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Table 1. Crystal data and structure refinement for 1.

Identification code	locreo
Empirical formula	$C_{52}H_{28}Au_3F_{15}FeP_2S$
Formula weight	1678.49
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 17.876(2) Å α = 90° b = 18.559(2) Å β = 104.074(8)° c = 17.896(2) Å γ = 90°
Volume	5759.0(11) $Å^3$
Z	4
Density (calculated)	1.936 Mg/m^3
Absorption coefficient	8.038 mm^{-1}
F(000)	3136
Crystal size	0.30 x 0.30 x 0.30 mm
θ range for data collection	3.07 to 22.50°
Index ranges	$0 \le h \le 19$, $-19 \le k \le 1$, $-19 \le \ell \le 18$
Reflections collected	7893
Independent reflections	7421 (R_{int} = 0.0407)
Absorption correction	SHELXA
Max. and min. transmission	0.56 and 0.31
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7404 / 238 / 407
Goodness-of-fit on F^2	0.911
Final R indices [I>2σ(I)]	R1 = 0.0470, wR2 = 0.1069
R indices (all data)	R1 = 0.0824, wR2 = 0.1327
Largest diff. peak and hole	1.582 and −0.955 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Au(1)	6255(1)	3121(1)	2347(1)	29(1)
Au(2)	6948(1)	1767(1)	2088(1)	27(1)
Au(3)	5846(1)	1913(1)	3623(1)	31(1)
Fe	5825(1)	2777(1)	-95(1)	31(1)
S	6964(2)	2330(2)	3263(2)	29(1)
P(1)	5619(2)	3854(2)	1408(2)	30(1)
P(2)	6912(2)	1387(2)	889(2)	28(1)
C(11)	5920(8)	3715(7)	548(8)	31(3)
C(12)	5501(8)	3823(7)	-257(8)	33(4)
C(13)	5986(9)	3660(8)	-732(9)	42(4)
C(14)	6694(9)	3424(8)	-277(8)	39(4)
C(15)	6662(8)	3460(7)	523(8)	31(3)
C(21)	6064(7)	1733(7)	221(7)	29(3)
C(22)	5391(8)	1956(7)	432(8)	34(4)
C(23)	4855(10)	2163(8)	-275(9)	49(4)
C(24)	5185(9)	2078(8)	-885(10)	48(4)
C(25)	5912(9)	1810(8)	-603(8)	41(4)
C(31)	6880(8)	417(8)	768(7)	40(4)
C(32)	7429(9)	24(7)	1279(8)	47(4)
C(33)	7458(9)	-722(8)	1177(9)	55(5)
C(34)	6941(9)	-1059(9)	599(8)	53(5)
C(35)	6404(10)	-674(8)	97(10)	65(5)
C(36)	6371(8)	79(7)	174(8)	39(4)
C(41)	7750(9)	1677(7)	560(8)	41(4)
C(42)	8218(8)	2215(7)	964(8)	44(4)
C(43)	8874(9)	2445(9)	741(10)	59(5)
C(44)	9046(11)	2128(9)	107(9)	67(5)
C(45)	8586(10)	1608(10)	-309(10)	68(5)
C(46)	7935(9)	1375(8)	-83(9)	50(4)
C(51)	4584(8)	3787(6)	1169(7)	34(4)
C(52)	4235(8)	3163(8)	1347(8)	47(4)
C(53)	3442(9)	3109(9)	1148(9)	61(5)
C(54)	3005(11)	3655(7)	756(9)	58(5)
C(55)	3330(8)	4270(8)	584(9)	49(4)
C(56)	4131(8)	4346(7)	780(8)	38(4)
C(61)	5817(7)	4799(8)	1644(7)	36(4)
C(62)	6311(7)	5197(6)	1308(7)	27(3)
C(63)	6457(9)	5912(7)	1522(8)	46(4)
C(64)	6140(8)	6230(8)	2052(8)	42(4)
C(65)	5674(9)	5842(7)	2397(8)	45(4)
C(66)	5503(9)	5137(8)	2201(9)	48(4)
C(71)	4944(8)	1526(7)	3996(7)	42(4)
C(72)	5067(9)	1151(7)	4687(8)	56(5)
C(73)	4482(9)	853(8)	4960(9)	56(5)
C(74)	3745(10)	931(10)	4532(8)	63(5)
C(75)	3580(10)	1277(10)	3836(10)	69(5)
C(76)	4175(9)	1597(9)	3597(9)	57(5)
F(1)	5788(5)	1086(5)	5116(5)	67(3)
F(2)	4621(6)	501(6)	5629(6)	92(4)
F(3)	3139(6)	625(6)	4774(8)	103(4)
F(4)	2847(6)	1365(9)	3447(7)	119(5)
F(5)	4011(5)	1937(7)	2927(6)	98(4)

C(81)	5820(7)	2896(7)	4152(7)	36(4)
C(82)	5331(9)	3473(8)	3833(9)	60(5)
C(83)	5413(10)	4140(9)	4175(10)	79(6)
C(84)	5943(10)	4249(11)	4776(10)	79(6)
C(85)	6368(12)	3756(9)	5157(11)	83(6)
C(86)	6344(10)	3071(9)	4841(10)	62(5)
F(6)	4785(6)	3333(6)	3193(6)	81(3)
F(7)	4910(9)	4663(6)	3802(8)	134(6)
F(8)	6000(9)	4946(6)	5116(9)	146(7)
F(9)	6923(8)	3865(8)	5827(8)	139(6)
F(10)	6828(7)	2573(6)	5182(6)	93(4)
C(91)	5882(6)	919(7)	3096(6)	28(3)
C(92)	5413(7)	750(7)	2377(7)	38(4)
C(93)	5455(8)	113(7)	2025(8)	50(4)
C(94)	5970(8)	-423(8)	2388(7)	46(4)
C(95)	6481(8)	-244(7)	3122(8)	42(4)
C(96)	6428(8)	399(7)	3440(8)	38(4)
F(11)	4899(5)	1231(5)	2007(5)	61(3)
F(12)	4981(6)	-46(6)	1344(6)	96(4)
F(13)	6008(6)	-1067(5)	2079(6)	77(3)
F(14)	6978(5)	-746(5)	3449(6)	72(3)
F(15)	6910(5)	537(5)	4109(4)	57(3)

Table 3. Selected bond lengths [Å] and angles [°] for 1.

Au(1)-P(1)	2.244(3)	Au(1)-S	2.332(3)
Au(1)-Au(2)	2.8889(8)	Au(2)-P(2)	2.245(4)
Au(2)-S	2.342(4)	Au(3)-C(71)	2.02(2)
Au(3)-C(81)	2.061(14)	Au(3)-C(91)	2.079(13)
Au(3)-S	2.374(4)	P(1)-C(11)	1.77(2)
P(1)-C(51)	1.80(2)	P(1)-C(61)	1.820(14)
P(2)-C(21)	1.805(13)	P(2)-C(31)	1.81(2)
P(2)-C(41)	1.82(2)		

P(1)-Au(1)-S	175.98(14)	P(1)-Au(1)-Au(2)	124.47(10)
S-Au(1)-Au(2)	51.97(9)	P(2)-Au(2)-S	171.72(12)
P(2)-Au(2)-Au(1)	120.84(9)	S-Au(2)-Au(1)	51.67(8)
C(71)-Au(3)-C(81)	93.1(5)	C(71)-Au(3)-C(91)	87.1(5)
C(81)-Au(3)-C(91)	179.5(4)	C(71)-Au(3)-S	176.0(3)
C(81)-Au(3)-S	87.2(4)	C(91)-Au(3)-S	92.6(4)
Au(1)-S-Au(2)	76.36(10)	Au(1)-S-Au(3)	92.64(12)
Au(2)-S-Au(3)	105.69(14)	C(11)-P(1)-C(51)	107.2(6)
C(11)-P(1)-C(61)	105.0(6)	C(51)-P(1)-C(61)	104.6(6)
C(11)-P(1)-Au(1)	111.0(5)	C(51)-P(1)-Au(1)	116.1(4)
C(61)-P(1)-Au(1)	112.1(4)	C(21)-P(2)-C(31)	106.1(6)
C(21)-P(2)-C(41)	107.8(6)	C(31)-P(2)-C(41)	105.0(7)
C(21)-P(2)-Au(2)	110.2(5)	C(31)-P(2)-Au(2)	114.8(5)
C(41)-P(2)-Au(2)	112.5(4)	C(72)-C(71)-C(76)	115(2)
C(86)-C(81)-C(82)	114(2)	C(92)-C(91)-C(96)	116.6(13)

Table 4. Bond lengths [Å] and angles [°] for 1.

Au(1)-P(1)	2.244(3)	Au(1)-S	2.332(3)
Au(1)-Au(2)	2.8889(8)	Au(2)-P(2)	2.245(4)
Au(2)-S	2.342(4)	Au(3)-C(71)	2.02(2)
Au(3)-C(81)	2.061(14)	Au(3)-C(91)	2.079(13)
Au(3)-S	2.374(4)	Fe-C(12)	2.026(13)
Fe-C(25)	2.03(2)	Fe-C(23)	2.03(2)
Fe-C(21)	2.035(13)	Fe-C(22)	2.041(14)
Fe-C(24)	2.05(2)	Fe-C(14)	2.05(2)
Fe-C(13)	2.06(2)	Fe-C(15)	2.064(13)
Fe-C(11)	2.071(13)	P(1)-C(11)	1.77(2)
P(1)-C(51)	1.80(2)	P(1)-C(61)	1.820(14)
P(2)-C(21)	1.805(13)	P(2)-C(31)	1.81(2)
P(2)-C(41)	1.82(2)	C(11)-C(15)	1.42(2)
C(11)-C(12)	1.47(2)	C(12)-C(13)	1.39(2)
C(13)-C(14)	1.40(2)	C(14)-C(15)	1.45(2)
C(21)-C(22)	1.41(2)	C(21)-C(25)	1.44(2)
C(22)-C(23)	1.44(2)	C(23)-C(24)	1.37(2)
C(24)-C(25)	1.37(2)	C(31)-C(36)	1.37(2)
C(31)-C(32)	1.38(2)	C(32)-C(33)	1.40(2)
C(33)-C(34)	1.36(2)	C(34)-C(35)	1.35(2)
C(35)-C(36)	1.41(2)	C(41)-C(42)	1.39(2)
C(41)-C(46)	1.39(2)	C(42)-C(43)	1.39(2)
C(43)-C(44)	1.38(2)	C(44)-C(45)	1.37(2)
C(45)-C(46)	1.39(2)	C(51)-C(52)	1.39(2)
C(51)-C(56)	1.39(2)	C(52)-C(53)	1.38(2)
C(53)-C(54)	1.36(2)	C(54)-C(55)	1.35(2)
C(55)-C(56)	1.40(2)	C(61)-C(62)	1.39(2)
C(61)-C(66)	1.41(2)	C(62)-C(63)	1.39(2)
C(63)-C(64)	1.35(2)	C(64)-C(65)	1.36(2)
C(65)-C(66)	1.37(2)	C(71)-C(72)	1.39(2)
C(71)-C(76)	1.39(2)	C(72)-F(1)	1.34(2)
C(72)-C(73)	1.37(2)	C(73)-F(2)	1.33(2)
C(73)-C(74)	1.36(2)	C(74)-C(75)	1.37(2)
C(74)-F(3)	1.38(2)	C(75)-F(4)	1.34(2)
C(75)-C(76)	1.37(2)	C(76)-F(5)	1.32(2)
C(81)-C(86)	1.39(2)	C(81)-C(82)	1.41(2)
C(82)-F(6)	1.34(2)	C(82)-C(83)	1.37(2)
C(83)-C(84)	1.27(2)	C(83)-F(7)	1.38(2)

C(84)-C(85)	1.28(2)	C(84)-F(8)	1.42(2)
C(85)-F(9)	1.37(2)	C(85)-C(86)	1.39(2)
C(86)-F(10)	1.31(2)	C(91)-C(92)	1.39(2)
C(91)-C(96)	1.40(2)	C(92)-F(11)	1.337(13)
C(92)-C(93)	1.35(2)	C(93)-F(12)	1.338(14)
C(93)-C(94)	1.40(2)	C(94)-F(13)	1.33(2)
C(94)-C(95)	1.44(2)	C(95)-F(14)	1.321(14)
C(95)-C(96)	1.34(2)	C(96)-F(15)	1.319(13)

P(1)-Au(1)-S	175.98(14)	P(1)-Au(1)-Au(2)	124.47(10)
S-Au(1)-Au(2)	51.97(9)	P(2)-Au(2)-S	171.72(12)
P(2)-Au(2)-Au(1)	120.84(9)	S-Au(2)-Au(1)	51.67(8)
C(71)-Au(3)-C(81)	93.1(5)	C(71)-Au(3)-C(91)	87.1(5)
C(81)-Au(3)-C(91)	179.5(4)	C(71)-Au(3)-S	176.0(3)
C(81)-Au(3)-S	87.2(4)	C(91)-Au(3)-S	92.6(4)
C(12)-Fe-C(25)	146.2(6)	C(12)-Fe-C(23)	108.1(6)
C(25)-Fe-C(23)	65.8(6)	C(12)-Fe-C(21)	170.2(6)
C(25)-Fe-C(21)	41.5(5)	C(23)-Fe-C(21)	67.9(6)
C(12)-Fe-C(22)	130.8(6)	C(25)-Fe-C(22)	68.1(6)
C(23)-Fe-C(22)	41.4(5)	C(21)-Fe-C(22)	40.4(5)
C(12)-Fe-C(24)	114.5(6)	C(25)-Fe-C(24)	39.2(6)
C(23)-Fe-C(24)	39.2(6)	C(21)-Fe-C(24)	68.5(6)
C(22)-Fe-C(24)	68.7(6)	C(12)-Fe-C(14)	67.5(6)
C(25)-Fe-C(14)	107.6(6)	C(23)-Fe-C(14)	162.2(6)
C(21)-Fe-C(14)	119.0(6)	C(22)-Fe-C(14)	153.8(5)
C(24)-Fe-C(14)	125.3(6)	C(12)-Fe-C(13)	39.7(6)
C(25)-Fe-C(13)	114.7(6)	C(23)-Fe-C(13)	126.0(6)
C(21)-Fe-C(13)	149.9(6)	C(22)-Fe-C(13)	166.2(6)
C(24)-Fe-C(13)	104.5(6)	C(14)-Fe-C(13)	39.8(5)
C(12)-Fe-C(15)	68.5(5)	C(25)-Fe-C(15)	131.0(6)
C(23)-Fe-C(15)	155.2(6)	C(21)-Fe-C(15)	111.1(5)
C(22)-Fe-C(15)	121.2(5)	C(24)-Fe-C(15)	165.4(6)
C(14)-Fe-C(15)	41.2(5)	C(13)-Fe-C(15)	68.1(6)
C(12)-Fe-C(11)	41.9(5)	C(25)-Fe-C(11)	170.0(6)
C(23)-Fe-C(11)	120.7(6)	C(21)-Fe-C(11)	131.5(5)
C(22)-Fe-C(11)	111.1(6)	C(24)-Fe-C(11)	150.6(6)
C(14)-Fe-C(11)	68.5(6)	C(13)-Fe-C(11)	68.6(6)
C(15)-Fe-C(11)	40.1(5)	Au(1)-S-Au(2)	76.36(10)
Au(1)-S-Au(3)	92.64(12)	Au(2)-S-Au(3)	105.69(14)
C(11)-P(1)-C(51)	107.2(6)	C(11)-P(1)-C(61)	105.0(6)
C(51)-P(1)-C(61)	104.6(6)	C(11)-P(1)-Au(1)	111.0(5)
C(51)-P(1)-Au(1)	116.1(4)	C(61)-P(1)-Au(1)	112.1(4)

C(21)-P(2)-C(31)	106.1(6)	C(21)-P(2)-C(41)	107.8(6)
C(31)-P(2)-C(41)	105.0(7)	C(21)-P(2)-Au(2)	110.2(5)
C(31)-P(2)-Au(2)	114.8(5)	C(41)-P(2)-Au(2)	112.5(4)
C(15)-C(11)-C(12)	105.8(12)	C(15)-C(11)-P(1)	124.1(10)
C(12)-C(11)-P(1)	130.1(11)	C(15)-C(11)-Fe	69.7(8)
C(12)-C(11)-Fe	67.4(7)	P(1)-C(11)-Fe	127.2(7)
C(13)-C(12)-C(11)	109.1(13)	C(13)-C(12)-Fe	71.3(8)
C(11)-C(12)-Fe	70.6(7)	C(12)-C(13)-C(14)	108.8(14)
C(12)-C(13)-Fe	68.9(8)	C(14)-C(13)-Fe	69.9(8)
C(13)-C(14)-C(15)	108.3(14)	C(13)-C(14)-Fe	70.3(9)
C(15)-C(14)-Fe	69.9(8)	C(11)-C(15)-C(14)	108.0(12)
C(11)-C(15)-Fe	70.2(8)	C(14)-C(15)-Fe	68.9(8)
C(22)-C(21)-C(25)	106.5(12)	C(22)-C(21)-P(2)	124.2(10)
C(25)-C(21)-P(2)	129.2(11)	C(22)-C(21)-Fe	70.0(7)
C(25)-C(21)-Fe	69.3(8)	P(2)-C(21)-Fe	127.5(7)
C(21)-C(22)-C(23)	105.8(13)	C(21)-C(22)-Fe	69.6(8)
C(23)-C(22)-Fe	69.0(8)	C(24)-C(23)-C(22)	110(2)
C(24)-C(23)-Fe	71.0(10)	C(22)-C(23)-Fe	69.5(8)
C(25)-C(24)-C(23)	108(2)	C(25)-C(24)-Fe	69.8(9)
C(23)-C(24)-Fe	69.8(9)	C(24)-C(25)-C(21)	109.9(14)
C(24)-C(25)-Fe	71.0(9)	C(21)-C(25)-Fe	69.3(8)
C(36)-C(31)-C(32)	120.3(14)	C(36)-C(31)-P(2)	122.9(10)
C(32)-C(31)-P(2)	116.7(10)	C(31)-C(32)-C(33)	118.7(14)
C(34)-C(33)-C(32)	121(2)	C(35)-C(34)-C(33)	120(2)
C(34)-C(35)-C(36)	120(2)	C(31)-C(36)-C(35)	119.7(14)
C(42)-C(41)-C(46)	119(2)	C(42)-C(41)-P(2)	118.9(11)
C(46)-C(41)-P(2)	122.0(11)	C(41)-C(42)-C(43)	120.8(14)
C(44)-C(43)-C(42)	119(2)	C(45)-C(44)-C(43)	122(2)
C(44)-C(45)-C(46)	120(2)	C(41)-C(46)-C(45)	120(2)
C(52)-C(51)-C(56)	119.8(14)	C(52)-C(51)-P(1)	119.7(10)
C(56)-C(51)-P(1)	120.4(10)	C(53)-C(52)-C(51)	119.5(14)
C(54)-C(53)-C(52)	120(2)	C(55)-C(54)-C(53)	121(2)
C(54)-C(55)-C(56)	120(2)	C(51)-C(56)-C(55)	119.0(13)
C(62)-C(61)-C(66)	118.3(13)	C(62)-C(61)-P(1)	121.2(10)
C(66)-C(61)-P(1)	120.4(10)	C(63)-C(62)-C(61)	118.9(13)
C(64)-C(63)-C(62)	121.8(14)	C(63)-C(64)-C(65)	120(2)
C(64)-C(65)-C(66)	121(2)	C(65)-C(66)-C(61)	120.3(14)
C(72)-C(71)-C(76)	115(2)	C(72)-C(71)-Au(3)	120.4(10)
C(76)-C(71)-Au(3)	124.4(10)	F(1)-C(72)-C(73)	118.0(13)
F(1)-C(72)-C(71)	118.6(13)	C(73)-C(72)-C(71)	123(2)
F(2)-C(73)-C(74)	120(2)	F(2)-C(73)-C(72)	121.6(14)
C(74)-C(73)-C(72)	118(2)	C(73)-C(74)-C(75)	122(2)

C(73)-C(74)-F(3)	120.3(13)	C(75)-C(74)-F(3)	117.8(13)
F(4)-C(75)-C(74)	120(2)	F(4)-C(75)-C(76)	121(2)
C(74)-C(75)-C(76)	118(2)	F(5)-C(76)-C(75)	118.1(14)
F(5)-C(76)-C(71)	118.9(14)	C(75)-C(76)-C(71)	123(2)
C(86)-C(81)-C(82)	114(2)	C(86)-C(81)-Au(3)	121.8(10)
C(82)-C(81)-Au(3)	124.5(9)	F(6)-C(82)-C(83)	122(2)
F(6)-C(82)-C(81)	116.8(13)	C(83)-C(82)-C(81)	121(2)
C(84)-C(83)-C(82)	120(2)	C(84)-C(83)-F(7)	124(2)
C(82)-C(83)-F(7)	116(2)	C(83)-C(84)-C(85)	124(2)
C(83)-C(84)-F(8)	118(2)	C(85)-C(84)-F(8)	117(2)
C(84)-C(85)-F(9)	125(2)	C(84)-C(85)-C(86)	119(2)
F(9)-C(85)-C(86)	116(2)	F(10)-C(86)-C(85)	120(2)
F(10)-C(86)-C(81)	118.3(13)	C(85)-C(86)-C(81)	122(2)
C(92)-C(91)-C(96)	116.6(13)	C(92)-C(91)-Au(3)	122.9(8)
C(96)-C(91)-Au(3)	120.4(8)	F(11)-C(92)-C(93)	117.6(12)
F(11)-C(92)-C(91)	119.6(11)	C(93)-C(92)-C(91)	122.8(12)
F(12)-C(93)-C(92)	121.6(13)	F(12)-C(93)-C(94)	117.7(12)
C(92)-C(93)-C(94)	120.6(13)	F(13)-C(94)-C(93)	122.7(11)
F(13)-C(94)-C(95)	120.1(10)	C(93)-C(94)-C(95)	117(2)
F(14)-C(95)-C(96)	123.4(12)	F(14)-C(95)-C(94)	116.7(11)
C(96)-C(95)-C(94)	119.9(13)	F(15)-C(96)-C(95)	117.5(12)
F(15)-C(96)-C(91)	119.7(11)	C(95)-C(96)-C(91)	122.8(12)

Table 5. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Au(1)	29(1)	27(1)	29(1)	5(1)	5(1)	2(1)
Au(2)	26(1)	28(1)	27(1)	2(1)	5(1)	1(1)
Au(3)	34(1)	31(1)	30(1)	4(1)	12(1)	3(1)
Fe	31(1)	29(1)	30(1)	4(1)	1(1)	-3(1)
S	29(2)	34(2)	22(2)	9(2)	3(2)	7(2)
P(1)	32(2)	25(2)	30(2)	4(2)	3(2)	3(2)
P(2)	26(2)	24(2)	33(2)	1(2)	3(2)	2(2)
F(1)	50(6)	82(7)	65(7)	33(6)	9(5)	5(6)
F(2)	94(9)	91(8)	115(10)	53(7)	73(8)	26(7)
F(3)	69(8)	70(8)	196(14)	16(8)	83(9)	-4(6)
F(4)	50(8)	206(15)	103(10)	6(10)	22(7)	-11(9)
F(5)	42(6)	177(13)	80(8)	40(8)	24(6)	17(8)
F(6)	97(8)	90(8)	64(7)	14(6)	34(6)	56(7)
F(7)	233(17)	68(8)	144(12)	55(8)	131(12)	96(10)
F(8)	234(18)	54(7)	204(15)	-61(9)	157(14)	-45(9)
F(9)	107(11)	147(13)	152(13)	-83(11)	10(10)	-26(10)
F(10)	94(9)	104(9)	66(7)	-37(7)	-11(7)	7(8)
F(11)	64(7)	61(6)	41(5)	11(5)	-19(5)	15(5)
F(12)	95(9)	105(9)	60(7)	-30(7)	-33(6)	4(7)
F(13)	94(8)	52(6)	74(7)	-43(5)	0(6)	-1(6)
F(14)	66(7)	50(6)	82(7)	-18(5)	-14(6)	21(5)
F(15)	64(6)	56(6)	31(5)	-17(4)	-26(4)	17(5)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(12)	4981(8)	3979(7)	-426(8)	39
H(13)	5858(9)	3702(8)	-1278(9)	51
H(14)	7123(9)	3267(8)	-460(8)	47
H(15)	7066(8)	3335(7)	955(8)	37
H(22)	5308(8)	1968(7)	936(8)	41
H(23)	4346(10)	2333(8)	-313(9)	58
H(24)	4952(9)	2186(8)	-1409(10)	58
H(25)	6265(9)	1692(8)	-905(8)	49
H(32)	7780(9)	255(7)	1694(8)	57
H(33)	7844(9)	-997(8)	1517(9)	66
H(34)	6958(9)	-1568(9)	548(8)	64
H(35)	6047(10)	-911(8)	-309(10)	78
H(36)	5999(8)	352(7)	-184(8)	46
H(42)	8089(8)	2431(7)	1398(8)	53
H(43)	9196(9)	2811(9)	1020(10)	70
H(44)	9496(11)	2276(9)	-45(9)	80
H(45)	8710(10)	1406(10)	-751(10)	81
H(46)	7617(9)	1010(8)	-368(9)	60
H(52)	4540(8)	2777(8)	1605(8)	57
H(53)	3199(9)	2691(9)	1284(9)	73
H(54)	2461(11)	3600(7)	601(9)	69
H(55)	3014(8)	4651(8)	330(9)	59
H(56)	4365(8)	4773(7)	649(8)	46
H(62)	6543(7)	4982(6)	938(7)	32
H(63)	6789(9)	6185(7)	1290(8)	55
H(64)	6242(8)	6723(8)	2182(8)	51
H(65)	5465(9)	6062(7)	2780(8)	54
H(66)	5169(9)	4876(8)	2442(9)	57

Table 1. Crystal data and structure refinement for 2.

Identification code	ogott
Empirical formula	$C_{84}H_{62}Au_5Cl_6F_{13}Fe_2O_3P_4S$
Formula weight	2895.63
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 18.214(3) Å α = 90° b = 22.444(3) Å β = 105.611(12)° c = 24.081(3) Å γ = 90°
Volume	9481(2) $Å^3$
Z	4
Density (calculated)	2.029 Mg/m^3
Absorption coefficient	8.377 mm^{-1}
F(000)	5456
Crystal size	0.60 x 0.30 x 0.20 mm
θ range for data collection	3.10 to 22.50°
Index ranges	$0 \le h \le 19$, $0 \le k \le 24$, $-25 \le \ell \le 24$
Reflections collected	12707
Independent reflections	12260 (R_{int} = 0.0415)
Absorption correction	Psi-scans
Max. and min. transmission	0.918 and 0.510
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12249 / 242 / 525
Goodness-of-fit on F^2	0.899
Final R indices [$I>2\sigma(I)$]	R1 = 0.0446, wR2 = 0.1015
R indices (all data)	R1 = 0.0834, wR2 = 0.1188
Largest diff. peak and hole	2.057 and -1.247 $eÅ^{-3}$

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

	x	y	z	U(eq)
Au(1)	4597(1)	4360(1)	1064(1)	24(1)
Au(2)	5953(1)	4368(1)	2041(1)	24(1)
Au(3)	3954(1)	3115(1)	754(1)	26(1)
Au(4)	3609(1)	2289(1)	1604(1)	26(1)
Au(5)	5567(1)	2973(1)	1827(1)	24(1)
Fe(1)	4386(1)	5672(1)	2312(1)	25(1)
Fe(2)	2829(1)	1519(1)	-75(1)	26(1)
P(1)	3560(2)	4929(2)	1032(2)	26(1)
P(2)	6095(2)	4973(2)	2803(2)	25(1)
P(3)	3647(2)	2886(2)	-191(2)	27(1)
P(4)	2950(2)	1434(2)	1354(2)	26(1)
S(1)	5722(2)	3782(2)	1218(2)	26(1)
S(2)	4264(2)	3186(2)	1768(2)	27(1)
C(11)	3583(6)	5166(4)	1748(3)	21(3)
C(12)	3900(5)	4834(3)	2258(4)	24(3)
C(13)	3766(6)	5154(4)	2730(3)	32(4)
C(14)	3364(6)	5683(4)	2511(4)	37(4)
C(15)	3252(6)	5691(4)	1904(4)	34(4)
C(16)	5552(5)	5646(3)	2581(4)	25(3)
C(17)	5265(6)	6038(4)	2935(3)	26(4)
C(18)	4847(6)	6496(4)	2579(4)	30(4)
C(19)	4877(6)	6386(4)	2005(3)	30(4)
C(20)	5312(6)	5861(4)	2006(3)	33(4)
C(21)	3417(6)	5594(3)	600(4)	33(4)
C(22)	2723(5)	5892(4)	470(4)	42(4)
C(23)	2650(5)	6442(4)	195(5)	49(5)
C(24)	3271(6)	6694(3)	51(4)	49(5)
C(25)	3965(5)	6396(4)	182(4)	38(4)
C(26)	4039(5)	5846(4)	456(4)	38(4)
C(31)	2706(5)	4493(4)	780(4)	27(4)
C(32)	2396(6)	4407(4)	191(4)	44(4)
C(33)	1790(6)	4016(5)	-4(3)	54(5)
C(34)	1494(5)	3711(4)	390(5)	52(5)
C(35)	1804(6)	3797(4)	978(4)	46(5)
C(36)	2410(6)	4188(4)	1173(3)	42(4)
C(41)	5775(5)	4661(4)	3395(3)	24(3)
C(42)	5278(5)	4179(4)	3284(3)	28(4)
C(43)	4968(5)	3964(3)	3713(4)	32(4)
C(44)	5156(5)	4232(4)	4254(3)	39(4)
C(45)	5653(6)	4714(4)	4365(3)	36(4)
C(46)	5963(5)	4928(3)	3936(4)	33(4)
C(51)	7076(5)	5198(4)	3133(4)	29(4)
C(52)	7623(6)	4751(3)	3216(4)	45(4)
C(53)	8382(5)	4882(4)	3480(5)	55(5)
C(54)	8595(5)	5460(5)	3660(5)	53(5)
C(55)	8049(6)	5907(4)	3577(5)	60(5)
C(56)	7289(6)	5776(4)	3313(5)	45(4)
C(61)	2858(5)	2368(4)	-370(4)	24(3)
C(62)	2297(6)	2324(4)	-61(3)	27(4)
C(63)	1758(5)	1886(4)	-336(4)	39(4)
C(64)	1986(6)	1660(4)	-814(4)	47(5)
C(65)	2666(6)	1958(4)	-835(4)	36(4)

C(66)	3144(5)	1128(4)	716(3)	26(3)
C(67)	3798(5)	1293(4)	538(4)	23(3)
C(68)	3773(5)	986(4)	17(4)	35(4)
C(69)	3103(6)	630(4)	-126(3)	34(4)
C(70)	2715(5)	718(4)	306(4)	28(4)
C(71)	3362(6)	3510(4)	-681(4)	33(4)
C(72)	2793(6)	3467(4)	-1196(5)	55(5)
C(73)	2623(6)	3954(5)	-1565(4)	69(6)
C(74)	3022(7)	4484(4)	-1418(4)	68(6)
C(75)	3590(6)	4528(4)	-903(5)	53(5)
C(76)	3760(5)	4041(4)	-534(4)	35(4)
C(81)	4428(5)	2545(4)	-412(4)	29(4)
C(82)	4446(5)	2554(4)	-985(3)	34(4)
C(83)	5027(6)	2262(4)	-1150(3)	39(4)
C(84)	5589(5)	1960(4)	-741(4)	46(5)
C(85)	5571(5)	1951(4)	-168(4)	33(4)
C(86)	4990(5)	2243(4)	-3(3)	33(4)
C(91)	1923(4)	1524(4)	1185(4)	27(4)
C(92)	1640(5)	2098(3)	1194(4)	37(4)
C(93)	858(6)	2197(3)	1029(5)	53(5)
C(94)	359(4)	1722(4)	856(5)	52(5)
C(95)	642(5)	1148(4)	847(4)	37(4)
C(96)	1424(5)	1049(3)	1012(4)	38(4)
C(101)	3197(6)	866(4)	1914(4)	28(4)
C(102)	3051(6)	265(4)	1793(3)	49(5)
C(103)	3228(7)	-152(3)	2236(5)	48(5)
C(104)	3551(7)	32(4)	2800(4)	61(5)
C(105)	3698(6)	633(5)	2921(3)	50(5)
C(106)	3520(6)	1050(3)	2478(4)	40(4)
C(111)	6708(8)	2823(5)	1930(4)	24(3)
C(112)	7245(7)	3019(5)	2417(6)	30(4)
C(113)	8007(8)	2945(6)	2484(6)	47(5)
C(114)	8273(11)	2669(7)	2075(5)	57(5)
C(115)	7751(8)	2467(7)	1595(6)	39(4)
C(116)	6981(7)	2540(6)	1528(6)	26(4)
F(1)	7014(5)	3296(4)	2839(3)	50(3)
F(2)	8518(6)	3174(5)	2959(4)	78(4)
F(3)	9012(6)	2601(5)	2145(5)	81(4)
F(4)	8000(6)	2212(5)	1173(5)	75(3)
F(5)	6499(5)	2362(4)	1028(4)	48(3)
C(121)	5553(8)	2248(6)	2350(5)	31(4)
C(122)	5645(7)	2302(6)	2928(6)	31(4)
C(123)	5671(8)	1818(6)	3283(6)	40(4)
C(124)	5570(9)	1261(6)	3049(5)	38(4)
C(125)	5461(9)	1193(6)	2477(6)	36(4)
C(126)	5466(9)	1682(6)	2129(6)	34(4)
F(6)	5703(6)	2851(3)	3173(3)	49(3)
F(7)	5792(6)	1879(4)	3855(4)	56(3)
F(8)	5593(6)	787(4)	3390(4)	65(3)
F(9)	5369(6)	645(4)	2233(4)	62(3)
F(10)	5357(5)	1595(3)	1561(4)	41(2)
S(3)	3009(3)	3985(2)	4317(2)	49(1)
O(1)	3314(7)	4571(4)	4440(5)	60(4)
O(2)	3501(6)	3554(5)	4188(6)	66(4)
O(3)	2234(6)	3963(5)	3947(5)	67(4)
C(1)	2842(9)	3730(7)	4972(9)	67(6)
F(11)	2563(7)	3192(5)	4938(5)	93(4)
F(12)	3483(6)	3726(4)	5412(5)	82(4)
F(13)	2363(7)	4086(6)	5147(5)	107(5)
C(2)	4305(13)	9691(9)	1112(9)	79(7)
Cl(1)	4785(4)	9285(3)	1703(3)	96(2)
Cl(2)	4674(3)	9638(2)	527(3)	78(2)
C(3)	9339(18)	2606(13)	9335(12)	139(11)

Cl(3)	8964(6)	2847(7)	8652(6)	308(10)
Cl(4)	9409(5)	3109(6)	9856(7)	277(8)
C(4)	2183(15)	2999(11)	3022(11)	103(8)
Cl(5)	2659(8)	3223(6)	2509(6)	132(3)
Cl(6)	1918(8)	2286(6)	2871(6)	132(3)
Cl(5′)	1227(13)	3088(9)	2525(9)	132(3)
Cl(6′)	1851(13)	2340(10)	3439(10)	132(3)

Table 3. Selected bond lengths [Å] and angles [°] for 2.

Au(1)-P(1)	2.266(4)	Au(1)-S(1)	2.368(4)
Au(1)-Au(2)	2.9158(9)	Au(1)-Au(3)	3.0436(8)
Au(2)-P(2)	2.243(4)	Au(2)-S(1)	2.321(4)
Au(2)-Au(5)	3.2195(8)	Au(3)-P(3)	2.252(4)
Au(3)-S(2)	2.360(4)	Au(3)-Au(4)	2.9511(9)
Au(3)-Au(5)	3.3661(10)	Au(4)-P(4)	2.258(4)
Au(4)-S(2)	2.319(4)	Au(5)-C(111)	2.053(14)
Au(5)-C(121)	2.062(14)	Au(5)-S(2)	2.387(4)
Au(5)-S(1)	2.397(4)		

P(1)-Au(1)-S(1)	173.20(14)	P(1)-Au(1)-Au(2)	122.78(10)
S(1)-Au(1)-Au(2)	50.83(9)	P(1)-Au(1)-Au(3)	104.31(10)
S(1)-Au(1)-Au(3)	78.19(9)	Au(2)-Au(1)-Au(3)	113.00(2)
P(2)-Au(2)-S(1)	175.62(14)	P(2)-Au(2)-Au(1)	123.39(10)
S(1)-Au(2)-Au(1)	52.27(10)	P(2)-Au(2)-Au(5)	133.77(10)
S(1)-Au(2)-Au(5)	47.97(9)	Au(1)-Au(2)-Au(5)	76.33(2)
P(3)-Au(3)-S(2)	170.70(13)	P(3)-Au(3)-Au(4)	121.13(10)
S(2)-Au(3)-Au(4)	50.29(9)	P(3)-Au(3)-Au(1)	115.57(10)
S(2)-Au(3)-Au(1)	73.40(9)	Au(4)-Au(3)-Au(1)	123.06(3)
P(3)-Au(3)-Au(5)	133.03(11)	S(2)-Au(3)-Au(5)	45.17(10)
Au(4)-Au(3)-Au(5)	73.32(2)	Au(1)-Au(3)-Au(5)	72.49(2)
P(4)-Au(4)-S(2)	174.55(13)	P(4)-Au(4)-Au(3)	123.05(10)
S(2)-Au(4)-Au(3)	51.51(9)	C(111)-Au(5)-C(121)	88.6(5)
C(111)-Au(5)-S(2)	176.1(3)	C(121)-Au(5)-S(2)	91.1(4)
C(111)-Au(5)-S(1)	85.2(3)	C(121)-Au(5)-S(1)	173.7(4)
S(2)-Au(5)-S(1)	95.19(13)	C(111)-Au(5)-Au(2)	88.3(3)
C(121)-Au(5)-Au(2)	135.1(3)	S(2)-Au(5)-Au(2)	89.17(8)
S(1)-Au(5)-Au(2)	45.99(9)	C(111)-Au(5)-Au(3)	139.0(3)
C(121)-Au(5)-Au(3)	113.1(4)	S(2)-Au(5)-Au(3)	44.51(9)
S(1)-Au(5)-Au(3)	71.36(9)	Au(2)-Au(5)-Au(3)	97.97(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [Å] and angles [°] for 2.

Au(1)-P(1)	2.266(4)	Au(1)-S(1)	2.368(4)
Au(1)-Au(2)	2.9158(9)	Au(1)-Au(3)	3.0436(8)
Au(2)-P(2)	2.243(4)	Au(2)-S(1)	2.321(4)
Au(2)-Au(5)	3.2195(8)	Au(3)-P(3)	2.252(4)
Au(3)-S(2)	2.360(4)	Au(3)-Au(4)	2.9511(9)
Au(3)-Au(5)	3.3661(10)	Au(4)-P(4)	2.258(4)
Au(4)-S(2)	2.319(4)	Au(5)-C(111)	2.053(14)
Au(5)-C(121)	2.062(14)	Au(5)-S(2)	2.387(4)
Au(5)-S(1)	2.397(4)	P(1)-C(11)	1.792(8)
P(1)-C(21)	1.797(7)	P(1)-C(31)	1.798(8)
P(2)-C(16)	1.806(7)	P(2)-C(41)	1.819(8)
P(2)-C(51)	1.820(8)	P(3)-C(61)	1.808(8)
P(3)-C(81)	1.816(8)	P(3)-C(71)	1.813(8)
P(4)-C(66)	1.803(8)	P(4)-C(91)	1.815(8)
P(4)-C(101)	1.823(8)	C(11)-C(12)	1.42
C(11)-C(15)	1.42	C(12)-C(13)	1.42
C(13)-C(14)	1.42	C(14)-C(15)	1.42
C(16)-C(17)	1.42	C(16)-C(20)	1.42
C(17)-C(18)	1.42	C(18)-C(19)	1.42
C(19)-C(20)	1.42	C(21)-C(22)	1.39
C(21)-C(26)	1.39	C(22)-C(23)	1.39
C(23)-C(24)	1.39	C(24)-C(25)	1.39
C(25)-C(26)	1.39	C(31)-C(32)	1.39
C(31)-C(36)	1.39	C(32)-C(33)	1.39
C(33)-C(34)	1.39	C(34)-C(35)	1.39
C(35)-C(36)	1.39	C(41)-C(42)	1.39
C(41)-C(46)	1.39	C(42)-C(43)	1.39
C(43)-C(44)	1.39	C(44)-C(45)	1.39
C(45)-C(46)	1.39	C(51)-C(52)	1.39
C(51)-C(56)	1.39	C(52)-C(53)	1.39
C(53)-C(54)	1.39	C(54)-C(55)	1.39
C(55)-C(56)	1.39	C(61)-C(65)	1.42
C(61)-C(62)	1.42	C(62)-C(63)	1.42
C(63)-C(64)	1.42	C(64)-C(65)	1.42
C(66)-C(67)	1.42	C(66)-C(70)	1.42
C(67)-C(68)	1.42	C(68)-C(69)	1.42
C(69)-C(70)	1.42	C(71)-C(72)	1.39
C(71)-C(76)	1.39	C(72)-C(73)	1.39

C(73)-C(74)	1.39	C(74)-C(75)	1.39
C(75)-C(76)	1.39	C(81)-C(82)	1.39
C(81)-C(86)	1.39	C(82)-C(83)	1.39
C(83)-C(84)	1.39	C(84)-C(85)	1.39
C(85)-C(86)	1.39	C(91)-C(92)	1.39
C(91)-C(96)	1.39	C(92)-C(93)	1.39
C(93)-C(94)	1.39	C(94)-C(95)	1.39
C(95)-C(96)	1.39	C(101)-C(102)	1.39
C(101)-C(106)	1.39	C(102)-C(103)	1.39
C(103)-C(104)	1.39	C(104)-C(105)	1.39
C(105)-C(106)	1.39	C(111)-C(116)	1.36(2)
C(111)-C(112)	1.38(2)	C(112)-F(1)	1.349(14)
C(112)-C(113)	1.36(2)	C(113)-C(114)	1.36(2)
C(113)-F(2)	1.37(2)	C(114)-F(3)	1.32(2)
C(114)-C(115)	1.36(2)	C(115)-F(4)	1.35(2)
C(115)-C(116)	1.38(2)	C(116)-F(5)	1.346(13)
C(121)-C(122)	1.36(2)	C(121)-C(126)	1.37(2)
C(122)-F(6)	1.357(14)	C(122)-C(123)	1.37(2)
C(123)-F(7)	1.34(2)	C(123)-C(124)	1.36(2)
C(124)-F(8)	1.34(2)	C(124)-C(125)	1.35(2)
C(125)-F(9)	1.354(14)	C(125)-C(126)	1.38(2)
C(126)-F(10)	1.342(14)	S(3)-O(2)	1.411(10)
S(3)-O(1)	1.428(10)	S(3)-O(3)	1.453(10)
S(3)-C(1)	1.78(2)	C(1)-F(11)	1.30(2)
C(1)-F(13)	1.33(2)	C(1)-F(12)	1.35(2)
C(2)-Cl(1)	1.72(2)	C(2)-Cl(2)	1.72(2)
C(3)-Cl(4)	1.67(3)	C(3)-Cl(3)	1.69(3)
C(4)-Cl(6)	1.68(3)	C(4)-Cl(5)	1.76(3)
C(4)-Cl(5')	1.84(3)	C(4)-Cl(6')	1.97(3)

P(1)-Au(1)-S(1)	173.20(14)	P(1)-Au(1)-Au(2)	122.78(10)
S(1)-Au(1)-Au(2)	50.83(9)	P(1)-Au(1)-Au(3)	104.31(10)
S(1)-Au(1)-Au(3)	78.19(9)	Au(2)-Au(1)-Au(3)	113.00(2)
P(2)-Au(2)-S(1)	175.62(14)	P(2)-Au(2)-Au(1)	123.39(10)
S(1)-Au(2)-Au(1)	52.27(10)	P(2)-Au(2)-Au(5)	133.77(10)
S(1)-Au(2)-Au(5)	47.97(9)	Au(1)-Au(2)-Au(5)	76.33(2)
P(3)-Au(3)-S(2)	170.70(13)	P(3)-Au(3)-Au(4)	121.13(10)
S(2)-Au(3)-Au(4)	50.29(9)	P(3)-Au(3)-Au(1)	115.57(10)
S(2)-Au(3)-Au(1)	73.40(9)	Au(4)-Au(3)-Au(1)	123.06(3)
P(3)-Au(3)-Au(5)	133.03(11)	S(2)-Au(3)-Au(5)	45.17(10)
Au(4)-Au(3)-Au(5)	73.32(2)	Au(1)-Au(3)-Au(5)	72.49(2)
P(4)-Au(4)-S(2)	174.55(13)	P(4)-Au(4)-Au(3)	123.05(10)

S(2)-Au(4)-Au(3)	51.51(9)	C(111)-Au(5)-C(121)	88.6(5)
C(111)-Au(5)-S(2)	176.1(3)	C(121)-Au(5)-S(2)	91.1(4)
C(111)-Au(5)-S(1)	85.2(3)	C(121)-Au(5)-S(1)	173.7(4)
S(2)-Au(5)-S(1)	95.19(13)	C(111)-Au(5)-Au(2)	88.3(3)
C(121)-Au(5)-Au(2)	135.1(3)	S(2)-Au(5)-Au(2)	89.17(8)
S(1)-Au(5)-Au(2)	45.99(9)	C(111)-Au(5)-Au(3)	139.0(3)
C(121)-Au(5)-Au(3)	113.1(4)	S(2)-Au(5)-Au(3)	44.51(9)
S(1)-Au(5)-Au(3)	71.36(9)	Au(2)-Au(5)-Au(3)	97.97(2)
C(11)-P(1)-C(21)	105.8(5)	C(11)-P(1)-C(31)	106.3(5)
C(21)-P(1)-C(31)	106.2(5)	C(11)-P(1)-Au(1)	109.3(4)
C(21)-P(1)-Au(1)	118.5(4)	C(31)-P(1)-Au(1)	110.0(4)
C(16)-P(2)-C(41)	106.9(5)	C(16)-P(2)-C(51)	107.0(5)
C(41)-P(2)-C(51)	104.4(5)	C(16)-P(2)-Au(2)	109.3(3)
C(41)-P(2)-Au(2)	114.7(3)	C(51)-P(2)-Au(2)	114.1(4)
C(61)-P(3)-C(81)	107.1(5)	C(61)-P(3)-C(71)	105.8(5)
C(81)-P(3)-C(71)	104.3(5)	C(61)-P(3)-Au(3)	110.6(4)
C(81)-P(3)-Au(3)	113.0(3)	C(71)-P(3)-Au(3)	115.5(4)
C(66)-P(4)-C(91)	106.1(5)	C(66)-P(4)-C(101)	107.3(5)
C(91)-P(4)-C(101)	106.1(5)	C(66)-P(4)-Au(4)	109.9(3)
C(91)-P(4)-Au(4)	114.0(3)	C(101)-P(4)-Au(4)	112.9(3)
Au(2)-S(1)-Au(1)	76.89(11)	Au(2)-S(1)-Au(5)	86.04(12)
Au(1)-S(1)-Au(5)	105.7(2)	Au(4)-S(2)-Au(3)	78.20(11)
Au(4)-S(2)-Au(5)	107.11(14)	Au(3)-S(2)-Au(5)	90.32(14)
C(12)-C(11)-C(15)	108.0	C(12)-C(11)-P(1)	125.1(5)
C(15)-C(11)-P(1)	126.8(6)	C(11)-C(12)-C(13)	108.0
C(12)-C(13)-C(14)	108.0	C(15)-C(14)-C(13)	108.0
C(14)-C(15)-C(11)	108.0	C(17)-C(16)-C(20)	108.0
C(17)-C(16)-P(2)	126.9(6)	C(20)-C(16)-P(2)	125.0(6)
C(16)-C(17)-C(18)	108.0	C(19)-C(18)-C(17)	108.0
C(20)-C(19)-C(18)	108.0	C(19)-C(20)-C(16)	108.0
C(22)-C(21)-C(26)	120.0	C(22)-C(21)-P(1)	120.7(6)
C(26)-C(21)-P(1)	118.9(6)	C(23)-C(22)-C(21)	120.0
C(22)-C(23)-C(24)	120.0	C(23)-C(24)-C(25)	120.0
C(24)-C(25)-C(26)	120.0	C(25)-C(26)-C(21)	120.0
C(32)-C(31)-C(36)	120.0	C(32)-C(31)-P(1)	119.8(6)
C(36)-C(31)-P(1)	119.7(6)	C(31)-C(32)-C(33)	120.0
C(34)-C(33)-C(32)	120.0	C(35)-C(34)-C(33)	120.0
C(36)-C(35)-C(34)	120.0	C(35)-C(36)-C(31)	120.0
C(42)-C(41)-C(46)	120.0	C(42)-C(41)-P(2)	118.6(5)
C(46)-C(41)-P(2)	121.1(5)	C(43)-C(42)-C(41)	120.0
C(44)-C(43)-C(42)	120.0	C(43)-C(44)-C(45)	120.0
C(44)-C(45)-C(46)	120.0	C(45)-C(46)-C(41)	120.0

C(52)-C(51)-C(56)	120.0	C(52)-C(51)-P(2)	116.4(6)
C(56)-C(51)-P(2)	123.6(6)	C(51)-C(52)-C(53)	120.0
C(54)-C(53)-C(52)	120.0	C(55)-C(54)-C(53)	120.0
C(54)-C(55)-C(56)	120.0	C(55)-C(56)-C(51)	120.0
C(65)-C(61)-C(62)	108.0	C(65)-C(61)-P(3)	128.0(6)
C(62)-C(61)-P(3)	123.9(6)	C(63)-C(62)-C(61)	108.0
C(64)-C(63)-C(62)	108.0	C(63)-C(64)-C(65)	108.0
C(64)-C(65)-C(61)	108.0	C(67)-C(66)-C(70)	108.0
C(67)-C(66)-P(4)	122.0(6)	C(70)-C(66)-P(4)	130.0(6)
C(66)-C(67)-C(68)	108.0	C(69)-C(68)-C(67)	108.0
C(68)-C(69)-C(70)	108.0	C(69)-C(70)-C(66)	108.0
C(72)-C(71)-C(76)	120.0	C(72)-C(71)-P(3)	122.7(6)
C(76)-C(71)-P(3)	117.2(6)	C(73)-C(72)-C(71)	120.0
C(74)-C(73)-C(72)	120.0	C(75)-C(74)-C(73)	120.0
C(74)-C(75)-C(76)	120.0	C(75)-C(76)-C(71)	120.0
C(82)-C(81)-C(86)	120.0	C(82)-C(81)-P(3)	120.9(5)
C(86)-C(81)-P(3)	119.0(5)	C(83)-C(82)-C(81)	120.0
C(82)-C(83)-C(84)	120.0	C(85)-C(84)-C(83)	120.0
C(86)-C(85)-C(84)	120.0	C(85)-C(86)-C(81)	120.0
C(92)-C(91)-C(96)	120.0	C(92)-C(91)-P(4)	117.6(5)
C(96)-C(91)-P(4)	122.3(5)	C(93)-C(92)-C(91)	120.0
C(92)-C(93)-C(94)	120.0	C(95)-C(94)-C(93)	120.0
C(94)-C(95)-C(96)	120.0	C(95)-C(96)-C(91)	120.0
C(102)-C(101)-C(106)	120.0	C(102)-C(101)-P(4)	121.9(5)
C(106)-C(101)-P(4)	118.1(5)	C(101)-C(102)-C(103)	120.0
C(104)-C(103)-C(102)	120.0	C(105)-C(104)-C(103)	120.0
C(104)-C(105)-C(106)	120.0	C(105)-C(106)-C(101)	120.0
C(116)-C(111)-C(112)	116.2(14)	C(116)-C(111)-Au(5)	123.0(9)
C(112)-C(111)-Au(5)	120.8(9)	F(1)-C(112)-C(113)	118.7(12)
F(1)-C(112)-C(111)	119.5(12)	C(113)-C(112)-C(111)	121.7(13)
C(114)-C(113)-C(112)	121(2)	C(114)-C(113)-F(2)	119.0(14)
C(112)-C(113)-F(2)	119.7(13)	F(3)-C(114)-C(113)	120.6(13)
F(3)-C(114)-C(115)	121.7(13)	C(113)-C(114)-C(115)	118(2)
F(4)-C(115)-C(114)	118.9(14)	F(4)-C(115)-C(116)	120.1(12)
C(114)-C(115)-C(116)	121(2)	F(5)-C(116)-C(111)	120.0(12)
F(5)-C(116)-C(115)	117.9(12)	C(111)-C(116)-C(115)	122.0(13)
C(122)-C(121)-C(126)	116.7(14)	C(122)-C(121)-Au(5)	122.4(9)
C(126)-C(121)-Au(5)	120.9(9)	F(6)-C(122)-C(121)	119.9(11)
F(6)-C(122)-C(123)	117.5(11)	C(121)-C(122)-C(123)	122.6(13)
F(7)-C(123)-C(124)	118.9(12)	F(7)-C(123)-C(122)	121.7(12)
C(124)-C(123)-C(122)	119.3(13)	F(8)-C(124)-C(125)	120.7(11)
F(8)-C(124)-C(123)	119.8(11)	C(125)-C(124)-C(123)	120(2)

C(124)-C(125)-F(9)	120.8(12)	C(124)-C(125)-C(126)	120.5(13)
F(9)-C(125)-C(126)	118.7(12)	F(10)-C(126)-C(121)	120.1(11)
F(10)-C(126)-C(125)	118.6(11)	C(121)-C(126)-C(125)	121.3(13)
O(2)-S(3)-O(1)	116.3(7)	O(2)-S(3)-O(3)	114.2(7)
O(1)-S(3)-O(3)	114.7(7)	O(2)-S(3)-C(1)	104.2(8)
O(1)-S(3)-C(1)	105.3(8)	O(3)-S(3)-C(1)	99.4(8)
F(11)-C(1)-F(13)	108(2)	F(11)-C(1)-F(12)	106.5(14)
F(13)-C(1)-F(12)	105.0(14)	F(11)-C(1)-S(3)	113.4(13)
F(13)-C(1)-S(3)	111.6(13)	F(12)-C(1)-S(3)	112.3(13)
Cl(1)-C(2)-Cl(2)	114.7(13)	Cl(4)-C(3)-Cl(3)	117(2)
Cl(6)-C(4)-Cl(5)	107(2)	Cl(5')-C(4)-Cl(6')	93(2)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters [$Å^2$ x 10^3] for 2.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Au(1)	24(1)	23(1)	25(1)	-1(1)	6(1)	0(1)
Au(2)	24(1)	23(1)	26(1)	-3(1)	7(1)	-2(1)
Au(3)	27(1)	23(1)	27(1)	0(1)	4(1)	-5(1)
Au(4)	27(1)	24(1)	28(1)	-1(1)	7(1)	-6(1)
Au(5)	25(1)	21(1)	24(1)	-1(1)	4(1)	-1(1)
Fe(1)	26(1)	24(1)	27(1)	-1(1)	9(1)	0(1)
Fe(2)	27(1)	26(1)	24(1)	-1(1)	7(1)	-9(1)
P(1)	22(2)	25(2)	31(2)	-2(2)	7(2)	-2(2)
P(2)	19(2)	25(2)	29(2)	0(2)	5(2)	0(2)
P(3)	25(2)	27(2)	27(2)	5(2)	3(2)	-6(2)
P(4)	36(3)	24(2)	21(2)	1(2)	11(2)	-9(2)
S(1)	29(2)	26(2)	24(2)	-1(2)	9(2)	-2(2)
S(2)	30(2)	23(2)	28(2)	-1(2)	7(2)	-3(2)
F(1)	40(6)	79(7)	24(5)	-3(5)	-1(4)	-5(5)
F(2)	40(7)	126(10)	55(7)	17(7)	-9(5)	-9(7)
F(3)	25(6)	108(9)	109(10)	3(8)	17(6)	29(6)
F(4)	57(8)	81(8)	97(9)	-15(7)	36(7)	12(6)
F(5)	46(6)	48(5)	52(6)	-17(5)	17(5)	5(5)
F(6)	75(8)	38(5)	31(5)	3(4)	6(5)	3(5)
F(7)	59(7)	74(7)	33(6)	20(5)	8(5)	-1(6)
F(8)	76(8)	45(6)	73(7)	49(5)	16(6)	8(5)
F(9)	81(8)	26(5)	83(8)	1(5)	28(6)	1(5)
F(10)	45(6)	28(5)	48(6)	-11(4)	9(5)	-4(4)
S(3)	49(3)	35(2)	66(3)	-8(2)	23(3)	4(2)
O(1)	74(10)	26(6)	74(9)	-9(6)	10(8)	-1(6)
O(2)	48(9)	44(7)	124(12)	-21(7)	56(8)	1(6)
O(3)	54(9)	73(9)	58(9)	-11(7)	-16(7)	1(7)
F(11)	100(10)	88(8)	86(9)	18(7)	15(8)	-54(8)
F(12)	79(9)	72(7)	75(8)	10(6)	-15(7)	0(7)
F(13)	91(10)	155(12)	87(10)	-10(9)	46(8)	38(9)
Cl(1)	99(5)	85(4)	102(5)	-17(4)	22(4)	-6(4)
Cl(2)	69(4)	66(3)	103(5)	5(3)	31(3)	13(3)
Cl(3)	133(9)	431(19)	298(14)	282(15)	-49(9)	-103(11)
Cl(4)	87(7)	266(13)	435(19)	-226(14)	-3(9)	-2(8)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 2.

	x	y	z	U(eq)
H(12)	4158(8)	4463(4)	2279(6)	29
H(13)	3917(9)	5034(6)	3122(3)	38
H(14)	3200(9)	5980(5)	2732(5)	44
H(15)	2999(9)	5994(5)	1648(5)	40
H(17)	5339(9)	6001(6)	3339(3)	31
H(18)	4593(8)	6818(5)	2703(6)	36
H(19)	4646(9)	6623(6)	1677(4)	36
H(20)	5423(9)	5685(6)	1679(4)	39
H(22)	2298(6)	5719(6)	568(6)	50
H(23)	2175(6)	6646(6)	106(7)	59
H(24)	3221(8)	7070(4)	-136(6)	58
H(25)	4390(6)	6569(6)	83(6)	46
H(26)	4513(5)	5643(6)	545(6)	46
H(32)	2599(8)	4616(6)	-77(5)	52
H(33)	1578(8)	3957(7)	-406(3)	64
H(34)	1080(7)	3443(6)	256(6)	62
H(35)	1602(8)	3588(6)	1247(5)	55
H(36)	2622(8)	4247(6)	1575(3)	50
H(42)	5150(8)	3996(5)	2915(3)	34
H(43)	4628(7)	3635(5)	3637(5)	38
H(44)	4944(8)	4085(6)	4547(4)	47
H(45)	5781(8)	4897(5)	4734(3)	43
H(46)	6303(7)	5258(4)	4012(5)	40
H(52)	7477(8)	4356(4)	3093(7)	54
H(53)	8756(7)	4576(5)	3537(7)	66
H(54)	9115(5)	5549(7)	3840(7)	63
H(55)	8194(8)	6302(4)	3700(7)	72
H(56)	6915(7)	6082(5)	3257(7)	54
H(62)	2284(8)	2548(6)	271(5)	33
H(63)	1322(6)	1766(7)	-220(7)	47
H(64)	1729(8)	1362(6)	-1075(6)	57
H(65)	2944(8)	1894(7)	-1112(5)	43
H(67)	4185(6)	1562(6)	732(6)	28
H(68)	4140(7)	1013(7)	-197(6)	42
H(69)	2943(8)	378(6)	-453(5)	41
H(70)	2249(6)	535(6)	318(6)	34
H(72)	2521(8)	3104(5)	-1297(7)	66
H(73)	2235(8)	3924(7)	-1918(5)	83
H(74)	2906(10)	4817(5)	-1670(6)	81
H(75)	3863(9)	4891(4)	-802(7)	64
H(76)	4149(7)	4071(6)	-181(5)	43
H(82)	4062(6)	2760(6)	-1264(4)	41
H(83)	5039(8)	2268(6)	-1541(3)	47
H(84)	5986(6)	1760(6)	-854(6)	55
H(85)	5955(6)	1745(6)	111(5)	40
H(86)	4978(8)	2237(6)	389(3)	39
H(92)	1982(7)	2422(4)	1312(6)	45
H(93)	665(8)	2589(4)	1035(7)	63
H(94)	-175(4)	1790(6)	744(7)	63
H(95)	300(6)	824(5)	729(6)	45
H(96)	1617(7)	656(3)	1005(6)	46
H(102)	2830(9)	140(6)	1407(4)	59
H(103)	3128(10)	-562(3)	2153(6)	58

H(104)	3672(10)	-253(5)	3103(5)	73
H(105)	3918(9)	758(6)	3307(4)	60
H(106)	3620(9)	1460(3)	2561(6)	47
H(2A)	4308(13)	10116(9)	1225(9)	95
H(2B)	3768(13)	9558(9)	995(9)	95
H(3A)	9023(18)	2272(13)	9407(12)	167
H(3B)	9854(18)	2447(13)	9364(12)	167