Table S1 Crystal data and structure refinement for $(PPh_4)[1]$.

Identification code	olem36
Empirical formula	$C_{43}\ H_{22}\ Co_5\ Fe\ O_{17}\ P$
Formula weight	1192.08
Temperature	293(2) K
Wavelength	0.71069 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 9.7070(10) Å α = 90 °. b = 31.3350(10) Å β = 96.7480(10) °. c = 15.2050(10) Å γ = 90 °.
Volume	4592.8(6) $Å^3$
Z, Calculated density	4, 1.724 Mg/m^3
Absorption coefficient	2.178 mm^{-1}
F(000)	2368
Crystal size	0.1 x 0.1 x 0.2 mm
Theta range for data collection	2.48 to 28.89 °.
Index ranges	0<=h<=13, 0<=k<=41, -9<=l<=9
Reflections collected / unique	10650 / 4940 [R(int) = 0.0446]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4940 / 0 / 608
Goodness-of-fit on F^2	1.052
Final R indices [$I>2\sigma(I)$]	R1 = 0.0524, wR2 = 0.1311
R indices (all data)	R1 = 0.1160, wR2 = 0.1525
Largest diff. peak and hole	0.435 and -0.408 $e.Å^{-3}$

Table S2 Fractional atomic coordinates of non-H atoms (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (PPh_4)[**1**].

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Co(1)	11638(1)	914(1)	9197(1)	51(1)
Co(2)	10840(1)	1207(1)	7679(1)	50(1)
Co(3)	9483(1)	1921(1)	7917(1)	51(1)
Co(4)	8763(1)	1948(1)	9465(1)	49(1)
Co(5)	7211(1)	1632(1)	8223(1)	55(1)
Fe	9684(1)	542(1)	8213(1)	53(1)
P	12552(2)	1123(1)	3970(2)	47(1)
O(3)	13642(7)	263(2)	8819(7)	132(4)
O(5)	11106(11)	745(4)	11014(9)	98(5)
O(6)	13621(6)	1350(3)	7204(6)	106(3)
O(4)	13400(6)	1667(2)	9474(5)	81(3)
O(7)	10362(7)	592(3)	6306(7)	78(4)
O(8)	9784(8)	1675(3)	6125(7)	83(4)
O(9)	12035(6)	2416(2)	8241(6)	112(3)
O(10)	7968(8)	2561(3)	6831(7)	119(4)
O(11)	11128(7)	1871(2)	10820(6)	95(3)
O(12)	8550(9)	2864(2)	9195(7)	130(4)
O(13)	6597(7)	1774(3)	10573(6)	100(3)
O(14)	5245(7)	2360(2)	8050(6)	109(3)
O(15)	5896(7)	946(2)	9132(6)	95(3)
O(16)	6780(8)	1287(3)	6423(7)	91(4)
O(17)	11069(7)	-254(2)	7806(6)	106(3)
O(18)	8522(8)	266(3)	9804(8)	92(4)
O(19)	6965(6)	404(2)	7242(6)	101(3)
C(1)	9844(7)	1112(3)	8699(7)	49(3)
C(2)	9062(6)	1471(2)	8739(7)	51(3)
C(3)	12873(8)	522(3)	8943(8)	78(4)
C(4)	12709(8)	1383(3)	9343(7)	56(3)
C(5)	11308(12)	797(4)	10329(13)	63(8)
C(6)	12538(9)	1300(3)	7358(7)	55(3)
C(7)	10382(9)	750(4)	6986(11)	64(5)
C(8)	9988(9)	1594(3)	6890(10)	57(5)
C(9)	11097(9)	2210(3)	8140(7)	63(4)
C(10)	8537(8)	2311(3)	7264(8)	67(4)
C(11)	10225(8)	1902(3)	10275(8)	55(4)
C(12)	8634(9)	2502(3)	9272(8)	78(4)
C(13)	7461(9)	1844(3)	10163(8)	55(4)
C(14)	6010(8)	2081(4)	8130(8)	81(4)
C(15)	6349(8)	1222(3)	8780(8)	60(4)
C(16)	6979(9)	1427(3)	7106(11)	60(5)
C(17)	10532(9)	48(3)	7979(8)	70(4)
C(18)	9003(10)	374(3)	9204(10)	68(5)
C(19)	8040(9)	470(3)	7600(8)	69(4)
C(20)	13209(8)	1586(2)	4568(7)	43(3)
C(21)	12349(9)	1841(3)	5004(8)	68(4)
C(22)	12885(12)	2172(3)	5517(8)	88(4)
C(23)	14273(15)	2270(4)	5572(10)	97(5)
C(24)	15100(13)	2038(5)	5120(11)	103(5)

C(25)	14624(9)	1688(3)	4603(7)	71(4)
C(26)	13444(7)	1058(3)	3028(8)	56(3)
C(27)	13639(10)	1411(3)	2498(10)	62(4)
C(28)	14286(11)	1365(4)	1754(10)	73(4)
C(29)	14751(10)	968(6)	1504(10)	98(5)
C(30)	14559(10)	622(4)	2018(11)	78(5)
C(31)	13919(9)	665(3)	2802(9)	62(4)
C(32)	12787(7)	669(2)	4665(7)	45(3)
C(33)	13734(8)	669(3)	5427(8)	57(4)
C(34)	13880(9)	319(3)	5958(8)	77(4)
C(35)	13124(9)	-45(3)	5752(9)	81(4)
C(36)	12179(10)	-60(3)	5012(9)	82(5)
C(37)	12041(8)	291(3)	4479(8)	58(3)
C(38)	10720(9)	1177(3)	3627(10)	57(4)
C(39)	10223(9)	1291(3)	2791(9)	65(4)
C(40)	8807(10)	1326(3)	2541(9)	78(4)
C(41)	7919(10)	1251(3)	3161(10)	63(5)
C(42)	8393(9)	1141(3)	4021(9)	62(4)
C(43)	9832(8)	1095(3)	4259(8)	53(3)

Table S3 Fractional coordinates of hydrogen atoms (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (PPh_4)[**1**].

	x	y	z	U(eq)
H(21)	11401	1787	4946	82
H(22)	12305	2332	5834	105
H(23)	14631	2496	5922	117
H(24)	16032	2112	5150	124
H(25)	15219	1529	4295	85
H(27)	13328	1679	2652	74
H(28)	14418	1603	1408	87
H(29)	15187	940	994	117
H(30)	14851	354	1851	93
H(31)	13821	430	3161	30(2)
H(33)	14270	910	5574	90(3)
H(34)	14504	326	6472	70(3)
H(35)	13256	-283	6118	60(3)
H(36)	11645	-303	4876	99
H(37)	11419	279	3966	69
H(39)	10838	1345	2379	79
H(40)	8466	1399	1963	93
H(41)	6968	1276	2997	75
H(42)	7775	1097	4436	74
H(43)	10181	1012	4828	64

Table S4 Anisotropic coefficients of non-H atoms ($Å^2 \times 10^3$) for $(PPh_4)[\mathbf{1}]$.

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}	U33	U_{23}	U_{13}	U_{12}
Co(1)	43(1)	54(1)	56(2)	-4(1)	1(1)	2(1)
Co(2)	46(1)	57(1)	46(2)	-5(1)	7(1)	-4(1)
Co(3)	48(1)	53(1)	55(2)	4(1)	9(1)	-2(1)
Co(4)	50(1)	48(1)	50(2)	-3(1)	7(1)	-2(1)
Co(5)	38(1)	63(1)	64(2)	-2(1)	2(1)	-1(1)
Fe	49(1)	47(1)	61(2)	-6(1)	3(1)	-5(1)
P	48(1)	54(1)	39(3)	3(1)	6(1)	2(1)
O(3)	76(4)	103(6)	215(13)	-69(7)	13(5)	23(4)
O(5)	127(7)	131(7)	35(15)	-6(9)	5(7)	-38(5)
O(6)	46(3)	174(8)	100(10)	-4(6)	17(4)	-32(4)
O(4)	76(4)	74(5)	88(9)	-7(4)	-11(4)	-30(3)
O(7)	105(5)	94(6)	39(12)	-26(5)	28(5)	-14(4)
O(8)	104(5)	106(6)	41(12)	26(7)	18(6)	28(4)
O(9)	72(4)	114(6)	151(11)	-2(6)	14(5)	-43(4)
O(10)	129(6)	114(7)	110(11)	54(6)	-4(6)	26(5)
O(11)	78(4)	125(6)	75(9)	-12(5)	-16(5)	3(4)
O(12)	213(9)	44(5)	133(12)	9(5)	22(7)	-2(5)
O(13)	75(4)	133(7)	99(10)	-24(6)	36(5)	-33(4)
O(14)	96(5)	109(6)	119(10)	-6(5)	5(5)	44(4)
O(15)	86(5)	72(5)	133(11)	12(5)	37(5)	-18(4)
O(16)	86(5)	121(7)	62(13)	-31(6)	-13(5)	-4(4)
O(17)	121(6)	63(5)	140(10)	-23(5)	44(5)	15(4)
O(18)	87(5)	99(6)	92(12)	34(6)	23(5)	-5(4)
O(19)	74(4)	99(5)	121(10)	-26(5)	-31(5)	-16(4)
C(1)	45(4)	65(6)	37(11)	-3(5)	12(4)	-7(4)
C(2)	35(4)	47(5)	71(11)	-16(5)	5(4)	-8(3)
C(3)	44(4)	67(6)	122(14)	-15(7)	9(6)	-3(4)
C(4)	56(5)	80(7)	32(12)	1(6)	3(5)	4(4)
C(5)	75(6)	67(7)	50(3)	2(10)	9(9)	-12(4)
C(6)	74(6)	66(6)	27(11)	-1(6)	9(6)	-14(4)
C(7)	59(5)	88(8)	49(19)	-29(8)	20(7)	1(5)
C(8)	65(6)	69(7)	42(17)	9(8)	27(7)	13(4)
C(9)	71(5)	75(6)	47(12)	10(6)	28(6)	-6(5)
C(10)	63(5)	71(7)	65(13)	15(7)	6(6)	2(4)
C(11)	45(4)	73(6)	49(12)	-2(6)	21(5)	1(4)
C(12)	89(6)	63(7)	79(14)	-9(7)	4(6)	-8(5)
C(13)	58(5)	68(6)	39(12)	-4(6)	0(6)	-15(4)
C(14)	55(5)	109(8)	76(14)	-15(8)	-3(6)	6(5)
C(15)	50(4)	69(6)	60(12)	2(7)	10(5)	1(4)
C(16)	55(5)	74(7)	46(19)	-6(8)	-15(7)	3(4)
C(17)	68(5)	55(6)	89(13)	-14(7)	16(6)	-7(4)
C(18)	68(6)	69(7)	68(19)	14(8)	7(7)	-10(5)
C(19)	77(6)	60(6)	67(13)	-11(6)	-6(6)	0(4)

C(20)	68(5)	40(5)	20(10)	-1(5)	0(5)	-6(4)
C(21)	71(5)	61(6)	71(13)	-8(7)	0(6)	8(5)
C(22)	121(9)	69(7)	73(14)	-30(8)	7(8)	-1(6)
C(23)	139(11)	66(8)	82(16)	6(8)	-11(10)	-33(7)
C(24)	104(9)	114(11)	87(17)	-20(10)	-5(9)	-45(8)
C(25)	68(5)	96(8)	49(12)	-2(7)	10(6)	-6(5)
C(26)	51(4)	63(6)	56(12)	-5(7)	13(5)	6(4)
C(27)	79(6)	84(8)	26(15)	-4(8)	24(7)	-4(5)
C(28)	87(7)	97(9)	38(16)	16(8)	26(8)	1(6)
C(29)	67(6)	163(14)	67(16)	-6(13)	27(7)	-18(8)
C(30)	75(6)	115(11)	50(17)	-27(10)	34(7)	4(6)
C(31)	77(6)	77(8)	36(14)	-8(8)	19(7)	5(5)
C(32)	49(4)	47(5)	42(11)	-1(5)	13(5)	9(3)
C(33)	57(5)	53(6)	59(12)	6(6)	-2(5)	-12(4)
C(34)	86(6)	57(6)	76(14)	23(7)	-44(7)	-2(5)
C(35)	83(7)	53(6)	100(14)	34(7)	-19(7)	-2(5)
C(36)	88(7)	50(6)	105(16)	23(7)	-4(7)	-14(5)
C(37)	61(5)	67(7)	43(11)	-10(7)	-2(5)	-2(4)
C(38)	47(5)	58(6)	65(15)	-5(6)	6(6)	4(4)
C(39)	57(5)	67(6)	70(15)	-2(7)	-1(6)	4(4)
C(40)	71(6)	112(9)	46(14)	4(8)	-11(7)	2(6)
C(41)	56(5)	76(7)	52(15)	-8(7)	-10(7)	4(5)
C(42)	64(5)	55(6)	69(15)	-16(7)	21(7)	2(4)
C(43)	56(5)	64(6)	39(12)	-5(6)	-1(5)	13(4)

Table S5 Listing of bond lengths (Å) and angles (deg) of for $(PPh_4)[1]$.

Co(1)-C(3)	1.790(10)
Co(1)-C(4)	1.799(10)
Co(1)-C(5)	1.825(19)
Co(1)-C(1)	1.918(8)
Co(1)-Co(2)	2.520(2)
Co(1)-Fe	2.5547(16)
Co(2)-C(6)	1.796(10)
Co(2)-C(7)	1.802(12)
Co(2)-C(8)	1.833(12)
Co(2)-C(1)	1.945(9)
Co(2)-Fe	2.5447(17)
Co(2)-Co(3)	2.6431(15)
Co(3)-C(10)	1.763(11)
Co(3)-C(9)	1.806(9)
Co(3)-C(2)	1.960(9)
Co(3)-C(8)	1.977(14)
Co(3)-Co(5)	2.4797(14)
Co(3)-Co(4)	2.535(2)
Co(4)-C(12)	1.763(11)
Co(4)-C(11)	1.773(10)
Co(4)-C(13)	1.774(11)
Co(4)-C(2)	1.901(8)
Co(4)-Co(5)	2.4804(18)
Co(5)-C(15)	1.796(11)
Co(5)-C(16)	1.805(15)
Co(5)-C(14)	1.824(11)
Co(5)-C(2)	1.940(7)
Fe-C(19)	1.765(10)
Fe-C(18)	1.795(14)
Fe-C(17)	1.809(10)
Fe-C(1)	1.930(8)
Fe-C(7)	2.160(16)
P-C(32)	1.771(9)
P-C(26)	1.771(11)
P-C(20)	1.789(8)
P-C(38)	1.802(9)
O(3)-C(3)	1.133(10)
O(5)-C(5)	1.095(17)
O(6)-C(6)	1.115(9)
O(4)-C(4)	1.119(9)
O(7)-C(7)	1.145(13)
O(8)-C(8)	1.184(13)
O(9)-C(9)	1.113(9)
O(10)-C(10)	1.125(10)
O(11)-C(11)	1.136(10)
O(12)-C(12)	1.140(11)
O(13)-C(13)	1.123(11)
O(14)-C(14)	1.143(10)
O(15)-C(15)	1.135(10)
O(16)-C(16)	1.123(14)
O(17)-C(17)	1.126(10)
O(18)-C(18)	1.124(14)
O(19)-C(19)	1.138(9)

C(1)-C(2)	1.363(10)
C(20)-C(21)	1.379(12)
C(20)-C(25)	1.406(11)
C(21)-C(22)	1.364(13)
C(22)-C(23)	1.375(15)
C(23)-C(24)	1.333(16)
C(24)-C(25)	1.395(15)
C(26)-C(31)	1.371(12)
C(26)-C(27)	1.396(13)
C(27)-C(28)	1.365(15)
C(28)-C(29)	1.392(16)
C(29)-C(30)	1.363(16)
C(30)-C(31)	1.414(15)
C(32)-C(33)	1.392(12)
C(32)-C(37)	1.399(11)
C(33)-C(34)	1.360(12)
C(34)-C(35)	1.373(12)
C(35)-C(36)	1.366(13)
C(36)-C(37)	1.364(12)
C(38)-C(39)	1.352(14)
C(38)-C(43)	1.388(14)
C(39)-C(40)	1.388(12)
C(40)-C(41)	1.371(15)
C(41)-C(42)	1.378(14)
C(42)-C(43)	1.409(11)

C(3)-Co(1)-C(4)	101.3(4)
C(3)-Co(1)-C(5)	105.2(6)
C(4)-Co(1)-C(5)	102.2(5)
C(3)-Co(1)-C(1)	137.4(5)
C(4)-Co(1)-C(1)	105.6(3)
C(5)-Co(1)-C(1)	100.7(5)
C(3)-Co(1)-Co(2)	101.2(4)
C(4)-Co(1)-Co(2)	85.8(3)
C(5)-Co(1)-Co(2)	150.2(4)
C(1)-Co(1)-Co(2)	49.8(3)
C(3)-Co(1)-Fe	91.8(3)
C(4)-Co(1)-Fe	145.5(3)
C(5)-Co(1)-Fe	105.0(4)
C(1)-Co(1)-Fe	48.6(3)
Co(2)-Co(1)-Fe	60.19(5)
C(6)-Co(2)-C(7)	98.2(5)
C(6)-Co(2)-C(8)	94.2(5)
C(7)-Co(2)-C(8)	94.7(6)
C(6)-Co(2)-C(1)	143.1(4)
C(7)-Co(2)-C(1)	103.4(5)
C(8)-Co(2)-C(1)	113.3(5)
C(6)-Co(2)-Co(1)	96.6(3)
C(7)-Co(2)-Co(1)	105.9(5)
C(8)-Co(2)-Co(1)	155.1(4)
C(1)-Co(2)-Co(1)	48.8(2)
C(6)-Co(2)-Fe	132.3(3)
C(7)-Co(2)-Fe	56.5(5)
C(8)-Co(2)-Fe	124.6(3)
C(1)-Co(2)-Fe	48.7(2)
Co(1)-Co(2)-Fe	60.59(5)
C(6)-Co(2)-Co(3)	112.8(3)
C(7)-Co(2)-Co(3)	131.3(3)

C(8)-Co(2)-Co(3)	48.4(4)
C(1)-Co(2)-Co(3)	73.6(2)
Co(1)-Co(2)-Co(3)	106.71(7)
Fe-Co(2)-Co(3)	113.80(6)
C(10)-Co(3)-C(9)	98.2(4)
C(10)-Co(3)-C(2)	136.4(4)
C(9)-Co(3)-C(2)	118.8(4)
C(10)-Co(3)-C(8)	94.3(5)
C(9)-Co(3)-C(8)	96.8(4)
C(2)-Co(3)-C(8)	102.7(4)
C(10)-Co(3)-Co(5)	86.8(3)
C(9)-Co(3)-Co(5)	156.8(4)
C(2)-Co(3)-Co(5)	50.17(19)
C(8)-Co(3)-Co(5)	105.5(3)
C(10)-Co(3)-Co(4)	108.5(4)
C(9)-Co(3)-Co(4)	97.9(4)
C(2)-Co(3)-Co(4)	48.0(3)
C(8)-Co(3)-Co(4)	150.7(3)
Co(5)-Co(3)-Co(4)	59.28(5)
C(10)-Co(3)-Co(2)	138.1(4)
C(9)-Co(3)-Co(2)	90.8(3)
C(2)-Co(3)-Co(2)	67.8(2)
C(8)-Co(3)-Co(2)	43.9(3)
Co(5)-Co(3)-Co(2)	100.62(5)
Co(4)-Co(3)-Co(2)	110.59(6)
C(12)-Co(4)-C(11)	103.4(4)
C(12)-Co(4)-C(13)	103.9(5)
C(11)-Co(4)-C(13)	97.9(4)
C(12)-Co(4)-C(2)	133.7(5)
C(11)-Co(4)-C(2)	100.1(4)
C(13)-Co(4)-C(2)	111.7(4)
C(12)-Co(4)-Co(5)	104.0(4)
C(11)-Co(4)-Co(5)	149.5(3)
C(13)-Co(4)-Co(5)	88.3(3)
C(2)-Co(4)-Co(5)	50.5(2)
C(12)-Co(4)-Co(3)	84.3(4)
C(11)-Co(4)-Co(3)	110.9(3)
C(13)-Co(4)-Co(3)	147.5(3)
C(2)-Co(4)-Co(3)	50.0(3)
Co(5)-Co(4)-Co(3)	59.25(5)
C(15)-Co(5)-C(16)	100.2(5)
C(15)-Co(5)-C(14)	105.0(4)
C(16)-Co(5)-C(14)	101.2(5)
C(15)-Co(5)-C(2)	94.9(4)
C(16)-Co(5)-C(2)	107.2(4)
C(14)-Co(5)-C(2)	141.7(4)
C(15)-Co(5)-Co(3)	145.5(3)
C(16)-Co(5)-Co(3)	88.2(3)
C(14)-Co(5)-Co(3)	106.1(3)
C(2)-Co(5)-Co(3)	50.9(3)
C(15)-Co(5)-Co(4)	101.6(4)
C(16)-Co(5)-Co(4)	148.9(3)
C(14)-Co(5)-Co(4)	94.3(3)
C(2)-Co(5)-Co(4)	49.1(3)
Co(3)-Co(5)-Co(4)	61.46(5)
C(19)-Fe-C(18)	90.4(5)
C(19)-Fe-C(17)	101.0(4)
C(18)-Fe-C(17)	97.7(5)

C(19)-Fe-C(1)	110.4(4)
C(18)-Fe-C(1)	88.4(5)
C(17)-Fe-C(1)	148.0(4)
C(19)-Fe-C(7)	86.5(5)
C(18)-Fe-C(7)	176.7(4)
C(17)-Fe-C(7)	83.8(5)
C(1)-Fe-C(7)	91.9(4)
C(19)-Fe-Co(2)	110.0(3)
C(18)-Fe-Co(2)	136.8(4)
C(17)-Fe-Co(2)	114.2(3)
C(1)-Fe-Co(2)	49.2(3)
C(7)-Fe-Co(2)	44.1(3)
C(19)-Fe-Co(1)	158.5(3)
C(18)-Fe-Co(1)	87.9(4)
C(17)-Fe-Co(1)	100.5(3)
C(1)-Fe-Co(1)	48.2(2)
C(7)-Fe-Co(1)	94.7(3)
Co(2)-Fe-Co(1)	59.23(5)
C(32)-P-C(26)	110.5(4)
C(32)-P-C(20)	109.6(4)
C(26)-P-C(20)	109.0(4)
C(32)-P-C(38)	107.6(4)
C(26)-P-C(38)	109.6(5)
C(20)-P-C(38)	110.5(4)
C(2)-C(1)-Co(1)	137.2(6)
C(2)-C(1)-Fe	139.4(6)
Co(1)-C(1)-Fe	83.2(3)
C(2)-C(1)-Co(2)	103.9(7)
Co(1)-C(1)-Co(2)	81.4(3)
Fe-C(1)-Co(2)	82.1(4)
C(1)-C(2)-Co(4)	143.0(7)
C(1)-C(2)-Co(5)	133.7(6)
Co(4)-C(2)-Co(5)	80.4(3)
C(1)-C(2)-Co(3)	114.0(7)
Co(4)-C(2)-Co(3)	82.0(3)
Co(5)-C(2)-Co(3)	79.0(3)
O(3)-C(3)-Co(1)	176.5(12)
O(4)-C(4)-Co(1)	176.6(9)
O(5)-C(5)-Co(1)	176.8(15)
O(6)-C(6)-Co(2)	176.1(10)
O(7)-C(7)-Co(2)	148.1(14)
O(7)-C(7)-Fe	132.5(11)
Co(2)-C(7)-Fe	79.4(6)
O(8)-C(8)-Co(2)	142.6(11)
O(8)-C(8)-Co(3)	129.6(9)
Co(2)-C(8)-Co(3)	87.8(7)
O(9)-C(9)-Co(3)	173.9(9)
O(10)-C(10)-Co(3)	177.7(10)
O(11)-C(11)-Co(4)	177.3(10)
O(12)-C(12)-Co(4)	176.4(12)
O(13)-C(13)-Co(4)	177.0(10)
O(14)-C(14)-Co(5)	178.3(11)
O(15)-C(15)-Co(5)	174.7(8)
O(16)-C(16)-Co(5)	176.4(13)
O(17)-C(17)-Fe	177.6(11)
O(18)-C(18)-Fe	177.0(12)
O(19)-C(19)-Fe	175.7(10)
C(21)-C(20)-C(25)	119.5(8)

C(21)-C(20)-P	120.9(6)
C(25)-C(20)-P	119.5(7)
C(22)-C(21)-C(20)	120.3(9)
C(21)-C(22)-C(23)	120.6(11)
C(24)-C(23)-C(22)	119.5(12)
C(23)-C(24)-C(25)	122.6(11)
C(24)-C(25)-C(20)	117.3(10)
C(31)-C(26)-C(27)	119.6(11)
C(31)-C(26)-P	121.1(10)
C(27)-C(26)-P	119.2(9)
C(28)-C(27)-C(26)	120.1(11)
C(27)-C(28)-C(29)	121.1(13)
C(30)-C(29)-C(28)	119.0(14)
C(29)-C(30)-C(31)	120.7(13)
C(26)-C(31)-C(30)	119.5(11)
C(33)-C(32)-C(37)	116.4(8)
C(33)-C(32)-P	121.5(6)
C(37)-C(32)-P	122.1(8)
C(34)-C(33)-C(32)	120.4(8)
C(33)-C(34)-C(35)	121.3(10)
C(36)-C(35)-C(34)	120.4(10)
C(37)-C(36)-C(35)	118.1(9)
C(36)-C(37)-C(32)	123.4(10)
C(39)-C(38)-C(43)	121.1(9)
C(39)-C(38)-P	121.9(9)
C(43)-C(38)-P	117.0(10)
C(38)-C(39)-C(40)	120.7(12)
C(41)-C(40)-C(39)	118.7(12)
C(40)-C(41)-C(42)	121.9(10)
C(41)-C(42)-C(43)	118.6(11)
C(38)-C(43)-C(42)	118.8(11)

Symmetry transformations used to generate equivalent atoms.

Table S6 Crystal data and structure refinement for **4**.

Empirical formula	$C_{71}\ H_{60}\ Au_3\ Fe_3\ O_{12}\ P_3$
Formula weight	1956.55
Temperature	293(2) K
Wavelength	0.71069 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 13.826(1) Å alpha = 90 °. b = 22.962(1) Å beta = 97.199(1) °. c = 21.907(1) Å gamma = 90 °.
Volume	6900.0(7) $Å^3$
Z, Calculated density	4, 1.883 Mg/m^3
Absorption coefficient	7.098 mm^{-1}
F(000) 3768	
Crystal size	0.1 x 0.1 x 0.2 mm
Theta range for data collection	2.53 to 31.63 °.
Index ranges	-19<=h<=15, 0<=k<=30, 0<=l<=30
Reflections collected / unique	19000 / 9411 [R(int) = 0.0407]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9411 / 235 / 782
Goodness-of-fit on F^2 1.064	
Final R indices [I>2σ(I)]	R1 = 0.0373, wR2 = 0.0951
R indices (all data)	R1 = 0.0666, wR2 = 0.1030
Largest diff. peak and hole	0.851 and -0.802 $e.Å^{-3}$

Table S7 Fractional atomic coordinates of non-H atoms (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Au(1)	119(1)	1423(1)	1821(1)	49(1)
Au(2)	1600(1)	1311(1)	2886(1)	45(1)
Au(3)	2186(1)	105(1)	2943(1)	46(1)
Fe(1)	-319(1)	1313(1)	2991(1)	41(1)
Fe(2)	860(1)	529(1)	3629(1)	39(1)
Fe(3)	324(1)	374(1)	2404(1)	38(1)
P(1)	3537(2)	-426(1)	2801(1)	48(1)
P(2)	2899(2)	1926(1)	2853(1)	50(1)
P(3)	-177(2)	1948(1)	929(1)	49(1)
O(1)	-1684(5)	-183(3)	2915(4)	87(3)
O(2)	-1547(4)	327(3)	3778(3)	68(2)
O(5)	-2316(5)	1366(3)	2404(5)	92(3)
O(6)	1628(4)	340(3)	1431(3)	75(2)
O(7)	1051(6)	-701(3)	3975(4)	87(2)
O(8)	208(5)	-888(3)	2535(3)	76(2)
O(9)	59(5)	704(3)	4775(4)	86(2)
O(10)	-994(8)	1727(4)	4111(5)	135(4)
O(11)	2723(5)	965(3)	4278(3)	65(2)
O(12)	128(5)	2550(2)	2793(4)	80(2)
O(13)	-1441(5)	300(3)	1543(4)	75(2)
C(1)	-367(6)	478(3)	3117(4)	43(1)
C(2)	-1264(6)	171(3)	3241(4)	43(2)
C(3)	-2409(7)	73(5)	3930(6)	80(3)
C(4)	-2444(8)	171(6)	4599(6)	105(5)
C(5)	-1527(6)	1347(3)	2593(5)	50(3)
C(6)	1177(6)	388(3)	1807(4)	43(1)
C(7)	1016(6)	-215(4)	3799(4)	51(2)
C(8)	311(6)	-394(3)	2493(4)	43(1)
C(9)	356(6)	663(4)	4322(5)	56(3)
C(10)	-680(7)	1541(4)	3701(6)	65(3)
C(11)	2037(6)	811(4)	3981(5)	48(2)
C(12)	42(7)	2052(4)	2860(5)	65(3)
C(13)	-768(7)	351(3)	1875(5)	43(1)
C(111)	4238(7)	-677(4)	3486(6)	73(1)
C(112)	4957(7)	-1128(4)	3493(6)	74(1)
C(113)	5500(7)	-1285(4)	4033(6)	74(2)
C(114)	5369(7)	-1053(4)	4547(6)	74(2)
C(115)	4676(7)	-635(4)	4568(6)	74(1)
C(116)	4153(7)	-435(4)	4063(6)	74(1)
C(121)	4414(7)	-71(4)	2384(6)	72(2)
C(122)	5393(7)	-94(4)	2533(6)	72(2)
C(123)	6026(7)	210(5)	2215(6)	72(2)
C(124)	2063(8)	3747(5)	3403(9)	118(6)
C(125)	4632(7)	575(4)	1534(6)	73(2)
C(126)	4037(7)	288(4)	1896(5)	73(2)
C(131)	3226(8)	-1096(5)	2406(7)	96(2)
C(132)	2579(8)	-1468(5)	2618(7)	96(2)
C(133)	2380(8)	-2008(5)	2399(7)	97(2)
C(134)	2794(8)	-2184(5)	1911(7)	97(2)

C(135)	3418(8)	-1822(5)	1645(7)	97(2)
C(136)	3646(8)	-1284(5)	1917(7)	96(2)
C(211)	4012(8)	1767(5)	3374(7)	97(2)
C(212)	4402(8)	1229(5)	3350(7)	98(2)
C(213)	5277(8)	1105(5)	3700(7)	98(2)
C(214)	5730(9)	1512(5)	4046(7)	98(2)
C(215)	5308(8)	2006(5)	4165(7)	98(2)
C(216)	4440(8)	2166(5)	3782(7)	97(2)
C(221)	2576(9)	2673(4)	3048(6)	88(2)
C(222)	2784(8)	3149(4)	2728(6)	88(2)
C(223)	2517(9)	3700(4)	2911(7)	89(2)
C(224)	5628(9)	517(5)	1709(6)	100(4)
C(225)	1898(8)	3274(4)	3777(6)	89(2)
C(226)	2122(8)	2741(4)	3571(6)	88(2)
C(231)	3416(8)	1996(4)	2158(6)	72(3)
C(232)	4316(7)	2215(5)	2104(6)	92(4)
C(233)	4659(10)	2255(7)	1536(9)	130(7)
C(234)	4073(10)	2125(6)	1016(7)	100(5)
C(235)	3152(10)	1889(5)	1054(6)	91(4)
C(236)	2861(8)	1846(4)	1629(6)	73(3)
C(311)	-1392(7)	2273(4)	848(6)	78(1)
C(312)	-1537(7)	2853(4)	701(6)	79(1)
C(313)	-2457(7)	3080(5)	653(6)	79(1)
C(314)	-3224(7)	2745(4)	735(6)	80(1)
C(315)	-3092(7)	2167(4)	858(6)	80(1)
C(316)	-2147(7)	1958(5)	979(6)	79(1)
C(321)	619(7)	2538(4)	832(5)	59(3)
C(322)	875(8)	2927(4)	1278(6)	80(3)
C(323)	1440(10)	3410(5)	1200(7)	100(4)
C(324)	1840(9)	3475(6)	653(9)	103(5)
C(325)	1661(10)	3093(6)	221(7)	102(4)
C(326)	1027(8)	2635(5)	275(6)	85(4)
C(331)	-230(9)	1521(5)	235(6)	83(2)
C(332)	314(9)	1048(5)	231(6)	83(2)
C(333)	321(9)	717(5)	-308(6)	83(2)
C(334)	-255(9)	880(5)	-818(6)	83(2)
C(335)	-730(9)	1372(5)	-809(6)	84(2)
C(336)	-782(9)	1699(5)	-298(5)	83(2)
C(14)	4218(18)	972(13)	-471(19)	346(8)
C(15)	5240(2)	1206(9)	-368(19)	346(8)
C(16)	6849(18)	820(10)	-98(19)	346(8)
C(17)	7353(19)	235(13)	-80(19)	346(8)
O(14)	5848(16)	690(8)	-324(12)	346(8)

Table S8 Fractional coordinates of hydrogen atoms (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **4**.

	x	y	z	U(eq)
H(3)	-2414	-341	3842	96
H(3A)	-2972	250	3692	96
H(4)	-3029	3	4716	126
H(4A)	-2438	582	4681	126
H(4B)	-1887	-7	4831	126
H(112)	5054	-1314	3128	88
H(113)	5977	-1570	4026	89
H(114)	5749	-1169	4907	89
H(115)	4566	-486	4947	89
H(116)	3721	-129	4093	88
H(122)	5648	-325	2864	87
H(123)	6695	208	2338	87
H(124)	1841	4112	3505	141
H(125)	4382	795	1193	88
H(126)	3365	335	1813	87
H(132)	2251	-1340	2939	115
H(133)	1965	-2253	2583	116
H(134)	2661	-2555	1750	116
H(135)	3680	-1935	1292	116
H(136)	4100	-1047	1759	116
H(212)	4081	944	3100	117
H(213)	5546	735	3690	118
H(214)	6373	1448	4214	118
H(215)	5569	2243	4489	118
H(216)	4171	2534	3811	117
H(222)	3108	3109	2383	106
H(223)	2657	4029	2691	107
H(224)	6049	697	1468	120
H(225)	1647	3322	4149	106
H(226)	1967	2412	3787	106
H(232)	4710	2340	2455	110
H(233)	5298	2372	1514	155
H(234)	4279	2193	634	120
H(235)	2753	1765	705	110
H(236)	2237	1705	1656	87
H(312)	-1012	3088	634	95
H(313)	-2552	3473	563	95
H(314)	-3845	2907	709	95
H(315)	-3623	1919	861	95
H(316)	-2039	1591	1154	94
H(322)	662	2869	1660	95
H(323)	1551	3689	1510	120
H(324)	2236	3793	597	124
H(325)	1964	3126	-133	123
H(326)	865	2387	-57	102
H(332)	696	932	590	99
H(333)	718	391	-311	100
H(334)	-314	650	-1170	100
H(335)	-1056	1507	-1179	100
H(336)	-1174	2028	-308	100

Table S9. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **4**.

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)	47(1)	48(1)	52(1)	9(1)	2(1)	-3(1)
Au(2)	33(1)	40(1)	62(1)	6(1)	3(1)	-3(1)
Au(3)	36(1)	44(1)	60(1)	0(1)	8(1)	7(1)
Fe(1)	33(1)	37(1)	51(1)	0(1)	6(1)	4(1)
Fe(2)	34(1)	39(1)	43(1)	1(1)	6(1)	1(1)
Fe(3)	34(1)	36(1)	44(1)	-2(1)	5(1)	2(1)
P(1)	36(1)	45(1)	65(2)	-4(1)	8(1)	6(1)
P(2)	37(1)	39(1)	72(2)	10(1)	-2(1)	-1(1)
P(3)	47(1)	43(1)	55(2)	7(1)	1(1)	1(1)
O(1)	60(4)	110(6)	94(6)	-39(5)	26(5)	-45(4)
O(2)	45(3)	94(5)	70(5)	-20(4)	28(4)	-27(3)
O(5)	49(5)	81(5)	142(9)	29(5)	-5(5)	8(3)
O(6)	59(4)	107(5)	66(5)	12(4)	34(4)	18(4)
O(7)	127(7)	50(4)	82(6)	14(4)	11(5)	-2(4)
O(8)	88(5)	44(4)	95(6)	-9(3)	11(5)	-1(3)
O(9)	83(5)	114(6)	64(6)	-5(4)	22(5)	6(4)
O(10)	195(11)	111(7)	102(8)	-22(6)	30(8)	63(7)
O(11)	47(4)	89(5)	54(5)	5(4)	-6(4)	-17(3)
O(12)	77(5)	29(3)	135(7)	0(3)	20(5)	-3(3)
O(13)	64(5)	60(4)	91(6)	-5(4)	-28(5)	-8(3)
C(1)	43(2)	39(2)	43(3)	-2(2)	-4(3)	-2(2)
C(2)	45(5)	45(5)	40(6)	-7(4)	7(5)	-5(4)
C(3)	39(6)	122(9)	78(9)	5(7)	8(6)	-19(5)
C(4)	56(7)	179(14)	81(10)	-11(9)	11(8)	-16(7)
C(5)	30(5)	54(5)	66(8)	-1(4)	5(6)	1(4)
C(6)	43(2)	39(2)	43(3)	-2(2)	-4(3)	-2(2)
C(7)	50(6)	70(6)	30(6)	11(4)	-4(5)	15(4)
C(8)	43(2)	39(2)	43(3)	-2(2)	-4(3)	-2(2)
C(9)	53(5)	62(6)	57(7)	7(4)	19(6)	11(4)
C(10)	63(6)	53(6)	74(9)	0(5)	-12(7)	15(5)
C(11)	24(4)	69(6)	51(7)	2(5)	3(5)	13(4)
C(12)	64(6)	43(5)	93(8)	4(5)	35(6)	14(4)
C(13)	43(2)	39(2)	43(3)	-2(2)	-4(3)	-2(2)
C(111)	44(3)	70(3)	100(4)	14(3)	-14(3)	8(2)
C(112)	44(3)	70(3)	100(4)	14(3)	-15(3)	9(2)
C(113)	45(3)	71(3)	101(4)	15(3)	-15(3)	8(2)
C(114)	45(3)	71(3)	101(4)	15(3)	-15(3)	8(2)
C(115)	46(3)	71(3)	100(4)	15(3)	-15(3)	8(2)
C(116)	44(3)	71(3)	100(4)	14(3)	-15(3)	8(2)
C(121)	42(3)	85(3)	91(4)	12(3)	14(3)	4(2)
C(122)	42(3)	85(3)	91(4)	12(3)	14(3)	4(2)
C(123)	42(3)	85(3)	91(4)	12(3)	14(3)	3(2)
C(124)	54(7)	62(7)	220(2)	-27(9)	-44(10)	18(5)
C(125)	44(3)	85(3)	91(4)	13(3)	14(3)	5(2)
C(126)	43(3)	85(3)	91(4)	12(3)	14(3)	5(2)
C(131)	79(3)	72(3)	138(5)	-30(3)	24(3)	-10(2)
C(132)	80(3)	72(3)	138(5)	-30(3)	24(3)	-11(2)
C(133)	81(3)	73(3)	139(5)	-30(3)	23(3)	-11(2)

C(134)	81(3)	73(3)	139(5)	-31(3)	23(3)	-11(2)
C(135)	81(3)	73(3)	139(5)	-31(3)	23(3)	-10(2)
C(136)	80(3)	73(3)	139(5)	-31(3)	24(3)	-10(2)
C(211)	72(3)	73(3)	137(6)	12(3)	-22(4)	3(3)
C(212)	73(3)	74(3)	137(6)	11(3)	-22(4)	4(3)
C(213)	73(3)	75(3)	138(6)	11(3)	-23(4)	5(3)
C(214)	73(3)	75(3)	138(6)	12(3)	-22(4)	4(3)
C(215)	73(3)	74(3)	138(6)	12(3)	-23(4)	3(3)
C(216)	72(3)	73(3)	137(6)	12(3)	-22(4)	3(3)
C(221)	101(4)	50(3)	114(5)	5(3)	17(3)	2(3)
C(222)	101(4)	50(3)	114(5)	5(3)	16(3)	2(3)
C(223)	102(4)	51(3)	115(5)	5(3)	15(4)	2(3)
C(224)	101(9)	85(8)	125(12)	27(7)	52(9)	-11(7)
C(225)	101(4)	51(3)	115(5)	3(3)	17(4)	2(3)
C(226)	101(4)	50(3)	115(5)	4(3)	17(3)	2(3)
C(231)	65(7)	66(6)	90(9)	-1(6)	36(7)	-12(5)
C(232)	47(6)	110(9)	121(11)	39(8)	21(7)	-21(5)
C(233)	62(8)	171(14)	164(17)	81(13)	47(10)	2(9)
C(234)	82(9)	142(11)	85(10)	50(9)	48(9)	19(8)
C(235)	115(10)	86(8)	75(9)	15(6)	19(8)	14(7)
C(236)	75(7)	69(7)	80(9)	23(6)	28(8)	9(5)
C(311)	55(3)	74(3)	104(4)	24(3)	5(3)	13(2)
C(312)	56(3)	75(3)	104(4)	24(3)	5(3)	13(2)
C(313)	56(3)	75(3)	105(4)	24(3)	5(3)	13(2)
C(314)	56(3)	76(3)	105(4)	24(3)	5(3)	13(2)
C(315)	56(3)	76(3)	105(4)	24(3)	5(3)	12(2)
C(316)	55(3)	75(3)	104(4)	24(3)	5(3)	12(2)
C(321)	48(6)	69(6)	52(7)	12(5)	-25(6)	-14(5)
C(322)	87(8)	69(7)	75(9)	17(6)	-19(7)	-19(6)
C(323)	122(11)	61(7)	103(12)	-5(7)	-44(10)	-40(7)
C(324)	77(8)	72(8)	161(16)	29(9)	18(10)	-26(6)
C(325)	115(11)	88(9)	105(12)	39(8)	22(9)	-25(8)
C(326)	102(9)	74(7)	82(9)	7(6)	27(8)	-11(6)
C(331)	92(4)	87(3)	67(4)	-12(3)	4(3)	3(3)
C(332)	92(4)	87(3)	67(4)	-12(3)	4(3)	2(3)
C(333)	93(4)	88(3)	68(4)	-12(3)	4(3)	2(3)
C(334)	93(4)	88(3)	68(4)	-12(3)	4(3)	2(3)
C(335)	93(4)	89(3)	68(4)	-12(3)	4(3)	2(3)
C(336)	92(4)	88(3)	68(4)	-12(3)	4(3)	3(3)

Table S10 Listing of bond lengths (Å) and angles (deg) of **4**.

Au(1)-P(3)	2.289(2)
Au(1)-C(12)	2.708(10)
Au(1)-Fe(1)	2.7174(12)
Au(1)-Fe(3)	2.7236(11)
Au(1)-Au(2)	2.9157(6)
Au(2)-P(2)	2.293(2)
Au(2)-C(11)	2.659(10)
Au(2)-Fe(1)	2.6916(10)
Au(2)-Fe(2)	2.7093(10)
Au(2)-Au(3)	2.8829(4)
Au(2)-Fe(3)	2.8953(11)
Au(3)-P(1)	2.2844(19)
Au(3)-Fe(2)	2.6956(10)
Au(3)-Fe(3)	2.7650(12)
Fe(1)-C(10)	1.771(12)
Fe(1)-C(5)	1.786(10)
Fe(1)-C(12)	1.800(9)
Fe(1)-C(1)	1.940(7)
Fe(1)-Fe(2)	2.6985(16)
Fe(1)-Fe(3)	2.7164(14)
Fe(2)-C(7)	1.756(9)
Fe(2)-C(9)	1.773(9)
Fe(2)-C(11)	1.829(10)
Fe(2)-C(1)	1.916(9)
Fe(2)-Fe(3)	2.7169(18)
Fe(3)-C(8)	1.776(8)
Fe(3)-C(13)	1.785(11)
Fe(3)-C(6)	1.869(8)
Fe(3)-C(1)	1.945(8)
P(1)-C(111)	1.777(12)
P(1)-C(131)	1.790(11)
P(1)-C(121)	1.803(9)
P(2)-C(231)	1.769(10)
P(2)-C(211)	1.833(13)
P(2)-C(221)	1.836(10)
P(3)-C(321)	1.775(9)
P(3)-C(331)	1.804(12)
P(3)-C(311)	1.826(10)
O(1)-C(2)	1.184(10)
O(2)-C(2)	1.334(9)
O(2)-C(3)	1.404(9)
O(5)-C(5)	1.119(10)
O(6)-C(6)	1.098(9)
O(7)-C(7)	1.179(10)
O(8)-C(8)	1.148(9)
O(9)-C(9)	1.124(10)
O(10)-C(10)	1.130(12)
O(11)-C(11)	1.138(10)
O(12)-C(12)	1.162(9)
O(13)-C(13)	1.113(10)
C(1)-C(2)	1.482(10)
C(3)-C(4)	1.489(16)
C(111)-C(116)	1.399(15)
C(111)-C(112)	1.433(12)
C(112)-C(113)	1.368(15)

C(113)-C(114)	1.279(15)
C(114)-C(115)	1.361(13)
C(115)-C(116)	1.325(14)
C(121)-C(122)	1.353(13)
C(123)-C(224)	1.369(16)
C(124)-C(223)	1.317(19)
C(124)-C(225)	1.399(18)
C(121)-C(126)	1.398(15)
C(122)-C(123)	1.377(12)
C(125)-C(126)	1.381(12)
C(125)-C(224)	1.388(15)
C(131)-C(136)	1.350(17)
C(131)-C(132)	1.361(15)
C(132)-C(133)	1.345(14)
C(133)-C(134)	1.337(15)
C(134)-C(135)	1.379(15)
C(135)-C(136)	1.392(14)
C(211)-C(212)	1.351(15)
C(213)-C(214)	1.311(17)
C(214)-C(215)	1.318(15)
C(215)-C(216)	1.423(16)
C(211)-C(216)	1.363(17)
C(212)-C(213)	1.378(16)
C(221)-C(222)	1.348(14)
C(221)-C(226)	1.384(15)
C(222)-C(223)	1.392(14)
C(225)-C(226)	1.354(14)
C(231)-C(236)	1.352(15)
C(231)-C(232)	1.361(12)
C(232)-C(233)	1.390(18)
C(233)-C(234)	1.346(19)
C(234)-C(235)	1.396(16)
C(235)-C(236)	1.373(14)
C(311)-C(316)	1.330(13)
C(311)-C(312)	1.379(13)
C(312)-C(313)	1.366(12)
C(313)-C(314)	1.341(13)
C(314)-C(315)	1.361(13)
C(315)-C(316)	1.387(13)
C(321)-C(322)	1.340(14)
C(321)-C(326)	1.425(14)
C(322)-C(323)	1.379(14)
C(323)-C(324)	1.391(18)
C(324)-C(325)	1.291(18)
C(325)-C(326)	1.383(14)
C(331)-C(332)	1.322(15)
C(331)-C(336)	1.375(16)
C(332)-C(333)	1.405(15)
C(333)-C(334)	1.342(15)
C(334)-C(335)	1.307(14)
C(335)-C(336)	1.356(14)
C(14)-C(15)	1.507(10)
C(15)-O(14)	1.445(10)
C(16)-O(14)	1.442(10)
C(16)-C(17)	1.510(10)

P(3)-Au(1)-C(12)	114.5(2)
P(3)-Au(1)-Fe(1)	144.76(6)

C(12)-Au(1)-Fe(1)	38.76(19)
P(3)-Au(1)-Fe(3)	149.62(6)
C(12)-Au(1)-Fe(3)	95.18(19)
Fe(1)-Au(1)-Fe(3)	59.90(3)
P(3)-Au(1)-Au(2)	139.66(6)
C(12)-Au(1)-Au(2)	58.2(2)
Fe(1)-Au(1)-Au(2)	56.96(3)
Fe(3)-Au(1)-Au(2)	61.67(3)
P(2)-Au(2)-C(11)	101.8(2)
P(2)-Au(2)-Fe(1)	141.75(6)
C(11)-Au(2)-Fe(1)	92.20(17)
P(2)-Au(2)-Fe(2)	141.58(7)
C(11)-Au(2)-Fe(2)	39.8(2)
Fe(1)-Au(2)-Fe(2)	59.95(3)
P(2)-Au(2)-Au(3)	112.09(5)
C(11)-Au(2)-Au(3)	61.06(18)
Fe(1)-Au(2)-Au(3)	105.86(2)
Fe(2)-Au(2)-Au(3)	57.54(2)
P(2)-Au(2)-Fe(3)	152.87(7)
C(11)-Au(2)-Fe(3)	93.9(2)
Fe(1)-Au(2)-Fe(3)	58.04(3)
Fe(2)-Au(2)-Fe(3)	57.88(3)
Au(3)-Au(2)-Fe(3)	57.18(2)
P(2)-Au(2)-Au(1)	113.24(7)
C(11)-Au(2)-Au(1)	144.8(2)
Fe(1)-Au(2)-Au(1)	57.81(3)
Fe(2)-Au(2)-Au(1)	105.01(3)
Au(3)-Au(2)-Au(1)	106.569(15)
Fe(3)-Au(2)-Au(1)	55.90(3)
P(1)-Au(3)-Fe(2)	153.37(7)
P(1)-Au(3)-Fe(3)	142.66(7)
Fe(2)-Au(3)-Fe(3)	59.66(4)
P(1)-Au(3)-Au(2)	137.48(5)
Fe(2)-Au(3)-Au(2)	58.00(2)
Fe(3)-Au(3)-Au(2)	61.64(2)
C(10)-Fe(1)-C(5)	93.8(4)
C(10)-Fe(1)-C(12)	88.7(4)
C(5)-Fe(1)-C(12)	98.2(4)
C(10)-Fe(1)-C(1)	98.5(4)
C(5)-Fe(1)-C(1)	93.7(4)
C(12)-Fe(1)-C(1)	165.6(3)
C(10)-Fe(1)-Au(2)	117.8(3)
C(5)-Fe(1)-Au(2)	146.1(3)
C(12)-Fe(1)-Au(2)	72.1(3)
C(1)-Fe(1)-Au(2)	93.5(2)
C(10)-Fe(1)-Fe(2)	87.7(3)
C(5)-Fe(1)-Fe(2)	138.4(3)
C(12)-Fe(1)-Fe(2)	123.4(3)
C(1)-Fe(1)-Fe(2)	45.2(3)
Au(2)-Fe(1)-Fe(2)	60.35(3)
C(10)-Fe(1)-Fe(3)	142.6(3)
C(5)-Fe(1)-Fe(3)	98.3(3)
C(12)-Fe(1)-Fe(3)	124.0(3)
C(1)-Fe(1)-Fe(3)	45.7(2)
Au(2)-Fe(1)-Fe(3)	64.74(3)
Fe(2)-Fe(1)-Fe(3)	60.23(4)
C(10)-Fe(1)-Au(1)	157.2(3)
C(5)-Fe(1)-Au(1)	80.8(3)

C(12)-Fe(1)-Au(1)	70.3(3)
C(1)-Fe(1)-Au(1)	104.0(2)
Au(2)-Fe(1)-Au(1)	65.24(3)
Fe(2)-Fe(1)-Au(1)	111.05(4)
Fe(3)-Fe(1)-Au(1)	60.16(3)
C(7)-Fe(2)-C(9)	92.3(4)
C(7)-Fe(2)-C(11)	100.2(4)
C(9)-Fe(2)-C(11)	90.1(4)
C(7)-Fe(2)-C(1)	98.1(4)
C(9)-Fe(2)-C(1)	95.6(4)
C(11)-Fe(2)-C(1)	160.6(4)
C(7)-Fe(2)-Au(3)	72.1(3)
C(9)-Fe(2)-Au(3)	155.1(3)
C(11)-Fe(2)-Au(3)	74.4(2)
C(1)-Fe(2)-Au(3)	105.4(2)
C(7)-Fe(2)-Fe(1)	144.0(3)
C(9)-Fe(2)-Fe(1)	92.9(3)
C(11)-Fe(2)-Fe(1)	115.4(3)
C(1)-Fe(2)-Fe(1)	45.9(2)
Au(3)-Fe(2)-Fe(1)	111.15(5)
C(7)-Fe(2)-Au(2)	136.5(3)
C(9)-Fe(2)-Au(2)	128.1(3)
C(11)-Fe(2)-Au(2)	68.6(3)
C(1)-Fe(2)-Au(2)	93.5(2)
Au(3)-Fe(2)-Au(2)	64.47(2)
Fe(1)-Fe(2)-Au(2)	59.70(3)
C(7)-Fe(2)-Fe(3)	95.3(3)
C(9)-Fe(2)-Fe(3)	141.3(3)
C(11)-Fe(2)-Fe(3)	125.5(3)
C(1)-Fe(2)-Fe(3)	45.7(2)
Au(3)-Fe(2)-Fe(3)	61.44(3)
Fe(1)-Fe(2)-Fe(3)	60.21(4)
Au(2)-Fe(2)-Fe(3)	64.50(3)
C(8)-Fe(3)-C(13)	91.3(4)
C(8)-Fe(3)-C(6)	96.2(3)
C(13)-Fe(3)-C(6)	95.9(4)
C(8)-Fe(3)-C(1)	91.2(3)
C(13)-Fe(3)-C(1)	93.7(4)
C(6)-Fe(3)-C(1)	167.7(4)
C(8)-Fe(3)-Fe(1)	136.8(2)
C(13)-Fe(3)-Fe(1)	91.8(2)
C(6)-Fe(3)-Fe(1)	126.2(2)
C(1)-Fe(3)-Fe(1)	45.6(2)
C(8)-Fe(3)-Fe(2)	91.6(3)
C(13)-Fe(3)-Fe(2)	138.5(3)
C(6)-Fe(3)-Fe(2)	124.9(3)
C(1)-Fe(3)-Fe(2)	44.8(3)
Fe(1)-Fe(3)-Fe(2)	59.56(4)
C(8)-Fe(3)-Au(1)	158.1(3)
C(13)-Fe(3)-Au(1)	72.1(2)
C(6)-Fe(3)-Au(1)	72.2(2)
C(1)-Fe(3)-Au(1)	103.6(2)
Fe(1)-Fe(3)-Au(1)	59.94(3)
Fe(2)-Fe(3)-Au(1)	110.30(4)
C(8)-Fe(3)-Au(3)	75.7(3)
C(13)-Fe(3)-Au(3)	159.6(2)
C(6)-Fe(3)-Au(3)	70.5(3)
C(1)-Fe(3)-Au(3)	102.1(3)

Fe(1)-Fe(3)-Au(3)	108.53(5)
Fe(2)-Fe(3)-Au(3)	58.90(3)
Au(1)-Fe(3)-Au(3)	115.75(4)
C(8)-Fe(3)-Au(2)	135.4(3)
C(13)-Fe(3)-Au(2)	133.3(2)
C(6)-Fe(3)-Au(2)	80.4(2)
C(1)-Fe(3)-Au(2)	87.4(2)
Fe(1)-Fe(3)-Au(2)	57.22(3)
Fe(2)-Fe(3)-Au(2)	57.63(3)
Au(1)-Fe(3)-Au(2)	62.43(2)
Au(3)-Fe(3)-Au(2)	61.18(3)
C(111)-P(1)-C(131)	101.7(6)
C(111)-P(1)-C(121)	104.1(5)
C(131)-P(1)-C(121)	106.2(6)
C(111)-P(1)-Au(3)	115.3(4)
C(131)-P(1)-Au(3)	111.9(4)
C(121)-P(1)-Au(3)	116.2(3)
C(231)-P(2)-C(211)	98.9(6)
C(231)-P(2)-C(221)	104.5(5)
C(211)-P(2)-C(221)	104.5(6)
C(231)-P(2)-Au(2)	119.1(4)
C(211)-P(2)-Au(2)	117.2(4)
C(221)-P(2)-Au(2)	110.8(4)
C(321)-P(3)-C(331)	105.9(5)
C(321)-P(3)-C(311)	104.7(5)
C(331)-P(3)-C(311)	101.6(6)
C(321)-P(3)-Au(1)	117.2(3)
C(331)-P(3)-Au(1)	114.7(4)
C(311)-P(3)-Au(1)	111.3(4)
C(2)-O(2)-C(3)	116.8(8)
C(2)-C(1)-Fe(2)	128.5(6)
C(2)-C(1)-Fe(1)	122.8(5)
Fe(2)-C(1)-Fe(1)	88.8(3)
C(2)-C(1)-Fe(3)	126.5(6)
Fe(2)-C(1)-Fe(3)	89.5(3)
Fe(1)-C(1)-Fe(3)	88.7(3)
O(1)-C(2)-O(2)	122.6(7)
O(1)-C(2)-C(1)	125.1(7)
O(2)-C(2)-C(1)	112.2(7)
O(2)-C(3)-C(4)	107.7(9)
O(5)-C(5)-Fe(1)	172.6(9)
O(6)-C(6)-Fe(3)	172.0(8)
O(7)-C(7)-Fe(2)	171.2(8)
O(8)-C(8)-Fe(3)	173.5(8)
O(9)-C(9)-Fe(2)	174.4(8)
O(10)-C(10)-Fe(1)	171.4(10)
O(11)-C(11)-Fe(2)	170.0(8)
O(11)-C(11)-Au(2)	117.5(7)
Fe(2)-C(11)-Au(2)	71.6(3)
O(12)-C(12)-Fe(1)	169.3(7)
O(12)-C(12)-Au(1)	113.8(7)
Fe(1)-C(12)-Au(1)	70.9(3)
O(13)-C(13)-Fe(3)	175.5(7)
C(116)-C(111)-C(112)	114.4(11)
C(116)-C(111)-P(1)	122.4(8)
C(112)-C(111)-P(1)	123.1(10)
C(113)-C(112)-C(111)	120.3(12)
C(113)-C(112)-H(112)	119.8

C(111)-C(112)-H(112)	119.8
C(114)-C(113)-C(112)	121.9(10)
C(113)-C(114)-C(115)	120.1(12)
C(116)-C(115)-C(114)	122.0(12)
C(115)-C(116)-C(111)	121.2(10)
C(122)-C(121)-C(126)	118.3(9)
C(122)-C(121)-P(1)	125.2(9)
C(126)-C(121)-P(1)	116.4(7)
C(121)-C(122)-C(123)	122.5(11)
C(224)-C(123)-C(122)	117.0(10)
C(223)-C(124)-C(225)	123.1(11)
C(126)-C(125)-C(224)	115.9(10)
C(125)-C(126)-C(121)	122.0(9)
C(136)-C(131)-C(132)	115.9(11)
C(136)-C(131)-P(1)	123.8(9)
C(132)-C(131)-P(1)	120.1(10)
C(133)-C(132)-C(131)	124.8(12)
C(134)-C(133)-C(132)	118.4(12)
C(133)-C(134)-C(135)	120.6(11)
C(134)-C(135)-C(136)	118.3(12)
C(131)-C(136)-C(135)	121.8(12)
C(212)-C(211)-C(216)	119.7(12)
C(212)-C(211)-P(2)	117.8(10)
C(216)-C(211)-P(2)	122.5(9)
C(211)-C(212)-C(213)	119.6(13)
C(214)-C(213)-C(212)	119.8(12)
C(213)-C(214)-C(215)	122.4(13)
C(214)-C(215)-C(216)	117.8(13)
C(211)-C(216)-C(215)	118.7(11)
C(222)-C(221)-C(226)	119.2(10)
C(222)-C(221)-P(2)	124.3(10)
C(226)-C(221)-P(2)	116.5(8)
C(221)-C(222)-C(223)	120.4(12)
C(124)-C(223)-C(222)	118.8(11)
C(123)-C(224)-C(125)	123.9(10)
C(226)-C(225)-C(124)	116.5(13)
C(225)-C(226)-C(221)	121.6(11)
C(236)-C(231)-C(232)	116.5(11)
C(236)-C(231)-P(2)	117.9(7)
C(232)-C(231)-P(2)	125.5(11)
C(231)-C(232)-C(233)	121.4(14)
C(234)-C(233)-C(232)	120.4(11)
C(233)-C(234)-C(235)	119.5(11)
C(236)-C(235)-C(234)	117.2(13)
C(231)-C(236)-C(235)	124.6(11)
C(316)-C(311)-C(312)	118.7(9)
C(316)-C(311)-P(3)	119.6(8)
C(312)-C(311)-P(3)	121.5(8)
C(313)-C(312)-C(311)	119.6(10)
C(314)-C(313)-C(312)	121.0(10)
C(313)-C(314)-C(315)	119.8(10)
C(314)-C(315)-C(316)	118.4(10)
C(311)-C(316)-C(315)	121.1(10)
C(322)-C(321)-C(326)	115.0(9)
C(322)-C(321)-P(3)	122.3(8)
C(326)-C(321)-P(3)	122.7(8)
C(321)-C(322)-C(323)	123.3(12)
C(322)-C(323)-C(324)	119.1(12)

C(325)-C(324)-C(323)	119.8(11)
C(324)-C(325)-C(326)	121.4(13)
C(325)-C(326)-C(321)	121.0(12)
C(332)-C(331)-C(336)	119.6(11)
C(332)-C(331)-P(3)	119.3(10)
C(336)-C(331)-P(3)	121.0(9)
C(331)-C(332)-C(333)	120.9(13)
C(334)-C(333)-C(332)	118.9(11)
C(335)-C(334)-C(333)	118.3(12)
C(334)-C(335)-C(336)	124.7(13)
C(335)-C(336)-C(331)	117.1(11)
O(14)-C(15)-C(14)	104.1(9)
O(14)-C(16)-C(17)	104.2(9)
C(16)-O(14)-C(15)	112.1(10)

Symmetry transformations used to generate equivalent atoms.