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SUPPORTING INFORMATION FOR

COMPLEX 3

Table 1. Crystal data and structure refinement for wondered.

Identification code	wondered	
Empirical formula	$C_{61}H_{32}Au_4Cl_2F_{20}P_2Se_2$	
Formula weight	2223.49	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P (-1)	
Unit cell dimensions	a = 9.4464(12) Å	α= 102.892(10)°.
	b = 12.4953(14) Å	β= 92.724(10)°.
	c = 14.279(2) Å	γ = 99.30(10)°.
Volume	1615.2(4) Å^3	
Z	1	
Density (calculated)	2.286 Mg/m^3	
Absorption coefficient	10.410 mm^{-1}	
F(000)	1026	
Crystal size	0.40 x 0.25 x 0.10 mm^3	
Theta range for data collection	3.00 to 25.00°.	
Index ranges	0<=h<=11, -14<=k<=14, -16<=l<=16	
Reflections collected	6025	
Independent reflections	5652 [R(int) = 0.0262]	
Completeness to theta = 25.00°	99.5 %	
Absorption correction	Psi-scans	
Max. and min. transmission	0.990 and 0.409	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5652 / 365 / 409	
Goodness-of-fit on F^2	0.878	
Final R indices [I>2sigma(I)]	R1 = 0.0318, wR2 = 0.0572	
R indices (all data)	R1 = 0.0559, wR2 = 0.0613	
Largest diff. peak and hole	1.196 and -0.720 e.Å^{-3}	

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

	x	y	z	U(eq)
Au(1)	555(1)	1732(1)	3821(1)	29(1)
Au(2)	1154(1)	1016(1)	5957(1)	24(1)
Se	-1018(1)	965(1)	4890(1)	26(1)
P	1942(2)	2583(2)	2846(2)	28(1)
C(11)	3714(8)	2203(5)	2695(5)	30(2)
C(12)	4511(8)	2132(6)	3502(6)	43(2)
C(13)	5914(9)	1923(6)	3440(6)	42(2)
C(14)	6500(9)	1807(6)	2579(6)	45(2)
C(15)	5710(9)	1859(7)	1765(7)	48(2)
C(16)	4299(8)	2056(6)	1821(6)	39(2)
C(21)	2311(7)	4089(6)	3303(5)	31(2)
C(22)	1373(9)	4630(6)	3883(6)	42(2)
C(23)	1643(11)	5778(6)	4201(6)	55(3)
C(24)	2795(9)	6415(7)	3947(6)	51(2)
C(25)	3744(9)	5918(6)	3366(8)	61(3)
C(26)	3503(8)	4748(6)	3043(7)	49(2)
C(31)	1020(7)	2316(5)	1657(5)	31(2)
C(32)	5(8)	1345(6)	1326(6)	43(2)
C(33)	-752(9)	1142(7)	431(6)	57(3)
C(34)	-499(9)	1886(7)	-135(7)	56(2)
C(35)	487(9)	2842(7)	176(6)	52(2)
C(36)	1228(9)	3072(6)	1068(6)	41(2)
C(41)	2945(8)	998(5)	6813(5)	30(2)
C(42)	2894(8)	987(5)	7777(6)	36(2)
C(43)	4090(9)	936(6)	8357(6)	47(2)
C(44)	5373(9)	904(7)	7961(6)	49(2)
C(45)	5486(8)	906(7)	7015(7)	46(2)
C(46)	4286(8)	978(6)	6455(6)	37(2)
F(1)	1635(5)	1038(4)	8192(3)	50(1)
F(2)	3973(6)	920(5)	9288(4)	72(2)
F(3)	6537(5)	809(4)	8505(4)	72(2)

F(4)	6755(5)	835(4)	6631(4)	69(2)
F(5)	4444(5)	989(4)	5517(4)	49(1)
C(51)	1229(7)	2678(5)	6620(5)	24(2)
C(52)	391(7)	3032(6)	7345(5)	36(2)
C(53)	436(8)	4126(6)	7778(5)	38(2)
C(54)	1377(8)	4924(6)	7472(6)	42(2)
C(55)	2240(8)	4622(6)	6742(6)	42(2)
C(56)	2164(8)	3496(6)	6329(6)	35(2)
F(6)	3026(5)	3220(3)	5612(4)	48(1)
F(7)	3118(5)	5401(4)	6431(4)	63(2)
F(8)	1435(6)	6015(3)	7883(4)	66(2)
F(9)	-395(5)	4434(4)	8483(4)	59(2)
F(10)	-557(5)	2262(3)	7624(3)	43(1)
C(99)	4570(40)	5200(20)	80(30)	148(13)
Cl(1)	3406(19)	6168(13)	197(13)	296(8)
Cl(2)	4430(30)	4046(18)	-928(17)	420(13)

Table 3. Bond lengths [Å] and angles [°] for wondered.

Au(1)-P	2.273(2)
Au(1)-Se	2.4225(9)
Au(2)-C(41)	2.046(8)
Au(2)-C(51)	2.070(7)
Au(2)-Se	2.4802(8)
Au(2)-Se#1	2.4801(8)
P-C(31)	1.807(8)
P-C(21)	1.819(7)
P-C(11)	1.822(8)
C(11)-C(16)	1.376(9)
C(11)-C(12)	1.374(9)
C(12)-C(13)	1.396(10)
C(13)-C(14)	1.360(10)
C(14)-C(15)	1.370(10)
C(15)-C(16)	1.397(10)
C(21)-C(22)	1.394(9)-
C(21)-C(26)	1.400(9)
C(22)-C(23)	1.381(9)
C(23)-C(24)	1.355(10)
C(24)-C(25)	1.379(10)
C(25)-C(26)	1.408(9)
C(31)-C(32)	1.393(9)
C(31)-C(36)	1.396(9)
C(32)-C(33)	1.386(10)
C(33)-C(34)	1.362(10)
C(34)-C(35)	1.362(10)
C(35)-C(36)	1.371(10)
C(41)-C(42)	1.382(9)
C(41)-C(46)	1.390(9)
C(42)-F(1)	1.358(8)
C(42)-C(43)	1.387(10)
C(43)-F(2)	1.344(9)
C(43)-C(44)	1.363(10)
C(44)-F(3)	1.353(9)

C(44)-C(45)	1.361(10)
C(45)-F(4)	1.350(9)
C(45)-C(46)	1.383(10)
C(46)-F(5)	1.357(8)
C(51)-C(52)	1.371(9)
C(51)-C(56)	1.390(8)
C(52)-F(10)	1.347(8)
C(52)-C(53)	1.362(9)
C(53)-F(9)	1.333(8)
C(53)-C(54)	1.385(9)
C(54)-F(8)	1.350(8)
C(54)-C(55)	1.378(10)
C(55)-F(7)	1.341(8)
C(55)-C(56)	1.387(9)
C(56)-F(6)	1.357(8)
C(99)-Cl(2)	1.78(3)
C(99)-Cl(1)	1.75(2)

P-Au(1)-Se	175.14(5)
C(41)-Au(2)-C(51)	89.7(2)
C(41)-Au(2)-Se	177.92(18)
C(51)-Au(2)-Se	92.37(17)
C(41)-Au(2)-Se#1	92.14(18)
C(51)-Au(2)-Se#1	177.94(18)
Se-Au(2)-Se#1	85.77(3)
Au(1)-Se-Au(2)	88.20(3)
Au(1)-Se-Au(2)#1	95.82(3)
Au(2)-Se-Au(2)#1	94.23(3)
C(31)-P-C(21)	106.6(3)
C(31)-P-C(11)	107.3(3)
C(21)-P-C(11)	104.4(3)
C(31)-P-Au(1)	110.5(2)
C(21)-P-Au(1)	111.3(2)
C(11)-P-Au(1)	116.3(2)
C(16)-C(11)-C(12)	119.8(8)
C(16)-C(11)-P	122.3(6)

C(12)-C(11)-P	117.8(6)
C(11)-C(12)-C(13)	120.3(8)
C(14)-C(13)-C(12)	119.7(8)
C(13)-C(14)-C(15)	120.7(8)
C(14)-C(15)-C(16)	119.9(8)
C(11)-C(16)-C(15)	119.7(8)
C(22)-C(21)-C(26)	117.8(7)
C(22)-C(21)-P	121.0(6)
C(26)-C(21)-P	121.2(6)
C(23)-C(22)-C(21)	120.3(8)
C(24)-C(23)-C(22)	121.8(8)
C(23)-C(24)-C(25)	119.9(8)
C(24)-C(25)-C(26)	119.4(8)
C(21)-C(26)-C(25)	120.8(8)
C(32)-C(31)-C(36)	118.0(8)
C(32)-C(31)-P	119.2(6)
C(36)-C(31)-P	122.7(5)
C(33)-C(32)-C(31)	120.2(8)
C(34)-C(33)-C(32)	120.2(8)
C(35)-C(34)-C(33)	120.5(9)
C(34)-C(35)-C(36)	120.3(8)
C(35)-C(36)-C(31)	120.7(8)
C(42)-C(41)-C(46)	115.9(8)
C(42)-C(41)-Au(2)	122.2(5)
C(46)-C(41)-Au(2)	121.9(5)
F(1)-C(42)-C(41)	119.7(7)
F(1)-C(42)-C(43)	117.5(7)
C(41)-C(42)-C(43)	122.8(8)
F(2)-C(43)-C(44)	121.3(8)
F(2)-C(43)-C(42)	120.1(8)
C(44)-C(43)-C(42)	118.6(8)
F(3)-C(44)-C(45)	119.2(7)
F(3)-C(44)-C(43)	119.4(7)
C(45)-C(44)-C(43)	121.2(8)
F(4)-C(45)-C(44)	120.2(7)
F(4)-C(45)-C(46)	120.6(8)

C(44)-C(45)-C(46)	119.2(8)
F(5)-C(46)-C(45)	117.5(7)
F(5)-C(46)-C(41)	120.2(7)
C(45)-C(46)-C(41)	122.2(8)
C(52)-C(51)-C(56)	116.9(7)
C(52)-C(51)-Au(2)	123.4(5)
C(56)-C(51)-Au(2)	119.6(5)
F(10)-C(52)-C(53)	118.1(7)
F(10)-C(52)-C(51)	118.4(6)
C(53)-C(52)-C(51)	123.4(7)
F(9)-C(53)-C(52)	121.4(7)
F(9)-C(53)-C(54)	120.2(7)
C(52)-C(53)-C(54)	118.4(7)
F(8)-C(54)-C(55)	119.3(7)
F(8)-C(54)-C(53)	119.6(7)
C(55)-C(54)-C(53)	121.0(8)
F(7)-C(55)-C(54)	120.6(7)
F(7)-C(55)-C(56)	121.0(7)
C(54)-C(55)-C(56)	118.4(7)
F(6)-C(56)-C(55)	117.3(7)
F(6)-C(56)-C(51)	120.9(6)
C(55)-C(56)-C(51)	121.8(7)
Cl(2)-C(99)-Cl(1)	123(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for wondered. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au(1)	26(1)	34(1)	27(1)	8(1)	-1(1)	7(1)
Au(2)	22(1)	26(1)	24(1)	5(1)	-2(1)	3(1)
Se	23(1)	28(1)	27(1)	6(1)	-1(1)	6(1)
P	25(1)	35(1)	26(1)	5(1)	0(1)	8(1)
C(11)	27(4)	26(4)	35(5)	6(3)	2(3)	2(3)
C(12)	43(5)	50(5)	37(5)	9(4)	-1(4)	12(4)
C(13)	45(5)	39(4)	41(5)	5(4)	-16(4)	14(4)
C(14)	31(5)	41(5)	67(6)	16(5)	2(4)	11(4)
C(15)	49(5)	57(5)	44(5)	15(5)	25(4)	22(4)
C(16)	41(5)	41(5)	39(5)	12(4)	6(4)	12(4)
C(21)	32(4)	31(4)	32(5)	8(3)	1(4)	6(3)
C(22)	49(5)	47(4)	38(5)	14(4)	19(4)	21(4)
C(23)	98(7)	39(4)	36(6)	8(4)	25(5)	33(5)
C(24)	63(6)	38(5)	43(6)	-4(4)	-20(5)	11(4)
C(25)	33(5)	34(4)	102(9)	0(5)	-4(5)	-7(4)
C(26)	32(5)	38(4)	67(7)	-5(4)	10(4)	3(4)
C(31)	29(4)	36(4)	25(4)	-1(3)	0(4)	7(3)
C(32)	47(5)	39(4)	36(5)	0(4)	1(4)	-1(4)
C(33)	45(6)	74(6)	34(5)	-6(4)	2(4)	-18(5)
C(34)	37(5)	96(7)	29(5)	4(4)	-14(4)	9(4)
C(35)	53(6)	72(6)	35(5)	26(5)	-10(5)	8(4)
C(36)	47(5)	43(5)	33(5)	10(4)	-3(4)	8(4)
C(41)	29(4)	32(4)	26(4)	7(3)	5(4)	1(3)
C(42)	46(5)	32(4)	31(4)	11(4)	-1(4)	6(4)
C(43)	55(5)	52(5)	30(5)	7(4)	-11(4)	8(4)
C(44)	35(4)	46(5)	63(6)	21(5)	-26(5)	1(4)
C(45)	21(4)	51(5)	62(6)	16(5)	-7(4)	-8(4)
C(46)	28(4)	41(4)	37(5)	8(4)	-5(4)	-3(4)
F(1)	53(3)	69(3)	31(3)	12(2)	7(3)	21(3)
F(2)	81(4)	96(4)	36(3)	18(3)	-29(3)	16(3)
F(3)	45(3)	81(4)	88(5)	34(3)	-39(3)	-3(3)

F(4)	26(3)	83(4)	104(5)	42(3)	1(3)	1(3)
F(5)	34(3)	74(3)	48(3)	29(3)	11(3)	12(2)
C(51)	23(4)	27(4)	21(4)	6(3)	-2(3)	3(3)
C(52)	41(5)	32(4)	36(5)	12(4)	3(4)	7(4)
C(53)	45(5)	38(4)	31(5)	1(3)	6(4)	18(4)
C(54)	43(5)	35(4)	44(6)	3(4)	-5(4)	11(4)
C(55)	31(5)	32(4)	55(6)	3(4)	-10(4)	-5(3)
C(56)	29(4)	36(4)	31(5)	2(3)	0(4)	-7(3)
F(6)	46(3)	34(3)	62(4)	7(2)	13(3)	3(2)
F(7)	54(3)	33(3)	97(5)	16(3)	18(3)	-9(2)
F(8)	74(4)	29(3)	85(5)	-10(3)	11(3)	11(2)
F(9)	69(4)	49(3)	60(4)	5(3)	21(3)	17(3)
F(10)	45(3)	41(3)	49(3)	16(2)	17(3)	13(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for wondered.

	x	y	z	U(eq)
H(12)	4104	2227	4105	52
H(13)	6458	1861	3997	51
H(14)	7467	1690	2542	54
H(15)	6122	1761	1165	57
H(16)	3746	2088	1258	47
H(22)	543	4207	4061	50
H(23)	1004	6130	4609	65
H(24)	2948	7204	4170	61
H(25)	4554	6360	3185	73
H(26)	4156	4402	2644	58
H(32)	-168	820	1715	52
H(33)	-1450	483	211	69
H(34)	-1014	1737	-751	68
H(35)	663	3351	-227	62
H(36)	1890	3753	1286	49
H(99A)	5557	5631	124	178
H(99B)	4508	4888	660	178

SUPPORTING INFORMATION FOR

COMPLEX 4

Table 1. Crystal data and structure refinement for complex **4**.

Identification code	concha31
Empirical formula	C60 H48 Au3 C12 F15 Fe O P2 Se
Formula weight	1928.53
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P(-1)
Unit cell dimensions	a = 12.344(2) A alpha= 97.780(10) deg. b = 17.362(2) A beta = 108.150(10) deg. c = 17.889(3) A gamma= 109.650(10) deg.
Volume	3305.2(9) A^3
Z, Calculated density	2, 1.938 Mg/m^3
Absorption coefficient	7.612 mm^-1
F(000)	1824
Crystal size	0.70 x 0.30 x 0.10 mm
Theta range for data collection	3.07 to 25.00 deg.
Limiting indices	-13<=h<=1, -19<=k<=19, -20<=l<=20
Reflections collected / unique	12286 / 11290 [R(int) = 0.0510]
Completeness to theta = 25.00	97.0 %
Absorption correction	Psi-scans
Max. and min. transmission	0.5165 and 0.0758
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11290 / 698 / 744
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0477, wR2 = 0.1151
R indices (all data)	R1 = 0.0804, wR2 = 0.1332
Largest diff. peak and hole	1.613 and -1.835 $e.A^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex **4**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Au(1)	84(1)	1766(1)	4582(1)	31(1)
Au(2)	-1815(1)	719(1)	2962(1)	32(1)
Au(3)	919(1)	1829(1)	2654(1)	30(1)
Se	349(1)	872(1)	3523(1)	33(1)
P(1)	-372(3)	2522(2)	5484(2)	29(1)
P(2)	-3771(2)	680(2)	2505(2)	31(1)
Fe	-3498(1)	1892(1)	4284(1)	30(1)
C(1)	-1705(9)	2737(6)	4967(6)	28(2)
C(2)	-2550(9)	2907(6)	5304(7)	40(2)
C(3)	-3408(10)	3088(7)	4688(8)	48(3)
C(4)	-3126(10)	3024(7)	3982(8)	43(3)
C(5)	-2074(9)	2816(6)	4144(7)	35(2)
C(6)	-4250(8)	818(6)	3353(6)	31(2)
C(7)	-5195(9)	1099(7)	3425(6)	39(2)
C(8)	-5210(10)	1094(7)	4214(7)	40(3)
C(9)	-4286(11)	835(7)	4633(7)	42(3)
C(10)	-3684(10)	667(6)	4120(6)	34(2)
C(11)	-758(10)	2013(6)	6254(6)	35(2)
C(12)	-683(12)	2493(8)	6975(7)	57(3)
C(13)	-1087(14)	2105(9)	7521(8)	66(4)
C(14)	-1562(13)	1223(8)	7357(8)	60(3)
C(15)	-1644(11)	747(8)	6634(8)	46(3)
C(16)	-1237(10)	1139(7)	6088(7)	40(2)
C(21)	893(9)	3572(7)	6078(6)	33(2)
C(22)	654(10)	4297(7)	6126(6)	42(3)
C(23)	1630(12)	5074(8)	6587(8)	58(3)
C(24)	2798(12)	5110(8)	6997(9)	64(4)
C(25)	3024(12)	4388(8)	6949(10)	70(4)
C(26)	2069(11)	3605(8)	6483(9)	60(4)
C(31)	-3868(8)	1525(7)	2027(6)	32(2)
C(32)	-5028(10)	1575(7)	1642(6)	39(2)
C(33)	-5084(11)	2240(7)	1302(7)	46(3)
C(34)	-3996(9)	2862(8)	1345(8)	48(3)
C(35)	-2851(11)	2820(7)	1711(7)	43(3)
C(36)	-2777(10)	2158(7)	2040(7)	37(2)
C(41)	-4955(9)	-283(7)	1738(6)	36(2)
C(42)	-5833(11)	-875(7)	1929(8)	61(4)
C(43)	-6717(13)	-1623(8)	1319(9)	78(5)
C(44)	-6688(12)	-1761(8)	560(8)	61(4)
C(45)	-5834(12)	-1194(8)	370(8)	56(3)
C(46)	-4949(12)	-440(8)	959(7)	53(3)
C(51)	138(8)	759(7)	1673(6)	35(2)
C(52)	-1109(9)	405(6)	1134(6)	38(3)
C(53)	-1623(10)	-316(7)	505(6)	44(3)
C(54)	-893(9)	-727(8)	380(7)	48(3)
C(55)	342(11)	-417(7)	896(7)	41(3)
C(56)	824(9)	308(7)	1518(6)	35(2)
F(1)	-1881(6)	788(5)	1233(4)	50(2)
F(2)	-2835(7)	-616(5)	14(4)	65(2)
F(3)	-1398(8)	-1451(5)	-225(4)	71(2)
F(4)	1055(8)	-813(5)	772(4)	61(2)
F(5)	2057(5)	622(4)	1998(4)	46(2)

C(61)	1426(8)	2589(6)	1926(6)	35(2)
C(62)	2657(10)	2988(6)	2020(6)	40(3)
C(63)	3019(11)	3491(7)	1523(8)	51(3)
C(64)	2130(9)	3593(9)	919(8)	56(3)
C(65)	917(12)	3225(8)	799(8)	56(3)
C(66)	581(10)	2724(7)	1301(7)	43(3)
F(6)	3578(6)	2893(5)	2611(5)	57(2)
F(7)	4239(7)	3885(5)	1651(6)	75(3)
F(8)	2456(9)	4075(7)	418(7)	92(3)
F(9)	28(8)	3307(7)	185(6)	96(3)
F(10)	-648(6)	2370(6)	1175(5)	65(2)
C(71)	1776(9)	2907(7)	3635(6)	37(3)
C(72)	1287(9)	3513(6)	3701(6)	34(2)
C(73)	1900(10)	4255(6)	4321(6)	43(3)
C(74)	3055(10)	4422(7)	4915(7)	44(3)
C(75)	3556(10)	3817(7)	4856(7)	47(3)
C(76)	2914(10)	3084(7)	4230(7)	43(3)
F(11)	165(6)	3388(4)	3148(4)	51(2)
F(12)	1392(8)	4829(5)	4375(5)	69(2)
F(13)	3683(8)	5142(4)	5510(5)	65(2)
F(14)	4694(7)	3988(5)	5423(4)	61(2)
F(15)	3465(6)	2537(4)	4212(4)	49(2)
C(99)	6017(18)	-1530(40)	3420(30)	170(20)
Cl(1)	4740(20)	-1886(10)	3654(11)	145(7)
Cl(2)	7259(18)	-1339(14)	4279(13)	156(9)
C(99')	6990(40)	-1720(50)	4310(50)	170(20)
Cl(1')	7920(20)	-956(13)	4020(10)	124(7)
Cl(2')	5480(40)	-2050(30)	3690(20)	266(17)
C(81)	7390(30)	4628(19)	7288(18)	169(12)
C(82)	8300(20)	4470(20)	7950(20)	206(14)
C(83)	9580(20)	4970(20)	8075(19)	204(14)
C(84)	10500(30)	4720(20)	8620(20)	225(16)
C(85)	11240(40)	5350(30)	9400(30)	370(30)
O(87)	6900(30)	8451(19)	1708(19)	267(14)
C(88)	7900(30)	8140(30)	1830(30)	260(20)
C(89)	7420(50)	7320(30)	1200(30)	370(30)

Table 4. Bond lengths [A] and angles [deg] for complex **4**.

Au(1)-P(1)	2.266(3)
Au(1)-Se	2.4569(11)
Au(1)-Au(2)	2.9457(9)
Au(2)-P(2)	2.269(3)
Au(2)-Se	2.4486(12)
Au(3)-C(61)	2.060(12)
Au(3)-C(71)	2.079(11)
Au(3)-C(51)	2.079(11)
Au(3)-Se	2.5038(13)
P(1)-C(1)	1.806(11)
P(1)-C(11)	1.834(12)
P(1)-C(21)	1.849(11)
P(2)-C(6)	1.808(11)
P(2)-C(31)	1.814(12)
P(2)-C(41)	1.817(11)
Fe-C(10)	2.031(11)
Fe-C(7)	2.032(10)
Fe-C(6)	2.036(10)
Fe-C(1)	2.047(9)
Fe-C(4)	2.048(11)
Fe-C(9)	2.048(12)
Fe-C(5)	2.053(10)
Fe-C(2)	2.053(10)
Fe-C(8)	2.055(10)
Fe-C(3)	2.058(11)
C(1)-C(5)	1.441(13)
C(1)-C(2)	1.445(12)
C(2)-C(3)	1.423(14)
C(3)-C(4)	1.410(18)
C(4)-C(5)	1.417(14)
C(6)-C(10)	1.436(13)
C(6)-C(7)	1.440(13)
C(7)-C(8)	1.419(14)
C(8)-C(9)	1.403(17)
C(9)-C(10)	1.406(13)
C(11)-C(16)	1.381(13)
C(11)-C(12)	1.396(13)
C(12)-C(13)	1.382(15)
C(13)-C(14)	1.394(15)
C(14)-C(15)	1.393(14)
C(15)-C(16)	1.388(15)
C(21)-C(22)	1.383(12)
C(21)-C(26)	1.384(13)
C(22)-C(23)	1.393(14)
C(23)-C(24)	1.375(14)
C(24)-C(25)	1.369(14)
C(25)-C(26)	1.391(14)
C(31)-C(36)	1.414(12)
C(31)-C(32)	1.420(12)
C(32)-C(33)	1.387(14)
C(33)-C(34)	1.383(13)
C(34)-C(35)	1.392(13)
C(35)-C(36)	1.378(14)
C(41)-C(46)	1.386(13)
C(41)-C(42)	1.388(13)
C(42)-C(43)	1.411(14)
C(43)-C(44)	1.360(15)
C(44)-C(45)	1.347(14)
C(45)-C(46)	1.401(14)

C(51)-C(56)	1.393(12)
C(51)-C(52)	1.398(12)
C(52)-F(1)	1.371(11)
C(52)-C(53)	1.370(13)
C(53)-F(2)	1.346(11)
C(53)-C(54)	1.374(13)
C(54)-F(3)	1.351(13)
C(54)-C(55)	1.379(13)
C(55)-F(4)	1.335(11)
C(55)-C(56)	1.372(13)
C(56)-F(5)	1.361(11)
C(61)-C(66)	1.379(13)
C(61)-C(62)	1.386(13)
C(62)-F(6)	1.364(12)
C(62)-C(63)	1.395(15)
C(63)-F(7)	1.356(12)
C(63)-C(64)	1.360(14)
C(64)-C(65)	1.347(14)
C(64)-F(8)	1.367(16)
C(65)-F(9)	1.351(13)
C(65)-C(66)	1.391(15)
C(66)-F(10)	1.361(11)
C(71)-C(76)	1.376(12)
C(71)-C(72)	1.385(12)
C(72)-F(11)	1.354(11)
C(72)-C(73)	1.378(13)
C(73)-F(12)	1.351(11)
C(73)-C(74)	1.393(13)
C(74)-F(13)	1.332(13)
C(74)-C(75)	1.395(13)
C(75)-F(14)	1.357(11)
C(75)-C(76)	1.372(13)
C(76)-F(15)	1.343(11)
C(99)-Cl(1)	1.69(3)
C(99)-Cl(2)	1.70(3)
C(99')-Cl(2')	1.69(3)
C(99')-Cl(1')	1.70(3)
C(81)-C(82)	1.49(2)
C(82)-C(83)	1.45(2)
C(83)-C(84)	1.47(2)
C(84)-C(85)	1.45(2)
O(87)-C(88)	1.48(2)
C(88)-C(89)	1.50(2)

P(1)-Au(1)-Se	174.16(7)
P(1)-Au(1)-Au(2)	121.34(7)
Se-Au(1)-Au(2)	52.97(3)
P(2)-Au(2)-Se	175.51(8)
P(2)-Au(2)-Au(1)	122.77(7)
Se-Au(2)-Au(1)	53.23(3)
C(61)-Au(3)-C(71)	88.8(4)
C(61)-Au(3)-C(51)	90.2(4)
C(71)-Au(3)-C(51)	177.5(3)
C(61)-Au(3)-Se	177.7(2)
C(71)-Au(3)-Se	92.4(3)
C(51)-Au(3)-Se	88.4(3)
Au(2)-Se-Au(1)	73.81(3)
Au(2)-Se-Au(3)	91.01(4)
Au(1)-Se-Au(3)	103.63(4)
C(1)-P(1)-C(11)	105.0(5)
C(1)-P(1)-C(21)	105.4(4)
C(11)-P(1)-C(21)	104.7(5)
C(1)-P(1)-Au(1)	111.0(3)

C(11)-P(1)-Au(1)	115.8(3)
C(21)-P(1)-Au(1)	113.9(3)
C(6)-P(2)-C(31)	106.8(5)
C(6)-P(2)-C(41)	107.8(4)
C(31)-P(2)-C(41)	104.3(5)
C(6)-P(2)-Au(2)	109.7(3)
C(31)-P(2)-Au(2)	112.3(3)
C(41)-P(2)-Au(2)	115.4(3)
C(10)-Fe-C(7)	69.3(5)
C(10)-Fe-C(6)	41.4(4)
C(7)-Fe-C(6)	41.5(4)
C(10)-Fe-C(1)	112.5(4)
C(7)-Fe-C(1)	169.3(4)
C(6)-Fe-C(1)	133.0(4)
C(10)-Fe-C(4)	153.4(5)
C(7)-Fe-C(4)	104.9(5)
C(6)-Fe-C(4)	117.2(5)
C(1)-Fe-C(4)	68.6(4)
C(10)-Fe-C(9)	40.3(4)
C(7)-Fe-C(9)	68.3(4)
C(6)-Fe-C(9)	68.5(4)
C(1)-Fe-C(9)	120.3(4)
C(4)-Fe-C(9)	163.2(5)
C(10)-Fe-C(5)	122.3(4)
C(7)-Fe-C(5)	128.5(4)
C(6)-Fe-C(5)	110.6(4)
C(1)-Fe-C(5)	41.2(4)
C(4)-Fe-C(5)	40.4(4)
C(9)-Fe-C(5)	155.3(5)
C(10)-Fe-C(2)	131.2(4)
C(7)-Fe-C(2)	145.6(4)
C(6)-Fe-C(2)	171.5(4)
C(1)-Fe-C(2)	41.3(3)
C(4)-Fe-C(2)	68.4(5)
C(9)-Fe-C(2)	108.1(5)
C(5)-Fe-C(2)	69.0(5)
C(10)-Fe-C(8)	68.1(4)
C(7)-Fe-C(8)	40.6(4)
C(6)-Fe-C(8)	68.7(4)
C(1)-Fe-C(8)	150.0(4)
C(4)-Fe-C(8)	125.1(5)
C(9)-Fe-C(8)	40.0(5)
C(5)-Fe-C(8)	164.5(5)
C(2)-Fe-C(8)	114.1(4)
C(10)-Fe-C(3)	166.4(5)
C(7)-Fe-C(3)	112.5(4)
C(6)-Fe-C(3)	147.8(4)
C(1)-Fe-C(3)	68.5(4)
C(4)-Fe-C(3)	40.1(5)
C(9)-Fe-C(3)	126.7(5)
C(5)-Fe-C(3)	67.9(4)
C(2)-Fe-C(3)	40.5(4)
C(8)-Fe-C(3)	104.0(5)
C(5)-C(1)-C(2)	107.4(10)
C(5)-C(1)-P(1)	125.3(7)
C(2)-C(1)-P(1)	127.3(8)
C(5)-C(1)-Fe	69.6(5)
C(2)-C(1)-Fe	69.6(5)
P(1)-C(1)-Fe	128.6(5)
C(3)-C(2)-C(1)	107.2(10)
C(3)-C(2)-Fe	69.9(6)
C(1)-C(2)-Fe	69.1(5)
C(4)-C(3)-C(2)	108.9(9)

C(4)-C(3)-Fe	69.5(6)
C(2)-C(3)-Fe	69.6(6)
C(3)-C(4)-C(5)	108.7(9)
C(3)-C(4)-Fe	70.3(6)
C(5)-C(4)-Fe	70.0(6)
C(4)-C(5)-C(1)	107.7(9)
C(4)-C(5)-Fe	69.6(6)
C(1)-C(5)-Fe	69.2(5)
C(10)-C(6)-C(7)	106.9(10)
C(10)-C(6)-P(2)	123.4(7)
C(7)-C(6)-P(2)	129.7(8)
C(10)-C(6)-Fe	69.1(6)
C(7)-C(6)-Fe	69.1(5)
P(2)-C(6)-Fe	125.7(5)
C(8)-C(7)-C(6)	107.6(9)
C(8)-C(7)-Fe	70.6(6)
C(6)-C(7)-Fe	69.4(5)
C(9)-C(8)-C(7)	108.5(9)
C(9)-C(8)-Fe	69.8(6)
C(7)-C(8)-Fe	68.8(6)
C(8)-C(9)-C(10)	109.0(9)
C(8)-C(9)-Fe	70.3(6)
C(10)-C(9)-Fe	69.2(6)
C(9)-C(10)-C(6)	108.0(9)
C(9)-C(10)-Fe	70.5(6)
C(6)-C(10)-Fe	69.5(6)
C(16)-C(11)-C(12)	119.4(12)
C(16)-C(11)-P(1)	119.6(8)
C(12)-C(11)-P(1)	120.7(8)
C(13)-C(12)-C(11)	120.9(11)
C(12)-C(13)-C(14)	119.8(12)
C(15)-C(14)-C(13)	119.0(13)
C(16)-C(15)-C(14)	120.9(11)
C(11)-C(16)-C(15)	119.9(11)
C(22)-C(21)-C(26)	121.5(11)
C(22)-C(21)-P(1)	120.5(7)
C(26)-C(21)-P(1)	118.0(8)
C(21)-C(22)-C(23)	118.7(11)
C(24)-C(23)-C(22)	120.1(12)
C(25)-C(24)-C(23)	120.8(12)
C(24)-C(25)-C(26)	120.3(12)
C(21)-C(26)-C(25)	118.7(12)
C(36)-C(31)-C(32)	118.5(11)
C(36)-C(31)-P(2)	120.2(8)
C(32)-C(31)-P(2)	121.3(8)
C(33)-C(32)-C(31)	120.6(10)
C(34)-C(33)-C(32)	119.5(10)
C(33)-C(34)-C(35)	120.8(12)
C(36)-C(35)-C(34)	120.6(11)
C(35)-C(36)-C(31)	119.9(10)
C(46)-C(41)-C(42)	119.7(11)
C(46)-C(41)-P(2)	119.2(8)
C(42)-C(41)-P(2)	121.0(8)
C(41)-C(42)-C(43)	119.0(11)
C(44)-C(43)-C(42)	119.9(12)
C(45)-C(44)-C(43)	121.5(12)
C(44)-C(45)-C(46)	120.0(12)
C(41)-C(46)-C(45)	119.7(11)
C(56)-C(51)-C(52)	114.0(10)
C(56)-C(51)-Au(3)	121.7(7)
C(52)-C(51)-Au(3)	124.3(7)
F(1)-C(52)-C(53)	117.1(9)
F(1)-C(52)-C(51)	119.2(9)

C(53)-C(52)-C(51)	123.7(9)
F(2)-C(53)-C(52)	120.0(10)
F(2)-C(53)-C(54)	120.5(10)
C(52)-C(53)-C(54)	119.5(10)
F(3)-C(54)-C(53)	119.9(9)
F(3)-C(54)-C(55)	120.3(9)
C(53)-C(54)-C(55)	119.7(11)
F(4)-C(55)-C(56)	121.1(10)
F(4)-C(55)-C(54)	119.8(10)
C(56)-C(55)-C(54)	119.1(10)
F(5)-C(56)-C(55)	118.1(9)
F(5)-C(56)-C(51)	117.9(9)
C(55)-C(56)-C(51)	124.0(9)
C(66)-C(61)-C(62)	114.9(11)
C(66)-C(61)-Au(3)	123.4(7)
C(62)-C(61)-Au(3)	121.7(8)
F(6)-C(62)-C(61)	120.4(10)
F(6)-C(62)-C(63)	116.9(9)
C(61)-C(62)-C(63)	122.8(10)
F(7)-C(63)-C(64)	120.5(11)
F(7)-C(63)-C(62)	120.6(11)
C(64)-C(63)-C(62)	118.8(11)
C(65)-C(64)-C(63)	121.2(13)
C(65)-C(64)-F(8)	118.6(10)
C(63)-C(64)-F(8)	120.2(10)
F(9)-C(65)-C(64)	121.4(12)
F(9)-C(65)-C(66)	119.9(11)
C(64)-C(65)-C(66)	118.7(11)
F(10)-C(66)-C(61)	118.9(10)
F(10)-C(66)-C(65)	117.5(10)
C(61)-C(66)-C(65)	123.6(10)
C(76)-C(71)-C(72)	116.2(10)
C(76)-C(71)-Au(3)	121.0(7)
C(72)-C(71)-Au(3)	122.7(7)
F(11)-C(72)-C(73)	117.2(9)
F(11)-C(72)-C(71)	120.3(9)
C(73)-C(72)-C(71)	122.6(9)
F(12)-C(73)-C(72)	121.1(10)
F(12)-C(73)-C(74)	118.7(9)
C(72)-C(73)-C(74)	120.2(9)
F(13)-C(74)-C(73)	121.6(9)
F(13)-C(74)-C(75)	120.6(9)
C(73)-C(74)-C(75)	117.8(10)
F(14)-C(75)-C(76)	122.1(10)
F(14)-C(75)-C(74)	117.8(9)
C(76)-C(75)-C(74)	120.2(9)
F(15)-C(76)-C(75)	116.5(9)
F(15)-C(76)-C(71)	120.4(9)
C(75)-C(76)-C(71)	123.1(9)
Cl(1)-C(99)-Cl(2)	107(3)
Cl(2')-C(99')-Cl(1')	110(4)
C(83)-C(82)-C(81)	112(2)
C(82)-C(83)-C(84)	114(3)
C(85)-C(84)-C(83)	112(2)
O(87)-C(88)-C(89)	109(2)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for complex **4**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Au(1)	28(1)	33(1)	31(1)	3(1)	9(1)	15(1)
Au(2)	25(1)	35(1)	33(1)	3(1)	8(1)	12(1)
Au(3)	22(1)	32(1)	31(1)	1(1)	7(1)	12(1)
Se	31(1)	37(1)	34(1)	5(1)	11(1)	20(1)
P(1)	27(1)	26(1)	31(1)	2(1)	10(1)	11(1)
P(2)	22(1)	34(2)	29(1)	2(1)	5(1)	9(1)
Fe	23(1)	27(1)	35(1)	4(1)	8(1)	9(1)
C(1)	24(5)	15(5)	32(5)	-5(4)	4(4)	3(4)
C(2)	28(6)	31(6)	49(6)	-2(5)	12(5)	8(5)
C(3)	32(6)	33(6)	75(8)	5(6)	18(5)	14(5)
C(4)	35(6)	25(6)	69(7)	27(6)	15(5)	12(5)
C(5)	23(5)	24(5)	50(6)	11(5)	11(5)	0(4)
C(6)	23(5)	24(5)	32(5)	-2(4)	8(4)	0(4)
C(7)	21(5)	40(6)	38(5)	1(5)	5(4)	3(4)
C(8)	25(5)	39(6)	44(6)	0(5)	12(5)	2(5)
C(9)	43(6)	37(6)	37(5)	5(5)	15(5)	10(5)
C(10)	37(6)	25(5)	35(5)	4(4)	14(4)	7(4)
C(11)	43(6)	37(5)	34(5)	16(5)	14(5)	27(5)
C(12)	89(10)	45(6)	53(7)	11(5)	44(7)	31(7)
C(13)	113(12)	56(7)	55(8)	21(6)	53(8)	41(8)
C(14)	73(9)	64(7)	69(8)	34(7)	40(7)	40(7)
C(15)	42(7)	45(6)	66(7)	26(5)	22(6)	27(6)
C(16)	40(6)	35(5)	46(6)	14(5)	13(5)	19(5)
C(21)	26(5)	37(5)	36(6)	6(5)	14(4)	10(4)
C(22)	35(6)	32(6)	47(7)	6(5)	5(5)	12(4)
C(23)	52(7)	41(6)	60(8)	-2(6)	12(6)	8(5)
C(24)	48(6)	43(6)	62(8)	-11(7)	6(6)	-3(6)
C(25)	39(7)	49(7)	85(10)	-5(7)	-5(7)	8(5)
C(26)	35(6)	44(6)	76(9)	-7(7)	2(6)	13(5)
C(31)	35(5)	32(5)	31(5)	4(4)	14(4)	14(4)
C(32)	32(5)	38(6)	35(6)	-3(5)	6(5)	11(5)
C(33)	34(5)	43(6)	38(6)	-4(5)	-8(5)	14(5)
C(34)	57(7)	36(6)	50(7)	14(5)	14(6)	22(5)
C(35)	37(5)	34(6)	47(7)	10(5)	12(5)	7(5)
C(36)	31(5)	39(6)	36(6)	7(5)	9(5)	12(4)
C(41)	26(5)	35(6)	47(6)	5(5)	15(5)	13(4)
C(42)	50(8)	48(7)	62(7)	-13(6)	32(6)	-8(6)
C(43)	66(9)	49(8)	81(9)	-21(7)	40(8)	-17(6)
C(44)	45(7)	46(7)	60(7)	-14(6)	9(6)	1(5)
C(45)	56(8)	50(7)	40(6)	0(5)	10(6)	8(6)
C(46)	52(7)	41(7)	48(6)	-1(5)	20(6)	2(5)
C(51)	36(5)	42(6)	30(5)	15(5)	22(4)	10(5)
C(52)	27(5)	54(7)	31(6)	5(5)	15(4)	14(5)
C(53)	38(6)	55(7)	31(6)	10(5)	13(5)	10(5)
C(54)	67(7)	42(7)	25(6)	-3(5)	13(5)	18(6)
C(55)	57(6)	42(6)	38(6)	15(5)	27(5)	25(6)
C(56)	38(6)	38(6)	33(6)	15(4)	16(5)	16(5)
F(1)	28(3)	64(5)	55(4)	4(4)	10(3)	22(3)
F(2)	47(4)	62(5)	44(4)	-5(4)	-4(4)	0(4)
F(3)	92(6)	56(5)	37(4)	-16(4)	15(4)	17(5)
F(4)	92(6)	61(5)	53(4)	13(4)	36(4)	51(5)
F(5)	27(3)	60(5)	50(4)	7(3)	12(3)	23(3)
C(61)	29(5)	32(6)	44(6)	3(5)	15(5)	14(4)

C(62)	33(5)	49(7)	36(6)	5(5)	15(5)	15(5)
C(63)	46(6)	37(7)	79(9)	15(6)	33(6)	17(6)
C(64)	66(7)	48(8)	64(8)	25(6)	33(6)	22(6)
C(65)	56(6)	47(8)	62(8)	23(6)	17(6)	21(6)
C(66)	33(6)	43(7)	51(7)	12(5)	13(5)	14(5)
F(6)	35(4)	64(5)	66(5)	15(4)	15(4)	19(4)
F(7)	52(5)	64(5)	119(8)	32(5)	51(5)	15(4)
F(8)	90(7)	100(8)	120(8)	78(7)	64(6)	39(6)
F(9)	69(6)	124(9)	100(7)	77(7)	20(5)	37(6)
F(10)	26(4)	95(6)	71(5)	47(5)	13(4)	16(4)
C(71)	35(6)	36(6)	35(6)	5(5)	10(4)	14(5)
C(72)	29(5)	32(6)	40(6)	7(4)	11(4)	15(4)
C(73)	51(7)	34(6)	50(7)	4(5)	20(5)	24(5)
C(74)	52(7)	22(5)	45(6)	0(5)	17(5)	6(5)
C(75)	27(6)	56(7)	46(7)	-4(5)	8(5)	14(5)
C(76)	34(6)	46(6)	48(7)	1(5)	10(5)	25(5)
F(11)	39(4)	43(4)	66(5)	9(4)	6(3)	26(3)
F(12)	75(6)	43(4)	87(6)	-6(4)	24(5)	35(4)
F(13)	78(6)	33(4)	62(5)	-9(4)	19(4)	12(4)
F(14)	46(4)	66(5)	48(4)	-6(4)	-4(3)	23(4)
F(15)	38(4)	48(4)	53(4)	-2(3)	2(3)	29(3)
Cl(1)	237(18)	135(11)	123(10)	47(8)	132(12)	83(11)
Cl(2)	138(13)	189(18)	153(13)	75(13)	22(11)	99(13)
Cl(1')	173(15)	159(15)	140(12)	99(10)	101(11)	123(13)
Cl(2')	260(30)	300(30)	200(20)	80(20)	70(20)	80(30)

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Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for complex **4**.

	x	y	z	U(eq)
H(2)	-2536	2899	5837	48
H(3)	-4063	3230	4743	58
H(4)	-3568	3106	3482	51
H(5)	-1682	2743	3775	42
H(7)	-5714	1259	3018	46
H(8)	-5754	1241	4424	48
H(9)	-4097	781	5176	50
H(10)	-3019	485	4257	41
H(12)	-349	3095	7093	68
H(13)	-1041	2439	8006	80
H(14)	-1826	950	7734	72
H(15)	-1983	145	6513	56
H(16)	-1288	807	5601	47
H(22)	-161	4265	5851	50
H(23)	1489	5581	6618	70
H(24)	3457	5641	7318	76
H(25)	3836	4422	7234	84
H(26)	2222	3103	6445	72
H(32)	-5773	1149	1617	46
H(33)	-5863	2268	1042	56
H(34)	-4031	3324	1123	58
H(35)	-2114	3253	1734	51
H(36)	-1995	2125	2274	44
H(42)	-5839	-778	2463	73
H(43)	-7331	-2031	1439	93
H(44)	-7285	-2268	155	74
H(45)	-5831	-1304	-164	67
H(46)	-4348	-39	825	63
H(99A)	6094	-1004	3244	204
H(99B)	5961	-1964	2971	204
H(99C)	7237	-2210	4291	199
H(99D)	7100	-1497	4881	199
H(81A)	6539	4279	7229	202
H(81B)	7489	4482	6773	202
H(81C)	7531	5229	7427	202
H(82A)	8177	4598	8466	248
H(82B)	8145	3857	7810	248
H(83A)	9779	5577	8308	244
H(83B)	9663	4921	7539	244
H(84A)	10056	4176	8708	270
H(84B)	11057	4644	8350	270
H(85A)	11822	5154	9749	445
H(85B)	10695	5439	9672	445
H(85C)	11715	5892	9320	445
H(88A)	8170	8054	2385	308
H(88B)	8633	8562	1781	308
H(89A)	7033	6847	1405	445
H(89B)	8114	7248	1083	445
H(89C)	6806	7320	699	445