Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting information

Stronger-together: the cooperativity of aurophilic interactions

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1. Supplementary tables and figures

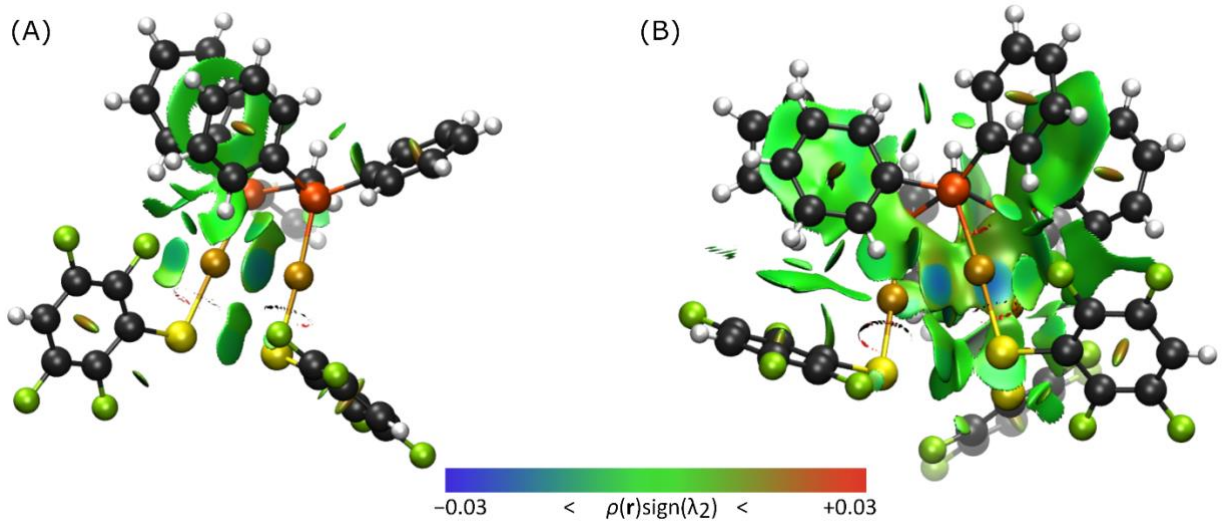


Figure S1. NCI-index plots showing the main noncovalent interactions within the structures of **2AuF4** (A) and **3AuF4** (B). Color code for the elements: H, white; C, black; F, lime; S, Yellow; P, orange; Au, golden. The considered isovalue is ρ = 0.03.

Table S1. Selected crystallographic distances in the studied compounds. All the values are given in Å.

Compound	Au-Au	Au-P	Au-X*	CCDC number
2AuF4	3.2075(4)	2.251(1) 2.257(1)	2.302(1) 2.294(1)	2104099
3AuF5	3.1177(6) 3.1041(7) 3.1398(6)	2.268(1) 2.270(1) 2.270(1)	2.301(1) 2.307(1) 2.309(1)	2104103
3AuF4	3.0849(7) 3.1055(4) 3.1405(6)	2.271(2) 2.259(2) 2.269(2)	2.303(2) 2.303(2) 2.311(2)	2104102
3AuF2	3.0498(6) 3.1126(6) 3.2888(6)	2.270(2) 2.256(2) 2.256(2)	2.301(2) 2.310(2) 2.310(3)	2104101
3AuF1	3.0777(5) 3.1259(6) 3.2896(5)	2.271(2) 2.259(2) 2.254(2)	2.301(2) 2.308(2) 2.304(2)	2104100
2AuCl[†]	3.341	2.238 2.238	2.287 2.287	1145302
3AuCl[ǂ]	3.2014(7)	2.253(3)	2.300(5)	1199414
B2Au	2.9960(3)	2.241(2) 2.236(2)	2.292(2) 2.292(2)	207994
B3Au	2.9671(5) 2.9249(6)	2.243(2) 2.228(2) 2.233(2)	2.296(2) 2.283(2) 2.303(2)	1237453

*X = S or Cl.
[†] Estimated standard deviations were not reported.
[ǂ] All distances are equal due to symmetry considerations.

Table S2. Selected QTAIM parameters of the bonds of Au in compounds **2AuF4** and **3AuFX** (X = 1, 2, 4, 5). All the values are given in atomic units. Average values with standard deviation (SD) are given. Full data are available in Section 3.

Bond		**2AuF4**	**3AuF5**	**3AuF4**	**3AuF2**	**3AuF1**
Au-Au	DI(Au|Au)	0.2713	0.2666	0.2693	0.2638	0.2571
	SD_{DI}	-	0.0105	0.0084	0.0472	0.0379
	$\rho(\mathbf{r}_{bcp})$	0.0223	0.0266	0.0271	0.0254	0.0246
	$SD_{\rho(\mathbf{r}_{bcp})}$	-	0.0008	0.0012	0.0048	0.0041
Au-P	DI(Au|P)	1.0220	0.9805	0.9840	0.9944	0.9943
	SD_{DI}	0.0057	0.0009	0.0043	0.0077	0.0089
	$\rho(\mathbf{r}_{bcp})$	0.1209	0.1180	0.1188	0.1190	0.1192
	$SD_{\rho(\mathbf{r}_{bcp})}$	0.0009	0.0004	0.0010	0.0009	0.0012
Au-S	DI(Au|S)	1.0904	1.0525	1.0436	1.0817	1.0847
	SD_{DI}	0.0198	0.0041	0.0058	0.0100	0.0050
	$\rho(\mathbf{r}_{bcp})$	0.1107	0.1094	0.1093	0.1094	0.1098
	$SD_{\rho(\mathbf{r}_{bcp})}$	0.0003	0.0007	0.0006	0.0012	0.0011

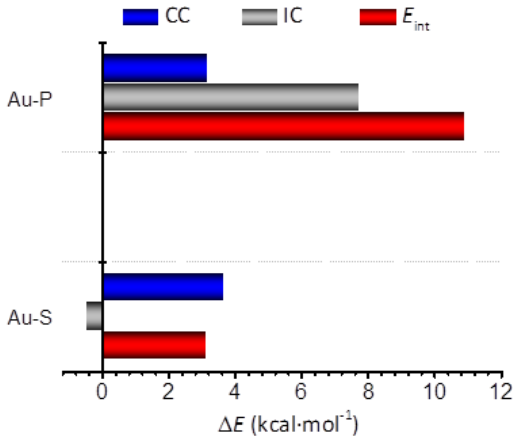


Figure S2. Changes in the energy contributions of the Au-P and Au-S bonds which result from the increase on the number of aurophilic interactions in the involved gold atoms in **3AuF4** with respect to **2AuF4**. Colour codes as in the main text.

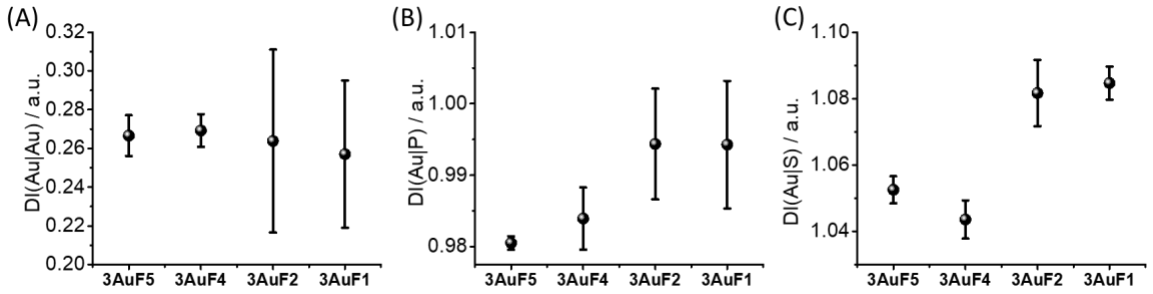


Figure S3. Change in the delocalization indexes (DI(A|B)) of the Au-Au (A), Au-P (B) and Au-S (C) bonds due to the modification of the fluorination pattern in the trimetallic complexes **3AuFX** (X = 1, 2, 3, 4).

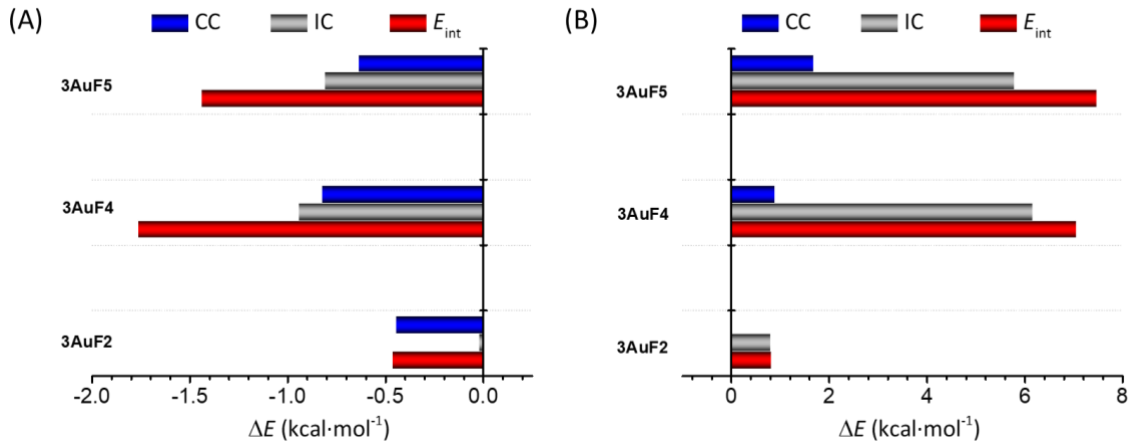


Figure S4. (A) Change in the mean energy contributions of the Au-Au interactions due to the modification of the fluorination pattern in the trimetallic complexes **3AuFX** (X = 1, 2, 4, 5) when compared with **3AuF1**. (B) Ditto for the Au-P bonds. Colour codes as in the main text.

Table S3. Selected QTAIM parameters of the bonds of Au atoms in compounds **2AuCl**, **3AuCl**, **B2Au**, and **B3Au**. All the values are given in atomic units. Average values with standard deviation (SD) are given. Full data are available in Section 3.

Bond		**2AuCl**	**3AuCl**	**B2Au**	**B3Au**
Au-Au	DI(Au|Au)	0.2015	0.2312	0.3698	0.3798
	SD_{DI}	-	0.0001	-	0.0093
	$\rho(\mathbf{r}_{bcp})$	0.0187	0.0230	0.0335	0.0370
	$SD_{\rho(\mathbf{r}_{bcp})}$	-	0.0000	-	0.0008
Au-P	DI(Au|P)	1.0430	1.0293	1.0492	1.0399
	SD_{DI}	0.0001	0.0003	0.0079	0.0156
	$\rho(\mathbf{r}_{bcp})$	0.1256	0.1215	0.1239	0.1248
	$SD_{\rho(\mathbf{r}_{bcp})}$	0.0000	0.0000	0.0004	0.0015
Au-S	DI(Au|S)	1.0741	1.0461	1.0565	1.0265
	SD_{DI}	0.0000	0.0001	0.0148	0.0137
	$\rho(\mathbf{r}_{bcp})$	0.1032	0.1032	0.1042	0.1039
	$SD_{\rho(\mathbf{r}_{bcp})}$	0.0000	0.0000	0.0002	0.0016

Table S4. Selected QTAIM parameters of the bonds of the Au atoms in model systems **Au2**, **Au3**, and **Au4**. All the values are given in atomic units. Average values with standard deviation (SD) are given. Full data are available in Section 3.

Bond		**Au2**	**Au3**	**Au4**
Au-Au	DI(Au|Au)	0.2915	0.3317	0.3716
	SD_{DI}	-	0.0020	0.0014
	$\rho(\mathbf{r}_{bcp})$	0.0242	0.0288	0.0350
	$SD_{\rho(\mathbf{r}_{bcp})}$	-	0.0003	0.0003
Au-P	DI(Au|P)	1.1027	1.0850	1.0626
	SD_{DI}	0.0000	0.0150	0.0341
	$\rho(\mathbf{r}_{bcp})$	0.1206	0.1201	0.1187
	$SD_{\rho(\mathbf{r}_{bcp})}$	0.0000	0.0011	0.0013
Au-Cl	DI(Au|S)	1.0250	1.0004	0.9793
	SD_{DI}	0.0003	0.0335	0.0420
	$\rho(\mathbf{r}_{bcp})$	0.0985	0.0973	0.0953
	$SD_{\rho(\mathbf{r}_{bcp})}$	0.0001	0.0025	0.0022

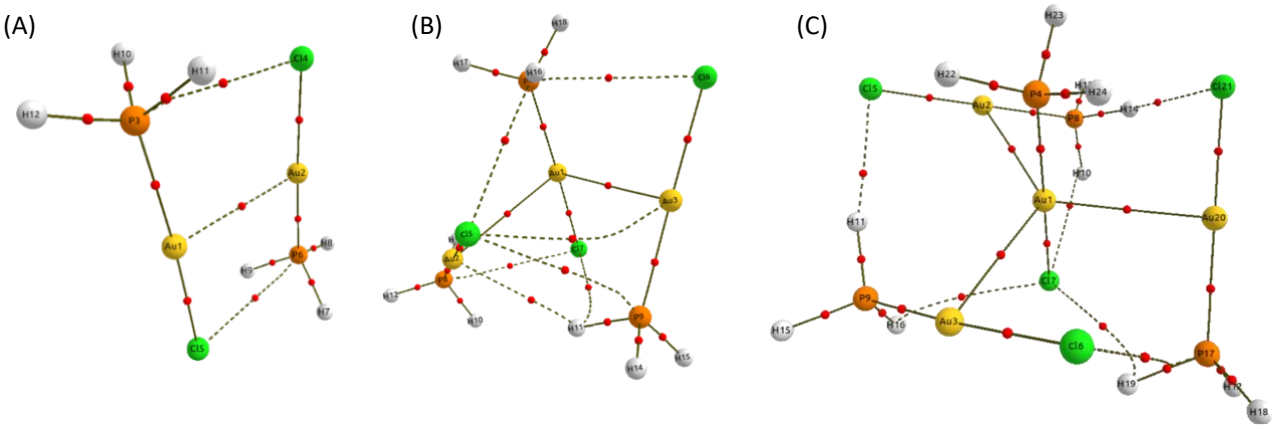


Figure S5. Molecular graphs of the optimised structures of model systems (A) **Au2**, (B) **Au3** and (C) **Au4**. Color code: H, white; Cl, green; P, orange; Au, golden; the red dots correspond to bond critical points.

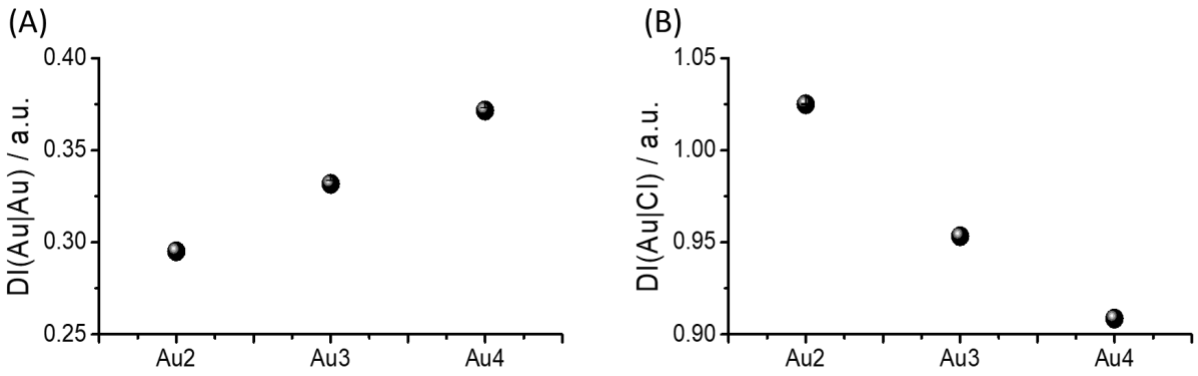


Figure S6. (A) Plot showing the mean DI(Au|Au) in the dimer, trimer and tetrameric model systems **Au2**, **Au3**, and **Au4**. (B) Ditto for the DI(Au|Cl) in the central Au-Cl bond of the same model systems.

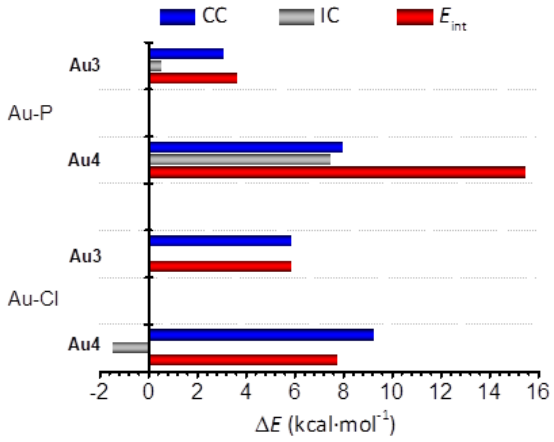


Figure S7. Change in the energy contribution of the Au-L bonds due to the increase in the number of aurophilic contacts in the model systems **Au3** and **Au4** with respect to **Au2**.

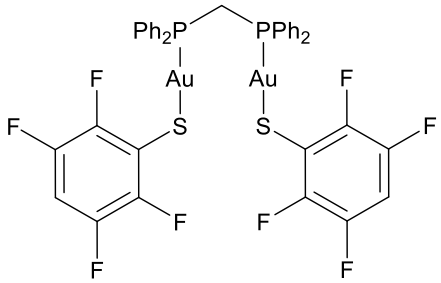
2. Experimental Part

2.1. Materials and methods

All the used solvents were obtained from JT Baker in analytical reagent grade and used without previous treatment. Bis(diphenylphosphino)methane (dppm), tris(diphenylphosphino)methane (CP_3), $K[AuCl_4]$, tetrahydrothiophene, and all the fluorinated thiols were purchased from Sigma-Aldrich and used as received. Lead fluorophenyl thiolates,[1] [AuCl(THT)],[2] [AuCl(dppm)] (**2AuCl**)[3] and [AuCl(CP_3)] (**3AuCl**)[4] were synthesised following previously reported protocols.

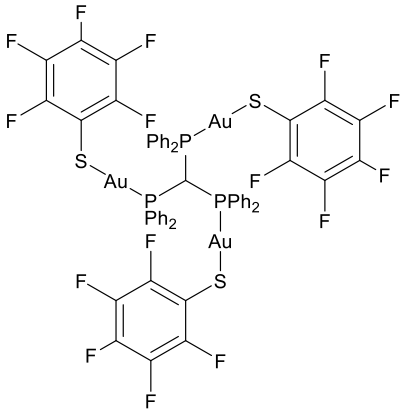
The Infrared spectra were recorded on a Perkin-Elmer FTIR/FIR Spectrum 400 spectrometer in the range of 4000 to 400 cm^{-1} using Attenuated Total Reflectance (ATR). Elemental analyses were determined using a Thermo Scientific Flash 2000 Analyzer at 950 °C. ^{1}H, ^{19}F and ^{31}P NMR spectra were registered on a 14 T Jeol ECZ600R spectrometer. Chemical shifts are in ppm relative to internal TMS δ = 0 (^{1}H) and to external references of $CFCl_3$ (for ^{19}F) and H_3PO_4 (for ^{31}P) at 0 ppm. *J* values are given in Hz. The mass spectra were obtained by Atmosphere Pressure Chemical Ionization (APCI) in a Perkin-Elmer DSA-AxION2 TOF.

2.2. Synthesis and characterization

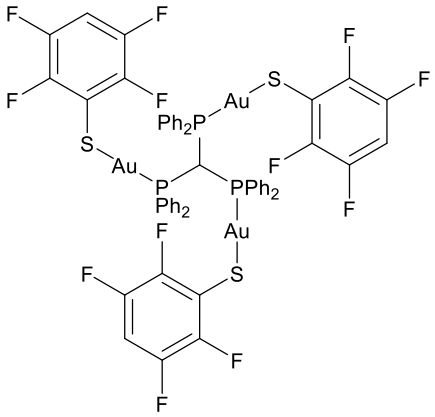


$[Au_2(p\text{-}SC_6HF_4)_2(dppm)]$, **2AuF4**. In a 50 mL round bottom flask, $Pb(p\text{-}SC_6HF_4)_2$ (135 mg, 0.235 mmol) was added to a solution of **2AuCl** (0.200 mg, 0.235 mmol) in 15 mL of CH_2Cl_2. The reaction mixture was left stirring for 2 h. After that time, the solution was filtered, and the volume was reduced *in vacuo* to approximately 2 mL. The product was precipitated out with the addition of *n*-hexane (20 mL). The desired compound was recovered by filtration, washed with hexane 2 x 20 mL and dried under vacuum yielding a pale-yellow powder (201 mg, 75 %); Elemental Analysis found: C 38.7, H 2.0 calcd. for $C_{37}H_{24}Au_2F_8P_2S_2$: C 39.0 H 2.1%; IR(ATR) ν_{max}/cm^{-1} 3053 (CH ar), 2920 (CH), 1598 (CC, ar_F), 1436 and 1320vs (CC, ar), 1086br and 1011vs (CF); $\delta^{1}H$ (600 MHz, CD_3OD) 7.71 – 7.58 (8H, m, Ph), 7.54 – 7.46 (4H, m, Ph),), 7.45 – 7.32 (12H, m, m-Ph), 6.65 (1H, m, 4-$SC_6F_4\mathit{H}$) 3.67 – 3.56 (m, 2H, CH_2); $\delta^{19}F$ NMR (565 MHz, $CDCl_3$) -132.17 – -133.48 (4F, m, 2,6-F), -140.69 – -143.13 (4F, m, 3,5-F); $\delta^{31}P$ NMR (243 MHz, CD_3OD) 33.17 (br s); MS(APCI) m/Z 959 ($[Au_2SC_6F_5(dppm)]^+$, 40%).

General procedure for the compounds of the type $[Au_3(SR_F)_3(CP_3)]$, **3AuFX**. In a 50 mL round bottom flask, $Pb(SR_F)_2$ (0.143 mmol) was added to a solution of **3AuCl** (120 mg, 0.095 mmol) in 15 mL of CH_2Cl_2. The reaction mixture was left stirring for 4 h. After that time the solution was filtered, and the remaining solid washed subsequently with acetone and tetrahydrofuran (3 x 10 mL each). The liquids were combined and dried under reduced pressure. The resulting white-yellow solids were washed with hot *n*-hexane (2 x 20 mL) and dried under vacuum.

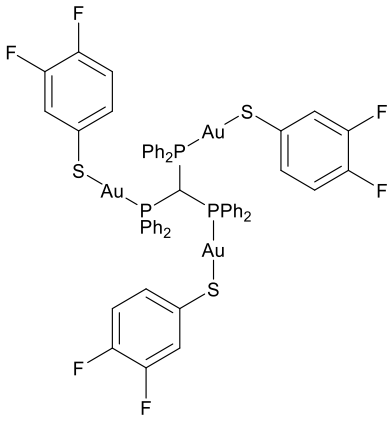


$[Au_3(SC_6F_5)_3(CP_3)]$, **3AuF5**. White crystalline powder (142 mg, 85 %); Elemental Analysis found: C 37.6, H 1.5 calcd. for $C_{55}H_{43}Au_3F_3P_3S_3$: C 37.6 H 1.8%; IR(ATR) ν_{max}/cm^{-1} 3063 (CH, ar), 2922 (CH,al) 1641 (CC, ar), 1472vs (CC, ar_F), 1074s (CF) and 967vs (CF); δ^1H (600 MHz, $CDCl_3$) 7.71 – 7.57 (12H, m, o-Ph), 7.22 – 7.15 (6H, m, p-Ph), 7.04 – 6.96 (12H, m, m-Ph), 5.62 (1H, q, $J_{H,P}$ = 9.2, CH); $\delta^{19}F$ NMR (565 MHz, $CDCl_3$) -131.20 – -132.14 (6F, m, 2,6-F), -163.04 – -163.92 (3F, m, 4-F) -164.55 – -165.02 (6F, m, 3,5-F); $\delta^{31}P$ NMR (243 MHz, $CDCl_3$) 37.34 (br s); MS(APCI) m/Z 1360 ($[Au_3(SC_6F_5)_2(CP_3)]^+$, 43%).

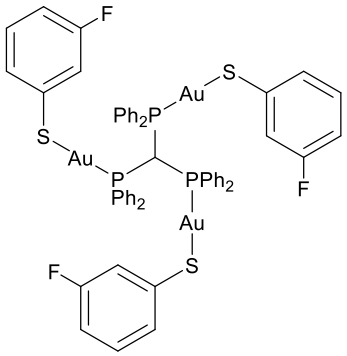


$[Au_3(p\text{-}SC_6F_4H)_3(CP_3)]$, **3AuF4**. Pale-yellow powder (89 mg, 55 %); Elemental Analysis found: C 38.7, H 1.8 calcd. for $C_{55}H_{43}Au_3F_3P_3S_3$: C 38.8 H 2.0%; IR(ATR) ν_{max}/cm^{-1} 3056 (CH, ar), 2893 (CH,al) 1623s (CC, ar),

1476vs and 1436vs (CC, ar_F) 1096s (CF) and 908vs (CF); δ^1H (600 MHz, $CDCl_3$) 7.91 – 7.72 (12H, m, o-Ph), 7.61 – 7.48 (6H, m, p-Ph), 7.49 – 7.28 (12H, m, m-Ph), 5.27 – 5.16 (3H, m, SC_6F_4H) 6.55 (1H, q, $J_{H,P}$ = 9.3, CH); δ^{19}F NMR (565 MHz, $CDCl_3$) -131.98 – -132.31 (6F, m, 2,6-F), -136.45 – -136.82 (6F, m, 3,5-F); δ^{31}P NMR (243 MHz, $CDCl_3$) 37.68 (br s); MS(APCI) m/Z 1521 ($[Au_3(SC_6F_4H)_2(CP_3)]^+$, 43%).



$[Au_3(3,4\text{-}SC_6F_2H_3)_3(CP_3)]$, **3AuF2**. Pale-yellow crystalline powder (129 mg, 85%); Elemental Analysis found: C 41.5, H 2.2 calcd. for $C_{55}H_{43}Au_3F_3P_3S_3$: C 41.4 H 2.5%; IR(ATR) ν_{max}/cm^{-1} 3052 (CH, ar), 2927 (CH,al) 1598vs and 1573vs (CC, ar), 1435s (CC, ar_F) and 1109s (CF); δ^1H (600 MHz, CD_3OD) 7.87 – 7.72 (12H, m, o-Ph), 7.49 – 7.43 (3H, m, SC_6FH_4), 7.25 – 7.12 (12H, m), 6.96 – 6.89 (12H, m, m-Ph), 6.83 (1H, q, $J_{H,P}$ = 9.4, CH); δ^{19}F NMR (565 MHz, CD_3OD) -134.75 – -135.04 (3F, m, 3-F), -137.46 – -137.66 (3F, m, 4-F); δ^{31}P NMR (243 MHz, CD_3OD) 38.28 (br s); MS(APCI) m/Z 1449 ($[Au_3(SC_6F_2H_3)_2(CP_3)]^+$, 36%).



$[Au_3(m\text{-}SC_6FH_4)_3(CP_3)]$, **3AuF1**. White crystalline powder (110 mg, 75%); Elemental Analysis found: C 42.6, H 2.6 calcd. for $C_{55}H_{43}Au_3F_3P_3S_3$: C 42.9 H 2.8%; IR(ATR) ν_{max}/cm^{-1} 3052 (CH, ar), 2921 (CH,al) 1590vs and 1566vs (CC, ar), 1462vs and 1434vs (CC, ar_F) and 1090s (CF); δ^1H (600 MHz, CD_3OD) 7.83 – 7.73 (12H, m, o-Ph), 7.70 – 7.61 (6H, m, SC_6FH_4), 7.58 – 7.53 (3H, m, SC_6FH_4), 7.18 – 7.13 (3H, m, SC_6FH_4), 7.01 – 6.97 (6H, m, p-Ph), 6.92 – 6.86 (12H, m, m-Ph), 6.76 (1H, q, $J_{H,P}$ = 9.3, CH); δ^{19}F NMR (565 MHz, CD_3OD) -120.98 (br s).; δ^{31}P NMR (243 MHz, CD_3OD) 40.84 (br s); MS(APCI) m/Z 1413 ($[Au_3(SC_6FH_4)_2(CP_3)]^+$, 25%).

3. Computational details

We carried out geometry optimizations of the model systems using the PBE exchange-correlation functional[5] in combination with the zora-def2-tzvp Gaussian basis sets of triple zeta valence quality[6,7] under the Zeroth Order Regular Approximation (ZORA), [8,9] as implemented in the ORCA program.[10] The electronic densities for the experimental systems were obtained at the same level of theory without altering the corresponding crystallographic geometries.

The Quantum Theory of Atoms in Molecules (QTAIM)[11] analyses were completed with the help of the AIMAll package[12] while the NCI-index study[13] was performed using the NCIPlot program.[14] The NCI-index results were visualised with the help of the VMD package.[15] Finally, the covalent (CC) and ionic (IC) contributions to the interaction energies (E_{int})[16] were approximated according to

$$\mathrm{CC} = \frac{-\mathrm{DI(A|B)}}{2\mathbf{r}_{\mathrm{A-B}}}$$

$$\mathrm{IC} = \frac{(q_{\mathrm{A}} \cdot q_{\mathrm{B}})}{\mathbf{r}_{\mathrm{A-B}}}$$

$$E_{int} = \mathrm{CC} + \mathrm{IC}$$

wherein DI(A|B), **r**, and *q* stand for the delocalization index, the interatomic distance and the QTAIM charges, respectively.[17] Covalent contributions approximated by the CC term provide an orbital-free measure whose fingerprint is the fluctuation of the electron population between the bonded fragments,[17,18] in the light envisioned by R. Feynman.[19] The index DI(A|B) in the contribution CC is computed by considering the covariance between the electron populations of A and B, that is to say, a correlation between the populations of both atomic basins[20] and hence an indication of covalency.

We point out that the inclusion of Grimme's dispersion corrections, i.e.:

$$E_{disp} = -\sum_{A<B}\sum_{n=6,8} s_n \frac{C_n^{AB}}{r_{AB}^n}$$

do not affect the computed electron density of a system, $\rho(\boldsymbol{r})$, because this expression is merely added to the electron energy of a given system. Therefore, DC does not change to any extent the Kohn-Sham spin orbitals $\chi(\boldsymbol{x})$, from which the electron density is computed:

$$\rho(\boldsymbol{r}) = \sum\nolimits_i \int |\chi(\boldsymbol{x})|^2 ds$$

wherein $\boldsymbol{x}$ represents jointly spatial and spin coordinates and the sum goes over all the occupied Kohn-Sham spin orbitals. Because our results are completely dependent on $\rho(\boldsymbol{r})$, the omission of DC does not change our conclusions in any way.

In order validate the choice of the exchange-correlation functional in our results, we have studied systems **2AuCl** and **3AuCl** using BLYP. The obtained values are not significantly different to those computed using PBE (Figure S7). This result demonstrates that, while the absolute computed DFT energy is highly dependent of the chosen functional, the electron density remains practically invariable and thus the QTAIM picture of the Au-Au interactions and the IQA-estimated energies are not significantly affected by the methods exploited in this investigation.

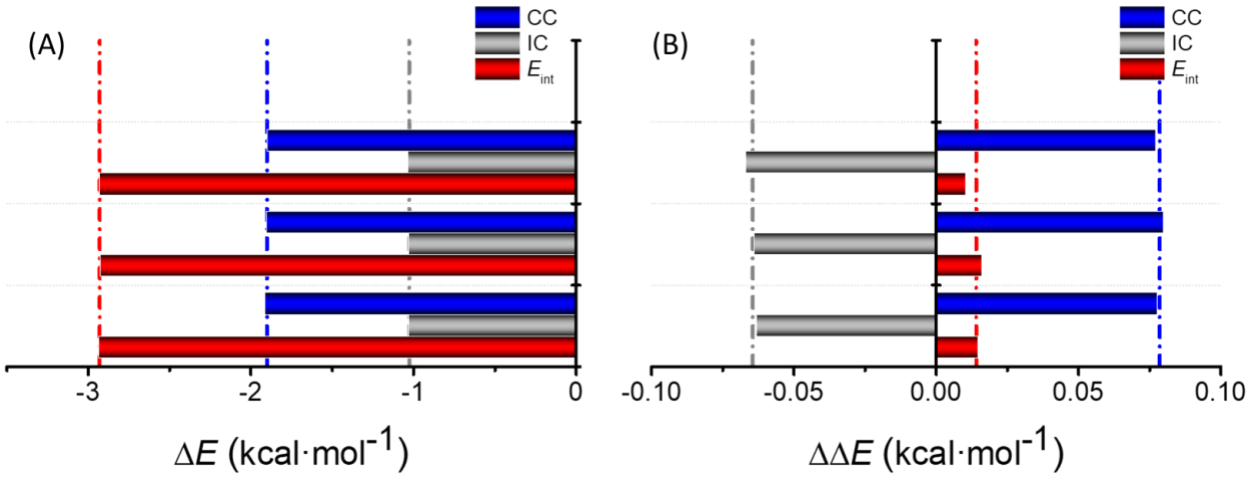


Figure S8. (A) Plot of the change in the energy contributions for the aurophilic interactions in the trinuclear compound **3AuCl** when compared with the single aurophilic interaction in the dinuclear compound **2AuCl** as estimated using the electron density calculated with the BLYP functional. (B) Differences between the Δ*E* values obtained with BLYP when compared with those computed with BPE for the different interaction components. The dashed lines represent the mean values from the different components in the trinuclear compounds for the ionic (grey) covalent (blue) and total energy (red).

3.1. QTAIM results of experimental structures

Table S5. QTAIM parameters in compound **2AuF4**.

Bond	DI(A|B)	$\rho(\mathbf{r}_{bcp})$	$\nabla^2\rho(\mathbf{r}_{bcp})$	Atom	*q*
Au1–Au2	0.2713	0.0223	0.0505	Au1	-0.1816
Au1–P1	1.0277	0.1218	0.0557	Au2	-0.2159
Au1–S1	1.0706	0.1104	0.1263	P1	1.8796
Au2–P2	1.0163	0.1199	0.0610	P2	1.8745
Au2–S2	1.1102	0.1110	0.1204	P3	-0.0084
				S1	-0.0447

Table S6. QTAIM parameters in compound **3AuF5**.

Bond	DI(A|B)	$\rho(\mathbf{r}_{bcp})$	$\nabla^2\rho(\mathbf{r}_{bcp})$	Atom	*q*
Au1–Au2	0.2660	0.0267	0.0588	Au1	-0.1861
Au1–Au3	0.2798	0.0275	0.0602	Au2	-0.1812
Au2–Au3	0.2540	0.0257	0.0567	Au3	-0.1821
Au1–P1	0.9817	0.1185	0.0636	P1	1.7847
Au1–S1	1.0582	0.1103	0.1201	P2	1.7817
Au2–P2	0.9804	0.1179	0.0658	P3	1.7952
Au2–S2	1.0489	0.1091	0.1192	S1	-0.0111
Au3–P3	0.9795	0.1177	0.0667	S2	-0.0070
Au3–S3	1.0505	0.1087	0.1169	S3	-0.0208

Table S7. QTAIM parameters in compound **3AuF4**.

Bond	DI(A|B)	$\rho(\mathbf{r}_{bcp})$	$\nabla^2\rho(\mathbf{r}_{bcp})$	Atom	*q*
Au1–Au2	0.2780	0.0284	0.0623	Au1	-0.1791
Au1–Au3	0.2719	0.0274	0.0604	Au2	-0.1826
Au2–Au3	0.2579	0.0254	0.0574	Au3	-0.1764
Au1–P1	0.9804	0.1179	0.0642	P1	1.7687
Au1–S1	1.0459	0.1098	0.1212	P2	1.7988
Au2–P2	0.9901	0.1202	0.0626	P3	1.8225
Au2–S2	1.0493	0.1097	0.1202	S1	-0.0025
Au3–P3	0.9814	0.1182	0.0646	S2	-0.0161
Au3–S3	1.0357	0.1085	0.1170	S3	-0.0150

Table S8. QTAIM parameters in compound **3AuF2**.

Bond	DI(A|B)	$\rho(\mathbf{r}_{bcp})$	$\nabla^2\rho(\mathbf{r}_{bcp})$	Atom	*q*
Au1–Au2	0.3167	0.0304	0.0647	Au1	-0.2043
Au1–Au3	0.2021	0.0190	0.0447	Au2	-0.2064
Au2–Au3	0.2727	0.0268	0.0586	Au3	-0.1988
Au1–P1	1.0012	0.1202	0.0672	P1	1.7682
Au1–S1	1.0676	0.1090	0.1091	P2	1.7526
Au2–P2	0.9836	0.1180	0.0668	P3	1.7700
Au2–S2	1.0876	0.1111	0.1155	S1	-0.1191
Au3–P3	0.9984	0.1188	0.0672	S2	-0.0851
Au3–S3	1.0898	0.1082	0.1137	S3	-0.1364

Table S9. QTAIM parameters in compound **3AuF1**.

Bond	DI(A|B)	$\rho(\mathbf{r}_{bcp})$	$\nabla^2\rho(\mathbf{r}_{bcp})$	Atom	*q*
Au1–Au2	0.2889	0.0286	0.0623	Au1	-0.2101
Au1–Au3	0.2785	0.0263	0.0570	Au2	-0.1971
Au2–Au3	0.2037	0.0190	0.0443	Au3	-0.2051
Au1–P1	0.9817	0.1177	0.0678	P1	1.7669
Au1–S1	1.0890	0.1111	0.1138	P2	1.7847
Au2–P2	1.0004	0.1194	0.0673	P3	1.7945
Au2–S2	1.0872	0.1084	0.1145	S1	-0.0808
Au3–P3	1.0008	0.1206	0.0650	S2	-0.1330
Au3–S3	1.0777	0.1100	0.1113	S3	-0.1217

Table S10. QTAIM parameters in compound **2AuCl**.

Bond	DI(A|B)	$\rho(\mathbf{r}_{bcp})$	$\nabla^2\rho(\mathbf{r}_{bcp})$	Atom	*q*
Au1–Au2	0.2015	0.0187	0.0417	Au1	-0.1445
Au1–Cl1	1.0741	0.1053	0.2070	Au2	-0.1446
Au1–P1	1.0431	0.1256	0.0282	Cl2	-0.4426
Au2–Cl2	1.0741	0.1053	0.2070	Cl1	-0.4426
Au2–P2	1.0429	0.1256	0.0282	P2	1.9757
				P1	1.9752

Table S11. QTAIM parameters in compound **3AuCl**.

Bond	DI(A|B)	$\rho(\mathbf{r}_{bcp})$	$\nabla^2\rho(\mathbf{r}_{bcp})$	Atom	*q*
Au1–Au2	0.2314	0.0230	0.0503	Au1	-0.1038
Au1–Au3	0.2312	0.0230	0.0503	Au2	-0.1035
Au2–Au3	0.2311	0.0230	0.0503	Au3	-0.1036
Au1–Cl1	1.0462	0.1032	0.1968	Cl1	-0.4174
Au1–P1	1.0291	0.1215	0.0491	Cl2	-0.4174
Au2–Cl2	1.0459	0.1032	0.1968	Cl3	-0.4174
Au2–P2	1.0292	0.1215	0.0491	P1	1.8325
Au3–Cl3	1.0460	0.1032	0.1968	P2	1.8324
Au3–P3	1.0297	0.1215	0.0491	P3	1.8320

Table S12. QTAIM parameters in compound **B2Au**.

Bond	DI(A|B)	$\rho(\mathbf{r}_{bcp})$	$\nabla^2\rho(\mathbf{r}_{bcp})$	Atom	*q*
Au1–Au2	0.3698	0.0335	0.0723	Au1	-0.1230
Au1–Cl1	1.0713	0.1040	0.2056	Au2	-0.1169
Au1–P1	1.0413	0.1236	0.0358	Cl1	-0.4312
Au2–Cl2	1.0418	0.1045	0.2023	Cl2	-0.4297
Au2–P2	1.0570	0.1244	0.0411	P1	1.9375
				P2	1.8996

Table S13. QTAIM parameters in compound **B3Au**.

Bond	DI(A|B)	$\rho(\mathbf{r}_{bcp})$	$\nabla^2\rho(\mathbf{r}_{bcp})$	Atom	*q*
Au1–Au2	0.3705	0.0361	0.0771	Au1	-0.0848
Au1–Au3	0.3891	0.0378	0.0846	Au2	-0.1371
Au1–Cl1	1.0108	0.1034	0.2052	Au3	-0.1237
Au1–P1	1.0180	0.1227	0.0401	Cl1	-0.4179
Au2–Cl2	1.0442	0.1060	0.2129	Cl2	-0.4469
Au2–P2	1.0481	0.1263	0.0261	Cl3	-0.4353
Au3–Cl3	1.0246	0.1022	0.1983	P1	1.9196
Au3–P3	1.0534	0.1252	0.0373	P2	1.9551
				P3	1.9173

3.2. QTAIM results of model systems

Table S14. QTAIM parameters in model **Au2**.

Bond	DI(A|B)	$\rho(\mathbf{r}_{bcp})$	$\nabla^2\rho(\mathbf{r}_{bcp})$	Atom	*q*
Au1–Au2	0.2951	0.0242	0.0575	Au1	-0.0818
Au1–Cl5	1.0247	0.0984	0.1966	Au2	-0.0819
Au1–P3	1.1027	0.1206	0.0543	Cl4	-0.4307
Au2–Cl4	1.0252	0.0986	0.1969	Cl5	-0.4309
Au2–P6	1.1028	0.1206	0.0542	P3	1.9035
				P6	1.9034

Table S15. QTAIM parameters in model **Au3**.

Bond	DI(A|B)	$\rho(\mathbf{r}_{bcp})$	$\nabla^2\rho(\mathbf{r}_{bcp})$	Atom	*q*
Au1–Au2	0.3297	0.0285	0.0655	Au1	-0.0798
Au1–Au3	0.3337	0.0291	0.0680	Au2	-0.0955
Au1–Cl7	0.9533	0.0938	0.1899	Au3	-0.0752
Au1–P4	1.0642	0.1190	0.0505	Cl5	-0.4143
Au2–Cl5	1.0289	0.0994	0.1934	Cl6	-0.4284
Au2–P8	1.0916	0.1198	0.0587	Cl7	-0.4485
Au3–Cl6	1.0191	0.0985	0.1947	P4	1.9134
Au3–P9	1.0991	0.1215	0.0539	P8	1.8951
				P9	1.8975

Table S16. QTAIM parameters in model **Au4**.

Bond	DI(A|B)	$\rho(\mathbf{r}_{bcp})$	$\nabla^2\rho(\mathbf{r}_{bcp})$	Atom	*q*
Au1–Au2	0.3710	0.0353	0.0817	Au1	-0.0555
Au1–Au20	0.3703	0.0350	0.0819	Au2	-0.0979
Au1–Au3	0.3736	0.0346	0.0819	Au20	-0.0871
Au1–Cl7	0.9086	0.0917	0.1843	Au3	-0.1051
Au1–P4	1.0037	0.1166	0.0464	Cl21	-0.4423
Au2–Cl5	1.0091	0.0966	0.1968	Cl5	-0.4356
Au2–P8	1.0826	0.1191	0.0482	Cl6	-0.4285
Au20–Cl21	0.9870	0.0957	0.1934	Cl7	-0.4548
Au3–Cl6	1.0127	0.0973	0.1947	P17	1.9091
Au3–P9	1.0787	0.1189	0.0494	P4	1.9119
P17–Au20	1.0853	0.1203	0.0474	P8	1.8721
				P9	1.8639

4. Crystallography

4.1. Crystal structures determination

Suitable single crystals of compounds **2AuF4**, **3AuF1**, **3AuF2**, **3AuF4** and **3AuF5** were obtained by slow evaporation of acetone solutions protected from light at 4-5°C. The crystals were mounted on a glass fiber and the crystallographic data were collected with an Oxford Diffraction Gemini "A" diffractometer with a CCD area detector at 130 K, with $\lambda_{MoK\alpha}$ = 0.71073 Å. Unit cell parameters were determined with a set of three runs of 15 frames (1° in ω). The double pass method of scanning was used to exclude any noise[21]. The collected frames were integrated by using an orientation matrix determined from the narrow frame scans. Final cell constants were established by a global refinement. Collected data were corrected for absorbance by using analytical numeric absorption corrections using a multifaceted crystal model based on expressions upon the Laue symmetry with equivalent reflections.[22] Structure's solutions and refinement were carried out with the SHELXS-2018 [23] and SHELXL-2018 [24] packages. The WinGX v2020.2 [25] software was used to prepare material for publication. Full-matrix least-squares refinement was carried out by minimizing $(Fo^2–Fc^2)^2$. All non-hydrogen atoms were refined anisotropically. H atoms of the water molecule (O-H) were located in a difference map and refined isotropically with Uiso(H) = 1.5 Ueq for H-O. H atoms attached to C atoms were placed in geometrically idealised positions and refined as riding on their parent atoms, with C–H = 0.95-1.00 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic, methylene and methine groups. In compound **3AuF1**, the atoms F2, F14 and F2P, F14P are disordered over two sites with occupancies 0.40:0.60. Crystallographic data for all complexes are presented in Table S17. The crystallographic data for the structures reported in this paper has been deposited in the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 2104099-2104103. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge, CB2 1EZ, UK (fax: (+44) 1223-336-033, e-mail: deposit@ccdc.cam.ac.uk).

Table S17. Crystal data and structure refinement for compounds **2AuF4**, **3AuF1**, **3AuF2**, **3AuF4** and **3AuF5**.

Identification code	**2AuF4**	**3AuF1**	**3AuF2**	**3AuF4**	**3AuF5**
Empirical formula	$C_{37}H_{24}Au_2F_8P_2S_2$	$C_{55}H_{43}Au_3F_3P_3S_3$	$C_{55}H_{40}Au_3F_6P_3S_3$	$C_{55}H_{34}Au_3F_{12}P_3S_3$	$C_{55}H_{33}Au_3F_{15}OP_3S_3$
Formula weight	1140.55	1540.88	1594.86	1702.81	1774.80
Temperature	130(2) K	130(2) K	130(2) K	130(2) K	130(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic	Monoclinic	Orthorhombic	Monoclinic
Space group	P 21/n	P 21/n	P 21/n	P c a 21	P 21/c
Unit cell dimensions	a = 13.3221(5) Å b = 11.4452(4) Å c = 22.9850(8) Å β= 91.484(3)°.	a = 15.2146(7) Å b = 20.9398(7) Å c = 15.5266(6) Å β= 99.295(4)°.	a = 15.1382(9) Å b = 21.3370(13) Å c = 15.6982(8) Å β= 99.988(6)°.	a = 12.2753(6) Å b = 20.840(3) Å c = 20.8414(12) Å	a = 10.8448(5) Å b = 23.3463(14) Å c = 21.4117(12) Å β= 96.897(5)°.
Volume	3503.4(2) $Å^3$	4881.7(3) $Å^3$	4993.7(5) $Å^3$	5331.6(9) $Å^3$	5381.9(5) $Å^3$
Z	4	4	4	4	4
Density (calculated)(Mg/m^3)	2.162 Mg/m^3	2.097 Mg/m^3	2.121 Mg/m^3	2.121 Mg/m^3	2.190 Mg/m^3
Absorption coefficient (mm^{-1})	8.647 mm^{-1}	9.271 mm^{-1}	9.075 mm^{-1}	8.523 mm^{-1}	8.457 mm^{-1}
F(000)	2152	2920	3016	3208	3344
Crystal size (mm^3)	0.390 x 0.300 x 0.290 mm^3	0.210 x 0.160 x 0.080 mm^3	0.140 x 0.120 x 0.035 mm^3	0.190 x 0.140 x 0.110 mm^3	0.280 x 0.060 x 0.050 mm^3
Theta range for data collection	3.496 to 29.423°.	3.320 to 29.531°.	3.348 to 29.548°.	3.370 to 29.466°.	3.362 to 29.527°.
Index ranges	-16<=h<=17, -12<=k<=15, -31<=l<=29	-13<=h<=20, -16<=k<=28, -20<=l<=20	-20<=h<=20, -29<=k<=27, -20<=l<=21	-16<=h<=12, -27<=k<=25, -26<=l<=26	-14<=h<=13, -30<=k<=31, -29<=l<=27
Reflections collected	20028	25954	54916	28367	71397
Independent reflections	8358 [R(int) = 0.0426]	11511 [R(int) = 0.0443]	12345 [R(int) = 0.0590]	12040 [R(int) = 0.0349]	13502 [R(int) = 0.0564]
Completeness to theta = 25.242°	99.8 %	99.8 %	99.7 %	99.7 %	99.8 %
Absorption correction	Analytical	Analytical	Analytical	Analytical	Analytical
Max. and min. transmission	0.187 and 0.089	0.476 and 0.248	0.735 and 0.337	0.485 and 0.400	0.655 and 0.308
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	8358 / 0 / 460	11511 / 0 / 593	12345 / 0 / 631	12040 / 1 / 637	13502 / 2 / 727
Goodness-of-fit on F^2	1.064	1.083	1.165	1.067	1.091
Final R indices [I>2sigma(I)]	R1 = 0.0380, wR2 = 0.0756	R1 = 0.0444, wR2 = 0.0929	R1 = 0.0498, wR2 = 0.1177	R1 = 0.0314, wR2 = 0.0432	R1 = 0.0327, wR2 = 0.0526
R indices (all data)	R1 = 0.0514, wR2 = 0.0829	R1 = 0.0634, wR2 = 0.1012	R1 = 0.0783, wR2 = 0.1299	R1 = 0.0442, wR2 = 0.0469	R1 = 0.0561, wR2 = 0.0608
Largest diff. peak and hole ($e.Å^{-3}$)	2.188 and -1.665 $e.Å^{-3}$	2.152 and -1.849 $e.Å^{-3}$	2.518 and -3.317 $e.Å^{-3}$	1.378 and -1.351 $e.Å^{-3}$	1.427 and -1.278 $e.Å^{-3}$

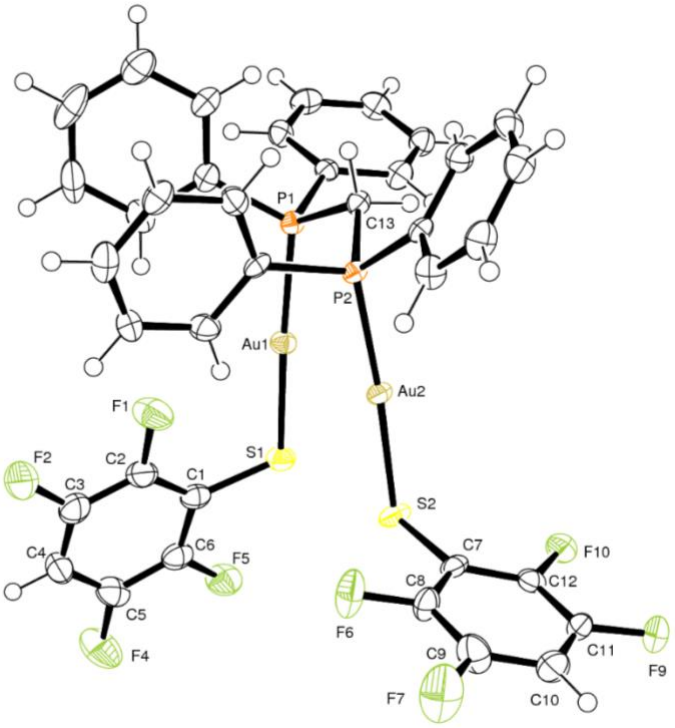


Figure S9. View on perspective of compound **2AuF4** with displacement ellipsoids at 50% probability level for non-H atoms.

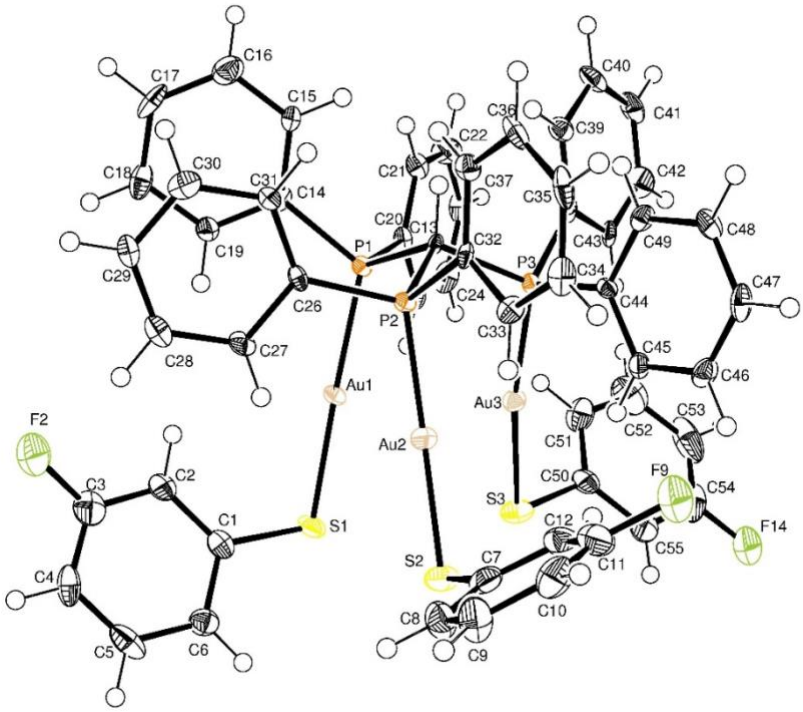


Figure S10. View on perspective of compound **3AuF1** with displacement ellipsoids at 50% probability level for non-H atoms

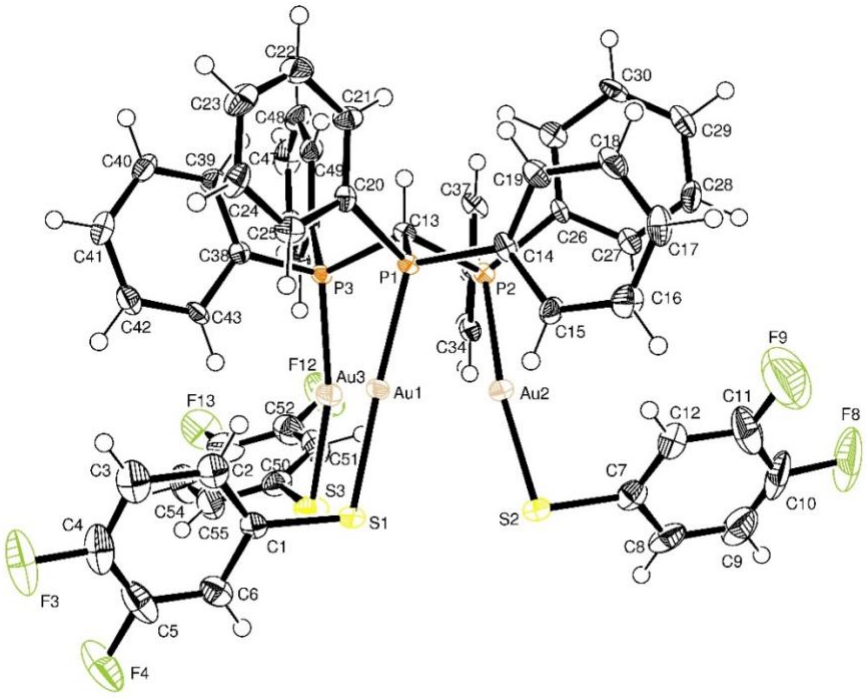


Figure S11. View on perspective of compound **3AuF2** with displacement ellipsoids at 50% probability level for non-H atoms.

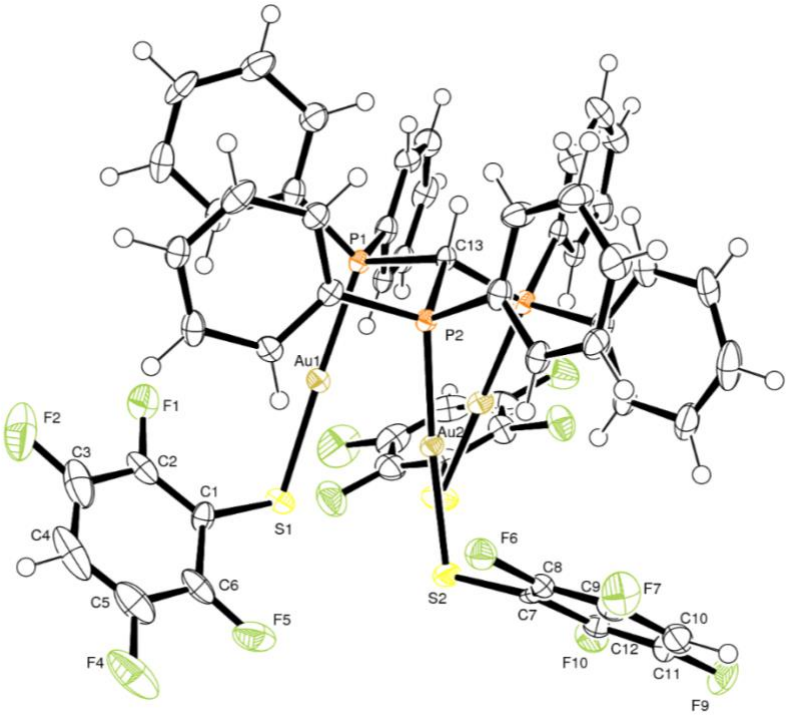


Figure S12. View on perspective of compound **3AuF4** with displacement ellipsoids at 50% probability level for non-H atoms.

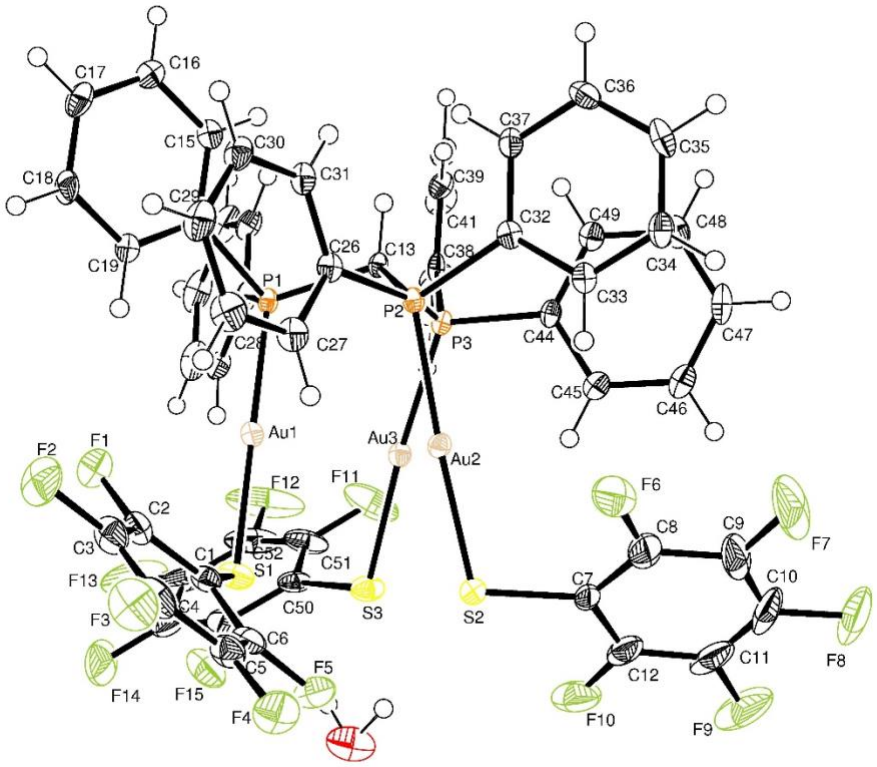


Figure S13. View on perspective of compound **3AuF5** with displacement ellipsoids at 50% probability level for non-H atoms.

4.3. Additional crystallographic tables

Table S18. Atomic coordinates in Å (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **2AuF4**. U(eq) is defined as one third of the trace of the orthogonalised U^{ij} tensor.

Atom	x	y	z	U(eq)
C(7)	7854(4)	4744(5)	3207(2)	22(1)
C(12)	8677(4)	4613(5)	2852(2)	22(1)
C(11)	8708(4)	3769(6)	2432(2)	27(1)
C(10)	7911(5)	3056(6)	2313(3)	35(2)
C(9)	7096(4)	3190(6)	2651(3)	37(2)
C(8)	7063(4)	3993(6)	3088(3)	28(1)
C(1)	6134(4)	8742(5)	4469(2)	26(1)
C(6)	5704(5)	9560(6)	4084(3)	31(1)
C(5)	4683(5)	9741(6)	4052(3)	37(2)
C(4)	4049(5)	9183(7)	4423(3)	42(2)
C(3)	4455(5)	8399(7)	4804(3)	37(2)
C(2)	5467(5)	8182(6)	4821(3)	33(2)
C(13)	9128(4)	5333(5)	6000(2)	19(1)
C(14)	7149(4)	4222(5)	5867(2)	19(1)
C(15)	6291(4)	4735(5)	5622(3)	27(1)
C(16)	5370(4)	4569(6)	5865(3)	30(1)
C(17)	5275(4)	3844(6)	6340(3)	34(2)
C(18)	6130(4)	3321(6)	6589(3)	31(1)
C(19)	7054(4)	3515(5)	6349(2)	26(1)
C(20)	8934(4)	2978(5)	5583(2)	16(1)
C(21)	9768(4)	2750(5)	5940(2)	24(1)
C(22)	10130(4)	1614(5)	5981(3)	27(1)
C(23)	9682(4)	715(5)	5683(3)	30(1)
C(24)	8867(5)	948(6)	5319(3)	31(1)
C(25)	8488(4)	2061(5)	5272(3)	27(1)
C(26)	7776(4)	6647(5)	6702(2)	23(1)
C(27)	6824(4)	7126(6)	6651(3)	33(2)
C(28)	6177(5)	7022(7)	7111(3)	45(2)
C(29)	6477(5)	6455(7)	7613(3)	47(2)
C(30)	7426(5)	5986(6)	7664(3)	38(2)
C(31)	8076(5)	6075(6)	7212(2)	30(1)
C(32)	9689(4)	7636(5)	6395(2)	19(1)
C(33)	9571(4)	8417(5)	6844(2)	24(1)
C(34)	10364(4)	9115(5)	7031(3)	29(1)
C(35)	11268(4)	9053(6)	6758(3)	30(1)
C(36)	11389(4)	8280(6)	6304(3)	29(1)
C(37)	10609(4)	7591(5)	6114(3)	26(1)
Au(2)	8123(1)	5126(1)	4616(1)	19(1)
Au(1)	7958(1)	7578(1)	5282(1)	21(1)
F(10)	9490(2)	5310(3)	2931(2)	32(1)
F(9)	9559(2)	3665(4)	2124(2)	38(1)
F(7)	6284(3)	2494(4)	2552(2)	65(1)
F(6)	6237(3)	4050(4)	3407(2)	45(1)
F(5)	6297(3)	10167(3)	3728(2)	42(1)
F(4)	4320(3)	10532(4)	3663(2)	64(1)
F(2)	3867(3)	7846(4)	5183(2)	55(1)
F(1)	5799(3)	7384(4)	5213(2)	48(1)
P(2)	8349(1)	4400(1)	5523(1)	17(1)
P(1)	8623(1)	6793(1)	6103(1)	18(1)
S(2)	7779(1)	5898(1)	3711(1)	26(1)
S(1)	7431(1)	8535(1)	4448(1)	28(1)

Table S19. Bond lengths [Å] and angles [°] for **2AuF4**.

C(7)-C(8)	1.382(8)	C(30)-C(31)	1.373(8)
C(7)-C(12)	1.390(8)	C(30)-H(30)	0.9500
C(7)-S(2)	1.762(6)	C(31)-H(31)	0.9500
C(12)-F(10)	1.354(6)	C(32)-C(33)	1.376(8)
C(12)-C(11)	1.368(8)	C(32)-C(37)	1.401(8)
C(11)-F(9)	1.357(6)	C(32)-P(1)	1.830(6)
C(11)-C(10)	1.361(9)	C(33)-C(34)	1.385(8)
C(10)-C(9)	1.361(9)	C(33)-H(33)	0.9500
C(10)-H(10)	0.9500	C(34)-C(35)	1.374(8)
C(9)-F(7)	1.358(7)	C(34)-H(34)	0.9500
C(9)-C(8)	1.362(9)	C(35)-C(36)	1.380(8)
C(8)-F(6)	1.340(6)	C(35)-H(35)	0.9500
C(1)-C(2)	1.376(9)	C(36)-C(37)	1.367(8)
C(1)-C(6)	1.400(8)	C(36)-H(36)	0.9500
C(1)-S(1)	1.745(6)	C(37)-H(37)	0.9500
C(6)-F(5)	1.346(7)	Au(2)-P(2)	2.2567(14)
C(6)-C(5)	1.377(9)	Au(2)-S(2)	2.2939(14)
C(5)-F(4)	1.353(8)	Au(2)-Au(1)	3.2076(3)
C(5)-C(4)	1.373(10)	Au(1)-P(1)	2.2511(14)
C(4)-C(3)	1.356(10)	Au(1)-S(1)	2.3014(15)
C(4)-H(4)	0.9500		
C(3)-F(2)	1.344(8)	C(8)-C(7)-C(12)	115.2(5)
C(3)-C(2)	1.371(9)	C(8)-C(7)-S(2)	122.7(4)
C(2)-F(1)	1.348(7)	C(12)-C(7)-S(2)	121.7(4)
C(13)-P(1)	1.819(6)	F(10)-C(12)-C(11)	118.1(5)
C(13)-P(2)	1.834(5)	F(10)-C(12)-C(7)	119.9(5)
C(13)-H(13A)	0.9900	C(11)-C(12)-C(7)	121.9(5)
C(13)-H(13B)	0.9900	F(9)-C(11)-C(10)	120.0(5)
C(14)-C(19)	1.379(8)	F(9)-C(11)-C(12)	118.2(5)
C(14)-C(15)	1.391(8)	C(10)-C(11)-C(12)	121.8(5)
C(14)-P(2)	1.814(5)	C(9)-C(10)-C(11)	116.6(6)
C(15)-C(16)	1.374(8)	C(9)-C(10)-H(10)	121.7
C(15)-H(15)	0.9500	C(11)-C(10)-H(10)	121.7
C(16)-C(17)	1.379(9)	F(7)-C(9)-C(10)	118.8(6)
C(16)-H(16)	0.9500	F(7)-C(9)-C(8)	118.6(6)
C(17)-C(18)	1.396(9)	C(10)-C(9)-C(8)	122.6(6)
C(17)-H(17)	0.9500	F(6)-C(8)-C(9)	118.6(5)
C(18)-C(19)	1.380(8)	F(6)-C(8)-C(7)	119.6(5)
C(18)-H(18)	0.9500	C(9)-C(8)-C(7)	121.8(5)
C(19)-H(19)	0.9500	C(2)-C(1)-C(6)	115.1(6)
C(20)-C(21)	1.389(7)	C(2)-C(1)-S(1)	127.4(5)
C(20)-C(25)	1.394(8)	C(6)-C(1)-S(1)	117.6(5)
C(20)-P(2)	1.808(5)	F(5)-C(6)-C(5)	119.0(6)
C(21)-C(22)	1.389(8)	F(5)-C(6)-C(1)	119.5(5)
C(21)-H(21)	0.9500	C(5)-C(6)-C(1)	121.5(6)
C(22)-C(23)	1.365(9)	F(4)-C(5)-C(4)	120.5(6)
C(22)-H(22)	0.9500	F(4)-C(5)-C(6)	118.1(6)
C(23)-C(24)	1.379(9)	C(4)-C(5)-C(6)	121.3(6)
C(23)-H(23)	0.9500	C(3)-C(4)-C(5)	117.8(6)
C(24)-C(25)	1.374(8)	C(3)-C(4)-H(4)	121.1
C(24)-H(24)	0.9500	C(5)-C(4)-H(4)	121.1
C(25)-H(25)	0.9500	F(2)-C(3)-C(4)	120.0(6)
C(26)-C(27)	1.384(8)	F(2)-C(3)-C(2)	119.0(6)
C(26)-C(31)	1.393(8)	C(4)-C(3)-C(2)	121.0(6)
C(26)-P(1)	1.809(5)	F(1)-C(2)-C(3)	116.6(6)
C(27)-C(28)	1.387(9)	F(1)-C(2)-C(1)	120.2(5)
C(27)-H(27)	0.9500	C(3)-C(2)-C(1)	123.2(6)
C(28)-C(29)	1.376(10)	P(1)-C(13)-P(2)	114.1(3)
C(28)-H(28)	0.9500	P(1)-C(13)-H(13A)	108.7
C(29)-C(30)	1.376(10)	P(2)-C(13)-H(13A)	108.7
C(29)-H(29)	0.9500	P(1)-C(13)-H(13B)	108.7

P(2)-C(13)-H(13B)	108.7	C(28)-C(29)-C(30)	120.1(6)
H(13A)-C(13)-H(13B)	107.6	C(28)-C(29)-H(29)	120.0
C(19)-C(14)-C(15)	118.8(5)	C(30)-C(29)-H(29)	120.0
C(19)-C(14)-P(2)	121.1(4)	C(31)-C(30)-C(29)	120.3(7)
C(15)-C(14)-P(2)	120.0(4)	C(31)-C(30)-H(30)	119.9
C(16)-C(15)-C(14)	120.6(6)	C(29)-C(30)-H(30)	119.9
C(16)-C(15)-H(15)	119.7	C(30)-C(31)-C(26)	119.9(6)
C(14)-C(15)-H(15)	119.7	C(30)-C(31)-H(31)	120.0
C(15)-C(16)-C(17)	120.4(6)	C(26)-C(31)-H(31)	120.0
C(15)-C(16)-H(16)	119.8	C(33)-C(32)-C(37)	119.2(5)
C(17)-C(16)-H(16)	119.8	C(33)-C(32)-P(1)	120.9(4)
C(16)-C(17)-C(18)	119.4(5)	C(37)-C(32)-P(1)	119.5(4)
C(16)-C(17)-H(17)	120.3	C(32)-C(33)-C(34)	120.4(5)
C(18)-C(17)-H(17)	120.3	C(32)-C(33)-H(33)	119.8
C(19)-C(18)-C(17)	119.6(6)	C(34)-C(33)-H(33)	119.8
C(19)-C(18)-H(18)	120.2	C(35)-C(34)-C(33)	119.9(6)
C(17)-C(18)-H(18)	120.2	C(35)-C(34)-H(34)	120.0
C(14)-C(19)-C(18)	121.1(5)	C(33)-C(34)-H(34)	120.0
C(14)-C(19)-H(19)	119.5	C(34)-C(35)-C(36)	119.9(5)
C(18)-C(19)-H(19)	119.5	C(34)-C(35)-H(35)	120.0
C(21)-C(20)-C(25)	119.0(5)	C(36)-C(35)-H(35)	120.0
C(21)-C(20)-P(2)	123.5(4)	C(37)-C(36)-C(35)	120.6(5)
C(25)-C(20)-P(2)	117.4(4)	C(37)-C(36)-H(36)	119.7
C(22)-C(21)-C(20)	119.2(6)	C(35)-C(36)-H(36)	119.7
C(22)-C(21)-H(21)	120.4	C(36)-C(37)-C(32)	119.9(6)
C(20)-C(21)-H(21)	120.4	C(36)-C(37)-H(37)	120.1
C(23)-C(22)-C(21)	121.7(6)	C(32)-C(37)-H(37)	120.1
C(23)-C(22)-H(22)	119.2	P(2)-Au(2)-S(2)	175.97(5)
C(21)-C(22)-H(22)	119.2	P(2)-Au(2)-Au(1)	83.72(4)
C(22)-C(23)-C(24)	119.0(6)	S(2)-Au(2)-Au(1)	94.65(4)
C(22)-C(23)-H(23)	120.5	P(1)-Au(1)-S(1)	173.31(5)
C(24)-C(23)-H(23)	120.5	P(1)-Au(1)-Au(2)	91.19(4)
C(25)-C(24)-C(23)	120.6(6)	S(1)-Au(1)-Au(2)	92.41(4)
C(25)-C(24)-H(24)	119.7	C(20)-P(2)-C(14)	104.4(2)
C(23)-C(24)-H(24)	119.7	C(20)-P(2)-C(13)	104.0(2)
C(24)-C(25)-C(20)	120.4(6)	C(14)-P(2)-C(13)	107.2(2)
C(24)-C(25)-H(25)	119.8	C(20)-P(2)-Au(2)	116.69(17)
C(20)-C(25)-H(25)	119.8	C(14)-P(2)-Au(2)	110.26(18)
C(27)-C(26)-C(31)	120.0(5)	C(13)-P(2)-Au(2)	113.46(19)
C(27)-C(26)-P(1)	119.2(5)	C(26)-P(1)-C(13)	104.7(3)
C(31)-C(26)-P(1)	120.9(4)	C(26)-P(1)-C(32)	105.3(3)
C(26)-C(27)-C(28)	119.3(6)	C(13)-P(1)-C(32)	104.2(2)
C(26)-C(27)-H(27)	120.4	C(26)-P(1)-Au(1)	115.78(19)
C(28)-C(27)-H(27)	120.4	C(13)-P(1)-Au(1)	113.33(18)
C(29)-C(28)-C(27)	120.5(6)	C(32)-P(1)-Au(1)	112.45(18)
C(29)-C(28)-H(28)	119.8	C(7)-S(2)-Au(2)	107.12(19)
C(27)-C(28)-H(28)	119.8	C(1)-S(1)-Au(1)	108.8(2)

Table S20. Anisotropic displacement parameters ($Å^2$ x 10^3)for **2AuF4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(7)	30(3)	22(3)	13(3)	2(2)	1(2)	4(3)
C(12)	24(3)	21(3)	22(3)	1(2)	-5(2)	4(2)
C(11)	30(3)	34(4)	18(3)	-1(3)	3(2)	10(3)
C(10)	38(4)	37(4)	30(4)	-12(3)	-4(3)	5(3)
C(9)	26(3)	35(4)	51(4)	-11(3)	-3(3)	-6(3)
C(8)	29(3)	26(3)	28(3)	-9(3)	6(2)	2(3)
C(1)	34(3)	23(3)	22(3)	-3(3)	-3(2)	0(3)
C(6)	41(4)	29(4)	24(3)	-6(3)	-1(3)	1(3)
C(5)	43(4)	29(4)	39(4)	-5(3)	-8(3)	14(3)
C(4)	26(3)	60(5)	38(4)	-13(4)	-4(3)	10(3)
C(3)	36(4)	47(5)	29(4)	-11(3)	1(3)	-3(3)
C(2)	36(3)	37(4)	25(3)	-2(3)	-4(3)	6(3)
C(13)	21(3)	18(3)	18(3)	1(2)	2(2)	1(2)
C(14)	28(3)	16(3)	13(3)	-4(2)	3(2)	-1(2)
C(15)	31(3)	26(3)	24(3)	6(3)	-2(2)	4(3)
C(16)	19(3)	39(4)	32(4)	0(3)	2(2)	3(3)
C(17)	25(3)	34(4)	42(4)	-9(3)	9(3)	-4(3)
C(18)	34(3)	33(4)	26(3)	5(3)	10(3)	-5(3)
C(19)	23(3)	27(3)	27(3)	3(3)	1(2)	3(3)
C(20)	21(3)	13(3)	14(3)	1(2)	5(2)	-3(2)
C(21)	25(3)	23(3)	24(3)	-3(3)	2(2)	0(2)
C(22)	28(3)	22(3)	32(4)	7(3)	4(2)	7(3)
C(23)	39(4)	17(3)	35(4)	2(3)	9(3)	6(3)
C(24)	36(3)	22(3)	34(4)	-11(3)	6(3)	-2(3)
C(25)	23(3)	23(3)	33(3)	-6(3)	1(2)	-6(3)
C(26)	22(3)	23(3)	24(3)	-5(3)	3(2)	-7(2)
C(27)	24(3)	35(4)	39(4)	0(3)	0(3)	0(3)
C(28)	24(3)	54(5)	58(5)	-16(4)	12(3)	3(3)
C(29)	51(4)	51(5)	38(4)	-11(4)	25(3)	-28(4)
C(30)	46(4)	39(4)	30(4)	-8(3)	6(3)	-7(3)
C(31)	35(3)	32(4)	22(3)	-1(3)	6(2)	0(3)
C(32)	23(3)	15(3)	19(3)	3(2)	0(2)	4(2)
C(33)	26(3)	18(3)	27(3)	-1(2)	2(2)	3(2)
C(34)	40(3)	23(3)	25(3)	-4(3)	-5(3)	-3(3)
C(35)	27(3)	27(4)	34(4)	-4(3)	-7(3)	-7(3)
C(36)	27(3)	31(4)	29(3)	2(3)	5(2)	0(3)
C(37)	29(3)	22(3)	27(3)	1(3)	5(2)	-5(3)
Au(2)	23(1)	19(1)	14(1)	0(1)	1(1)	1(1)
Au(1)	24(1)	19(1)	21(1)	0(1)	-2(1)	2(1)
F(10)	25(2)	39(2)	31(2)	-2(2)	-2(1)	-2(2)
F(9)	34(2)	49(3)	33(2)	-5(2)	11(2)	10(2)
F(7)	52(3)	56(3)	89(4)	-43(3)	14(2)	-24(2)
F(6)	36(2)	45(3)	56(3)	-18(2)	22(2)	-9(2)
F(5)	49(2)	36(2)	40(2)	14(2)	-2(2)	4(2)
F(4)	54(3)	60(3)	78(3)	16(3)	-15(2)	22(2)
F(2)	31(2)	86(4)	49(3)	7(2)	5(2)	-10(2)
F(1)	36(2)	60(3)	47(3)	25(2)	-7(2)	-12(2)
P(2)	21(1)	16(1)	14(1)	0(1)	2(1)	-1(1)
P(1)	21(1)	15(1)	18(1)	-2(1)	0(1)	1(1)
S(2)	43(1)	21(1)	13(1)	-2(1)	-1(1)	5(1)
S(1)	31(1)	29(1)	23(1)	4(1)	-2(1)	3(1)

Table S21. Atomic coordinates in Å (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **3AuF1**. U(eq) is defined as one third of the trace of the orthogonalised U^{ij} tensor.

Atom	x	y	z	U(eq)
Au(1)	6(1)	1544(1)	62(1)	14(1)
Au(2)	650(1)	2510(1)	-1195(1)	19(1)
Au(3)	-642(1)	2951(1)	206(1)	16(1)
C(1)	-456(5)	633(4)	-1661(5)	20(2)
C(2)	221(5)	247(4)	-1233(5)	22(2)
C(3)	553(6)	-236(4)	-1679(6)	31(2)
C(4)	239(6)	-376(4)	-2534(6)	26(2)
C(5)	-422(7)	1(4)	-2945(6)	31(2)
C(6)	-777(6)	511(4)	-2532(5)	23(2)
C(13)	1508(5)	2613(3)	1013(4)	10(1)
C(7)	438(6)	3080(4)	-3061(5)	26(2)
C(12)	649(6)	3687(5)	-2787(5)	29(2)
C(11)	1229(7)	4048(5)	-3187(6)	36(2)
C(10)	1612(7)	3832(5)	-3865(6)	36(2)
C(9)	1377(7)	3230(5)	-4158(6)	36(2)
C(8)	806(7)	2843(5)	-3769(6)	32(2)
C(26)	2457(5)	1761(4)	-99(5)	14(2)
C(27)	2119(5)	1295(4)	-702(5)	17(2)
C(28)	2591(6)	734(4)	-779(5)	24(2)
C(29)	3405(6)	628(4)	-245(5)	22(2)
C(30)	3743(6)	1091(4)	349(5)	27(2)
C(31)	3268(5)	1655(4)	434(5)	16(2)
C(32)	2621(5)	3128(3)	-170(5)	14(2)
C(33)	2494(5)	3500(4)	-922(5)	17(2)
C(34)	3087(6)	3985(4)	-1016(5)	25(2)
C(35)	3818(6)	4084(4)	-399(6)	24(2)
C(36)	3956(6)	3714(4)	352(5)	23(2)
C(37)	3359(5)	3239(4)	475(5)	17(2)
C(50)	-2604(6)	3259(4)	290(5)	25(2)
C(55)	-3253(6)	3694(4)	-51(6)	31(2)
C(54)	-3660(6)	4065(5)	540(8)	40(3)
C(53)	-3447(7)	4020(5)	1408(9)	52(3)
C(52)	-2791(8)	3570(6)	1738(8)	50(3)
C(51)	-2380(6)	3205(5)	1192(6)	31(2)
C(44)	1079(5)	3978(3)	411(4)	12(1)
C(45)	570(5)	4190(4)	-380(5)	17(2)
C(46)	795(6)	4746(4)	-749(5)	21(2)
C(47)	1496(6)	5107(4)	-347(5)	24(2)
C(48)	1992(5)	4910(4)	436(5)	21(2)
C(49)	1788(5)	4348(4)	818(5)	17(2)
C(38)	698(5)	3546(3)	2045(5)	16(1)
C(43)	-94(5)	3759(3)	2258(5)	16(1)
C(42)	-130(6)	3992(4)	3094(5)	27(2)
C(41)	616(6)	4012(4)	3704(5)	25(2)
C(40)	1419(6)	3796(4)	3505(5)	24(2)
C(39)	1464(5)	3564(4)	2675(5)	18(2)
C(20)	328(5)	2033(3)	2171(4)	14(2)
C(25)	-594(5)	2002(3)	2004(5)	16(2)
C(24)	-1079(6)	2129(4)	2673(5)	24(2)
C(23)	-660(6)	2289(4)	3487(6)	25(2)
C(22)	262(6)	2308(4)	3663(5)	27(2)
C(21)	744(5)	2177(4)	3011(5)	17(2)
C(14)	1827(5)	1315(3)	1719(4)	13(2)
C(19)	1776(5)	699(4)	1416(5)	19(2)
C(18)	2427(6)	247(4)	1724(6)	25(2)
C(17)	3139(6)	444(4)	2343(5)	28(2)
C(16)	3186(6)	1066(4)	2658(5)	28(2)

C(15)	2554(5)	1496(4)	2344(5)	19(2)
F(2)	1238(7)	-574(4)	-1329(6)	46(1)
F(14)	-4287(7)	4478(4)	222(6)	46(1)
F(2P)	-691(10)	-153(7)	-3739(10)	46(1)
F(14P)	-2607(11)	3514(7)	2478(10)	46(1)
F(9)	1432(4)	4651(3)	-2885(4)	46(1)
P(1)	935(1)	1861(1)	1282(1)	12(1)
P(2)	1822(1)	2497(1)	-98(1)	12(1)
P(3)	689(1)	3273(1)	929(1)	12(1)
S(1)	-983(1)	1247(1)	-1153(1)	22(1)
S(2)	-262(2)	2579(1)	-2533(1)	27(1)
S(3)	-2098(1)	2769(1)	-425(1)	26(1)

Table S22. Bond lengths [Å] and angles [°] for **3AuF1**.

Au(1)-P(1)	2.2714(18)	C(29)-H(29)	0.9500
Au(1)-S(1)	2.3014(18)	C(30)-C(31)	1.402(11)
Au(1)-Au(2)	3.0777(4)	C(30)-H(30)	0.9500
Au(1)-Au(3)	3.1259(4)	C(31)-H(31)	0.9500
Au(2)-P(2)	2.2589(18)	C(32)-C(33)	1.391(10)
Au(2)-S(2)	2.308(2)	C(32)-C(37)	1.398(10)
Au(2)-Au(3)	3.2897(5)	C(32)-P(2)	1.811(8)
Au(3)-P(3)	2.2545(19)	C(33)-C(34)	1.383(11)
Au(3)-S(3)	2.304(2)	C(33)-H(33)	0.9500
C(1)-C(6)	1.385(11)	C(34)-C(35)	1.361(12)
C(1)-C(2)	1.391(11)	C(34)-H(34)	0.9500
C(1)-S(1)	1.767(8)	C(35)-C(36)	1.387(12)
C(2)-C(3)	1.367(12)	C(35)-H(35)	0.9500
C(2)-H(2)	0.9500	C(36)-C(37)	1.381(11)
C(3)-F(2)	1.306(13)	C(36)-H(36)	0.9500
C(3)-C(4)	1.367(12)	C(37)-H(37)	0.9500
C(3)-H(3)	0.9500	C(50)-C(55)	1.385(12)
C(4)-C(5)	1.354(13)	C(50)-C(51)	1.391(12)
C(4)-H(4)	0.9500	C(50)-S(3)	1.776(9)
C(5)-F(2P)	1.277(16)	C(55)-C(54)	1.419(15)
C(5)-C(6)	1.398(12)	C(55)-H(55)	0.9500
C(5)-H(5)	0.9500	C(54)-F(14)	1.323(13)
C(6)-H(6)	0.9500	C(54)-C(53)	1.337(16)
C(13)-P(3)	1.852(7)	C(54)-H(54)	0.9500
C(13)-P(2)	1.878(7)	C(53)-C(52)	1.408(16)
C(13)-P(1)	1.878(7)	C(53)-H(53)	0.9500
C(13)-H(13)	1.0000	C(52)-F(14P)	1.143(17)
C(7)-C(12)	1.362(13)	C(52)-C(51)	1.366(14)
C(7)-C(8)	1.403(12)	C(52)-H(52)	0.9500
C(7)-S(2)	1.787(9)	C(51)-H(51)	0.9500
C(12)-C(11)	1.383(13)	C(44)-C(49)	1.394(10)
C(12)-H(12)	0.9500	C(44)-C(45)	1.414(10)
C(11)-C(10)	1.359(14)	C(44)-P(3)	1.826(8)
C(11)-F(9)	1.365(11)	C(45)-C(46)	1.366(11)
C(10)-C(9)	1.369(13)	C(45)-H(45)	0.9500
C(10)-H(10)	0.9500	C(46)-C(47)	1.372(12)
C(9)-C(8)	1.394(13)	C(46)-H(46)	0.9500
C(9)-H(9)	0.9500	C(47)-C(48)	1.387(11)
C(8)-H(8)	0.9500	C(47)-H(47)	0.9500
C(26)-C(31)	1.387(10)	C(48)-C(49)	1.375(10)
C(26)-C(27)	1.393(10)	C(48)-H(48)	0.9500
C(26)-P(2)	1.819(8)	C(49)-H(49)	0.9500
C(27)-C(28)	1.392(11)	C(38)-C(43)	1.374(11)
C(27)-H(27)	0.9500	C(38)-C(39)	1.396(11)
C(28)-C(29)	1.393(12)	C(38)-P(3)	1.822(7)
C(28)-H(28)	0.9500	C(43)-C(42)	1.396(11)
C(29)-C(30)	1.379(11)	C(43)-H(43)	0.9500

C(42)-C(41)	1.357(12)
C(42)-H(42)	0.9500
C(41)-C(40)	1.384(12)
C(41)-H(41)	0.9500
C(40)-C(39)	1.388(11)
C(40)-H(40)	0.9500
C(39)-H(39)	0.9500
C(20)-C(25)	1.386(10)
C(20)-C(21)	1.389(10)
C(20)-P(1)	1.815(7)
C(25)-C(24)	1.394(11)
C(25)-H(25)	0.9500
C(24)-C(23)	1.362(12)
C(24)-H(24)	0.9500
C(23)-C(22)	1.386(12)
C(23)-H(23)	0.9500
C(22)-C(21)	1.370(11)
C(22)-H(22)	0.9500
C(21)-H(21)	0.9500
C(14)-C(19)	1.370(11)
C(14)-C(15)	1.401(10)
C(14)-P(1)	1.821(7)
C(19)-C(18)	1.398(11)
C(19)-H(19)	0.9500
C(18)-C(17)	1.389(12)
C(18)-H(18)	0.9500
C(17)-C(16)	1.389(13)
C(17)-H(17)	0.9500
C(16)-C(15)	1.350(11)
C(16)-H(16)	0.9500
C(15)-H(15)	0.9500

P(1)-Au(1)-S(1)	177.51(7)
P(1)-Au(1)-Au(2)	96.77(5)
S(1)-Au(1)-Au(2)	83.73(6)
P(1)-Au(1)-Au(3)	79.96(5)
S(1)-Au(1)-Au(3)	98.11(5)
Au(2)-Au(1)-Au(3)	64.044(10)
P(2)-Au(2)-S(2)	164.99(8)
P(2)-Au(2)-Au(1)	78.89(5)
S(2)-Au(2)-Au(1)	113.92(6)
P(2)-Au(2)-Au(3)	89.31(5)
S(2)-Au(2)-Au(3)	103.93(6)
Au(1)-Au(2)-Au(3)	58.690(10)
P(3)-Au(3)-S(3)	170.27(8)
P(3)-Au(3)-Au(1)	92.82(5)
S(3)-Au(3)-Au(1)	96.11(6)
P(3)-Au(3)-Au(2)	80.17(5)
S(3)-Au(3)-Au(2)	107.96(6)
Au(1)-Au(3)-Au(2)	57.266(9)
C(6)-C(1)-C(2)	118.4(8)
C(6)-C(1)-S(1)	117.2(6)
C(2)-C(1)-S(1)	124.3(6)
C(3)-C(2)-C(1)	119.5(8)
C(3)-C(2)-H(2)	120.2
C(1)-C(2)-H(2)	120.2
F(2)-C(3)-C(2)	121.7(9)
F(2)-C(3)-C(4)	114.7(9)
C(2)-C(3)-C(4)	123.4(9)
C(2)-C(3)-H(3)	118.3
C(4)-C(3)-H(3)	118.3
C(5)-C(4)-C(3)	116.6(8)
C(5)-C(4)-H(4)	121.7
C(3)-C(4)-H(4)	121.7
F(2P)-C(5)-C(4)	114.0(10)
F(2P)-C(5)-C(6)	123.2(11)
C(4)-C(5)-C(6)	122.8(8)
C(4)-C(5)-H(5)	118.6
C(6)-C(5)-H(5)	118.6
C(1)-C(6)-C(5)	119.2(8)
C(1)-C(6)-H(6)	120.4
C(5)-C(6)-H(6)	120.4
P(3)-C(13)-P(2)	107.5(3)
P(3)-C(13)-P(1)	108.1(4)
P(2)-C(13)-P(1)	107.0(3)
P(3)-C(13)-H(13)	111.4
P(2)-C(13)-H(13)	111.4
P(1)-C(13)-H(13)	111.4
C(12)-C(7)-C(8)	118.1(8)
C(12)-C(7)-S(2)	122.2(7)
C(8)-C(7)-S(2)	119.7(7)
C(7)-C(12)-C(11)	120.3(9)
C(7)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(10)-C(11)-F(9)	118.2(9)
C(10)-C(11)-C(12)	123.4(9)
F(9)-C(11)-C(12)	118.4(9)
C(11)-C(10)-C(9)	116.2(9)
C(11)-C(10)-H(10)	121.9
C(9)-C(10)-H(10)	121.9
C(10)-C(9)-C(8)	122.6(9)
C(10)-C(9)-H(9)	118.7
C(8)-C(9)-H(9)	118.7
C(9)-C(8)-C(7)	119.3(9)
C(9)-C(8)-H(8)	120.3
C(7)-C(8)-H(8)	120.3
C(31)-C(26)-C(27)	119.1(7)
C(31)-C(26)-P(2)	123.8(6)
C(27)-C(26)-P(2)	117.1(6)
C(28)-C(27)-C(26)	120.6(7)
C(28)-C(27)-H(27)	119.7
C(26)-C(27)-H(27)	119.7
C(27)-C(28)-C(29)	120.4(7)
C(27)-C(28)-H(28)	119.8
C(29)-C(28)-H(28)	119.8
C(30)-C(29)-C(28)	119.0(8)
C(30)-C(29)-H(29)	120.5
C(28)-C(29)-H(29)	120.5
C(29)-C(30)-C(31)	120.9(8)
C(29)-C(30)-H(30)	119.6
C(31)-C(30)-H(30)	119.6
C(26)-C(31)-C(30)	120.0(7)
C(26)-C(31)-H(31)	120.0
C(30)-C(31)-H(31)	120.0
C(33)-C(32)-C(37)	119.6(7)
C(33)-C(32)-P(2)	117.2(6)
C(37)-C(32)-P(2)	123.2(6)
C(34)-C(33)-C(32)	119.7(7)
C(34)-C(33)-H(33)	120.1
C(32)-C(33)-H(33)	120.1
C(35)-C(34)-C(33)	120.7(8)
C(35)-C(34)-H(34)	119.7
C(33)-C(34)-H(34)	119.7
C(34)-C(35)-C(36)	120.1(8)

C(34)-C(35)-H(35)	119.9	C(39)-C(40)-H(40)	120.0
C(36)-C(35)-H(35)	119.9	C(40)-C(39)-C(38)	120.0(8)
C(37)-C(36)-C(35)	120.3(8)	C(40)-C(39)-H(39)	120.0
C(37)-C(36)-H(36)	119.8	C(38)-C(39)-H(39)	120.0
C(35)-C(36)-H(36)	119.8	C(25)-C(20)-C(21)	118.6(7)
C(36)-C(37)-C(32)	119.4(7)	C(25)-C(20)-P(1)	118.2(6)
C(36)-C(37)-H(37)	120.3	C(21)-C(20)-P(1)	123.2(6)
C(32)-C(37)-H(37)	120.3	C(20)-C(25)-C(24)	119.6(7)
C(55)-C(50)-C(51)	118.7(9)	C(20)-C(25)-H(25)	120.2
C(55)-C(50)-S(3)	119.7(7)	C(24)-C(25)-H(25)	120.2
C(51)-C(50)-S(3)	121.5(7)	C(23)-C(24)-C(25)	120.9(8)
C(50)-C(55)-C(54)	118.2(9)	C(23)-C(24)-H(24)	119.5
C(50)-C(55)-H(55)	120.9	C(25)-C(24)-H(24)	119.5
C(54)-C(55)-H(55)	120.9	C(24)-C(23)-C(22)	119.8(8)
F(14)-C(54)-C(53)	117.7(11)	C(24)-C(23)-H(23)	120.1
F(14)-C(54)-C(55)	118.8(11)	C(22)-C(23)-H(23)	120.1
C(53)-C(54)-C(55)	123.6(9)	C(21)-C(22)-C(23)	119.6(8)
C(53)-C(54)-H(54)	118.2	C(21)-C(22)-H(22)	120.2
C(55)-C(54)-H(54)	118.2	C(23)-C(22)-H(22)	120.2
C(54)-C(53)-C(52)	117.2(10)	C(22)-C(21)-C(20)	121.4(8)
C(54)-C(53)-H(53)	121.4	C(22)-C(21)-H(21)	119.3
C(52)-C(53)-H(53)	121.4	C(20)-C(21)-H(21)	119.3
F(14P)-C(52)-C(51)	120.2(14)	C(19)-C(14)-C(15)	119.2(7)
F(14P)-C(52)-C(53)	118.6(13)	C(19)-C(14)-P(1)	117.7(6)
C(51)-C(52)-C(53)	121.1(11)	C(15)-C(14)-P(1)	123.0(6)
C(51)-C(52)-H(52)	119.4	C(14)-C(19)-C(18)	121.5(7)
C(53)-C(52)-H(52)	119.4	C(14)-C(19)-H(19)	119.3
C(52)-C(51)-C(50)	121.2(9)	C(18)-C(19)-H(19)	119.3
C(52)-C(51)-H(51)	119.4	C(17)-C(18)-C(19)	117.8(8)
C(50)-C(51)-H(51)	119.4	C(17)-C(18)-H(18)	121.1
C(49)-C(44)-C(45)	119.7(7)	C(19)-C(18)-H(18)	121.1
C(49)-C(44)-P(3)	122.2(5)	C(18)-C(17)-C(16)	120.8(8)
C(45)-C(44)-P(3)	117.7(5)	C(18)-C(17)-H(17)	119.6
C(46)-C(45)-C(44)	119.5(7)	C(16)-C(17)-H(17)	119.6
C(46)-C(45)-H(45)	120.2	C(15)-C(16)-C(17)	120.4(8)
C(44)-C(45)-H(45)	120.2	C(15)-C(16)-H(16)	119.8
C(45)-C(46)-C(47)	120.5(7)	C(17)-C(16)-H(16)	119.8
C(45)-C(46)-H(46)	119.7	C(16)-C(15)-C(14)	120.3(7)
C(47)-C(46)-H(46)	119.7	C(16)-C(15)-H(15)	119.8
C(46)-C(47)-C(48)	120.5(7)	C(14)-C(15)-H(15)	119.8
C(46)-C(47)-H(47)	119.8	C(20)-P(1)-C(14)	106.3(3)
C(48)-C(47)-H(47)	119.8	C(20)-P(1)-C(13)	108.4(3)
C(49)-C(48)-C(47)	120.3(7)	C(14)-P(1)-C(13)	105.3(3)
C(49)-C(48)-H(48)	119.8	C(20)-P(1)-Au(1)	111.6(3)
C(47)-C(48)-H(48)	119.8	C(14)-P(1)-Au(1)	116.9(2)
C(48)-C(49)-C(44)	119.4(7)	C(13)-P(1)-Au(1)	107.9(2)
C(48)-C(49)-H(49)	120.3	C(32)-P(2)-C(26)	104.8(3)
C(44)-C(49)-H(49)	120.3	C(32)-P(2)-C(13)	103.6(3)
C(43)-C(38)-C(39)	119.2(7)	C(26)-P(2)-C(13)	108.9(3)
C(43)-C(38)-P(3)	117.3(6)	C(32)-P(2)-Au(2)	113.6(2)
C(39)-C(38)-P(3)	123.5(6)	C(26)-P(2)-Au(2)	111.4(2)
C(38)-C(43)-C(42)	120.3(7)	C(13)-P(2)-Au(2)	113.8(2)
C(38)-C(43)-H(43)	119.9	C(38)-P(3)-C(44)	102.2(3)
C(42)-C(43)-H(43)	119.9	C(38)-P(3)-C(13)	105.5(3)
C(41)-C(42)-C(43)	120.4(8)	C(44)-P(3)-C(13)	111.8(3)
C(41)-C(42)-H(42)	119.8	C(38)-P(3)-Au(3)	115.9(3)
C(43)-C(42)-H(42)	119.8	C(44)-P(3)-Au(3)	110.6(2)
C(42)-C(41)-C(40)	120.2(7)	C(13)-P(3)-Au(3)	110.6(2)
C(42)-C(41)-H(41)	119.9	C(1)-S(1)-Au(1)	106.2(3)
C(40)-C(41)-H(41)	119.9	C(7)-S(2)-Au(2)	97.7(3)
C(41)-C(40)-C(39)	119.9(8)	C(50)-S(3)-Au(3)	97.0(3)
C(41)-C(40)-H(40)	120.0		

Table S23. Anisotropic displacement parameters ($Å^2$ x 10^3)for **3AuF1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au(1)	14(1)	14(1)	15(1)	-2(1)	1(1)	-4(1)
Au(2)	19(1)	20(1)	16(1)	0(1)	0(1)	1(1)
Au(3)	14(1)	16(1)	18(1)	1(1)	2(1)	0(1)
C(1)	18(4)	17(4)	25(4)	-1(3)	6(3)	-9(3)
C(2)	20(4)	17(4)	28(4)	-2(3)	0(3)	-10(3)
C(3)	18(4)	27(5)	48(6)	-4(4)	4(4)	-8(4)
C(4)	28(5)	16(4)	41(5)	0(4)	21(4)	1(4)
C(5)	46(6)	29(5)	22(4)	-10(4)	15(4)	-16(5)
C(6)	25(4)	25(5)	20(4)	1(3)	4(3)	-2(4)
C(13)	13(3)	7(3)	9(3)	3(3)	3(3)	2(3)
C(7)	21(4)	32(5)	23(4)	3(4)	-2(3)	7(4)
C(12)	31(5)	37(5)	18(4)	-5(4)	4(4)	2(4)
C(11)	45(6)	32(6)	27(5)	-1(4)	-4(4)	-6(5)
C(10)	42(6)	33(6)	34(5)	13(4)	9(4)	3(5)
C(9)	56(7)	27(5)	30(5)	3(4)	20(5)	2(5)
C(8)	46(6)	25(5)	27(5)	-3(4)	10(4)	2(4)
C(26)	17(4)	12(4)	15(4)	-5(3)	7(3)	0(3)
C(27)	16(4)	15(4)	20(4)	-1(3)	1(3)	-8(3)
C(28)	30(5)	18(4)	24(4)	-6(3)	7(4)	-5(4)
C(29)	28(5)	14(4)	26(4)	-5(3)	6(4)	2(3)
C(30)	23(5)	31(5)	25(4)	2(4)	-1(4)	2(4)
C(31)	19(4)	14(4)	16(4)	-2(3)	-1(3)	-1(3)
C(32)	13(4)	9(4)	20(4)	1(3)	4(3)	5(3)
C(33)	13(4)	20(4)	19(4)	3(3)	5(3)	1(3)
C(34)	31(5)	20(4)	28(4)	2(3)	14(4)	2(4)
C(35)	28(5)	9(4)	40(5)	-2(3)	19(4)	-4(3)
C(36)	19(4)	17(4)	34(5)	-15(4)	9(4)	-5(3)
C(37)	20(4)	18(4)	14(4)	-2(3)	6(3)	1(3)
C(50)	21(4)	22(5)	30(5)	-2(3)	-3(4)	-10(4)
C(55)	19(4)	23(5)	49(6)	1(4)	-5(4)	-10(4)
C(54)	9(4)	22(5)	86(8)	0(5)	-2(5)	-1(4)
C(53)	28(6)	38(7)	95(10)	-32(6)	23(6)	-5(5)
C(52)	55(7)	48(7)	48(7)	-9(5)	16(6)	-6(6)
C(51)	23(5)	31(5)	41(5)	2(4)	11(4)	7(4)
C(44)	12(3)	12(4)	12(3)	-3(3)	2(3)	0(3)
C(45)	18(4)	12(4)	21(4)	0(3)	2(3)	1(3)
C(46)	28(5)	19(4)	16(4)	6(3)	5(3)	4(4)
C(47)	33(5)	11(4)	29(4)	6(3)	14(4)	1(4)
C(48)	21(4)	14(4)	29(4)	0(3)	5(3)	-11(3)
C(49)	20(4)	17(4)	14(4)	4(3)	5(3)	3(3)
C(38)	26(3)	7(2)	15(3)	3(2)	6(2)	3(2)
C(43)	26(3)	7(2)	15(3)	3(2)	6(2)	3(2)
C(42)	31(5)	31(5)	22(4)	-2(4)	12(4)	5(4)
C(41)	40(5)	20(4)	17(4)	-8(3)	12(4)	-2(4)
C(40)	39(5)	18(4)	15(4)	-1(3)	1(3)	-15(4)
C(39)	20(4)	17(4)	18(4)	0(3)	3(3)	-4(3)
C(20)	19(4)	11(4)	14(4)	1(3)	9(3)	0(3)
C(25)	16(4)	8(4)	24(4)	3(3)	8(3)	-1(3)
C(24)	19(4)	23(5)	33(5)	8(4)	15(4)	2(4)
C(23)	29(5)	20(4)	32(5)	4(4)	20(4)	0(4)
C(22)	34(5)	32(5)	15(4)	3(3)	4(3)	-1(4)
C(21)	21(4)	14(4)	18(4)	1(3)	8(3)	-5(3)
C(14)	14(4)	11(3)	15(4)	8(3)	5(3)	-1(3)
C(19)	18(4)	18(4)	20(4)	-4(3)	1(3)	2(3)
C(18)	22(4)	16(4)	39(5)	8(3)	14(4)	3(3)

C(17)	24(5)	30(5)	29(5)	18(4)	6(4)	15(4)
C(16)	30(5)	32(5)	22(4)	5(4)	0(4)	5(4)
C(15)	19(4)	13(4)	22(4)	-1(3)	1(3)	5(3)
F(2)	54(3)	28(2)	55(3)	-1(2)	7(2)	-2(2)
F(14)	54(3)	28(2)	55(3)	-1(2)	7(2)	-2(2)
F(2P)	54(3)	28(2)	55(3)	-1(2)	7(2)	-2(2)
F(14P)	54(3)	28(2)	55(3)	-1(2)	7(2)	-2(2)
F(9)	54(3)	28(2)	55(3)	-1(2)	7(2)	-2(2)
P(1)	13(1)	11(1)	12(1)	0(1)	3(1)	-2(1)
P(2)	12(1)	13(1)	10(1)	0(1)	2(1)	-1(1)
P(3)	13(1)	10(1)	12(1)	-1(1)	3(1)	0(1)
S(1)	17(1)	25(1)	22(1)	-9(1)	-2(1)	-2(1)
S(2)	26(1)	33(1)	21(1)	2(1)	-3(1)	-3(1)
S(3)	17(1)	37(1)	24(1)	2(1)	-1(1)	-1(1)

Table S24. Atomic coordinates in Å (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **3AuF2**. U(eq) is defined as one third of the trace of the orthogonalised U^{ij} tensor.

x	y	z	U(eq)
C(1)	5498(6)	4317(4)	6512(6)	21(2)
C(2)	4820(7)	4689(5)	6056(8)	30(2)
C(3)	4440(8)	5187(5)	6455(8)	38(3)
C(4)	4777(9)	5302(5)	7303(9)	42(3)
C(5)	5439(10)	4948(6)	7752(8)	43(3)
C(6)	5812(8)	4449(5)	7377(7)	31(2)
C(7)	7619(7)	1738(5)	4756(8)	29(2)
C(8)	8223(7)	1296(5)	5162(9)	38(3)
C(9)	8619(9)	875(6)	4674(12)	54(4)
C(10)	8441(9)	887(6)	3829(13)	57(4)
C(11)	7855(11)	1319(7)	3390(9)	54(4)
C(12)	7446(8)	1752(6)	3864(9)	42(3)
C(13)	3486(6)	2353(4)	3901(6)	15(2)
C(14)	4672(6)	2905(4)	2757(6)	16(2)
C(15)	5611(6)	2931(5)	2917(6)	22(2)
C(16)	6097(7)	2809(5)	2275(7)	31(2)
C(17)	5650(7)	2633(5)	1447(7)	30(2)
C(18)	4729(8)	2613(5)	1284(7)	29(2)
C(19)	4241(7)	2748(4)	1929(6)	22(2)
C(20)	3179(6)	3628(4)	3202(6)	16(2)
C(21)	2444(6)	3463(5)	2570(6)	22(2)
C(22)	1800(7)	3903(5)	2271(7)	30(2)
C(23)	1863(7)	4500(5)	2595(7)	30(2)
C(24)	2568(7)	4669(5)	3222(7)	27(2)
C(25)	3233(6)	4233(4)	3532(6)	21(2)
C(26)	4308(6)	1421(4)	2909(5)	15(2)
C(27)	5122(7)	1211(4)	2713(6)	23(2)
C(28)	5157(7)	970(5)	1900(7)	28(2)
C(29)	4389(8)	936(5)	1286(7)	31(2)
C(30)	3582(7)	1133(5)	1472(6)	24(2)
C(31)	3541(7)	1381(4)	2278(6)	21(2)
C(32)	3924(6)	1018(4)	4534(6)	16(2)
C(33)	4435(6)	824(4)	5323(6)	20(2)
C(34)	4215(7)	275(5)	5711(6)	27(2)
C(35)	3523(7)	-86(4)	5315(7)	27(2)
C(36)	3016(7)	101(5)	4532(7)	25(2)
C(37)	3219(7)	645(4)	4149(6)	22(2)
C(38)	2537(6)	3203(4)	4990(5)	15(2)
C(39)	1714(6)	3313(4)	4470(7)	23(2)
C(40)	1247(6)	3868(5)	4551(7)	25(2)
C(41)	1609(7)	4308(5)	5158(7)	27(2)
C(42)	2415(7)	4199(5)	5676(6)	26(2)

C(43)	2897(6)	3659(4)	5600(6)	19(2)
C(44)	2344(6)	1856(4)	5042(6)	14(2)
C(45)	2443(7)	1500(4)	5802(6)	21(2)
C(46)	1826(7)	1042(5)	5908(7)	30(2)
C(47)	1087(8)	952(5)	5268(8)	36(3)
C(48)	973(7)	1302(5)	4515(8)	28(2)
C(49)	1612(6)	1745(5)	4394(7)	24(2)
C(50)	4520(7)	1930(5)	7972(7)	31(2)
C(51)	4319(9)	1320(6)	7706(8)	40(3)
C(52)	3773(9)	957(5)	8113(8)	39(3)
C(53)	3428(9)	1186(6)	8790(8)	41(3)
C(54)	3624(9)	1790(6)	9084(9)	44(3)
C(55)	4175(8)	2155(6)	8677(8)	40(3)
Au(1)	5025(1)	3398(1)	4843(1)	16(1)
Au(2)	5649(1)	2046(1)	4735(1)	19(1)
Au(3)	4334(1)	2462(1)	6100(1)	23(1)
F(3)	4425(7)	5765(3)	7728(6)	68(3)
F(4)	5738(7)	5095(4)	8588(5)	69(3)
F(8)	8777(7)	458(5)	3328(8)	98(4)
F(9)	7683(9)	1320(6)	2560(7)	117(4)
F(12)	3555(6)	367(4)	7836(5)	64(2)
F(13)	2872(6)	822(4)	9177(5)	59(2)
P(1)	4076(2)	3084(1)	3638(1)	13(1)
P(2)	4318(2)	1705(1)	4009(1)	14(1)
P(3)	3163(2)	2470(1)	4988(1)	14(1)
S(1)	6038(2)	3707(1)	6036(2)	27(1)
S(2)	7104(2)	2277(1)	5371(2)	26(1)
S(3)	5230(2)	2422(1)	7449(2)	34(1)

Table S25. Bond lengths [Å] and angles [°] for **3AuF2**.

C(1)-C(6)	1.387(14)	C(13)-H(13)	1.0000
C(1)-C(2)	1.392(15)	C(14)-C(19)	1.390(13)
C(1)-S(1)	1.771(10)	C(14)-C(15)	1.401(13)
C(2)-C(3)	1.407(16)	C(14)-P(1)	1.818(9)
C(2)-H(2)	0.9500	C(15)-C(16)	1.373(14)
C(3)-C(4)	1.362(18)	C(15)-H(15)	0.9500
C(3)-H(3)	0.9500	C(16)-C(17)	1.407(15)
C(4)-F(3)	1.352(13)	C(16)-H(16)	0.9500
C(4)-C(5)	1.353(19)	C(17)-C(18)	1.373(16)
C(5)-F(4)	1.348(14)	C(17)-H(17)	0.9500
C(5)-C(6)	1.383(16)	C(18)-C(19)	1.384(14)
C(6)-H(6)	0.9500	C(18)-H(18)	0.9500
C(7)-C(12)	1.379(17)	C(19)-H(19)	0.9500
C(7)-C(8)	1.389(15)	C(20)-C(25)	1.388(13)
C(7)-S(2)	1.768(11)	C(20)-C(21)	1.400(13)
C(8)-C(9)	1.384(18)	C(20)-P(1)	1.827(9)
C(8)-H(8)	0.9500	C(21)-C(22)	1.376(14)
C(9)-C(10)	1.31(2)	C(21)-H(21)	0.9500
C(9)-H(9)	0.9500	C(22)-C(23)	1.370(15)
C(10)-F(8)	1.362(15)	C(22)-H(22)	0.9500
C(10)-C(11)	1.38(2)	C(23)-C(24)	1.369(15)
C(11)-F(9)	1.284(17)	C(23)-H(23)	0.9500
C(11)-C(12)	1.397(18)	C(24)-C(25)	1.395(13)
C(12)-H(12)	0.9500	C(24)-H(24)	0.9500
C(13)-P(2)	1.859(9)	C(25)-H(25)	0.9500
C(13)-P(3)	1.872(9)	C(26)-C(31)	1.392(13)
C(13)-P(1)	1.880(9)	C(26)-C(27)	1.394(13)

C(26)-P(2)	1.828(9)	C(54)-H(54)	0.9500
C(27)-C(28)	1.386(14)	C(55)-H(55)	0.9500
C(27)-H(27)	0.9500	Au(1)-P(1)	2.270(2)
C(28)-C(29)	1.378(15)	Au(1)-S(1)	2.301(2)
C(28)-H(28)	0.9500	Au(1)-Au(2)	3.0499(5)
C(29)-C(30)	1.370(15)	Au(1)-Au(3)	3.1126(5)
C(29)-H(29)	0.9500	Au(2)-P(2)	2.256(2)
C(30)-C(31)	1.383(13)	Au(2)-S(2)	2.310(2)
C(30)-H(30)	0.9500	Au(2)-Au(3)	3.2887(6)
C(31)-H(31)	0.9500	Au(3)-P(3)	2.262(2)
C(32)-C(37)	1.383(13)	Au(3)-S(3)	2.310(3)
C(32)-C(33)	1.404(12)		
C(32)-P(2)	1.831(9)	C(6)-C(1)-C(2)	118.9(10)
C(33)-C(34)	1.386(13)	C(6)-C(1)-S(1)	117.2(8)
C(33)-H(33)	0.9500	C(2)-C(1)-S(1)	123.7(8)
C(34)-C(35)	1.361(15)	C(1)-C(2)-C(3)	121.6(11)
C(34)-H(34)	0.9500	C(1)-C(2)-H(2)	119.2
C(35)-C(36)	1.390(14)	C(3)-C(2)-H(2)	119.2
C(35)-H(35)	0.9500	C(4)-C(3)-C(2)	117.3(12)
C(36)-C(37)	1.368(13)	C(4)-C(3)-H(3)	121.4
C(36)-H(36)	0.9500	C(2)-C(3)-H(3)	121.4
C(37)-H(37)	0.9500	F(3)-C(4)-C(5)	118.1(12)
C(38)-C(39)	1.387(13)	F(3)-C(4)-C(3)	120.1(12)
C(38)-C(43)	1.407(12)	C(5)-C(4)-C(3)	121.8(11)
C(38)-P(3)	1.827(9)	F(4)-C(5)-C(4)	118.0(12)
C(39)-C(40)	1.396(13)	F(4)-C(5)-C(6)	120.1(13)
C(39)-H(39)	0.9500	C(4)-C(5)-C(6)	121.9(11)
C(40)-C(41)	1.381(15)	C(5)-C(6)-C(1)	118.5(11)
C(40)-H(40)	0.9500	C(5)-C(6)-H(6)	120.7
C(41)-C(42)	1.363(15)	C(1)-C(6)-H(6)	120.7
C(41)-H(41)	0.9500	C(12)-C(7)-C(8)	118.4(11)
C(42)-C(43)	1.381(14)	C(12)-C(7)-S(2)	121.0(9)
C(42)-H(42)	0.9500	C(8)-C(7)-S(2)	120.6(9)
C(43)-H(43)	0.9500	C(9)-C(8)-C(7)	120.0(13)
C(44)-C(49)	1.389(13)	C(9)-C(8)-H(8)	120.0
C(44)-C(45)	1.400(13)	C(7)-C(8)-H(8)	120.0
C(44)-P(3)	1.817(9)	C(10)-C(9)-C(8)	121.1(14)
C(45)-C(46)	1.381(14)	C(10)-C(9)-H(9)	119.5
C(45)-H(45)	0.9500	C(8)-C(9)-H(9)	119.5
C(46)-C(47)	1.382(16)	C(9)-C(10)-F(8)	122.7(15)
C(46)-H(46)	0.9500	C(9)-C(10)-C(11)	121.6(13)
C(47)-C(48)	1.383(16)	F(8)-C(10)-C(11)	115.6(16)
C(47)-H(47)	0.9500	F(9)-C(11)-C(10)	120.6(14)
C(48)-C(49)	1.388(14)	F(9)-C(11)-C(12)	120.6(15)
C(48)-H(48)	0.9500	C(10)-C(11)-C(12)	118.8(13)
C(49)-H(49)	0.9500	C(7)-C(12)-C(11)	120.2(12)
C(50)-C(51)	1.385(16)	C(7)-C(12)-H(12)	119.9
C(50)-C(55)	1.389(16)	C(11)-C(12)-H(12)	119.9
C(50)-S(3)	1.799(11)	P(2)-C(13)-P(3)	107.3(4)
C(51)-C(52)	1.369(18)	P(2)-C(13)-P(1)	107.3(5)
C(51)-H(51)	0.9500	P(3)-C(13)-P(1)	107.3(4)
C(52)-F(12)	1.353(13)	P(2)-C(13)-H(13)	111.6
C(52)-C(53)	1.354(18)	P(3)-C(13)-H(13)	111.6
C(53)-F(13)	1.362(14)	P(1)-C(13)-H(13)	111.6
C(53)-C(54)	1.384(17)	C(19)-C(14)-C(15)	118.4(9)
C(54)-C(55)	1.377(18)	C(19)-C(14)-P(1)	123.1(7)

C(15)-C(14)-P(1)	118.5(7)	C(34)-C(33)-H(33)	120.1
C(16)-C(15)-C(14)	121.0(9)	C(32)-C(33)-H(33)	120.1
C(16)-C(15)-H(15)	119.5	C(35)-C(34)-C(33)	120.2(9)
C(14)-C(15)-H(15)	119.5	C(35)-C(34)-H(34)	119.9
C(15)-C(16)-C(17)	119.8(10)	C(33)-C(34)-H(34)	119.9
C(15)-C(16)-H(16)	120.1	C(34)-C(35)-C(36)	120.3(9)
C(17)-C(16)-H(16)	120.1	C(34)-C(35)-H(35)	119.9
C(18)-C(17)-C(16)	119.4(10)	C(36)-C(35)-H(35)	119.9
C(18)-C(17)-H(17)	120.3	C(37)-C(36)-C(35)	120.1(9)
C(16)-C(17)-H(17)	120.3	C(37)-C(36)-H(36)	120.0
C(17)-C(18)-C(19)	120.7(10)	C(35)-C(36)-H(36)	120.0
C(17)-C(18)-H(18)	119.7	C(36)-C(37)-C(32)	120.8(9)
C(19)-C(18)-H(18)	119.7	C(36)-C(37)-H(37)	119.6
C(18)-C(19)-C(14)	120.7(9)	C(32)-C(37)-H(37)	119.6
C(18)-C(19)-H(19)	119.6	C(39)-C(38)-C(43)	119.0(9)
C(14)-C(19)-H(19)	119.6	C(39)-C(38)-P(3)	123.9(7)
C(25)-C(20)-C(21)	119.1(9)	C(43)-C(38)-P(3)	117.0(7)
C(25)-C(20)-P(1)	117.3(7)	C(38)-C(39)-C(40)	120.5(9)
C(21)-C(20)-P(1)	123.6(7)	C(38)-C(39)-H(39)	119.7
C(22)-C(21)-C(20)	119.9(9)	C(40)-C(39)-H(39)	119.7
C(22)-C(21)-H(21)	120.0	C(41)-C(40)-C(39)	119.5(9)
C(20)-C(21)-H(21)	120.0	C(41)-C(40)-H(40)	120.2
C(23)-C(22)-C(21)	120.6(10)	C(39)-C(40)-H(40)	120.2
C(23)-C(22)-H(22)	119.7	C(42)-C(41)-C(40)	120.2(9)
C(21)-C(22)-H(22)	119.7	C(42)-C(41)-H(41)	119.9
C(24)-C(23)-C(22)	120.5(9)	C(40)-C(41)-H(41)	119.9
C(24)-C(23)-H(23)	119.8	C(41)-C(42)-C(43)	121.5(9)
C(22)-C(23)-H(23)	119.8	C(41)-C(42)-H(42)	119.2
C(23)-C(24)-C(25)	120.1(10)	C(43)-C(42)-H(42)	119.2
C(23)-C(24)-H(24)	120.0	C(42)-C(43)-C(38)	119.2(9)
C(25)-C(24)-H(24)	120.0	C(42)-C(43)-H(43)	120.4
C(20)-C(25)-C(24)	119.8(9)	C(38)-C(43)-H(43)	120.4
C(20)-C(25)-H(25)	120.1	C(49)-C(44)-C(45)	119.1(9)
C(24)-C(25)-H(25)	120.1	C(49)-C(44)-P(3)	123.6(7)
C(31)-C(26)-C(27)	118.9(8)	C(45)-C(44)-P(3)	117.3(7)
C(31)-C(26)-P(2)	124.2(7)	C(46)-C(45)-C(44)	120.8(9)
C(27)-C(26)-P(2)	116.9(7)	C(46)-C(45)-H(45)	119.6
C(28)-C(27)-C(26)	120.0(9)	C(44)-C(45)-H(45)	119.6
C(28)-C(27)-H(27)	120.0	C(45)-C(46)-C(47)	119.3(10)
C(26)-C(27)-H(27)	120.0	C(45)-C(46)-H(46)	120.4
C(29)-C(28)-C(27)	120.0(10)	C(47)-C(46)-H(46)	120.4
C(29)-C(28)-H(28)	120.0	C(46)-C(47)-C(48)	120.8(10)
C(27)-C(28)-H(28)	120.0	C(46)-C(47)-H(47)	119.6
C(30)-C(29)-C(28)	120.7(9)	C(48)-C(47)-H(47)	119.6
C(30)-C(29)-H(29)	119.7	C(47)-C(48)-C(49)	119.9(10)
C(28)-C(29)-H(29)	119.7	C(47)-C(48)-H(48)	120.1
C(29)-C(30)-C(31)	119.8(9)	C(49)-C(48)-H(48)	120.1
C(29)-C(30)-H(30)	120.1	C(48)-C(49)-C(44)	120.1(10)
C(31)-C(30)-H(30)	120.1	C(48)-C(49)-H(49)	119.9
C(30)-C(31)-C(26)	120.6(9)	C(44)-C(49)-H(49)	119.9
C(30)-C(31)-H(31)	119.7	C(51)-C(50)-C(55)	118.1(11)
C(26)-C(31)-H(31)	119.7	C(51)-C(50)-S(3)	121.9(9)
C(37)-C(32)-C(33)	118.8(8)	C(55)-C(50)-S(3)	120.0(9)
C(37)-C(32)-P(2)	123.4(7)	C(52)-C(51)-C(50)	120.6(11)
C(33)-C(32)-P(2)	117.4(7)	C(52)-C(51)-H(51)	119.7
C(34)-C(33)-C(32)	119.9(9)	C(50)-C(51)-H(51)	119.7

F(12)-C(52)-C(53)	118.8(12)	S(3)-Au(3)-Au(1)	113.36(7)
F(12)-C(52)-C(51)	120.6(11)	P(3)-Au(3)-Au(2)	88.96(6)
C(53)-C(52)-C(51)	120.6(11)	S(3)-Au(3)-Au(2)	105.15(8)
C(52)-C(53)-F(13)	119.8(11)	Au(1)-Au(3)-Au(2)	56.827(12)
C(52)-C(53)-C(54)	120.5(12)	C(14)-P(1)-C(20)	106.5(4)
F(13)-C(53)-C(54)	119.6(12)	C(14)-P(1)-C(13)	108.1(4)
C(55)-C(54)-C(53)	118.9(12)	C(20)-P(1)-C(13)	105.0(4)
C(55)-C(54)-H(54)	120.5	C(14)-P(1)-Au(1)	111.7(3)
C(53)-C(54)-H(54)	120.5	C(20)-P(1)-Au(1)	116.5(3)
C(54)-C(55)-C(50)	121.1(12)	C(13)-P(1)-Au(1)	108.6(3)
C(54)-C(55)-H(55)	119.5	C(26)-P(2)-C(32)	102.2(4)
C(50)-C(55)-H(55)	119.5	C(26)-P(2)-C(13)	105.4(4)
P(1)-Au(1)-S(1)	177.56(9)	C(32)-P(2)-C(13)	111.5(4)
P(1)-Au(1)-Au(2)	80.32(6)	C(26)-P(2)-Au(2)	116.4(3)
S(1)-Au(1)-Au(2)	98.45(7)	C(32)-P(2)-Au(2)	111.3(3)
P(1)-Au(1)-Au(3)	96.03(6)	C(13)-P(2)-Au(2)	109.8(3)
S(1)-Au(1)-Au(3)	85.29(7)	C(44)-P(3)-C(38)	105.0(4)
Au(2)-Au(1)-Au(3)	64.498(13)	C(44)-P(3)-C(13)	103.5(4)
P(2)-Au(2)-S(2)	171.40(9)	C(38)-P(3)-C(13)	109.5(4)
P(2)-Au(2)-Au(1)	94.34(6)	C(44)-P(3)-Au(3)	114.1(3)
S(2)-Au(2)-Au(1)	93.14(7)	C(38)-P(3)-Au(3)	110.0(3)
P(2)-Au(2)-Au(3)	80.11(6)	C(13)-P(3)-Au(3)	114.1(3)
S(2)-Au(2)-Au(3)	107.49(7)	C(1)-S(1)-Au(1)	105.2(3)
Au(1)-Au(2)-Au(3)	58.675(11)	C(7)-S(2)-Au(2)	95.9(4)
P(3)-Au(3)-S(3)	164.72(10)	C(50)-S(3)-Au(3)	97.9(4)
P(3)-Au(3)-Au(1)	79.11(6)		

Table S26. Anisotropic displacement parameters ($Å^2$ x 10^3)for **3AuF2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	20(5)	16(4)	29(5)	-5(4)	7(4)	-11(4)
C(2)	29(6)	23(5)	41(6)	-3(5)	15(5)	-13(4)
C(3)	46(7)	24(6)	51(8)	-2(5)	23(6)	-11(5)
C(4)	60(8)	16(5)	59(8)	0(5)	38(7)	-5(5)
C(5)	68(9)	36(7)	33(6)	-12(5)	27(7)	-22(6)
C(6)	36(6)	30(6)	28(6)	-3(5)	6(5)	-7(5)
C(7)	24(5)	22(5)	41(6)	2(5)	6(5)	-2(4)
C(8)	20(5)	29(6)	63(8)	2(6)	0(6)	-4(4)
C(9)	31(7)	39(7)	94(12)	-16(8)	13(8)	-3(5)
C(10)	38(7)	36(7)	106(14)	-21(8)	40(9)	3(6)
C(11)	75(10)	54(9)	42(8)	-7(7)	37(8)	-9(7)
C(12)	32(6)	49(8)	47(8)	-6(6)	12(6)	8(5)
C(13)	18(4)	13(4)	14(4)	1(3)	2(4)	-1(3)
C(14)	27(5)	10(4)	15(4)	1(3)	11(4)	-5(3)
C(15)	17(5)	29(5)	20(5)	3(4)	8(4)	0(4)
C(16)	26(5)	40(6)	30(6)	6(5)	13(5)	-9(5)
C(17)	39(6)	29(6)	30(6)	5(4)	24(5)	0(5)
C(18)	44(7)	29(6)	16(5)	0(4)	6(5)	5(5)
C(19)	31(5)	20(5)	17(5)	2(4)	5(4)	-2(4)
C(20)	20(5)	16(4)	16(4)	4(3)	8(4)	1(3)
C(21)	21(5)	28(5)	16(4)	6(4)	1(4)	-1(4)
C(22)	29(6)	38(6)	21(5)	4(4)	-1(5)	3(5)
C(23)	28(6)	30(6)	31(6)	16(5)	2(5)	10(4)
C(24)	22(5)	19(5)	43(6)	3(4)	10(5)	6(4)
C(25)	22(5)	20(5)	23(5)	3(4)	4(4)	-7(4)
C(26)	23(5)	11(4)	12(4)	-2(3)	7(4)	0(3)
C(27)	28(5)	22(5)	18(5)	-2(4)	6(4)	1(4)

C(28)	28(5)	28(6)	32(6)	-4(4)	12(5)	10(4)
C(29)	45(7)	29(6)	20(5)	-10(4)	9(5)	1(5)
C(30)	29(5)	28(5)	15(4)	-7(4)	2(4)	-13(4)
C(31)	25(5)	17(4)	20(5)	3(4)	6(4)	-8(4)
C(32)	18(4)	14(4)	16(4)	2(3)	3(4)	0(3)
C(33)	24(5)	21(5)	16(4)	0(4)	6(4)	0(4)
C(34)	37(6)	25(5)	18(5)	10(4)	5(5)	12(4)
C(35)	36(6)	14(5)	33(6)	5(4)	10(5)	6(4)
C(36)	26(5)	25(5)	26(5)	-2(4)	7(5)	-7(4)
C(37)	31(5)	19(5)	17(5)	-1(4)	6(4)	-6(4)
C(38)	16(4)	22(5)	10(4)	3(3)	6(4)	-1(3)
C(39)	18(5)	21(5)	28(5)	-4(4)	2(4)	-3(4)
C(40)	17(5)	29(5)	29(5)	2(4)	5(4)	7(4)
C(41)	24(5)	26(5)	34(6)	2(4)	12(5)	8(4)
C(42)	30(6)	27(5)	22(5)	-7(4)	10(5)	-3(4)
C(43)	22(5)	19(5)	15(4)	-7(4)	3(4)	-4(4)
C(44)	11(4)	18(4)	16(4)	-2(3)	8(4)	-1(3)
C(45)	26(5)	21(5)	20(5)	0(4)	12(4)	0(4)
C(46)	38(6)	22(5)	34(6)	10(4)	20(5)	4(4)
C(47)	32(6)	22(5)	60(8)	-6(5)	23(6)	-12(4)
C(48)	15(5)	28(5)	42(6)	-7(5)	5(5)	-4(4)
C(49)	18(5)	25(5)	29(5)	-5(4)	6(4)	-2(4)
C(50)	25(5)	41(7)	27(6)	5(5)	1(5)	1(5)
C(51)	55(8)	36(7)	30(6)	-4(5)	7(6)	9(6)
C(52)	48(7)	28(6)	39(7)	-2(5)	0(6)	3(5)
C(53)	47(7)	40(7)	33(6)	11(5)	1(6)	-8(6)
C(54)	58(8)	38(7)	42(7)	-1(6)	23(7)	-5(6)
C(55)	47(7)	41(7)	35(6)	-8(5)	10(6)	5(6)
Au(1)	15(1)	17(1)	16(1)	-3(1)	2(1)	-3(1)
Au(2)	17(1)	20(1)	19(1)	1(1)	1(1)	1(1)
Au(3)	24(1)	26(1)	19(1)	0(1)	1(1)	1(1)
F(3)	111(7)	32(4)	80(6)	-10(4)	66(6)	-2(4)
F(4)	117(8)	58(5)	33(4)	-16(4)	15(5)	6(5)
F(8)	81(7)	71(6)	163(11)	-50(7)	74(7)	4(5)
F(9)	149(11)	141(11)	66(7)	-15(7)	36(7)	15(9)
F(12)	101(7)	35(4)	58(5)	-12(4)	22(5)	-19(4)
F(13)	76(6)	50(5)	52(5)	7(4)	19(4)	-16(4)
P(1)	15(1)	13(1)	12(1)	0(1)	2(1)	-2(1)
P(2)	17(1)	12(1)	13(1)	1(1)	2(1)	0(1)
P(3)	15(1)	17(1)	11(1)	0(1)	3(1)	-2(1)
S(1)	18(1)	35(1)	27(1)	-12(1)	-3(1)	-1(1)
S(2)	18(1)	34(1)	25(1)	-3(1)	-1(1)	0(1)
S(3)	32(2)	41(2)	25(1)	3(1)	-4(1)	-4(1)

Table S27. Atomic coordinates in Å (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **3auf4**. U(eq) is defined as one third of the trace of the orthogonalised U^{ij} tensor.

Atom	x	y	z	U(eq)
C(1)	10849(6)	2497(5)	-1451(4)	21(1)
C(2)	11734(7)	2313(6)	-1085(4)	34(3)
C(3)	12737(8)	2605(7)	-1127(5)	49(3)
C(4)	12910(9)	3099(7)	-1552(6)	55(4)
C(5)	12036(10)	3289(7)	-1911(5)	44(3)
C(6)	11033(8)	3012(5)	-1877(4)	32(2)
C(7)	6759(7)	4199(5)	-1456(3)	21(2)
C(8)	7009(7)	4766(5)	-1137(3)	21(2)
C(9)	6299(7)	5265(5)	-1097(4)	27(2)
C(10)	5283(7)	5246(5)	-1388(4)	30(2)
C(11)	5023(7)	4690(6)	-1713(4)	28(2)
C(12)	5722(7)	4185(5)	-1737(3)	22(2)
C(13)	7670(6)	2484(4)	911(3)	14(2)
C(14)	9705(6)	1795(5)	1246(4)	21(1)
C(15)	9538(7)	1816(5)	1913(4)	27(2)
C(16)	10426(8)	1774(6)	2316(4)	34(3)
C(17)	11464(7)	1712(5)	2083(4)	34(3)
C(18)	11638(7)	1687(5)	1431(4)	34(2)
C(19)	10764(6)	1733(5)	1003(4)	22(2)
C(20)	7863(7)	1063(5)	753(4)	21(1)
C(21)	7530(7)	827(5)	1342(4)	21(2)
C(22)	6936(7)	255(5)	1378(4)	28(2)
C(23)	6698(9)	-71(5)	822(4)	28(2)
C(24)	7042(7)	147(5)	235(4)	21(1)
C(25)	7635(6)	712(5)	196(4)	19(2)
C(26)	9707(6)	3261(4)	800(3)	16(2)
C(27)	10486(6)	3268(4)	308(4)	18(2)
C(28)	11586(7)	3278(5)	467(4)	24(2)
C(29)	11911(8)	3290(5)	1097(4)	21(1)
C(30)	11155(7)	3294(5)	1575(4)	29(2)
C(31)	10047(7)	3283(5)	1441(4)	21(2)
C(32)	7652(6)	3900(5)	1025(4)	21(1)
C(33)	7309(6)	4431(5)	673(4)	21(1)
C(34)	6873(7)	4961(5)	964(4)	25(2)
C(35)	6776(7)	4978(5)	1632(4)	29(2)
C(36)	7103(7)	4450(5)	1986(4)	31(2)
C(37)	7540(7)	3916(5)	1691(3)	26(2)
C(38)	5573(6)	1795(5)	997(3)	18(2)
C(39)	5528(7)	1818(5)	1669(4)	26(2)
C(40)	4905(7)	1374(5)	1997(4)	30(2)
C(41)	4318(7)	915(5)	1681(4)	31(2)
C(42)	4348(7)	890(5)	1015(4)	28(2)
C(43)	4967(6)	1331(5)	681(4)	20(2)
C(44)	5556(7)	3103(5)	555(4)	21(1)
C(45)	5260(6)	3412(5)	-5(4)	21(1)
C(46)	4685(7)	3984(5)	11(5)	34(2)
C(47)	4380(7)	4243(6)	590(5)	43(3)
C(48)	4645(7)	3941(5)	1158(5)	32(2)
C(49)	5224(7)	3375(5)	1139(4)	26(2)
C(50)	6352(7)	887(5)	-1496(4)	22(2)
C(51)	5369(7)	712(5)	-1226(4)	26(2)
C(52)	5045(8)	90(6)	-1178(4)	34(3)
C(53)	5660(10)	-400(6)	-1408(4)	46(3)
C(54)	6634(11)	-242(6)	-1685(4)	41(3)
C(55)	6965(8)	388(6)	-1737(4)	34(3)
Au(1)	9112(1)	1988(1)	-370(1)	18(1)
Au(2)	7997(1)	3310(1)	-483(1)	16(1)
Au(3)	6597(1)	2049(1)	-519(1)	19(1)

F(1)	11629(4)	1821(3)	-663(2)	43(2)
F(2)	13557(4)	2389(4)	-754(3)	69(2)
F(4)	12158(5)	3795(4)	-2326(3)	66(2)
F(5)	10234(5)	3224(3)	-2243(2)	44(2)
F(6)	7989(4)	4827(3)	-843(2)	28(1)
F(7)	6597(4)	5794(3)	-773(2)	38(1)
F(9)	4036(4)	4634(3)	-1990(2)	41(2)
F(10)	5405(4)	3656(3)	-2057(2)	32(2)
F(11)	4693(4)	1165(3)	-995(2)	37(2)
F(12)	4074(5)	-45(3)	-888(2)	56(2)
F(14)	7299(6)	-708(4)	-1928(3)	70(2)
F(15)	7944(4)	508(3)	-2021(2)	47(2)
P(1)	8604(2)	1813(1)	663(1)	15(1)
P(2)	8269(2)	3242(1)	587(1)	15(1)
P(3)	6318(2)	2363(1)	511(1)	17(1)
S(1)	9558(2)	2141(1)	-1433(1)	24(1)
S(2)	7664(2)	3545(1)	-1544(1)	25(1)
S(3)	6828(2)	1683(1)	-1556(1)	31(1)

Table S28. Bond lengths [Å] and angles [°] for **3auf4**.

C(1)-C(2)	1.382(12)	C(17)-C(18)	1.377(12)
C(1)-C(6)	1.411(13)	C(17)-H(17)	0.9500
C(1)-S(1)	1.750(9)	C(18)-C(19)	1.398(11)
C(2)-F(1)	1.358(11)	C(18)-H(18)	0.9500
C(2)-C(3)	1.376(14)	C(19)-H(19)	0.9500
C(3)-F(2)	1.351(12)	C(20)-C(21)	1.383(11)
C(3)-C(4)	1.373(17)	C(20)-C(25)	1.401(11)
C(4)-C(5)	1.366(17)	C(20)-P(1)	1.818(10)
C(4)-H(4)	0.9500	C(21)-C(22)	1.399(13)
C(5)-C(6)	1.361(15)	C(21)-H(21)	0.9500
C(5)-F(4)	1.372(14)	C(22)-C(23)	1.375(12)
C(6)-F(5)	1.318(11)	C(22)-H(22)	0.9500
C(7)-C(8)	1.390(13)	C(23)-C(24)	1.371(12)
C(7)-C(12)	1.402(11)	C(23)-H(23)	0.9500
C(7)-S(2)	1.768(9)	C(24)-C(25)	1.385(12)
C(8)-F(6)	1.355(9)	C(24)-H(24)	0.9500
C(8)-C(9)	1.359(13)	C(25)-H(25)	0.9500
C(9)-F(7)	1.346(11)	C(26)-C(31)	1.400(10)
C(9)-C(10)	1.387(12)	C(26)-C(27)	1.402(10)
C(10)-C(11)	1.380(14)	C(26)-P(2)	1.821(8)
C(10)-H(10)	0.9500	C(27)-C(28)	1.391(11)
C(11)-F(9)	1.348(9)	C(27)-H(27)	0.9500
C(11)-C(12)	1.359(13)	C(28)-C(29)	1.372(11)
C(12)-F(10)	1.345(10)	C(28)-H(28)	0.9500
C(13)-P(2)	1.868(9)	C(29)-C(30)	1.360(12)
C(13)-P(3)	1.875(7)	C(29)-H(29)	0.9500
C(13)-P(1)	1.881(8)	C(30)-C(31)	1.388(12)
C(13)-H(13)	1.0000	C(30)-H(30)	0.9500
C(14)-C(19)	1.401(11)	C(31)-H(31)	0.9500
C(14)-C(15)	1.407(11)	C(32)-C(33)	1.393(12)
C(14)-P(1)	1.818(8)	C(32)-C(37)	1.395(10)
C(15)-C(16)	1.380(12)	C(32)-P(2)	1.812(9)
C(15)-H(15)	0.9500	C(33)-C(34)	1.368(12)
C(16)-C(17)	1.370(13)	C(33)-H(33)	0.9500
C(16)-H(16)	0.9500	C(34)-C(35)	1.398(11)

C(34)-H(34)	0.9500
C(35)-C(36)	1.385(13)
C(35)-H(35)	0.9500
C(36)-C(37)	1.380(12)
C(36)-H(36)	0.9500
C(37)-H(37)	0.9500
C(38)-C(43)	1.387(12)
C(38)-C(39)	1.402(10)
C(38)-P(3)	1.807(9)
C(39)-C(40)	1.382(13)
C(39)-H(39)	0.9500
C(40)-C(41)	1.367(13)
C(40)-H(40)	0.9500
C(41)-C(42)	1.389(11)
C(41)-H(41)	0.9500
C(42)-C(43)	1.381(12)
C(42)-H(42)	0.9500
C(43)-H(43)	0.9500
C(44)-C(45)	1.383(11)
C(44)-C(49)	1.403(12)
C(44)-P(3)	1.806(10)
C(45)-C(46)	1.385(13)
C(45)-H(45)	0.9500
C(46)-C(47)	1.373(13)
C(46)-H(46)	0.9500
C(47)-C(48)	1.377(14)
C(47)-H(47)	0.9500
C(48)-C(49)	1.379(14)
C(48)-H(48)	0.9500
C(49)-H(49)	0.9500
C(50)-C(55)	1.380(14)
C(50)-C(51)	1.380(12)
C(50)-S(3)	1.762(10)
C(51)-F(11)	1.345(11)
C(51)-C(52)	1.359(14)
C(52)-C(53)	1.357(15)
C(52)-F(12)	1.366(10)
C(53)-C(54)	1.368(16)
C(53)-H(53)	0.9500
C(54)-F(14)	1.366(13)
C(54)-C(55)	1.379(16)
C(55)-F(15)	1.362(10)
Au(1)-P(1)	2.271(2)
Au(1)-S(1)	2.303(2)
Au(1)-Au(2)	3.0847(6)
Au(1)-Au(3)	3.1054(4)
Au(2)-P(2)	2.259(2)
Au(2)-S(2)	2.303(2)
Au(2)-Au(3)	3.1405(5)
Au(3)-P(3)	2.268(2)
Au(3)-S(3)	2.311(2)

C(2)-C(1)-C(6)	115.6(8)
C(2)-C(1)-S(1)	125.6(7)
C(6)-C(1)-S(1)	118.8(7)
F(1)-C(2)-C(3)	117.4(10)
F(1)-C(2)-C(1)	119.5(8)
C(3)-C(2)-C(1)	123.1(10)
F(2)-C(3)-C(4)	120.4(10)
F(2)-C(3)-C(2)	118.8(12)
C(4)-C(3)-C(2)	120.7(11)
C(5)-C(4)-C(3)	116.6(11)
C(5)-C(4)-H(4)	121.7
C(3)-C(4)-H(4)	121.7
C(6)-C(5)-C(4)	124.0(12)
C(6)-C(5)-F(4)	117.2(12)
C(4)-C(5)-F(4)	118.8(11)
F(5)-C(6)-C(5)	120.1(10)
F(5)-C(6)-C(1)	119.9(8)
C(5)-C(6)-C(1)	120.0(11)
C(8)-C(7)-C(12)	114.7(8)
C(8)-C(7)-S(2)	124.5(7)
C(12)-C(7)-S(2)	120.7(7)
F(6)-C(8)-C(9)	118.0(8)
F(6)-C(8)-C(7)	119.5(8)
C(9)-C(8)-C(7)	122.5(8)
F(7)-C(9)-C(8)	118.9(8)
F(7)-C(9)-C(10)	119.1(9)
C(8)-C(9)-C(10)	122.0(9)
C(11)-C(10)-C(9)	116.4(9)
C(11)-C(10)-H(10)	121.8
C(9)-C(10)-H(10)	121.8
F(9)-C(11)-C(12)	119.0(10)
F(9)-C(11)-C(10)	119.4(9)
C(12)-C(11)-C(10)	121.6(8)
F(10)-C(12)-C(11)	118.1(8)
F(10)-C(12)-C(7)	119.1(8)
C(11)-C(12)-C(7)	122.8(9)
P(2)-C(13)-P(3)	107.6(4)
P(2)-C(13)-P(1)	106.9(4)
P(3)-C(13)-P(1)	108.5(4)
P(2)-C(13)-H(13)	111.2
P(3)-C(13)-H(13)	111.2
P(1)-C(13)-H(13)	111.2
C(19)-C(14)-C(15)	119.7(7)
C(19)-C(14)-P(1)	116.8(6)
C(15)-C(14)-P(1)	123.4(6)
C(16)-C(15)-C(14)	119.0(8)
C(16)-C(15)-H(15)	120.5
C(14)-C(15)-H(15)	120.5
C(17)-C(16)-C(15)	121.7(9)
C(17)-C(16)-H(16)	119.2
C(15)-C(16)-H(16)	119.2
C(16)-C(17)-C(18)	119.9(8)
C(16)-C(17)-H(17)	120.0
C(18)-C(17)-H(17)	120.0
C(17)-C(18)-C(19)	120.5(8)
C(17)-C(18)-H(18)	119.7

C(19)-C(18)-H(18)	119.7	C(35)-C(36)-H(36)	119.5
C(18)-C(19)-C(14)	119.2(8)	C(36)-C(37)-C(32)	120.1(9)
C(18)-C(19)-H(19)	120.4	C(36)-C(37)-H(37)	119.9
C(14)-C(19)-H(19)	120.4	C(32)-C(37)-H(37)	119.9
C(21)-C(20)-C(25)	119.4(9)	C(43)-C(38)-C(39)	118.5(8)
C(21)-C(20)-P(1)	123.0(7)	C(43)-C(38)-P(3)	117.5(6)
C(25)-C(20)-P(1)	117.6(6)	C(39)-C(38)-P(3)	123.9(7)
C(20)-C(21)-C(22)	120.3(8)	C(40)-C(39)-C(38)	119.5(9)
C(20)-C(21)-H(21)	119.9	C(40)-C(39)-H(39)	120.2
C(22)-C(21)-H(21)	119.9	C(38)-C(39)-H(39)	120.2
C(23)-C(22)-C(21)	119.1(8)	C(41)-C(40)-C(39)	121.5(8)
C(23)-C(22)-H(22)	120.4	C(41)-C(40)-H(40)	119.3
C(21)-C(22)-H(22)	120.4	C(39)-C(40)-H(40)	119.3
C(24)-C(23)-C(22)	121.5(10)	C(40)-C(41)-C(42)	119.6(9)
C(24)-C(23)-H(23)	119.3	C(40)-C(41)-H(41)	120.2
C(22)-C(23)-H(23)	119.3	C(42)-C(41)-H(41)	120.2
C(23)-C(24)-C(25)	119.7(9)	C(43)-C(42)-C(41)	119.6(9)
C(23)-C(24)-H(24)	120.1	C(43)-C(42)-H(42)	120.2
C(25)-C(24)-H(24)	120.1	C(41)-C(42)-H(42)	120.2
C(24)-C(25)-C(20)	119.9(8)	C(42)-C(43)-C(38)	121.3(8)
C(24)-C(25)-H(25)	120.0	C(42)-C(43)-H(43)	119.3
C(20)-C(25)-H(25)	120.0	C(38)-C(43)-H(43)	119.3
C(31)-C(26)-C(27)	119.6(7)	C(45)-C(44)-C(49)	117.9(9)
C(31)-C(26)-P(2)	121.5(6)	C(45)-C(44)-P(3)	119.4(6)
C(27)-C(26)-P(2)	118.9(5)	C(49)-C(44)-P(3)	122.7(7)
C(28)-C(27)-C(26)	119.2(7)	C(44)-C(45)-C(46)	120.9(8)
C(28)-C(27)-H(27)	120.4	C(44)-C(45)-H(45)	119.5
C(26)-C(27)-H(27)	120.4	C(46)-C(45)-H(45)	119.5
C(29)-C(28)-C(27)	120.7(8)	C(47)-C(46)-C(45)	119.9(9)
C(29)-C(28)-H(28)	119.7	C(47)-C(46)-H(46)	120.1
C(27)-C(28)-H(28)	119.7	C(45)-C(46)-H(46)	120.1
C(30)-C(29)-C(28)	120.1(8)	C(46)-C(47)-C(48)	120.7(10)
C(30)-C(29)-H(29)	119.9	C(46)-C(47)-H(47)	119.6
C(28)-C(29)-H(29)	119.9	C(48)-C(47)-H(47)	119.6
C(29)-C(30)-C(31)	121.4(8)	C(47)-C(48)-C(49)	119.2(9)
C(29)-C(30)-H(30)	119.3	C(47)-C(48)-H(48)	120.4
C(31)-C(30)-H(30)	119.3	C(49)-C(48)-H(48)	120.4
C(30)-C(31)-C(26)	118.9(8)	C(48)-C(49)-C(44)	121.3(9)
C(30)-C(31)-H(31)	120.5	C(48)-C(49)-H(49)	119.4
C(26)-C(31)-H(31)	120.5	C(44)-C(49)-H(49)	119.4
C(33)-C(32)-C(37)	118.3(9)	C(55)-C(50)-C(51)	115.2(9)
C(33)-C(32)-P(2)	117.5(6)	C(55)-C(50)-S(3)	120.2(8)
C(37)-C(32)-P(2)	124.1(7)	C(51)-C(50)-S(3)	124.6(8)
C(34)-C(33)-C(32)	121.8(8)	F(11)-C(51)-C(52)	117.5(9)
C(34)-C(33)-H(33)	119.1	F(11)-C(51)-C(50)	119.9(9)
C(32)-C(33)-H(33)	119.1	C(52)-C(51)-C(50)	122.5(10)
C(33)-C(34)-C(35)	119.7(9)	C(53)-C(52)-C(51)	121.9(10)
C(33)-C(34)-H(34)	120.2	C(53)-C(52)-F(12)	119.1(11)
C(35)-C(34)-H(34)	120.2	C(51)-C(52)-F(12)	119.0(10)
C(36)-C(35)-C(34)	119.1(9)	C(52)-C(53)-C(54)	117.1(11)
C(36)-C(35)-H(35)	120.4	C(52)-C(53)-H(53)	121.5
C(34)-C(35)-H(35)	120.4	C(54)-C(53)-H(53)	121.5
C(37)-C(36)-C(35)	121.0(8)	F(14)-C(54)-C(53)	120.6(12)
C(37)-C(36)-H(36)	119.5	F(14)-C(54)-C(55)	118.1(12)

C(53)-C(54)-C(55)	121.3(11)	C(20)-P(1)-C(14)	106.6(4)
F(15)-C(55)-C(54)	117.9(11)	C(20)-P(1)-C(13)	107.8(4)
F(15)-C(55)-C(50)	120.1(11)	C(14)-P(1)-C(13)	106.5(4)
C(54)-C(55)-C(50)	121.9(10)	C(20)-P(1)-Au(1)	112.0(3)
P(1)-Au(1)-S(1)	177.37(8)	C(14)-P(1)-Au(1)	115.6(3)
P(1)-Au(1)-Au(2)	95.39(6)	C(13)-P(1)-Au(1)	107.9(3)
S(1)-Au(1)-Au(2)	84.81(7)	C(32)-P(2)-C(26)	105.4(4)
P(1)-Au(1)-Au(3)	80.09(5)	C(32)-P(2)-C(13)	107.1(4)
S(1)-Au(1)-Au(3)	97.75(6)	C(26)-P(2)-C(13)	108.1(4)
Au(2)-Au(1)-Au(3)	60.971(10)	C(32)-P(2)-Au(2)	112.8(3)
P(2)-Au(2)-S(2)	171.11(9)	C(26)-P(2)-Au(2)	112.5(2)
P(2)-Au(2)-Au(1)	78.67(6)	C(13)-P(2)-Au(2)	110.5(2)
S(2)-Au(2)-Au(1)	109.96(6)	C(44)-P(3)-C(38)	105.6(4)
P(2)-Au(2)-Au(3)	93.00(6)	C(44)-P(3)-C(13)	108.7(4)
S(2)-Au(2)-Au(3)	93.31(7)	C(38)-P(3)-C(13)	106.7(4)
Au(1)-Au(2)-Au(3)	59.840(12)	C(44)-P(3)-Au(3)	111.9(3)
P(3)-Au(3)-S(3)	177.01(9)	C(38)-P(3)-Au(3)	114.7(3)
P(3)-Au(3)-Au(1)	93.87(5)	C(13)-P(3)-Au(3)	109.0(2)
S(3)-Au(3)-Au(1)	87.59(6)	C(1)-S(1)-Au(1)	107.1(3)
P(3)-Au(3)-Au(2)	79.56(6)	C(7)-S(2)-Au(2)	100.1(2)
S(3)-Au(3)-Au(2)	103.43(7)	C(50)-S(3)-Au(3)	101.7(3)
Au(1)-Au(3)-Au(2)	59.189(11)		

Table S29. Anisotropic displacement parameters ($Å^2$ x 10^3) for **3auf4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	18(1)	15(2)	31(2)	-1(1)	-2(1)	1(1)
C(2)	32(5)	40(8)	30(5)	-4(5)	16(4)	-6(5)
C(3)	30(6)	61(10)	56(7)	-26(7)	14(5)	-2(7)
C(4)	42(7)	56(10)	66(8)	-33(7)	33(6)	-23(7)
C(5)	52(8)	35(8)	45(6)	-15(6)	26(6)	-10(7)
C(6)	37(6)	29(7)	30(5)	-11(5)	20(4)	-5(6)
C(7)	27(5)	22(6)	12(4)	9(4)	3(3)	9(4)
C(8)	16(4)	30(7)	18(4)	5(4)	3(3)	1(5)
C(9)	28(5)	28(7)	24(4)	-2(4)	0(4)	-4(5)
C(10)	34(6)	24(7)	33(5)	9(4)	10(4)	8(5)
C(11)	17(4)	40(8)	27(5)	8(5)	1(4)	5(5)
C(12)	25(5)	30(7)	11(4)	-2(4)	1(3)	3(5)
C(13)	14(4)	8(5)	21(4)	0(3)	0(3)	2(4)
C(14)	18(1)	15(2)	31(2)	-1(1)	-2(1)	1(1)
C(15)	21(4)	29(7)	31(5)	7(4)	-3(4)	-7(5)
C(16)	35(6)	32(8)	35(5)	13(5)	-13(4)	-8(5)
C(17)	26(5)	32(7)	44(5)	15(5)	-22(4)	-8(5)
C(18)	19(4)	26(7)	57(6)	-1(5)	-3(4)	4(5)
C(19)	22(4)	8(5)	37(5)	-2(4)	-1(4)	4(4)
C(20)	18(1)	15(2)	31(2)	-1(1)	-2(1)	1(1)
C(21)	26(5)	12(6)	25(4)	4(4)	0(4)	1(4)
C(22)	26(5)	22(6)	36(5)	10(4)	2(4)	-3(5)
C(23)	23(5)	12(6)	49(5)	3(5)	-8(4)	-2(5)
C(24)	18(1)	15(2)	31(2)	-1(1)	-2(1)	1(1)
C(25)	16(4)	15(6)	27(4)	-2(4)	-1(3)	2(4)
C(26)	19(4)	6(5)	22(4)	-1(4)	-3(3)	-1(4)
C(27)	22(4)	10(5)	22(4)	3(4)	4(3)	-1(4)
C(28)	15(4)	16(6)	40(5)	0(4)	2(4)	-2(4)
C(29)	18(1)	15(2)	31(2)	-1(1)	-2(1)	1(1)
C(30)	29(5)	21(6)	35(5)	2(4)	-16(4)	-4(5)

C(31)	20(4)	22(6)	21(4)	0(4)	-3(3)	-1(5)
C(32)	18(1)	15(2)	31(2)	-1(1)	-2(1)	1(1)
C(33)	18(1)	15(2)	31(2)	-1(1)	-2(1)	1(1)
C(34)	25(5)	19(6)	32(5)	7(4)	2(4)	8(5)
C(35)	36(6)	18(6)	34(5)	-6(4)	0(4)	7(5)
C(36)	46(6)	26(6)	23(4)	-1(4)	-3(4)	15(5)
C(37)	39(5)	21(6)	19(4)	0(4)	-3(4)	7(5)
C(38)	11(4)	16(6)	26(4)	0(4)	-1(3)	1(4)
C(39)	26(5)	22(6)	29(4)	-6(4)	0(4)	-4(5)
C(40)	32(5)	26(7)	32(4)	-3(5)	13(4)	-1(5)
C(41)	30(5)	22(7)	39(5)	4(4)	12(4)	-7(5)
C(42)	18(4)	27(7)	38(5)	-9(5)	1(4)	-3(4)
C(43)	15(4)	20(6)	25(4)	1(4)	-1(3)	1(4)
C(44)	18(1)	15(2)	31(2)	-1(1)	-2(1)	1(1)
C(45)	18(1)	15(2)	31(2)	-1(1)	-2(1)	1(1)
C(46)	22(5)	29(7)	50(6)	7(5)	0(4)	9(5)
C(47)	22(5)	19(7)	87(8)	7(6)	9(5)	5(5)
C(48)	23(5)	24(7)	49(5)	-3(5)	13(4)	6(5)
C(49)	15(4)	20(7)	43(5)	-1(4)	6(4)	-8(5)
C(50)	30(5)	12(6)	23(4)	-6(4)	-8(4)	-6(4)
C(51)	28(5)	23(7)	28(4)	-10(4)	0(4)	-6(5)
C(52)	44(6)	33(8)	25(5)	3(5)	-2(4)	-19(6)
C(53)	86(9)	22(7)	31(5)	0(5)	-17(6)	-15(7)
C(54)	61(8)	31(8)	31(5)	-18(5)	-13(5)	19(7)
C(55)	34(6)	47(9)	22(5)	-4(5)	-4(4)	-6(6)
Au(1)	19(1)	14(1)	20(1)	-1(1)	2(1)	0(1)
Au(2)	17(1)	15(1)	17(1)	2(1)	-1(1)	0(1)
Au(3)	21(1)	17(1)	20(1)	0(1)	-4(1)	-3(1)
F(1)	30(3)	57(5)	42(3)	1(3)	-3(2)	1(3)
F(2)	29(3)	86(7)	91(5)	-24(4)	-7(3)	2(4)
F(4)	83(5)	38(5)	77(4)	-2(4)	50(4)	-17(4)
F(5)	63(4)	34(5)	35(3)	10(3)	12(3)	2(4)
F(6)	25(3)	32(4)	27(2)	1(2)	0(2)	-4(3)
F(7)	40(3)	20(4)	53(3)	-2(3)	4(2)	-3(3)
F(9)	25(3)	55(5)	42(3)	1(3)	-14(2)	8(3)
F(10)	33(3)	37(4)	26(3)	-9(3)	-2(2)	-4(3)
F(11)	30(3)	40(4)	41(3)	-13(3)	4(2)	-3(3)
F(12)	57(4)	61(5)	50(3)	3(3)	6(3)	-38(4)
F(14)	99(5)	50(5)	60(4)	-32(4)	-10(4)	31(5)
F(15)	37(3)	67(6)	36(3)	-14(3)	7(2)	2(4)
P(1)	17(1)	11(1)	19(1)	0(1)	-1(1)	1(1)
P(2)	15(1)	12(1)	18(1)	1(1)	-1(1)	1(1)
P(3)	15(1)	14(1)	21(1)	1(1)	-3(1)	-1(1)
S(1)	26(1)	27(2)	20(1)	0(1)	4(1)	-3(1)
S(2)	31(1)	26(2)	19(1)	3(1)	2(1)	11(1)
S(3)	43(1)	31(2)	21(1)	-2(1)	-2(1)	-14(1)

Table S30 Atomic coordinates in Å (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **3auf5**. U(eq) is defined as one third of the trace of the orthogonalised U^{ij} tensor.

Atom	x	y	z	U(eq)
C(1)	5761(4)	1461(2)	2042(2)	21(1)
C(2)	5101(4)	968(2)	1863(2)	26(1)
C(3)	5318(5)	456(2)	2171(3)	31(1)
C(4)	6215(5)	419(2)	2686(3)	30(1)
C(5)	6891(4)	897(2)	2876(3)	28(1)
C(6)	6668(4)	1404(2)	2552(3)	26(1)
C(7)	5995(4)	3518(2)	3706(2)	27(1)
C(8)	5422(5)	3438(3)	4249(3)	39(2)
C(9)	5521(6)	3837(4)	4734(3)	62(2)

C(10)	6224(7)	4317(4)	4682(4)	69(3)
C(11)	6835(6)	4398(3)	4170(4)	64(2)
C(12)	6712(5)	4005(3)	3690(3)	44(2)
C(13)	985(4)	2921(2)	2033(2)	13(1)
C(14)	397(4)	1933(2)	1180(2)	16(1)
C(15)	-887(4)	1983(2)	1177(2)	20(1)
C(16)	-1641(4)	1514(2)	1020(2)	25(1)
C(17)	-1124(5)	996(2)	892(2)	27(1)
C(18)	145(4)	939(2)	903(2)	25(1)
C(19)	913(4)	1408(2)	1049(2)	18(1)
C(20)	1087(4)	2995(2)	641(2)	19(1)
C(21)	-125(4)	3170(2)	428(2)	23(1)
C(22)	-364(5)	3464(2)	-133(3)	33(1)
C(23)	569(6)	3575(2)	-496(3)	36(1)
C(24)	1772(5)	3407(2)	-292(2)	32(1)
C(25)	2035(4)	3119(2)	277(2)	22(1)
C(26)	1496(4)	1781(2)	2662(2)	16(1)
C(27)	2530(4)	1416(2)	2722(2)	23(1)
C(28)	2367(5)	832(2)	2704(3)	30(1)
C(29)	1193(5)	595(2)	2614(2)	29(1)
C(30)	158(5)	952(2)	2552(2)	25(1)
C(31)	316(4)	1540(2)	2583(2)	21(1)
C(32)	948(4)	2757(2)	3402(2)	17(1)
C(33)	1650(4)	2931(2)	3951(2)	19(1)
C(34)	1073(4)	3077(2)	4474(2)	24(1)
C(35)	-195(5)	3039(2)	4456(2)	24(1)
C(36)	-901(4)	2853(2)	3904(2)	25(1)
C(37)	-340(4)	2719(2)	3384(2)	21(1)
C(38)	561(4)	4101(2)	1524(2)	18(1)
C(39)	-713(4)	4084(2)	1528(2)	21(1)
C(40)	-1468(4)	4473(2)	1171(2)	25(1)
C(41)	-950(5)	4880(2)	815(2)	28(1)
C(42)	314(4)	4897(2)	806(3)	29(1)
C(43)	1076(4)	4507(2)	1151(2)	22(1)
C(44)	1608(4)	3974(2)	2799(2)	16(1)
C(45)	2726(4)	4137(2)	3146(2)	20(1)
C(46)	2726(5)	4392(2)	3732(2)	25(1)
C(47)	1624(5)	4469(2)	3982(2)	27(1)
C(48)	508(5)	4314(2)	3640(2)	24(1)
C(49)	491(4)	4067(2)	3054(2)	20(1)
C(50)	5349(4)	3767(2)	618(2)	26(1)
C(51)	4619(5)	4185(3)	301(3)	38(2)
C(52)	4506(5)	4239(4)	-341(3)	60(2)
C(53)	5129(6)	3874(4)	-693(3)	62(2)
C(54)	5880(5)	3458(3)	-399(3)	51(2)
C(55)	5989(5)	3407(3)	246(3)	32(1)
Au(1)	3488(1)	2315(1)	1506(1)	17(1)
Au(2)	3817(1)	2782(1)	2880(1)	16(1)
Au(3)	3589(1)	3628(1)	1733(1)	17(1)
F(1)	4195(3)	982(1)	1374(1)	35(1)
F(2)	4648(3)	-10(1)	1985(2)	46(1)
F(3)	6392(3)	-71(1)	3000(2)	45(1)
F(4)	7734(3)	866(2)	3385(2)	42(1)
F(5)	7363(2)	1853(1)	2759(2)	35(1)
F(6)	4748(3)	2967(2)	4322(2)	49(1)
F(7)	4923(4)	3745(3)	5234(2)	98(2)

F(8)	6311(4)	4706(2)	5156(2)	113(2)
F(9)	7541(4)	4866(2)	4138(3)	103(2)
F(10)	7325(3)	4104(2)	3195(2)	56(1)
F(11)	3986(3)	4557(2)	616(2)	61(1)
F(12)	3774(3)	4643(3)	-636(2)	102(2)
F(13)	5012(3)	3919(3)	-1321(2)	106(2)
F(14)	6525(4)	3101(2)	-733(2)	79(2)
F(15)	6739(3)	3003(2)	523(2)	49(1)
O(1W)	7983(4)	2985(2)	2066(2)	49(1)
P(1)	1442(1)	2542(1)	1330(1)	14(1)
P(2)	1771(1)	2547(1)	2747(1)	15(1)
P(3)	1646(1)	3657(1)	2025(1)	15(1)
S(1)	5584(1)	2124(1)	1649(1)	26(1)
S(2)	5887(1)	3029(1)	3077(1)	26(1)
S(3)	5566(1)	3702(1)	1442(1)	29(1)

Table S31. Bond lengths [Å] and angles [°] for **3auf5**.

C(1)-C(2)	1.385(7)	C(30)-C(31)	1.383(7)
C(1)-C(6)	1.386(7)	C(30)-H(30)	0.9500
C(1)-S(1)	1.761(5)	C(31)-H(31)	0.9500
C(2)-F(1)	1.349(6)	C(32)-C(33)	1.384(6)
C(2)-C(3)	1.371(7)	C(32)-C(37)	1.396(6)
C(3)-F(2)	1.341(6)	C(32)-P(2)	1.818(5)
C(3)-C(4)	1.383(8)	C(33)-C(34)	1.388(6)
C(4)-F(3)	1.330(6)	C(33)-H(33)	0.9500
C(4)-C(5)	1.370(8)	C(34)-C(35)	1.374(7)
C(5)-F(4)	1.338(6)	C(34)-H(34)	0.9500
C(5)-C(6)	1.377(7)	C(35)-C(36)	1.399(7)
C(6)-F(5)	1.337(6)	C(35)-H(35)	0.9500
C(7)-C(12)	1.380(8)	C(36)-C(37)	1.368(7)
C(7)-C(8)	1.394(8)	C(36)-H(36)	0.9500
C(7)-S(2)	1.759(5)	C(37)-H(37)	0.9500
C(8)-F(6)	1.341(7)	C(38)-C(39)	1.383(6)
C(8)-C(9)	1.389(9)	C(38)-C(43)	1.398(7)
C(9)-F(7)	1.334(8)	C(38)-P(3)	1.819(5)
C(9)-C(10)	1.368(12)	C(39)-C(40)	1.388(7)
C(10)-F(8)	1.356(7)	C(39)-H(39)	0.9500
C(10)-C(11)	1.361(12)	C(40)-C(41)	1.379(7)
C(11)-F(9)	1.340(9)	C(40)-H(40)	0.9500
C(11)-C(12)	1.371(9)	C(41)-C(42)	1.375(7)
C(12)-F(10)	1.338(8)	C(41)-H(41)	0.9500
C(13)-P(3)	1.863(4)	C(42)-C(43)	1.382(7)
C(13)-P(1)	1.865(4)	C(42)-H(42)	0.9500
C(13)-P(2)	1.874(4)	C(43)-H(43)	0.9500
C(13)-H(13)	1.0000	C(44)-C(45)	1.396(6)
C(14)-C(19)	1.390(6)	C(44)-C(49)	1.404(6)
C(14)-C(15)	1.396(6)	C(44)-P(3)	1.820(5)
C(14)-P(1)	1.821(4)	C(45)-C(46)	1.389(7)
C(15)-C(16)	1.384(7)	C(45)-H(45)	0.9500
C(15)-H(15)	0.9500	C(46)-C(47)	1.379(7)
C(16)-C(17)	1.374(7)	C(46)-H(46)	0.9500
C(16)-H(16)	0.9500	C(47)-C(48)	1.385(7)
C(17)-C(18)	1.381(7)	C(47)-H(47)	0.9500
C(17)-H(17)	0.9500	C(48)-C(49)	1.379(7)
C(18)-C(19)	1.389(6)	C(48)-H(48)	0.9500
C(18)-H(18)	0.9500	C(49)-H(49)	0.9500
C(19)-H(19)	0.9500	C(50)-C(51)	1.381(7)
C(20)-C(25)	1.392(6)	C(50)-C(55)	1.399(7)
C(20)-C(21)	1.399(6)	C(50)-S(3)	1.758(5)
C(20)-P(1)	1.819(5)	C(51)-F(11)	1.338(7)
C(21)-C(22)	1.381(7)	C(51)-C(52)	1.371(8)
C(21)-H(21)	0.9500	C(52)-F(12)	1.341(8)
C(22)-C(23)	1.373(8)	C(52)-C(53)	1.369(11)
C(22)-H(22)	0.9500	C(53)-F(13)	1.341(7)
C(23)-C(24)	1.382(8)	C(53)-C(54)	1.372(11)
C(23)-H(23)	0.9500	C(54)-F(14)	1.347(8)
C(24)-C(25)	1.390(7)	C(54)-C(55)	1.377(8)
C(24)-H(24)	0.9500	C(55)-F(15)	1.337(6)
C(25)-H(25)	0.9500	Au(1)-P(1)	2.2680(11)
C(26)-C(31)	1.390(6)	Au(1)-S(1)	2.3014(12)
C(26)-C(27)	1.403(6)	Au(1)-Au(3)	3.1041(3)
C(26)-P(2)	1.818(5)	Au(1)-Au(2)	3.1178(3)
C(27)-C(28)	1.375(7)	Au(2)-P(2)	2.2703(11)
C(27)-H(27)	0.9500	Au(2)-S(2)	2.3070(12)
C(28)-C(29)	1.380(7)	Au(2)-Au(3)	3.1398(3)
C(28)-H(28)	0.9500	Au(3)-P(3)	2.2704(11)
C(29)-C(30)	1.393(7)	Au(3)-S(3)	2.3089(12)
C(29)-H(29)	0.9500	O(1W)-H(2W)	0.89(2)

O(1W)-H(1W)	0.89(2)
C(2)-C(1)-C(6)	115.5(5)
C(2)-C(1)-S(1)	125.2(4)
C(6)-C(1)-S(1)	119.2(4)
F(1)-C(2)-C(3)	117.4(5)
F(1)-C(2)-C(1)	119.9(5)
C(3)-C(2)-C(1)	122.7(5)
F(2)-C(3)-C(2)	120.6(5)
F(2)-C(3)-C(4)	119.3(5)
C(2)-C(3)-C(4)	120.0(5)
F(3)-C(4)-C(5)	120.8(5)
F(3)-C(4)-C(3)	120.1(5)
C(5)-C(4)-C(3)	119.1(5)
F(4)-C(5)-C(4)	119.1(5)
F(4)-C(5)-C(6)	121.2(5)
C(4)-C(5)-C(6)	119.7(5)
F(5)-C(6)-C(5)	116.7(5)
F(5)-C(6)-C(1)	120.3(5)
C(5)-C(6)-C(1)	123.0(5)
C(12)-C(7)-C(8)	116.0(5)
C(12)-C(7)-S(2)	120.2(5)
C(8)-C(7)-S(2)	123.8(5)
F(6)-C(8)-C(9)	117.2(6)
F(6)-C(8)-C(7)	120.7(5)
C(9)-C(8)-C(7)	122.1(7)
F(7)-C(9)-C(10)	121.8(7)
F(7)-C(9)-C(8)	119.3(8)
C(10)-C(9)-C(8)	118.9(7)
F(8)-C(10)-C(11)	120.9(9)
F(8)-C(10)-C(9)	118.5(9)
C(11)-C(10)-C(9)	120.6(7)
F(9)-C(11)-C(10)	119.4(8)
F(9)-C(11)-C(12)	120.8(9)
C(10)-C(11)-C(12)	119.8(7)
F(10)-C(12)-C(11)	117.6(7)
F(10)-C(12)-C(7)	119.8(5)
C(11)-C(12)-C(7)	122.6(7)
P(3)-C(13)-P(1)	106.9(2)
P(3)-C(13)-P(2)	107.4(2)
P(1)-C(13)-P(2)	107.3(2)
P(3)-C(13)-H(13)	111.6
P(1)-C(13)-H(13)	111.6
P(2)-C(13)-H(13)	111.6
C(19)-C(14)-C(15)	119.9(4)
C(19)-C(14)-P(1)	117.8(3)
C(15)-C(14)-P(1)	122.3(4)
C(16)-C(15)-C(14)	119.6(5)
C(16)-C(15)-H(15)	120.2
C(14)-C(15)-H(15)	120.2
C(17)-C(16)-C(15)	120.1(4)
C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(16)-C(17)-C(18)	120.7(5)
C(16)-C(17)-H(17)	119.6
C(18)-C(17)-H(17)	119.6
C(17)-C(18)-C(19)	119.9(5)
C(17)-C(18)-H(18)	120.1
C(19)-C(18)-H(18)	120.1
C(18)-C(19)-C(14)	119.7(4)
C(18)-C(19)-H(19)	120.1
C(14)-C(19)-H(19)	120.1
C(25)-C(20)-C(21)	119.1(4)
C(25)-C(20)-P(1)	118.4(4)
C(21)-C(20)-P(1)	122.2(4)
C(22)-C(21)-C(20)	119.9(5)
C(22)-C(21)-H(21)	120.1
C(20)-C(21)-H(21)	120.1
C(23)-C(22)-C(21)	120.8(5)
C(23)-C(22)-H(22)	119.6
C(21)-C(22)-H(22)	119.6
C(22)-C(23)-C(24)	119.9(5)
C(22)-C(23)-H(23)	120.0
C(24)-C(23)-H(23)	120.0
C(23)-C(24)-C(25)	120.1(5)
C(23)-C(24)-H(24)	120.0
C(25)-C(24)-H(24)	120.0
C(24)-C(25)-C(20)	120.2(5)
C(24)-C(25)-H(25)	119.9
C(20)-C(25)-H(25)	119.9
C(31)-C(26)-C(27)	118.6(5)
C(31)-C(26)-P(2)	123.3(4)
C(27)-C(26)-P(2)	118.0(3)
C(28)-C(27)-C(26)	120.1(5)
C(28)-C(27)-H(27)	119.9
C(26)-C(27)-H(27)	119.9
C(27)-C(28)-C(29)	121.0(5)
C(27)-C(28)-H(28)	119.5
C(29)-C(28)-H(28)	119.5
C(28)-C(29)-C(30)	119.5(5)
C(28)-C(29)-H(29)	120.2
C(30)-C(29)-H(29)	120.2
C(31)-C(30)-C(29)	119.7(5)
C(31)-C(30)-H(30)	120.1
C(29)-C(30)-H(30)	120.1
C(30)-C(31)-C(26)	121.0(5)
C(30)-C(31)-H(31)	119.5
C(26)-C(31)-H(31)	119.5
C(33)-C(32)-C(37)	119.2(4)
C(33)-C(32)-P(2)	117.7(3)
C(37)-C(32)-P(2)	123.0(4)
C(32)-C(33)-C(34)	120.2(4)
C(32)-C(33)-H(33)	119.9
C(34)-C(33)-H(33)	119.9
C(35)-C(34)-C(33)	120.5(5)
C(35)-C(34)-H(34)	119.7
C(33)-C(34)-H(34)	119.7
C(34)-C(35)-C(36)	119.3(5)
C(34)-C(35)-H(35)	120.4
C(36)-C(35)-H(35)	120.4
C(37)-C(36)-C(35)	120.4(4)
C(37)-C(36)-H(36)	119.8
C(35)-C(36)-H(36)	119.8
C(36)-C(37)-C(32)	120.4(4)
C(36)-C(37)-H(37)	119.8
C(32)-C(37)-H(37)	119.8
C(39)-C(38)-C(43)	119.4(4)
C(39)-C(38)-P(3)	123.8(4)
C(43)-C(38)-P(3)	116.6(3)
C(38)-C(39)-C(40)	120.1(5)
C(38)-C(39)-H(39)	119.9
C(40)-C(39)-H(39)	119.9
C(41)-C(40)-C(39)	120.2(5)
C(41)-C(40)-H(40)	119.9

C(39)-C(40)-H(40)	119.9	F(15)-C(55)-C(54)	118.7(6)
C(42)-C(41)-C(40)	120.1(5)	F(15)-C(55)-C(50)	119.3(5)
C(42)-C(41)-H(41)	120.0	C(54)-C(55)-C(50)	122.0(6)
C(40)-C(41)-H(41)	120.0	P(1)-Au(1)-S(1)	176.94(5)
C(41)-C(42)-C(43)	120.4(5)	P(1)-Au(1)-Au(3)	79.13(3)
C(41)-C(42)-H(42)	119.8	S(1)-Au(1)-Au(3)	98.92(3)
C(43)-C(42)-H(42)	119.8	P(1)-Au(1)-Au(2)	94.28(3)
C(42)-C(43)-C(38)	119.9(4)	S(1)-Au(1)-Au(2)	86.75(4)
C(42)-C(43)-H(43)	120.1	Au(3)-Au(1)-Au(2)	60.614(6)
C(38)-C(43)-H(43)	120.1	P(2)-Au(2)-S(2)	176.67(4)
C(45)-C(44)-C(49)	119.0(4)	P(2)-Au(2)-Au(1)	78.29(3)
C(45)-C(44)-P(3)	118.8(3)	S(2)-Au(2)-Au(1)	104.99(3)
C(49)-C(44)-P(3)	122.1(3)	P(2)-Au(2)-Au(3)	93.99(3)
C(46)-C(45)-C(44)	120.2(4)	S(2)-Au(2)-Au(3)	88.24(4)
C(46)-C(45)-H(45)	119.9	Au(1)-Au(2)-Au(3)	59.477(7)
C(44)-C(45)-H(45)	119.9	P(3)-Au(3)-S(3)	174.03(5)
C(47)-C(46)-C(45)	120.0(5)	P(3)-Au(3)-Au(1)	93.18(3)
C(47)-C(46)-H(46)	120.0	S(3)-Au(3)-Au(1)	92.76(4)
C(45)-C(46)-H(46)	120.0	P(3)-Au(3)-Au(2)	77.94(3)
C(46)-C(47)-C(48)	120.3(5)	S(3)-Au(3)-Au(2)	105.65(3)
C(46)-C(47)-H(47)	119.8	Au(1)-Au(3)-Au(2)	59.909(7)
C(48)-C(47)-H(47)	119.8	H(2W)-O(1W)-H(1W)	97(6)
C(49)-C(48)-C(47)	120.3(5)	C(20)-P(1)-C(14)	104.1(2)
C(49)-C(48)-H(48)	119.8	C(20)-P(1)-C(13)	109.1(2)
C(47)-C(48)-H(48)	119.8	C(14)-P(1)-C(13)	107.0(2)
C(48)-C(49)-C(44)	120.1(4)	C(20)-P(1)-Au(1)	112.22(16)
C(48)-C(49)-H(49)	120.0	C(14)-P(1)-Au(1)	115.05(15)
C(44)-C(49)-H(49)	120.0	C(13)-P(1)-Au(1)	109.01(14)
C(51)-C(50)-C(55)	116.1(5)	C(26)-P(2)-C(32)	104.6(2)
C(51)-C(50)-S(3)	123.6(4)	C(26)-P(2)-C(13)	108.9(2)
C(55)-C(50)-S(3)	120.2(4)	C(32)-P(2)-C(13)	106.6(2)
F(11)-C(51)-C(52)	117.1(6)	C(26)-P(2)-Au(2)	113.36(15)
F(11)-C(51)-C(50)	120.6(5)	C(32)-P(2)-Au(2)	113.60(15)
C(52)-C(51)-C(50)	122.3(6)	C(13)-P(2)-Au(2)	109.42(14)
F(12)-C(52)-C(53)	118.8(6)	C(38)-P(3)-C(44)	102.8(2)
F(12)-C(52)-C(51)	121.0(7)	C(38)-P(3)-C(13)	107.9(2)
C(53)-C(52)-C(51)	120.3(6)	C(44)-P(3)-C(13)	108.4(2)
F(13)-C(53)-C(52)	120.7(7)	C(38)-P(3)-Au(3)	114.23(16)
F(13)-C(53)-C(54)	119.7(8)	C(44)-P(3)-Au(3)	112.72(15)
C(52)-C(53)-C(54)	119.6(6)	C(13)-P(3)-Au(3)	110.28(14)
F(14)-C(54)-C(53)	120.8(6)	C(1)-S(1)-Au(1)	106.43(15)
F(14)-C(54)-C(55)	119.5(7)	C(7)-S(2)-Au(2)	106.01(16)
C(53)-C(54)-C(55)	119.8(6)	C(50)-S(3)-Au(3)	105.11(15)

Table S32. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **3auf5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	19(2)	18(3)	27(3)	2(2)	8(2)	1(2)
C(2)	28(3)	24(3)	26(3)	-3(2)	6(2)	7(2)
C(3)	37(3)	16(3)	43(4)	0(3)	14(3)	0(2)
C(4)	40(3)	17(3)	37(3)	8(2)	15(3)	13(2)
C(5)	26(3)	21(3)	36(3)	2(2)	4(2)	8(2)
C(6)	19(2)	21(3)	39(3)	0(2)	12(2)	2(2)
C(7)	16(2)	35(3)	29(3)	-14(3)	-7(2)	8(2)
C(8)	30(3)	52(4)	31(3)	-9(3)	-11(2)	12(3)
C(9)	49(4)	106(7)	26(4)	-30(4)	-16(3)	39(4)
C(10)	52(5)	70(6)	71(6)	-52(5)	-44(4)	37(4)
C(11)	27(3)	47(5)	108(7)	-39(5)	-31(4)	14(3)
C(12)	22(3)	38(4)	67(5)	-23(3)	-16(3)	9(3)
C(13)	19(2)	10(2)	12(2)	0(2)	2(2)	-1(2)

C(14)	19(2)	16(3)	13(2)	0(2)	-2(2)	-6(2)
C(15)	25(3)	17(3)	18(3)	2(2)	4(2)	1(2)
C(16)	22(3)	25(3)	27(3)	-3(2)	1(2)	-3(2)
C(17)	36(3)	16(3)	28(3)	-1(2)	1(2)	-9(2)
C(18)	34(3)	12(3)	30(3)	-5(2)	6(2)	-2(2)
C(19)	23(2)	15(3)	15(2)	1(2)	1(2)	0(2)
C(20)	31(3)	12(2)	14(2)	-1(2)	1(2)	-2(2)
C(21)	29(3)	17(3)	20(3)	2(2)	-5(2)	-3(2)
C(22)	47(3)	18(3)	29(3)	3(2)	-14(3)	-1(2)
C(23)	66(4)	19(3)	19(3)	8(2)	-7(3)	-9(3)
C(24)	59(4)	22(3)	17(3)	6(2)	9(2)	-16(3)
C(25)	28(3)	21(3)	16(3)	-1(2)	2(2)	-8(2)
C(26)	23(2)	17(3)	9(2)	5(2)	2(2)	0(2)
C(27)	30(3)	17(3)	23(3)	5(2)	3(2)	1(2)
C(28)	38(3)	17(3)	36(3)	6(2)	4(2)	5(2)
C(29)	43(3)	15(3)	28(3)	2(2)	4(2)	-6(2)
C(30)	33(3)	18(3)	24(3)	-1(2)	7(2)	-10(2)
C(31)	27(3)	18(3)	17(2)	-1(2)	3(2)	0(2)
C(32)	22(2)	14(2)	14(2)	4(2)	3(2)	1(2)
C(33)	24(2)	17(3)	16(2)	0(2)	2(2)	2(2)
C(34)	33(3)	24(3)	15(3)	-1(2)	1(2)	2(2)
C(35)	39(3)	19(3)	17(3)	2(2)	11(2)	9(2)
C(36)	22(2)	23(3)	31(3)	0(2)	11(2)	2(2)
C(37)	26(3)	20(3)	18(3)	-3(2)	4(2)	-1(2)
C(38)	27(3)	10(2)	14(2)	-4(2)	-1(2)	3(2)
C(39)	24(3)	17(3)	20(3)	0(2)	0(2)	-3(2)
C(40)	26(3)	25(3)	21(3)	-1(2)	-3(2)	1(2)
C(41)	33(3)	19(3)	28(3)	10(2)	-7(2)	4(2)
C(42)	30(3)	22(3)	32(3)	9(2)	-4(2)	-7(2)
C(43)	21(2)	22(3)	21(3)	0(2)	-3(2)	0(2)
C(44)	23(2)	11(2)	14(2)	0(2)	-1(2)	0(2)
C(45)	23(2)	15(3)	22(3)	2(2)	-1(2)	0(2)
C(46)	32(3)	20(3)	21(3)	0(2)	-5(2)	-1(2)
C(47)	49(3)	17(3)	15(3)	-4(2)	2(2)	2(2)
C(48)	34(3)	15(3)	26(3)	0(2)	9(2)	0(2)
C(49)	24(2)	15(3)	21(3)	1(2)	0(2)	3(2)
C(50)	15(2)	38(3)	26(3)	8(2)	6(2)	-6(2)
C(51)	21(3)	60(4)	35(3)	25(3)	12(2)	6(3)
C(52)	21(3)	109(7)	49(4)	41(4)	2(3)	2(3)
C(53)	26(3)	136(8)	22(3)	20(4)	-3(3)	-28(4)
C(54)	37(3)	83(6)	34(4)	-17(4)	12(3)	-32(4)
C(55)	28(3)	37(4)	33(3)	0(3)	10(2)	-7(2)
Au(1)	19(1)	15(1)	15(1)	-1(1)	3(1)	0(1)
Au(2)	17(1)	17(1)	14(1)	0(1)	0(1)	0(1)
Au(3)	20(1)	14(1)	17(1)	0(1)	3(1)	-2(1)
F(1)	39(2)	31(2)	34(2)	-1(2)	-1(1)	-4(1)
F(2)	58(2)	18(2)	62(2)	-2(2)	3(2)	-7(2)
F(3)	59(2)	24(2)	52(2)	16(2)	8(2)	9(2)
F(4)	41(2)	42(2)	41(2)	9(2)	-7(2)	11(2)
F(5)	25(2)	25(2)	53(2)	3(2)	-3(1)	-1(1)
F(6)	42(2)	79(3)	25(2)	7(2)	4(2)	5(2)
F(7)	97(3)	171(6)	23(2)	-30(3)	-8(2)	60(3)
F(8)	80(3)	128(5)	115(4)	-101(4)	-61(3)	59(3)
F(9)	51(2)	52(3)	192(6)	-60(3)	-39(3)	1(2)
F(10)	29(2)	41(2)	99(3)	-6(2)	7(2)	-8(2)
F(11)	52(2)	61(3)	78(3)	40(2)	36(2)	29(2)
F(12)	32(2)	186(6)	89(3)	105(4)	12(2)	22(3)
F(13)	48(2)	246(7)	23(2)	27(3)	-4(2)	-49(3)
F(14)	77(3)	111(4)	55(3)	-48(3)	38(2)	-35(3)
F(15)	49(2)	39(2)	62(2)	0(2)	25(2)	11(2)
O(1W)	35(2)	58(3)	54(3)	15(3)	11(2)	4(2)
P(1)	19(1)	12(1)	12(1)	0(1)	2(1)	-1(1)

P(2)	18(1)	15(1)	11(1)	0(1)	2(1)	1(1)
P(3)	19(1)	13(1)	13(1)	-1(1)	0(1)	-1(1)
S(1)	20(1)	21(1)	37(1)	9(1)	8(1)	2(1)
S(2)	19(1)	32(1)	26(1)	-10(1)	2(1)	-1(1)
S(3)	20(1)	44(1)	22(1)	7(1)	4(1)	-4(1)

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