	H12B	51.1
H12C	C12	H12C	61.4
H12A	C12	H12B	110
H12A	C12	H12C	109
H12B	C12	H12C	110
C16	C17	H17A	109
C16	C17	H17B	110
C16	C17	H17C	110
C16	C17	H17A	109
C16	C17	H17B	110
C16	C17	H17C	110
H17A	C17	H17B	110
H17A	C17	H17C	109
H17A	C17	H17A	45.3
H17A	C17	H17B	67.1
H17A	C17	H17C	139
H17B	C17	H17C	109
H17B	C17	H17A	67.1
H17B	C17	H17B	139
H17B	C17	H17C	45.2
H17C	C17	H17A	139
H17C	C17	H17B	45.2
H17C	C17	H17C	67.1
H17A	C17	H17B	110
H17A	C17	H17C	109
H17B	C17	H17C	109
C3	P1	C1	99.8(3)
C3	P1	C2	99.7(3)
C3	P1	Au1	116.5(2)
C1	P1	C2	105.0(3)
C1	P1	Au1	116.5(2)
C2	P1	Au1	116.7(2)
C3	N3	C7	117.0(6)
C13	C14	H14	120.6
C13	C14	C15	118.8
H14	C14	C15	120.6
P1	C3	N3	113.4(5)
P1	C3	C4	123.7(6)
N3	C3	C4	122.9(7)
N1	C1	P1	116.1
N1	C1	H1A	108.3

Atom 1	Atom 2	Atom 3	Angle
N1	C1	H1B	108.2
P1	C1	H1A	108.3
P1	C1	H1B	108.2
H1A	C1	H1B	107.5
C8	C9	H9	120.3
C8	C9	C10	119.4
H9	C9	C10	120.3
N2	C2	P1	117.1
N2	C2	H2A	108.1
N2	C2	H2B	108.1
P1	C2	H2A	108.0
P1	C2	H2B	108.0
H2A	C2	H2B	107.3
C16	C15	C14	123.8
C16	C15	H15	118.1
C14	C15	H15	118.1
C3	C4	H4	120.5
C3	C4	C5	119.1(7)
H4	C4	C5	120.5
C4	C5	H5	121.2
C4	C5	C6	117.6(8)
H5	C5	C6	121.2
N3	C7	H7	118.1
N3	C7	C6	123.7(7)
H7	C7	C6	118.2
C11	C10	C9	122.7
C11	C10	H10	118.7
C9	C10	H10	118.6
C5	C6	C7	119.8(8)
C5	C6	H6	120.2
C7	C6	H6	120.0
P1	Au1	Cl1	178.96(7)
O1	C18	C19	120
O1	C18	C20	122
C19	C18	C20	119
C18	C19	H19A	109
C18	C19	H19B	110
C18	C19	H19C	109
C18	C19	H19A	109
C18	C19	H19B	110
C18	C19	H19C	109
H19A	C19	H19B	109
H19A	C19	H19C	109
H19A	C19	H19A	140
H19A	C19	H19B	47.8
H19A	C19	H19C	65
H19B	C19	H19C	109
H19B	C19	H19A	47.8
H19B	C19	H19B	65
H19B	C19	H19C	140
H19C	C19	H19A	65
H19C	C19	H19B	140
H19C	C19	H19C	47.8
H19A	C19	H19B	109
H19A	C19	H19C	109
H19B	C19	H19C	109
C18	C20	H20A	109
C18	C20	H20B	109
C18	C20	H20C	109
C18	C20	H20A	109
C18	C20	H20B	109
C18	C20	H20C	109
H20A	C20	H20B	109

Atom 1	Atom 2	Atom 3	Angle
H20A	C20	H20C	110
H20A	C20	H20A	43.0
H20A	C20	H20B	139
H20A	C20	H20C	69
H20B	C20	H20C	109
H20B	C20	H20A	139
H20B	C20	H20B	69
H20B	C20	H20C	42.9
H20C	C20	H20A	69
H20C	C20	H20B	42.9
H20C	C20	H20C	139
H20A	C20	H20B	109
H20A	C20	H20C	110
H20B	C20	H20C	109
O2	C21	C23	127(2)
O2	C21	C22	126(2)
C23	C21	C22	107(2)
C21	C23	H23A	110
C21	C23	H23B	109
C21	C23	H23C	109
H23A	C23	H23B	110
H23A	C23	H23C	110
H23B	C23	H23C	109
C21	C22	H22A	110
C21	C22	H22B	109
C21	C22	H22C	110
H22A	C22	H22B	110
H22A	C22	H22C	109
H22B	C22	H22C	109

Table S13. Torsions for **1c**, °.

Atom1	Atom2	Atom3	Atom4	Torsion
Cl1	Au1	P1	C3	126(4)
Cl1	Au1	P1	C1	8(4)
Cl1	Au1	P1	C2	-117(4)
Au1	P1	C3	N3	-175.1(4)
Au1	P1	C3	C4	3.9(7)
C1	P1	C3	N3	-48.8(6)
C1	P1	C3	C4	130.2(6)
C2	P1	C3	N3	58.4(6)
C2	P1	C3	C4	-122.6(7)
Au1	P1	C1	N1	-60.6
Au1	P1	C1	H1A	61.4
Au1	P1	C1	H1B	177.6
C3	P1	C1	N1	173.1
C3	P1	C1	H1A	-64.9
C3	P1	C1	H1B	51.3
C2	P1	C1	N1	70.3
C2	P1	C1	H1A	-167.7
C2	P1	C1	H1B	-51.5
Au1	P1	C2	N2	61.7
Au1	P1	C2	H2A	-176.1
Au1	P1	C2	H2B	-60.4
C3	P1	C2	N2	-172.0
C3	P1	C2	H2A	-49.8
C3	P1	C2	H2B	65.9
C1	P1	C2	N2	-69.0
C1	P1	C2	H2A	53.1
C1	P1	C2	H2B	168.8
C7	N3	C3	P1	178.4(5)
C7	N3	C3	C4	-1(1)
C3	N3	C7	H7	-179.5
C3	N3	C7	C6	1(1)
C2	N2	C8	C9	8
C2	N2	C8	C9	-170.5
C2	N2	C8	C9	170.5
C2	N2	C8	C9	-8
C8	N2	C2	P1	-88.8
C8	N2	C2	H2A	149.1
C8	N2	C2	H2B	33
C2	N2	C2	P1	108.7
C2	N2	C2	H2A	-13.4
C2	N2	C2	H2B	-129.2
C8	N2	C2	P1	88.8
C8	N2	C2	H2A	-149.1
C8	N2	C2	H2B	-33
C2	N2	C2	P1	-108.7
C2	N2	C2	H2A	13.4
C2	N2	C2	H2B	129.2
C13	N1	C1	P1	97.1
C13	N1	C1	H1A	-25
C13	N1	C1	H1B	-141.1
C1	N1	C1	P1	-110.7
C1	N1	C1	H1A	127.3
C1	N1	C1	H1B	11.1
C1	N1	C13	C14	-14
C1	N1	C13	C14	165.3
C1	N1	C13	C14	-165.3
C1	N1	C13	C14	14
C1	N1	C1	P1	110.7
C1	N1	C1	H1A	-127.3
C1	N1	C1	H1B	-11.1
C13	N1	C1	P1	-97.1

Atom1	Atom2	Atom3	Atom4	Torsion
C13	N1	C1	H1A	25
C13	N1	C1	H1B	141.1
N2	C8	C9	H9	1
N2	C8	C9	C10	-179.4
C9	C8	C9	H9	179.4
C9	C8	C9	C10	-1
N2	C8	C9	H9	-1
N2	C8	C9	C10	179.4
C9	C8	C9	H9	-179.4
C9	C8	C9	C10	1
H14	C14	C13	N1	-5
H14	C14	C13	C14	175.0
C15	C14	C13	N1	174.7
C15	C14	C13	C14	-5
H14	C14	C15	H15	1
H14	C14	C15	C16	-178.6
C13	C14	C15	H15	-178.7
C13	C14	C15	C16	1
P1	C3	C4	H4	1
P1	C3	C4	C5	-179.1(6)
N3	C3	C4	H4	179.6
N3	C3	C4	C5	-0(1)
C8	C9	C10	H10	179.6
C8	C9	C10	C11	-0
H9	C9	C10	H10	-0
H9	C9	C10	C11	179.7
N1	C13	C14	H14	5
N1	C13	C14	C15	-174.7
C14	C13	C14	H14	-175.0
C14	C13	C14	C15	5
C14	C15	C16	C17	-177
C14	C15	C16	C15	2
H15	C15	C16	C17	4
H15	C15	C16	C15	-177.7
C3	C4	C5	H5	-178.9
C3	C4	C5	C6	1(1)
H4	C4	C5	H5	1
H4	C4	C5	C6	-178.8
C4	C5	C6	C7	-1(1)
C4	C5	C6	H6	178.7
H5	C5	C6	C7	178.9
H5	C5	C6	H6	-1
N3	C7	C6	C5	0(1)
N3	C7	C6	H6	-179.5
H7	C7	C6	C5	-179.6
H7	C7	C6	H6	1
C15	C16	C17	H17A	-67
C15	C16	C17	H17B	173
C15	C16	C17	H17C	53
C15	C16	C17	H17A	-115
C15	C16	C17	H17B	5
C15	C16	C17	H17C	125
C15	C16	C17	H17A	115
C15	C16	C17	H17B	-5
C15	C16	C17	H17C	-125
C15	C16	C17	H17A	67
C15	C16	C17	H17B	-173
C15	C16	C17	H17C	-53
C15	C16	C15	C14	-2
C15	C16	C15	H15	177.7
C17	C16	C15	C14	177

Atom1	Atom2	Atom3	Atom4	Torsion
C17	C16	C15	H15	-4
C9	C10	C11	C12	-177
C9	C10	C11	C10	1
H10	C10	C11	C12	3
H10	C10	C11	C10	-178.8
C10	C11	C12	H12A	-63
C10	C11	C12	H12B	177
C10	C11	C12	H12C	57
C10	C11	C12	H12A	-118
C10	C11	C12	H12B	2
C10	C11	C12	H12C	122
C10	C11	C12	H12A	118
C10	C11	C12	H12B	-2
C10	C11	C12	H12C	-122
C10	C11	C12	H12A	63
C10	C11	C12	H12B	-177
C10	C11	C12	H12C	-57
C10	C11	C10	C9	-1
C10	C11	C10	H10	178.8
C12	C11	C10	C9	177
C12	C11	C10	H10	-3
C1	P1	C3	N3	48.8(6)
C1	P1	C3	C4	-130.2(6)
C2	P1	C3	N3	-58.4(6)
C2	P1	C3	C4	122.6(7)
Au1	P1	C3	N3	175.1(4)
Au1	P1	C3	C4	-3.9(7)
C3	P1	C1	N1	-173.1
C3	P1	C1	H1A	64.9
C3	P1	C1	H1B	-51.3
C2	P1	C1	N1	-70.3
C2	P1	C1	H1A	167.7
C2	P1	C1	H1B	51.5
Au1	P1	C1	N1	60.6
Au1	P1	C1	H1A	-61.4
Au1	P1	C1	H1B	-177.6
C3	P1	C2	N2	172.0
C3	P1	C2	H2A	49.8
C3	P1	C2	H2B	-65.9
C1	P1	C2	N2	69.0
C1	P1	C2	H2A	-53.1
C1	P1	C2	H2B	-168.8
Au1	P1	C2	N2	-61.7
Au1	P1	C2	H2A	176.1
Au1	P1	C2	H2B	60.4
C3	P1	Au1	Cl1	-126(4)
C1	P1	Au1	Cl1	-8(4)
C2	P1	Au1	Cl1	117(4)
C7	N3	C3	P1	-178.4(5)
C7	N3	C3	C4	1(1)
C3	N3	C7	H7	179.5
C3	N3	C7	C6	-1(1)
C13	C14	C15	C16	-1
C13	C14	C15	H15	178.7
H14	C14	C15	C16	178.6
H14	C14	C15	H15	-1
P1	C3	C4	H4	-1
P1	C3	C4	C5	179.1(6)
N3	C3	C4	H4	-179.6
N3	C3	C4	C5	0(1)
C8	C9	C10	C11	0
C8	C9	C10	H10	-179.6
H9	C9	C10	C11	-179.7

Atom1	Atom2	Atom3	Atom4	Torsion
H9	C9	C10	H10	0
C3	C4	C5	H5	178.9
C3	C4	C5	C6	-1(1)
H4	C4	C5	H5	-1
H4	C4	C5	C6	178.8
C4	C5	C6	C7	1(1)
C4	C5	C6	H6	-178.7
H5	C5	C6	C7	-178.9
H5	C5	C6	H6	1
N3	C7	C6	C5	-0(1)
N3	C7	C6	H6	179.5
H7	C7	C6	C5	179.6
H7	C7	C6	H6	-1
O1	C18	C19	H19A	-94
O1	C18	C19	H19B	145
O1	C18	C19	H19C	25
O1	C18	C19	H19A	94
O1	C18	C19	H19B	-145
O1	C18	C19	H19C	-25
C20	C18	C19	H19A	86
C20	C18	C19	H19B	-35
C20	C18	C19	H19C	-155
C20	C18	C19	H19A	-86
C20	C18	C19	H19B	35
C20	C18	C19	H19C	155
O1	C18	C20	H20A	-23
O1	C18	C20	H20B	-143
O1	C18	C20	H20C	97
O1	C18	C20	H20A	23
O1	C18	C20	H20B	143
O1	C18	C20	H20C	-97
C19	C18	C20	H20A	157
C19	C18	C20	H20B	37
C19	C18	C20	H20C	-83
C19	C18	C20	H20A	-157
C19	C18	C20	H20B	-37
C19	C18	C20	H20C	83
O2	C21	C23	H23A	-117
O2	C21	C23	H23B	123
O2	C21	C23	H23C	4
C22	C21	C23	H23A	64
C22	C21	C23	H23B	-57
C22	C21	C23	H23C	-176
O2	C21	C22	H22A	-32
O2	C21	C22	H22B	-152
O2	C21	C22	H22C	88
C23	C21	C22	H22A	148
C23	C21	C22	H22B	28
C23	C21	C22	H22C	-92