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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 Uij tensor.

	x	y	z	U(eq)
Zr	304(1)	725(1)	1384(1)	42(1)
Co(1)	-543(2)	1853(1)	3240(1)	53(1)
C(111)	-679(16)	2732(8)	3694(12)	84(6)
C(112)	50(16)	2411(9)	4182(11)	76(5)
C(113)	-1658(13)	2439(8)	3695(11)	74(5)
C(114)	-1540(15)	1930(9)	4194(11)	84(6)
C(115)	-460(16)	1934(9)	4513(10)	77(5)
P(1)	848(3)	1969(2)	2558(3)	62(1)
P(2)	-281(3)	869(2)	3349(2)	52(1)
P(3)	-1475(3)	1757(2)	2100(3)	60(1)
Co(2)	2656(1)	-512(1)	890(1)	45(1)
C(211)	3799(13)	-1116(9)	1379(11)	72(5)
C(212)	3047(13)	-1179(8)	80(11)	68(5)
C(213)	3848(14)	-735(8)	116(11)	74(5)
C(214)	3054(14)	-1410(7)	871(14)	75(6)
C(215)	4290(12)	-704(8)	933(12)	74(5)
P(4)	923(3)	-659(2)	672(2)	51(1)
P(5)	2525(3)	386(2)	386(3)	57(1)
P(6)	2403(3)	-179(2)	2089(2)	56(1)
O(11)	1062(7)	1518(4)	1879(6)	51(2)
O(12)	809(10)	2619(4)	2169(8)	84(4)
C(12)	1760(2)	2788(12)	1802(18)	31(7)
C(13)	1300(4)	2772(17)	850(3)	76(14)
C(12')	1410(3)	2849(13)	1420(2)	56(10)
C(13')	980(6)	3060(4)	710(4)	190(4)
O(14)	1951(9)	2033(5)	3116(8)	79(4)
C(14)	2608(16)	1526(11)	3375(14)	101(7)
C(15)	3280(3)	1618(16)	4040(2)	260(3)
O(20)	665(8)	709(5)	3884(6)	64(3)
O(21)	-321(6)	552(4)	2498(5)	47(2)
O(22)	-1354(8)	608(5)	3744(6)	65(3)
C(22)	-1300(15)	70(9)	4182(12)	94(6)
C(23)	-2315(16)	-74(10)	4511(14)	115(8)
O(31)	-1023(8)	1403(4)	1411(6)	58(3)
O(32)	-1715(11)	2443(6)	1774(7)	88(4)
C(32)	-2310(2)	2586(9)	1049(13)	112(8)
C(33)	-2620(8)	3150(3)	1060(6)	200(6)
C(33')	-2920(5)	3110(4)	1210(4)	220(5)
O(34)	-2690(10)	1569(8)	2175(9)	101(4)
C(34)	-2994(18)	971(11)	2218(13)	107(7)
C(35)	-3950(3)	932(17)	2880(2)	70(10)
C(35')	-3770(5)	890(4)	2590(4)	270(7)
O(40)	580(7)	-733(4)	-235(6)	57(3)
O(41)	259(7)	-203(4)	1129(6)	52(2)
O(42)	639(8)	-1280(4)	1129(7)	64(3)
C(42)	63(17)	-1749(9)	749(14)	101(7)
C(43)	-240(2)	-2177(12)	1348(17)	148(11)
O(51)	1557(7)	768(4)	545(5)	53(2)

O(52)	2594(12)	352(7)	-564(8)	91(5)
C(52)	2420(3)	865(10)	-1070(19)	48(8)
C(53)	2552(18)	677(10)	-1968(11)	103(7)
C(52')	2230(4)	490(4)	-1080(4)	190(4)
O(54)	3573(8)	794(6)	641(10)	92(4)
C(54)	3720(6)	1310(4)	1020(6)	250(7)
C(55)	4220(6)	1700(2)	1160(3)	71(18)
C(54')	3630(4)	1120(3)	1240(3)	85(15)
C(55')	4110(4)	1790(2)	850(3)	87(18)
O(61)	1726(7)	388(4)	2137(5)	50(2)
O(62)	1996(8)	-709(5)	2660(6)	65(3)
C(62)	988(13)	-693(8)	3033(10)	75(5)
C(63)	874(19)	-1249(11)	3497(16)	132(9)
O(64)	3565(7)	-35(5)	2549(6)	57(3)
C(64)	3684(16)	78(10)	3395(11)	96(6)
C(65)	4380(5)	-170(5)	3830(5)	400(11)
C(65')	4280(4)	-430(17)	3880(2)	66(12)

Bond lengths (Å) and angles (deg) for **1**.

Zr-O(21)	2.064(8)	P(4)-O(41)	1.537(9)
Zr-O(41)	2.100(9)	P(4)-O(42)	1.617(10)
Zr-O(40)#1	2.105(10)	P(5)-C(53')	0.897(4)
Zr-O(11)	2.130(8)	P(5)-O(51)	1.520(9)
Zr-O(51)	2.159(8)	P(5)-O(52)	1.558(13)
Zr-O(61)	2.224(9)	P(5)-O(54)	1.627(12)
Zr-O(31)	2.247(9)	P(6)-O(61)	1.523(9)
Co(1)-C(114)	2.070(14)	P(6)-O(62)	1.605(10)
Co(1)-C(115)	2.076(16)	P(6)-O(64)	1.625(10)
Co(1)-C(112)	2.068(17)	O(12)-C(12)	1.42(3)
Co(1)-C(113)	2.086(15)	O(12)-C(12')	1.57(3)
Co(1)-C(111)	2.097(16)	C(12)-C(13)	1.62(4)
Co(1)-P(3)	2.133(5)	C(12')-C(13')	1.33(5)
Co(1)-P(1)	2.153(4)	O(14)-C(14)	1.44(2)
Co(1)-P(2)	2.211(4)	C(14)-C(15)	1.34(3)
C(111)-C(112)	1.37(3)	O(22)-C(22)	1.389(19)
C(111)-C(113)	1.39(2)	C(22)-C(23)	1.45(2)
C(112)-C(115)	1.37(2)	O(32)-C(32)	1.39(2)
C(113)-C(114)	1.39(2)	C(32)-C(33)	1.31(6)
C(114)-C(115)	1.42(3)	C(32)-C(33')	1.43(5)
P(1)-O(11)	1.529(9)	O(34)-C(34)	1.38(2)
P(1)-O(12)	1.573(11)	C(34)-C(35')	1.20(5)
P(1)-O(14)	1.608(13)	C(34)-C(35)	1.68(3)
P(2)-O(20)	1.465(11)	O(40)-Zr#1	2.105(10)
P(2)-O(21)	1.551(9)	O(42)-C(42)	1.39(2)
P(2)-O(22)	1.640(9)	C(42)-C(43)	1.43(3)
P(3)-O(31)	1.513(9)	O(51)-C(53')	1.603(8)
P(3)-O(34)	1.596(13)	O(52)-C(52')	0.98(8)
P(3)-O(32)	1.632(13)	O(52)-C(53')	1.165(14)
Co(2)-C(214)	2.054(15)	O(52)-C(52)	1.41(3)
Co(2)-C(212)	2.064(15)	C(52)-C(53)	1.54(3)
Co(2)-C(213)	2.085(14)	C(52')-C(53')	1.83(6)
Co(2)-C(211)	2.080(15)	C(53')-O(54)	1.614(14)

Co(2)-C(215)	2.093(15)	O(54)-C(54')	1.20(4)
Co(2)-P(6)	2.132(4)	O(54)-C(54)	1.31(6)
Co(2)-P(5)	2.154(4)	C(54)-C(55)	1.08(7)
Co(2)-P(4)	2.206(4)	C(54')-C(55')	1.74(6)
C(211)-C(215)	1.34(2)	O(62)-C(62)	1.444(17)
C(211)-C(214)	1.37(2)	C(62)-C(63)	1.46(2)
C(212)-C(214)	1.39(2)	O(64)-C(64)	1.40(2)
C(212)-C(213)	1.41(2)	C(64)-C(65)	1.21(7)
C(213)-C(215)	1.41(2)	C(64)-C(65')	1.54(5)
P(4)-O(40)	1.517(10)		

O(21)-Zr-O(41)	89.1(3)	C(212)-Co(2)-P(4)	93.9(5)
O(21)-Zr-O(40)#1	124.9(4)	C(213)-Co(2)-P(4)	127.7(6)
O(41)-Zr-O(40)#1	80.1(4)	C(211)-Co(2)-P(4)	127.8(6)
O(21)-Zr-O(11)	90.5(3)	C(215)-Co(2)-P(4)	158.4(6)
O(41)-Zr-O(11)	152.7(4)	P(6)-Co(2)-P(4)	89.32(16)
O(40)#1-Zr-O(11)	121.5(4)	P(5)-Co(2)-P(4)	91.60(16)
O(21)-Zr-O(51)	154.8(3)	C(215)-C(211)-C(214)	108.5(17)
O(41)-Zr-O(51)	85.9(3)	C(215)-C(211)-Co(2)	71.7(9)
O(40)#1-Zr-O(51)	78.5(4)	C(214)-C(211)-Co(2)	69.6(9)
O(11)-Zr-O(51)	82.9(3)	C(214)-C(212)-C(213)	105.2(16)
O(21)-Zr-O(61)	78.1(3)	C(214)-C(212)-Co(2)	70.0(9)
O(41)-Zr-O(61)	77.8(3)	C(213)-C(212)-Co(2)	71.0(9)
O(40)#1-Zr-O(61)	147.6(3)	C(212)-C(213)-C(215)	107.9(16)
O(11)-Zr-O(61)	75.4(3)	C(212)-C(213)-Co(2)	69.4(8)
O(51)-Zr-O(61)	76.7(3)	C(215)-C(213)-Co(2)	70.7(8)
O(21)-Zr-O(31)	77.2(3)	C(211)-C(214)-C(212)	110.1(16)
O(41)-Zr-O(31)	130.6(4)	C(211)-C(214)-Co(2)	71.7(10)
O(40)#1-Zr-O(31)	70.6(3)	C(212)-C(214)-Co(2)	70.7(9)
O(11)-Zr-O(31)	75.7(4)	C(211)-C(215)-C(213)	108.2(18)
O(51)-Zr-O(31)	124.0(3)	C(211)-C(215)-Co(2)	70.7(9)
O(61)-Zr-O(31)	141.5(3)	C(213)-C(215)-Co(2)	70.0(9)
C(114)-Co(1)-C(115)	40.0(7)	O(40)-P(4)-O(41)	114.6(5)
C(114)-Co(1)-C(112)	66.4(7)	O(40)-P(4)-O(42)	107.4(6)
C(115)-Co(1)-C(112)	38.5(7)	O(41)-P(4)-O(42)	101.1(5)
C(114)-Co(1)-C(113)	39.1(7)	O(40)-P(4)-Co(2)	112.4(4)
C(115)-Co(1)-C(113)	65.1(8)	O(41)-P(4)-Co(2)	112.9(4)
C(112)-Co(1)-C(113)	65.1(7)	O(42)-P(4)-Co(2)	107.5(4)
C(114)-Co(1)-C(111)	65.8(7)	C(53')-P(5)-O(51)	78.4(4)
C(115)-Co(1)-C(111)	64.3(8)	C(53')-P(5)-O(52)	47.9(6)
C(112)-Co(1)-C(111)	38.4(7)	O(51)-P(5)-O(52)	107.4(6)
C(113)-Co(1)-C(111)	38.9(6)	C(53')-P(5)-O(54)	73.1(6)
C(114)-Co(1)-P(3)	109.7(6)	O(51)-P(5)-O(54)	106.8(6)
C(115)-Co(1)-P(3)	149.6(6)	O(52)-P(5)-O(54)	100.3(9)
C(112)-Co(1)-P(3)	148.3(6)	C(53')-P(5)-Co(2)	156.3(4)
C(113)-Co(1)-P(3)	91.7(5)	O(51)-P(5)-Co(2)	119.4(4)
C(111)-Co(1)-P(3)	110.2(7)	O(52)-P(5)-Co(2)	109.0(6)
C(114)-Co(1)-P(1)	159.1(5)	O(54)-P(5)-Co(2)	112.2(5)
C(115)-Co(1)-P(1)	121.3(6)	O(61)-P(6)-O(62)	111.8(5)
C(112)-Co(1)-P(1)	92.7(5)	O(61)-P(6)-O(64)	107.6(6)
C(113)-Co(1)-P(1)	134.4(5)	O(62)-P(6)-O(64)	100.9(6)
C(111)-Co(1)-P(1)	99.2(5)	O(61)-P(6)-Co(2)	117.0(4)
P(3)-Co(1)-P(1)	88.79(17)	O(62)-P(6)-Co(2)	110.6(4)

C(114)-Co(1)-P(2)	96.7(6)	O(64)-P(6)-Co(2)	107.5(4)
C(115)-Co(1)-P(2)	90.5(6)	P(1)-O(11)-Zr	135.8(5)
C(112)-Co(1)-P(2)	119.2(6)	C(12)-O(12)-P(1)	114.0(14)
C(113)-Co(1)-P(2)	133.3(5)	C(12)-O(12)-C(12')	28.4(12)
C(111)-Co(1)-P(2)	154.8(6)	P(1)-O(12)-C(12')	127.5(14)
P(3)-Co(1)-P(2)	92.37(17)	O(12)-C(12)-C(13)	98(3)
P(1)-Co(1)-P(2)	92.16(15)	C(13')-C(12')-O(12)	127(4)
C(112)-C(111)-C(113)	108.1(19)	C(14)-O(14)-P(1)	123.3(11)
C(112)-C(111)-Co(1)	69.7(10)	C(15)-C(14)-O(14)	116(2)
C(113)-C(111)-Co(1)	70.1(9)	P(2)-O(21)-Zr	135.3(5)
C(111)-C(112)-C(115)	108.5(18)	C(22)-O(22)-P(2)	119.5(10)
C(111)-C(112)-Co(1)	72.0(10)	O(22)-C(22)-C(23)	111.5(17)
C(115)-C(112)-Co(1)	71.0(10)	P(3)-O(31)-Zr	132.8(6)
C(111)-C(113)-C(114)	108.8(18)	C(32)-O(32)-P(3)	124.5(13)
C(111)-C(113)-Co(1)	71.0(9)	C(33)-C(32)-O(32)	110(5)
C(114)-C(113)-Co(1)	69.8(9)	C(33)-C(32)-C(33')	19(7)
C(113)-C(114)-C(115)	105.5(16)	O(32)-C(32)-C(33')	107(3)
C(113)-C(114)-Co(1)	71.1(9)	C(34)-O(34)-P(3)	121.6(14)
C(115)-C(114)-Co(1)	70.2(9)	C(35')-C(34)-O(34)	114(5)
C(112)-C(115)-C(114)	108.9(19)	C(35')-C(34)-C(35)	11(5)
C(112)-C(115)-Co(1)	70.4(10)	O(34)-C(34)-C(35)	107(2)
C(114)-C(115)-Co(1)	69.8(9)	P(4)-O(40)-Zr#1	163.5(6)
O(11)-P(1)-O(12)	108.0(6)	P(4)-O(41)-Zr	137.2(5)
O(11)-P(1)-O(14)	106.1(6)	C(42)-O(42)-P(4)	123.9(12)
O(12)-P(1)-O(14)	98.5(7)	O(42)-C(42)-C(43)	110(2)
O(11)-P(1)-Co(1)	119.1(4)	P(5)-O(51)-C(53')	33.2(2)
O(12)-P(1)-Co(1)	108.3(4)	P(5)-O(51)-Zr	135.4(5)
O(14)-P(1)-Co(1)	114.8(5)	C(53')-O(51)-Zr	168.6(5)
O(20)-P(2)-O(21)	113.2(5)	C(52')-O(52)-C(53')	116(5)
O(20)-P(2)-O(22)	109.7(6)	C(52')-O(52)-C(52)	37(4)
O(21)-P(2)-O(22)	102.5(5)	C(53')-O(52)-C(52)	87.4(14)
O(20)-P(2)-Co(1)	113.4(5)	C(52')-O(52)-P(5)	142(4)
O(21)-P(2)-Co(1)	112.3(4)	C(53')-O(52)-P(5)	34.8(4)
O(22)-P(2)-Co(1)	104.9(4)	C(52)-O(52)-P(5)	121.5(15)
O(31)-P(3)-O(34)	109.4(7)	O(52)-C(52)-C(53)	108.2(17)
O(31)-P(3)-O(32)	108.2(6)	O(52)-C(52')-C(53')	35(3)
O(34)-P(3)-O(32)	96.5(8)	P(5)-C(53')-O(52)	97.3(7)
O(31)-P(3)-Co(1)	119.0(4)	P(5)-C(53')-O(51)	68.3(4)
O(34)-P(3)-Co(1)	115.4(6)	O(52)-C(53')-O(51)	126.6(9)
O(32)-P(3)-Co(1)	105.5(5)	P(5)-C(53')-O(54)	74.7(5)
C(214)-Co(2)-C(212)	39.3(7)	O(52)-C(53')-O(54)	122.4(9)
C(214)-Co(2)-C(213)	64.8(7)	O(51)-C(53')-O(54)	103.6(6)
C(212)-Co(2)-C(213)	39.6(6)	P(5)-C(53')-C(52')	120(3)
C(214)-Co(2)-C(211)	38.7(7)	O(52)-C(53')-C(52')	29(3)
C(212)-Co(2)-C(211)	66.0(7)	O(51)-C(53')-C(52')	115.7(15)
C(213)-Co(2)-C(211)	64.6(6)	O(54)-C(53')-C(52')	140.7(15)
C(214)-Co(2)-C(215)	64.1(7)	C(54')-O(54)-C(54)	26(5)
C(212)-Co(2)-C(215)	66.3(7)	C(54')-O(54)-C(53')	128(3)
C(213)-Co(2)-C(215)	39.3(7)	C(54)-O(54)-C(53')	122(5)
C(211)-Co(2)-C(215)	37.6(6)	C(54')-O(54)-P(5)	123(2)
C(214)-Co(2)-P(6)	113.7(6)	C(54)-O(54)-P(5)	134(3)
C(212)-Co(2)-P(6)	153.0(6)	C(53')-O(54)-P(5)	32.1(3)
C(213)-Co(2)-P(6)	142.8(6)	C(55)-C(54)-O(54)	149(8)

C(211)-Co(2)-P(6)	91.0(5)	O(54)-C(54')-C(55')	102(3)
C(215)-Co(2)-P(6)	104.5(6)	P(6)-O(61)-Zr	132.8(6)
C(214)-Co(2)-P(5)	154.4(6)	C(62)-O(62)-P(6)	123.5(9)
C(212)-Co(2)-P(5)	115.7(6)	O(62)-C(62)-C(63)	108.6(15)
C(213)-Co(2)-P(5)	91.6(5)	C(64)-O(64)-P(6)	121.2(10)
C(211)-Co(2)-P(5)	140.6(6)	C(65)-C(64)-O(64)	121(5)
C(215)-Co(2)-P(5)	104.4(5)	C(65)-C(64)-C(65')	21(5)
P(6)-Co(2)-P(5)	90.92(17)	O(64)-C(64)-C(65')	113.1(19)
C(214)-Co(2)-P(4)	95.3(6)		

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z

Anisotropic displacement parameters ($Å^2 \times 10^3$) for **1**. 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
Zr	34(1)	46(1)	48(1)	-3(1)	16(1)	0(1)
Co(1)	47(1)	58(1)	58(1)	-10(1)	27(1)	-6(1)
C(111)	90(14)	59(11)	108(15)	-24(10)	48(12)	-13(10)
C(112)	79(12)	76(13)	74(12)	-35(10)	20(10)	0(11)
C(113)	56(10)	96(13)	74(12)	-22(10)	20(9)	17(9)
C(114)	86(13)	89(14)	85(13)	-34(11)	56(11)	-35(11)
C(115)	85(14)	99(14)	50(10)	-14(9)	26(9)	-17(11)
P(1)	57(2)	54(2)	81(3)	-19(2)	38(2)	-16(2)
P(2)	46(2)	62(2)	51(2)	1(2)	22(2)	-1(2)
P(3)	50(2)	68(3)	63(3)	-5(2)	22(2)	11(2)
Co(2)	35(1)	52(1)	48(1)	4(1)	12(1)	7(1)
C(211)	49(10)	105(13)	63(11)	16(10)	8(9)	32(10)
C(212)	50(10)	82(12)	74(12)	-19(10)	12(9)	24(9)
C(213)	64(11)	89(12)	73(14)	20(9)	40(10)	45(10)
C(214)	58(10)	51(10)	121(18)	14(11)	38(11)	30(8)
C(215)	40(9)	84(12)	101(15)	6(10)	24(9)	22(8)
P(4)	47(2)	51(2)	56(3)	1(2)	14(2)	-1(2)
P(5)	47(2)	65(2)	64(3)	8(2)	28(2)	8(2)
P(6)	44(2)	66(2)	59(3)	3(2)	13(2)	2(2)
O(11)	46(5)	41(5)	69(6)	-7(4)	34(5)	-10(4)
O(12)	101(9)	39(6)	122(10)	-16(6)	71(8)	-13(6)
C(12)	33(19)	34(14)	26(18)	9(11)	11(14)	-8(13)
C(13)	150(4)	70(3)	10(2)	27(17)	-30(2)	-20(2)
C(12')	64(19)	78(17)	20(2)	52(17)	-17(17)	-35(14)
C(13')	190(7)	230(10)	160(6)	150(6)	20(5)	-20(6)
O(14)	56(7)	74(8)	110(9)	-44(7)	34(7)	-21(6)
C(14)	67(12)	120(2)	113(17)	-43(15)	10(12)	-28(13)
C(15)	330(6)	170(4)	270(5)	-150(4)	-130(5)	50(4)
O(20)	59(7)	79(7)	55(6)	-2(5)	5(5)	6(6)
O(21)	33(5)	53(5)	58(6)	3(4)	17(4)	-11(4)
O(22)	57(6)	82(7)	61(6)	16(5)	39(5)	1(5)
C(22)	76(13)	114(15)	95(14)	44(12)	26(11)	-11(11)
C(23)	100(16)	121(17)	126(19)	68(15)	23(14)	-17(13)
O(31)	60(6)	62(6)	55(6)	-9(5)	18(5)	14(5)
O(32)	113(10)	91(9)	64(8)	-10(7)	33(7)	30(8)
C(32)	180(2)	80(13)	78(16)	19(11)	22(16)	15(14)

C(33)	310(17)	50(4)	230(9)	-40(5)	0(10)	30(6)
C(33')	200(5)	350(10)	90(4)	-60(4)	-80(3)	260(7)
O(34)	58(7)	138(13)	109(11)	-15(10)	9(7)	-6(8)
C(34)	117(17)	107(18)	102(15)	2(13)	44(13)	-20(14)
C(35)	50(2)	120(3)	50(2)	45(17)	39(17)	2(19)
C(35')	100(5)	610(18)	120(6)	140(8)	110(5)	180(8)
O(40)	45(6)	68(6)	58(7)	-11(5)	5(5)	21(5)
O(41)	40(5)	51(5)	66(6)	-8(5)	21(5)	-7(4)
O(42)	65(7)	47(6)	82(8)	4(5)	16(6)	-9(5)
C(42)	96(15)	79(13)	127(18)	25(12)	15(13)	-21(11)
C(43)	170(2)	110(2)	170(3)	30(19)	50(2)	-47(18)
O(51)	56(6)	53(6)	53(6)	10(4)	22(5)	17(5)
O(52)	105(11)	117(11)	55(8)	28(8)	34(7)	65(9)
C(52)	70(2)	21(12)	55(19)	7(11)	39(17)	18(12)
C(53)	117(17)	132(19)	65(12)	22(12)	30(11)	29(14)
C(52')	60(3)	400(12)	110(5)	-40(7)	40(3)	-120(6)
O(54)	44(6)	89(9)	146(14)	18(9)	25(7)	-18(6)
C(54)	120(5)	180(8)	470(16)	-230(9)	160(7)	-130(6)
C(55)	110(4)	30(3)	80(4)	20(2)	50(3)	30(3)
C(54')	80(3)	150(4)	20(2)	-40(2)	40(2)	-60(3)
C(55')	100(3)	80(2)	100(3)	50(3)	80(3)	-20(2)
O(61)	37(5)	59(6)	55(6)	-6(4)	13(4)	5(4)
O(62)	57(6)	73(6)	70(7)	19(5)	32(5)	12(5)
C(62)	54(9)	105(13)	67(10)	26(9)	26(8)	3(9)
C(63)	120(19)	130(2)	150(2)	44(18)	80(17)	4(16)
O(64)	42(5)	87(8)	42(6)	-4(5)	1(4)	-8(5)
C(64)	83(13)	147(18)	58(14)	13(12)	12(10)	-11(13)
C(65)	80(3)	900(3)	250(9)	410(14)	-60(4)	-80(8)
C(65')	100(3)	60(2)	30(2)	-14(18)	0(2)	0(2)

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

	x	y	z	U(eq)
H(111)	-542	3089	3408	53(13)
H(112)	779	2503	4274	53(13)
H(113)	-2295	2564	3407	53(13)
H(114)	-2065	1643	4296	53(13)
H(115)	-146	1655	4892	53(13)
H(211)	3942	-1190	1944	53(13)
H(212)	2602	-1294	-382	53(13)
H(213)	4052	-501	-327	53(13)
H(214)	2612	-1723	1035	53(13)
H(215)	4834	-441	1133	53(13)
H(12A)	2335	2495	1918	139(13)
H(12B)	2004	3191	1974	139(13)
H(13A)	1023	2374	714	139(13)
H(13B)	1877	2864	498	139(13)
H(13C)	742	3070	758	139(13)
H(12C)	1895	3166	1641	139(13)
H(12D)	1870	2513	1273	139(13)
H(13D)	623	2738	402	139(13)
H(13E)	1539	3228	394	139(13)

H(13F)	473	3375	816	139(13)
H(14A)	2140	1187	3490	139(13)
H(14B)	3025	1406	2916	139(13)
H(15A)	3570	2023	4023	139(13)
H(15B)	3861	1328	4044	139(13)
H(15C)	2904	1569	4535	139(13)
H(22A)	-748	102	4636	139(13)
H(22B)	-1099	-257	3819	139(13)
H(23A)	-2503	242	4887	139(13)
H(23B)	-2256	-455	4804	139(13)
H(23C)	-2864	-105	4063	139(13)
H(32A)	-1881	2521	579	139(13)
H(32B)	-2937	2322	985	139(13)
H(33A)	-3103	3204	1495	139(13)
H(33B)	-2988	3250	534	139(13)
H(33C)	-2005	3408	1161	139(13)
H(33D)	-2562	3335	1666	139(13)
H(33E)	-3624	2996	1354	139(13)
H(33F)	-2976	3367	725	139(13)
H(34A)	-2384	720	2411	139(13)
H(34B)	-3266	827	1674	139(13)
H(35A)	-4533	685	2650	139(13)
H(35B)	-4212	1335	2987	139(13)
H(35C)	-3661	755	3395	139(13)
H(35D)	-3657	1055	3143	139(13)
H(35E)	-3901	455	2634	139(13)
H(35F)	-4385	1078	2308	139(13)
H(42A)	498	-1949	353	139(13)
H(42B)	-578	-1589	447	139(13)
H(43A)	400	-2366	1605	139(13)
H(43B)	-692	-2482	1081	139(13)
H(43C)	-616	-1972	1764	139(13)
H(52A)	2941	1181	-904	139(13)
H(52B)	1704	1025	-1017	139(13)
H(53A)	3255	505	-2011	139(13)
H(53B)	2468	1028	-2323	139(13)
H(53C)	2014	379	-2136	139(13)
H(52C)	1521	331	-1256	139(13)
H(52D)	2643	672	-1507	139(13)
H(54A)	3059	1519	819	139(13)
H(54B)	3581	1190	1581	139(13)
H(55A)	4960	1591	1114	139(13)
H(55B)	4123	1838	1715	139(13)
H(55C)	4026	2023	773	139(13)
H(54C)	4129	951	1673	139(13)
H(54D)	2933	1172	1456	139(13)
H(55D)	4787	1714	619	139(13)
H(55E)	4203	2081	1290	139(13)
H(55F)	3600	1940	423	139(13)
H(62A)	402	-655	2606	139(13)
H(62B)	966	-344	3402	139(13)
H(63A)	1057	-1591	3163	139(13)
H(63B)	142	-1289	3642	139(13)

H(63C)	1346	-1238	3995	139(13)
H(64A)	3789	513	3465	139(13)
H(64B)	3003	-20	3621	139(13)
H(65A)	4317	-604	3760	139(13)
H(65B)	4305	-66	4400	139(13)
H(65C)	5073	-40	3670	139(13)
H(65D)	4972	-492	3673	139(13)
H(65E)	3867	-800	3828	139(13)
H(65F)	4369	-319	4462	139(13)

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

	x	y	z	U(eq)
Zr(1)	0	10000	0	22(1)
Zr(2)	5000	5000	5000	23(1)
Co(1)	-174(1)	7837(1)	1609(1)	23(1)
Co(2)	7509(1)	2461(1)	5291(1)	25(1)
P(1)	616(1)	7628(1)	440(1)	26(1)
P(2)	599(1)	8767(1)	1713(1)	24(1)
P(3)	-1587(1)	9074(1)	1257(1)	27(1)
P(4)	7307(1)	3395(1)	4198(1)	29(1)
P(5)	7083(1)	3655(1)	5948(1)	27(1)
P(6)	5858(1)	2593(1)	5473(1)	28(1)
S(1)	7713(1)	-4317(1)	11087(1)	43(1)
S(2)	8110(1)	-1568(1)	4535(1)	46(1)
O(100)	7034(3)	-3489(2)	11499(2)	90(1)
O(200)	7486(3)	-5175(2)	11397(2)	78(1)
O(300)	8851(3)	-4508(3)	10975(2)	87(1)
O(400)	7180(3)	-1520(3)	4252(2)	93(1)
O(500)	9005(3)	-2525(3)	4529(2)	88(1)
O(600)	8430(3)	-776(3)	4184(2)	88(1)
O(1)	754(2)	8518(2)	-81(1)	31(1)
O(2)	488(2)	9644(2)	1077(1)	28(1)
O(3)	-1367(2)	9766(2)	544(2)	32(1)
O(4)	6223(2)	4288(2)	4159(1)	32(1)
O(5)	6212(2)	4641(2)	5658(1)	30(1)
O(6)	4978(2)	3645(2)	5437(2)	32(1)
O(10)	-26(3)	7277(2)	23(2)	47(1)
O(13)	1781(2)	6786(2)	458(2)	38(1)
O(20)	1852(2)	8119(2)	1720(2)	33(1)
O(23)	277(2)	9209(2)	2500(1)	34(1)
O(30)	-2163(2)	9678(2)	1964(2)	37(1)
O(33)	-2547(2)	8860(2)	1109(2)	36(1)
O(40)	7478(2)	2840(2)	3486(2)	42(1)
O(43)	8234(2)	3776(2)	3963(2)	42(1)
O(50)	8041(2)	3900(2)	6064(2)	36(1)
O(53)	6658(2)	3364(2)	6824(1)	34(1)
O(60)	5532(2)	2031(2)	6263(2)	38(1)
O(63)	5749(2)	2069(2)	4836(2)	37(1)
C(21)	2580(3)	8580(3)	1712(2)	40(1)
C(7)	8471(4)	1476(3)	6073(3)	49(1)

C(1)	-1010(4)	7453(3)	2650(2)	35(1)
C(2)	79(4)	7157(3)	2723(2)	41(1)
C(3)	727(4)	6508(3)	2180(3)	39(1)
C(4)	34(3)	6385(3)	1779(2)	34(1)
C(5)	-1024(3)	6957(3)	2062(2)	33(1)
C(6)	7996(4)	1005(3)	5772(3)	49(1)
C(8)	9109(3)	1809(3)	5477(3)	45(1)
C(9)	9028(3)	1560(3)	4798(3)	44(1)
C(10)	8327(4)	1073(3)	4962(3)	48(1)
C(11)	242(5)	7063(7)	-747(4)	133(4)
C(12)	-504(7)	7302(8)	-1173(4)	158(4)
C(14)	2663(4)	6631(4)	-158(3)	53(1)
C(15)	3664(4)	5943(4)	116(4)	69(2)
C(22)	3285(4)	8548(4)	945(3)	66(2)
C(24)	-543(3)	10188(3)	2626(2)	40(1)
C(25)	-14(4)	10763(3)	2820(3)	72(2)
C(31)	-3223(4)	10470(4)	2000(3)	63(2)
C(32)	-3665(4)	10581(4)	2811(3)	78(2)
C(34)	-2591(4)	8564(3)	398(3)	43(1)
C(35)	-3742(4)	8902(4)	322(3)	71(2)
C(41)	6639(4)	2874(5)	3112(3)	67(2)
C(42)	6979(4)	2860(4)	2282(2)	54(1)
C(44)	8268(4)	4439(4)	3247(3)	73(2)
C(45)	9289(5)	4432(5)	3017(4)	111(3)
C(51)	8485(4)	4506(3)	5486(3)	46(1)
C(52)	8809(5)	5089(4)	5879(3)	66(2)
C(54)	6311(4)	4058(4)	7387(3)	52(1)
C(55)	5186(5)	4286(4)	7727(3)	81(2)
C(61)	4642(5)	2478(4)	6855(3)	76(2)
C(62)	4138(8)	1948(7)	7239(6)	215(7)
C(64)	4747(4)	1977(4)	4811(3)	55(1)
C(65)	4085(4)	2751(4)	4272(3)	70(2)
C(100)	6683(5)	-888(5)	7912(3)	86(2)
C(101)	7025(5)	-1052(4)	7062(3)	56(2)
C(102)	6388(4)	-492(4)	6506(3)	55(1)
C(103)	6707(4)	-652(3)	5743(3)	50(1)
C(104)	7684(4)	-1391(3)	5529(2)	40(1)
C(105)	8333(4)	-1966(4)	6075(3)	52(1)
C(106)	8005(5)	-1801(4)	6835(3)	63(2)
C(108)	6367(5)	-3302(4)	7881(3)	80(2)
C(110)	6708(5)	-3524(4)	8667(3)	53(1)
C(111)	7755(5)	-4068(3)	8780(3)	54(1)
C(112)	8085(4)	-4300(3)	9500(3)	50(1)
C(113)	7339(4)	-3984(3)	10139(2)	39(1)
C(114)	6272(4)	-3419(4)	10040(3)	52(1)
C(115)	5967(4)	-3194(4)	9304(3)	57(1)

Bond lengths (Å) and angles (deg) for **3**.

Zr(1)-O(1)#1	2.066(3)	Zr(2)-O(6)#2	2.067(3)
Zr(1)-O(1)	2.067(3)	Zr(2)-O(6)	2.067(3)
Zr(1)-O(2)	2.068(3)	Zr(2)-O(5)	2.074(3)
Zr(1)-O(2)#1	2.068(3)	Zr(2)-O(5)#2	2.074(3)

Zr(1)-O(3)#1	2.077(3)	Zr(2)-O(4)#2	2.077(2)
Zr(1)-O(3)	2.077(3)	Zr(2)-O(4)	2.077(2)
Co(1)-C(3)	2.063(4)	Co(2)-C(7)	2.056(4)
Co(1)-C(4)	2.074(4)	Co(2)-C(10)	2.070(4)
Co(1)-C(2)	2.078(4)	Co(2)-C(8)	2.077(4)
Co(1)-C(5)	2.086(4)	Co(2)-C(6)	2.079(4)
Co(1)-C(1)	2.090(4)	Co(2)-C(9)	2.080(4)
Co(1)-P(1)	2.1587(12)	Co(2)-P(4)	2.165(1)
Co(1)-P(3)	2.1621(13)	Co(2)-P(6)	2.166(1)
Co(1)-P(2)	2.1646(13)	Co(2)-P(5)	2.168(1)
P(1)-O(1)	1.544(3)	P(4)-O(4)	1.541(3)
P(1)-O(10)	1.575(3)	P(4)-O(43)	1.573(3)
P(1)-O(13)	1.578(3)	P(4)-O(40)	1.590(3)
P(2)-O(2)	1.544(3)	P(5)-O(5)	1.545(3)
P(2)-O(23)	1.580(3)	P(5)-O(50)	1.587(3)
P(2)-O(20)	1.591(3)	P(5)-O(53)	1.594(3)
P(3)-O(3)	1.548(3)	P(6)-O(6)	1.545(3)
P(3)-O(30)	1.579(3)	P(6)-O(63)	1.582(3)
P(3)-O(33)	1.583(3)	P(6)-O(60)	1.583(3)
S(1)-O(100)	1.445(3)	S(2)-O(600)	1.443(3)
S(1)-O(200)	1.450(3)	S(2)-O(400)	1.450(3)
S(1)-O(300)	1.452(4)	S(2)-O(500)	1.456(4)
S(1)-C(113)	1.787(5)	S(2)-C(104)	1.787(4)
O(10)-C(11)	1.414(6)	O(40)-C(41)	1.436(6)
O(13)-C(14)	1.431(5)	O(43)-C(44)	1.468(5)
O(20)-C(21)	1.451(5)	O(50)-C(51)	1.459(5)
O(23)-C(24)	1.467(5)	O(53)-C(54)	1.469(5)
O(30)-C(31)	1.448(5)	O(60)-C(61)	1.456(5)
O(33)-C(34)	1.453(5)	O(63)-C(64)	1.465(5)
C(21)-C(22)	1.500(6)	C(11)-C(12)	1.296(9)
C(7)-C(6)	1.396(7)	C(14)-C(15)	1.451(7)
C(7)-C(8)	1.393(6)	C(24)-C(25)	1.488(6)
C(1)-C(2)	1.405(6)	C(31)-C(32)	1.463(7)
C(1)-C(5)	1.423(6)	C(34)-C(35)	1.481(6)
C(2)-C(3)	1.409(6)	C(41)-C(42)	1.460(6)
C(3)-C(4)	1.406(6)	C(44)-C(45)	1.383(7)
C(4)-C(5)	1.392(6)	C(51)-C(52)	1.488(6)
C(6)-C(10)	1.420(6)	C(54)-C(55)	1.463(7)
C(8)-C(9)	1.383(6)	C(61)-C(62)	1.291(7)
C(9)-C(10)	1.409(6)	C(64)-C(65)	1.468(7)
C(100)-C(101)	1.529(6)	C(108)-C(110)	1.505(7)
C(101)-C(102)	1.372(7)	C(110)-C(111)	1.365(7)
C(101)-C(106)	1.394(7)	C(110)-C(115)	1.377(7)
C(102)-C(103)	1.379(6)	C(111)-C(112)	1.385(7)
C(103)-C(104)	1.378(6)	C(112)-C(113)	1.378(6)
C(104)-C(105)	1.373(7)	C(113)-C(114)	1.387(7)
C(105)-C(106)	1.375(6)	C(114)-C(115)	1.398(7)

O(1)#1-Zr(1)-O(1)	180.0	O(3)#1-Zr(1)-O(3)	180.0
O(1)#1-Zr(1)-O(2)	94.05(10)	O(6)#2-Zr(2)-O(5)	92.85(10)
O(1)-Zr(1)-O(2)	85.95(10)	O(6)-Zr(2)-O(5)	87.15(10)
O(1)#1-Zr(1)-O(2)#1	85.95(10)	O(6)#2-Zr(2)-O(5)#2	87.15(10)
O(1)-Zr(1)-O(2)#1	94.05(10)	O(6)-Zr(2)-O(5)#2	92.85(10)

O(2)-Zr(1)-O(2)#1	180.0	O(5)-Zr(2)-O(5)#2	180.0
O(1)#1-Zr(1)-O(3)#1	87.38(10)	O(6)#2-Zr(2)-O(4)#2	86.15(10)
O(1)-Zr(1)-O(3)#1	92.62(10)	O(6)-Zr(2)-O(4)#2	93.85(10)
O(2)-Zr(1)-O(3)#1	93.14(10)	O(5)-Zr(2)-O(4)#2	93.88(10)
O(2)#1-Zr(1)-O(3)#1	86.86(10)	O(5)#2-Zr(2)-O(4)#2	86.12(10)
O(1)#1-Zr(1)-O(3)	92.62(10)	O(6)#2-Zr(2)-O(4)	93.85(10)
O(1)-Zr(1)-O(3)	87.38(10)	O(6)-Zr(2)-O(4)	86.15(10)
O(2)-Zr(1)-O(3)	86.86(10)	O(5)-Zr(2)-O(4)	86.12(10)
O(2)#1-Zr(1)-O(3)	93.14(10)	O(5)#2-Zr(2)-O(4)	93.88(10)
O(6)#2-Zr(2)-O(6)	179.999(1)	O(4)#2-Zr(2)-O(4)	179.998(1)
C(3)-Co(1)-C(4)	39.7(2)	C(7)-Co(2)-C(10)	66.6(2)
C(3)-Co(1)-C(2)	39.8(2)	C(7)-Co(2)-C(8)	39.4(2)
C(4)-Co(1)-C(2)	66.3(2)	C(10)-Co(2)-C(8)	66.5(2)
C(3)-Co(1)-C(5)	66.3(2)	C(7)-Co(2)-C(6)	39.4(2)
C(4)-Co(1)-C(5)	39.1(2)	C(10)-Co(2)-C(6)	40.0(2)
C(2)-Co(1)-C(5)	66.0(2)	C(8)-Co(2)-C(6)	66.3(2)
C(3)-Co(1)-C(1)	66.9(2)	C(7)-Co(2)-C(9)	65.7(2)
C(4)-Co(1)-C(1)	66.6(2)	C(10)-Co(2)-C(9)	39.7(2)
C(2)-Co(1)-C(1)	39.4(2)	C(8)-Co(2)-C(9)	38.9(2)
C(5)-Co(1)-C(1)	39.8(2)	C(6)-Co(2)-C(9)	66.3(2)
C(3)-Co(1)-P(1)	99.88(13)	C(7)-Co(2)-P(4)	151.09(15)
C(4)-Co(1)-P(1)	87.77(12)	C(10)-Co(2)-P(4)	103.03(15)
C(2)-Co(1)-P(1)	138.50(14)	C(8)-Co(2)-P(4)	111.83(14)
C(5)-Co(1)-P(1)	113.41(12)	C(6)-Co(2)-P(4)	142.3(2)
C(1)-Co(1)-P(1)	152.63(12)	C(9)-Co(2)-P(4)	88.92(13)
C(3)-Co(1)-P(3)	158.68(12)	C(7)-Co(2)-P(6)	115.9(2)
C(4)-Co(1)-P(3)	125.73(13)	C(10)-Co(2)-P(6)	100.84(14)
C(2)-Co(1)-P(3)	127.44(14)	C(8)-Co(2)-P(6)	154.50(14)
C(5)-Co(1)-P(3)	93.35(12)	C(6)-Co(2)-P(6)	89.58(14)
C(1)-Co(1)-P(3)	93.66(13)	C(9)-Co(2)-P(6)	139.08(15)
P(1)-Co(1)-P(3)	93.88(5)	P(4)-Co(2)-P(6)	92.19(4)
C(3)-Co(1)-P(2)	103.19(13)	C(7)-Co(2)-P(5)	91.89(14)
C(4)-Co(1)-P(2)	141.87(13)	C(10)-Co(2)-P(5)	158.09(14)
C(2)-Co(1)-P(2)	89.82(12)	C(8)-Co(2)-P(5)	94.49(13)
C(5)-Co(1)-P(2)	153.04(12)	C(6)-Co(2)-P(5)	123.6(2)
C(1)-Co(1)-P(2)	113.48(12)	C(9)-Co(2)-P(5)	128.58(15)
P(1)-Co(1)-P(2)	92.45(5)	P(4)-Co(2)-P(5)	93.93(5)
P(3)-Co(1)-P(2)	92.32(5)	P(6)-Co(2)-P(5)	92.17(4)
O(1)-P(1)-O(10)	107.3(2)	O(4)-P(4)-O(43)	107.9(2)
O(1)-P(1)-O(13)	106.7(2)	O(4)-P(4)-O(40)	106.0(2)
O(10)-P(1)-O(13)	106.9(2)	O(43)-P(4)-O(40)	101.8(2)
O(1)-P(1)-Co(1)	116.98(11)	O(4)-P(4)-Co(2)	116.46(11)
O(10)-P(1)-Co(1)	109.29(13)	O(43)-P(4)-Co(2)	109.51(11)
O(13)-P(1)-Co(1)	109.19(11)	O(40)-P(4)-Co(2)	114.09(12)
O(2)-P(2)-O(23)	105.23(14)	O(5)-P(5)-O(50)	105.7(2)
O(2)-P(2)-O(20)	107.42(14)	O(5)-P(5)-O(53)	107.29(15)
O(23)-P(2)-O(20)	101.3(2)	O(50)-P(5)-O(53)	100.3(2)
O(2)-P(2)-Co(1)	116.63(11)	O(5)-P(5)-Co(2)	115.72(11)
O(23)-P(2)-Co(1)	116.25(11)	O(50)-P(5)-Co(2)	116.81(12)
O(20)-P(2)-Co(1)	108.61(11)	O(53)-P(5)-Co(2)	109.59(11)
O(3)-P(3)-O(30)	108.9(2)	O(6)-P(6)-O(63)	108.4(2)
O(3)-P(3)-O(33)	106.1(2)	O(6)-P(6)-O(60)	105.91(15)
O(30)-P(3)-O(33)	99.9(2)	O(63)-P(6)-O(60)	104.1(2)

O(3)-P(3)-Co(1)	115.30(11)	O(6)-P(6)-Co(2)	116.04(11)
O(30)-P(3)-Co(1)	107.70(11)	O(63)-P(6)-Co(2)	107.47(11)
O(33)-P(3)-Co(1)	117.58(12)	O(60)-P(6)-Co(2)	114.12(12)
O(100)-S(1)-O(200)	112.6(2)	O(600)-S(2)-O(400)	113.2(2)
O(100)-S(1)-O(300)	113.5(2)	O(600)-S(2)-O(500)	113.2(2)
O(200)-S(1)-O(300)	113.7(2)	O(400)-S(2)-O(500)	113.5(2)
O(100)-S(1)-C(113)	105.8(2)	O(600)-S(2)-C(104)	104.7(2)
O(200)-S(1)-C(113)	104.8(2)	O(400)-S(2)-C(104)	106.0(2)
O(300)-S(1)-C(113)	105.4(2)	O(500)-S(2)-C(104)	105.3(2)
P(1)-O(1)-Zr(1)	132.13(15)	P(4)-O(4)-Zr(2)	133.0(2)
P(2)-O(2)-Zr(1)	132.9(2)	P(5)-O(5)-Zr(2)	132.6(2)
P(3)-O(3)-Zr(1)	133.5(2)	P(6)-O(6)-Zr(2)	133.4(2)
C(11)-O(10)-P(1)	126.1(4)	C(41)-O(40)-P(4)	125.9(3)
C(14)-O(13)-P(1)	125.8(3)	C(44)-O(43)-P(4)	120.1(3)
C(21)-O(20)-P(2)	120.0(2)	C(51)-O(50)-P(5)	123.2(3)
C(24)-O(23)-P(2)	124.5(3)	C(54)-O(53)-P(5)	120.0(3)
C(31)-O(30)-P(3)	124.3(3)	C(61)-O(60)-P(6)	125.1(3)
C(34)-O(33)-P(3)	124.5(2)	C(64)-O(63)-P(6)	122.2(3)
O(20)-C(21)-C(22)	110.1(4)	C(12)-C(11)-O(10)	120.8(7)
C(6)-C(7)-C(8)	109.2(4)	O(13)-C(14)-C(15)	110.5(4)
C(6)-C(7)-Co(2)	71.2(3)	O(23)-C(24)-C(25)	108.5(4)
C(8)-C(7)-Co(2)	71.1(3)	O(30)-C(31)-C(32)	108.4(4)
C(2)-C(1)-C(5)	106.6(4)	O(33)-C(34)-C(35)	107.4(4)
C(2)-C(1)-Co(1)	69.8(2)	O(40)-C(41)-C(42)	111.0(4)
C(5)-C(1)-Co(1)	69.9(2)	C(45)-C(44)-O(43)	110.7(5)
C(1)-C(2)-C(3)	108.9(4)	O(50)-C(51)-C(52)	109.4(4)
C(1)-C(2)-Co(1)	70.8(2)	C(55)-C(54)-O(53)	110.6(4)
C(3)-C(2)-Co(1)	69.6(2)	C(62)-C(61)-O(60)	116.6(5)
C(2)-C(3)-C(4)	107.5(4)	C(65)-C(64)-O(63)	112.3(4)
C(2)-C(3)-Co(1)	70.7(2)	C(102)-C(101)-C(106)	117.9(5)
C(4)-C(3)-Co(1)	70.6(2)	C(102)-C(101)-C(100)	122.2(5)
C(5)-C(4)-C(3)	108.3(4)	C(106)-C(101)-C(100)	119.9(6)
C(5)-C(4)-Co(1)	70.9(2)	C(101)-C(102)-C(103)	121.4(5)
C(3)-C(4)-Co(1)	69.7(2)	C(104)-C(103)-C(102)	119.7(5)
C(4)-C(5)-C(1)	108.6(4)	C(105)-C(104)-C(103)	120.0(4)
C(4)-C(5)-Co(1)	70.0(2)	C(105)-C(104)-S(2)	120.6(4)
C(1)-C(5)-Co(1)	70.2(2)	C(103)-C(104)-S(2)	119.4(4)
C(7)-C(6)-C(10)	107.1(4)	C(104)-C(105)-C(106)	119.8(5)
C(7)-C(6)-Co(2)	69.4(3)	C(105)-C(106)-C(101)	121.1(5)
C(10)-C(6)-Co(2)	69.6(3)	C(111)-C(110)-C(115)	117.3(5)
C(9)-C(8)-C(7)	107.8(4)	C(111)-C(110)-C(108)	121.6(5)
C(9)-C(8)-Co(2)	70.7(3)	C(115)-C(110)-C(108)	121.0(5)
C(7)-C(8)-Co(2)	69.5(3)	C(110)-C(111)-C(112)	122.7(5)
C(8)-C(9)-C(10)	108.9(4)	C(113)-C(112)-C(111)	119.9(5)
C(8)-C(9)-Co(2)	70.4(2)	C(112)-C(113)-C(114)	118.6(4)
C(10)-C(9)-Co(2)	69.7(2)	C(112)-C(113)-S(1)	121.5(4)
C(9)-C(10)-C(6)	106.9(4)	C(114)-C(113)-S(1)	119.8(4)
C(9)-C(10)-Co(2)	70.6(3)	C(113)-C(114)-C(115)	120.1(5)
C(6)-C(10)-Co(2)	70.3(3)	C(110)-C(115)-C(114)	121.4(5)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+2,-z #2 -x+1,-y+1,-z+1

Anisotropic displacement parameters ($Å^2 \times 10^3$) for **3**. 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
Zr(1)	22(1)	20(1)	19(1)	3(1)	-6(1)	-6(1)
Zr(2)	21(1)	25(1)	22(1)	2(1)	-6(1)	-8(1)
Co(1)	24(1)	23(1)	22(1)	0(1)	-5(1)	-8(1)
Co(2)	24(1)	30(1)	22(1)	1(1)	-6(1)	-10(1)
P(1)	28(1)	24(1)	23(1)	-4(1)	-5(1)	-5(1)
P(2)	26(1)	24(1)	21(1)	-2(1)	-7(1)	-8(1)
P(3)	22(1)	28(1)	29(1)	-1(1)	-6(1)	-8(1)
P(4)	29(1)	36(1)	20(1)	1(1)	-3(1)	-12(1)
P(5)	27(1)	33(1)	24(1)	1(1)	-8(1)	-13(1)
P(6)	26(1)	31(1)	28(1)	2(1)	-4(1)	-14(1)
S(1)	59(1)	41(1)	37(1)	-10(1)	-5(1)	-25(1)
S(2)	41(1)	68(1)	39(1)	-14(1)	3(1)	-32(1)
O(100)	117(3)	75(2)	75(2)	-32(2)	-6(2)	-30(2)
O(200)	109(3)	73(2)	65(2)	-3(2)	-12(2)	-51(2)
O(300)	89(3)	109(3)	82(2)	-11(2)	-19(2)	-55(2)
O(400)	76(2)	155(4)	70(2)	-29(2)	-3(2)	-63(2)
O(500)	81(3)	95(3)	83(2)	-36(2)	2(2)	-25(2)
O(600)	93(3)	113(3)	70(2)	-4(2)	0(2)	-62(2)
O(1)	37(2)	26(2)	22(2)	0(1)	-1(1)	-7(1)
O(2)	33(2)	27(2)	26(2)	2(1)	-8(1)	-14(1)
O(3)	25(2)	31(2)	36(2)	7(1)	-10(1)	-9(1)
O(4)	31(2)	37(2)	21(2)	1(1)	-4(1)	-9(1)
O(5)	32(2)	32(2)	28(2)	-1(1)	-10(1)	-13(1)
O(6)	23(2)	31(2)	42(2)	1(1)	-6(1)	-12(1)
O(10)	57(2)	51(2)	41(2)	-15(2)	-17(2)	-20(2)
O(13)	29(2)	31(2)	35(2)	-2(1)	4(1)	2(1)
O(20)	26(2)	31(2)	41(2)	-3(1)	-11(1)	-10(1)
O(23)	49(2)	29(2)	23(2)	-5(1)	-11(1)	-12(1)
O(30)	25(2)	36(2)	42(2)	-13(1)	-4(1)	-2(1)
O(33)	28(2)	42(2)	40(2)	-2(1)	-10(1)	-17(1)
O(40)	39(2)	52(2)	25(2)	-10(1)	-6(1)	-7(2)
O(43)	38(2)	56(2)	29(2)	14(1)	-6(1)	-25(2)
O(50)	35(2)	42(2)	37(2)	3(1)	-16(1)	-21(1)
O(53)	42(2)	41(2)	21(2)	-5(1)	-2(1)	-18(1)
O(60)	34(2)	36(2)	34(2)	6(1)	4(1)	-13(1)
O(63)	35(2)	45(2)	38(2)	-4(1)	-9(1)	-23(2)
C(21)	31(2)	45(3)	50(3)	-1(2)	-14(2)	-19(2)
C(7)	44(3)	46(3)	33(3)	-1(2)	-15(2)	6(2)
C(1)	41(3)	35(3)	25(2)	2(2)	-1(2)	-16(2)
C(2)	68(3)	45(3)	25(2)	14(2)	-23(2)	-38(3)
C(3)	32(3)	28(2)	46(3)	17(2)	-10(2)	-9(2)
C(4)	44(3)	23(2)	32(2)	1(2)	-2(2)	-12(2)
C(5)	37(3)	31(2)	34(2)	7(2)	-9(2)	-19(2)
C(6)	30(3)	30(3)	68(4)	13(2)	-4(2)	-4(2)
C(8)	26(3)	46(3)	65(3)	-13(3)	-15(2)	-9(2)
C(9)	29(3)	40(3)	40(3)	3(2)	2(2)	-1(2)
C(10)	39(3)	35(3)	67(4)	-20(3)	-22(2)	0(2)
C(11)	66(5)	223(9)	111(6)	-124(7)	-25(4)	-8(5)

C(12)	177(9)	289(13)	52(4)	-26(6)	-40(5)	-122(9)
C(14)	36(3)	54(3)	50(3)	-4(3)	6(2)	-9(2)
C(15)	32(3)	49(3)	108(5)	-1(3)	-1(3)	-7(2)
C(22)	47(3)	82(4)	73(4)	-4(3)	-2(3)	-35(3)
C(24)	37(3)	38(3)	35(3)	-12(2)	2(2)	-7(2)
C(25)	73(4)	35(3)	108(5)	-26(3)	-39(3)	-2(3)
C(31)	41(3)	49(3)	84(4)	-28(3)	-9(3)	6(3)
C(32)	42(3)	66(4)	110(5)	-35(4)	22(3)	-11(3)
C(34)	44(3)	48(3)	46(3)	1(2)	-15(2)	-24(2)
C(35)	57(4)	92(5)	81(4)	1(3)	-37(3)	-37(3)
C(41)	64(4)	97(5)	52(3)	-31(3)	-3(3)	-35(3)
C(42)	72(4)	66(4)	34(3)	-6(2)	-12(2)	-36(3)
C(44)	61(4)	100(5)	45(3)	41(3)	-11(3)	-41(3)
C(45)	90(5)	159(7)	86(5)	60(5)	-22(4)	-82(5)
C(51)	44(3)	56(3)	46(3)	0(2)	-6(2)	-31(3)
C(52)	88(4)	66(4)	66(4)	11(3)	-23(3)	-56(3)
C(54)	64(4)	56(3)	38(3)	-15(2)	0(2)	-24(3)
C(55)	65(4)	89(5)	78(4)	-41(4)	4(3)	-14(4)
C(61)	93(5)	62(4)	50(3)	-9(3)	35(3)	-31(3)
C(62)	240(12)	199(10)	241(11)	-174(9)	216(10)	-172(9)
C(64)	53(3)	64(3)	65(4)	6(3)	-26(3)	-38(3)
C(65)	58(4)	68(4)	98(5)	12(3)	-41(3)	-35(3)
C(100)	117(6)	104(5)	55(4)	-31(4)	11(4)	-63(5)
C(101)	66(4)	71(4)	48(3)	-22(3)	15(3)	-46(3)
C(102)	59(4)	48(3)	57(4)	-19(3)	18(3)	-27(3)
C(103)	49(3)	48(3)	48(3)	-6(2)	5(2)	-21(3)
C(104)	43(3)	49(3)	36(3)	-10(2)	6(2)	-30(2)
C(105)	42(3)	69(4)	44(3)	-15(3)	2(2)	-21(3)
C(106)	64(4)	86(4)	44(3)	-8(3)	-9(3)	-35(3)
C(108)	110(5)	71(4)	66(4)	9(3)	-42(4)	-37(4)
C(110)	72(4)	45(3)	48(3)	2(3)	-18(3)	-29(3)
C(111)	70(4)	44(3)	36(3)	-10(2)	1(3)	-16(3)
C(112)	50(3)	44(3)	42(3)	-7(2)	-5(2)	-7(2)
C(113)	52(3)	31(2)	39(3)	-7(2)	-7(2)	-20(2)
C(114)	52(3)	53(3)	50(3)	-10(3)	3(3)	-22(3)
C(115)	53(3)	50(3)	65(4)	8(3)	-18(3)	-21(3)

Atomic coordinates (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 Uij tensor.

	x	y	z	U(eq)
Zr	5513(1)	-27(1)	2375(1)	15(1)
Co	4144(1)	-2360(1)	2354(1)	18(1)
P(3)	3132(1)	-1282(1)	2594(1)	18(1)
P(2)	5911(1)	-1946(1)	3058(1)	17(1)
P(1)	4625(1)	-1770(1)	1405(1)	19(1)
Cl(2)	4416(1)	952(1)	1449(1)	33(1)
Cl(3)	7666(1)	259(1)	2218(1)	33(1)
Cl(1)	5716(1)	903(1)	3431(1)	32(1)
O(3)	3372(2)	-1652(1)	774(1)	28(1)
O(8)	5302(2)	-934(1)	1556(1)	24(1)
O(5)	7030(2)	-2425(1)	2819(1)	23(1)

O(9)	6199(2)	-1017(1)	3076(1)	21(1)
O(2)	1725(2)	-1237(1)	2108(1)	30(1)
O(7)	3745(2)	-443(1)	2514(1)	23(1)
O(4)	5468(2)	-2321(1)	996(1)	26(1)
O(1)	2947(2)	-1350(1)	3418(1)	30(1)
O(6)	6071(2)	-2214(1)	3896(1)	25(1)
C(15)	9198(4)	-2029(2)	2824(2)	41(1)
C(14)	8338(3)	-2386(2)	3265(2)	28(1)
C(4)	4476(4)	-3508(2)	2851(2)	36(1)
C(12)	6827(4)	-2226(2)	1065(2)	37(1)
C(3)	4476(4)	-3575(2)	2113(2)	36(1)
C(16)	6044(4)	-1653(2)	4500(2)	36(1)
C(8)	2249(4)	-702(2)	3721(2)	43(1)
C(10)	3453(4)	-1308(2)	60(2)	46(1)
C(5)	3296(5)	-3210(2)	2918(2)	47(1)
C(2)	3293(4)	-3332(2)	1703(2)	45(1)
C(1)	2544(4)	-3104(2)	2190(3)	56(1)
C(6)	1192(5)	-553(2)	1661(3)	70(2)
C(9)	3096(5)	-255(2)	4324(3)	55(1)
C(17)	5461(5)	-2068(3)	5049(2)	52(1)
C(13)	7083(5)	-2220(3)	300(2)	64(1)
C(7)	60(4)	-762(3)	1124(3)	61(1)
C(11)	2702(9)	-616(4)	-133(3)	144(4)
C(101)	4783(4)	-4162(2)	-60(2)	35(1)
C(102)	5692(3)	-4469(2)	520(2)	33(1)
C(100)	4089(4)	-4686(2)	-586(2)	36(1)

Bond lengths (Å) and angles (deg) for **4**.

Zr-O(7)	2.088(2)	Zr-Cl(3)	2.4414(10)
Zr-O(8)	2.094(2)	Zr-Cl(2)	2.4433(10)
Zr-O(9)	2.098(2)	Zr-Cl(1)	2.4460(9)
O(3)-C(10)	1.457(4)	O(4)-C(12)	1.447(4)
O(5)-C(14)	1.465(4)	O(1)-C(8)	1.476(4)
O(2)-C(6)	1.427(4)	O(6)-C(16)	1.450(4)
Co-C(5)	2.065(3)	P(3)-O(7)	1.537(2)
Co-C(1)	2.068(4)	P(3)-O(2)	1.581(2)
Co-C(2)	2.073(3)	P(3)-O(1)	1.589(2)
Co-C(3)	2.074(3)	P(2)-O(9)	1.539(2)
Co-C(4)	2.077(3)	P(2)-O(5)	1.579(2)
Co-P(2)	2.1589(11)	P(2)-O(6)	1.586(2)
Co-P(3)	2.1611(9)	P(1)-O(8)	1.537(2)
Co-P(1)	2.1678(9)	P(1)-O(4)	1.583(2)
C(15)-C(14)	1.482(5)	P(1)-O(3)	1.587(3)
C(4)-C(3)	1.376(5)	C(8)-C(9)	1.467(6)
C(4)-C(5)	1.389(6)	C(10)-C(11)	1.385(6)
C(12)-C(13)	1.505(5)	C(5)-C(1)	1.422(6)
C(3)-C(2)	1.385(6)	C(2)-C(1)	1.389(6)
C(16)-C(17)	1.474(5)	C(6)-C(7)	1.432(6)
C(101)-C(102)	1.376(5)	C(102)-C(100)#1	1.395(5)
C(101)-C(100)	1.382(5)	C(100)-C(102)#1	1.395(5)
O(7)-Zr-O(8)	84.66(8)	O(9)-Zr-Cl(3)	90.54(6)

O(7)-Zr-O(9)	82.98(8)	O(7)-Zr-Cl(2)	89.33(6)
O(8)-Zr-O(9)	82.84(8)	O(8)-Zr-Cl(2)	89.51(6)
O(7)-Zr-Cl(3)	172.03(5)	O(9)-Zr-Cl(2)	169.61(6)
O(8)-Zr-Cl(3)	89.94(7)	Cl(3)-Zr-Cl(2)	96.50(4)
O(7)-Zr-Cl(1)	91.27(6)	Cl(3)-Zr-Cl(1)	93.51(4)
O(8)-Zr-Cl(1)	173.17(6)	Cl(2)-Zr-Cl(1)	95.95(4)
O(9)-Zr-Cl(1)	91.23(6)	C(10)-O(3)-P(1)	120.2(2)
P(3)-O(7)-Zr	136.25(12)	P(1)-O(8)-Zr	136.55(13)
C(12)-O(4)-P(1)	124.9(2)	C(14)-O(5)-P(2)	121.0(2)
C(8)-O(1)-P(3)	120.0(2)	P(2)-O(9)-Zr	134.28(13)
C(16)-O(6)-P(2)	124.6(2)	C(6)-O(2)-P(3)	125.2(2)
C(5)-Co-C(1)	40.2(2)	C(2)-Co-C(3)	39.0(2)
C(5)-Co-C(2)	66.3(2)	C(5)-Co-C(4)	39.2(2)
C(1)-Co-C(2)	39.2(2)	C(1)-Co-C(4)	66.1(2)
C(5)-Co-C(3)	65.74(14)	C(2)-Co-C(4)	65.41(15)
C(1)-Co-C(3)	65.74(15)	C(3)-Co-C(4)	38.70(15)
C(5)-Co-P(2)	109.26(14)	C(4)-Co-P(3)	132.88(11)
C(1)-Co-P(2)	149.48(15)	P(2)-Co-P(3)	92.16(3)
C(2)-Co-P(2)	143.56(13)	C(5)-Co-P(1)	157.07(12)
C(3)-Co-P(2)	104.91(11)	C(1)-Co-P(1)	118.7(2)
C(4)-Co-P(2)	88.32(11)	C(2)-Co-P(1)	91.03(12)
C(5)-Co-P(3)	97.88(11)	C(3)-Co-P(1)	99.32(11)
C(1)-Co-P(3)	93.62(11)	C(4)-Co-P(1)	135.26(11)
C(2)-Co-P(3)	124.13(13)	P(2)-Co-P(1)	90.95(4)
C(3)-Co-P(3)	159.30(11)	P(3)-Co-P(1)	91.86(4)
O(7)-P(3)-O(2)	106.21(11)	O(8)-P(1)-O(4)	106.84(12)
O(7)-P(3)-O(1)	107.69(12)	O(8)-P(1)-O(3)	108.47(12)
O(2)-P(3)-O(1)	104.09(14)	O(4)-P(1)-O(3)	101.38(12)
O(7)-P(3)-Co	116.89(9)	O(8)-P(1)-Co	115.54(9)
O(2)-P(3)-Co	112.47(8)	O(4)-P(1)-Co	113.95(9)
O(1)-P(3)-Co	108.66(8)	O(3)-P(1)-Co	109.62(9)
O(9)-P(2)-O(5)	109.13(12)	O(9)-P(2)-Co	117.67(9)
O(9)-P(2)-O(6)	105.71(11)	O(5)-P(2)-Co	107.35(8)
O(5)-P(2)-O(6)	102.59(12)	O(6)-P(2)-Co	113.33(9)
O(5)-C(14)-C(15)	110.1(3)	C(4)-C(5)-Co	70.9(2)
C(3)-C(4)-C(5)	108.7(4)	C(1)-C(5)-Co	70.0(2)
C(3)-C(4)-Co	70.5(2)	C(3)-C(2)-C(1)	108.3(4)
C(5)-C(4)-Co	69.9(2)	C(3)-C(2)-Co	70.5(2)
O(4)-C(12)-C(13)	108.1(3)	C(1)-C(2)-Co	70.2(2)
C(4)-C(3)-C(2)	108.6(4)	C(2)-C(1)-C(5)	107.3(3)
C(4)-C(3)-Co	70.8(2)	C(2)-C(1)-Co	70.6(2)
C(2)-C(3)-Co	70.5(2)	C(5)-C(1)-Co	69.7(2)
O(6)-C(16)-C(17)	109.4(3)	O(2)-C(6)-C(7)	112.8(3)
C(9)-C(8)-O(1)	111.3(3)	C(102)-C(101)-C(100)	120.4(3)
C(11)-C(10)-O(3)	113.4(4)	C(101)-C(102)-C(100)#1	120.1(3)
C(4)-C(5)-C(1)	107.1(3)	C(101)-C(100)-C(102)#1	119.5(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y-1,-z

Anisotropic displacement parameters ($Å^2 \times 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,[\,h^2\,a^{*2}\,U11 + ... + 2\,h\,k\,a^*\,b^*\,U12\,]$

	U11	U22	U33	U23	U13	U12

Zr	16(1)	10(1)	20(1)	0(1)	4(1)	-2(1)
Co	17(1)	11(1)	25(1)	-2(1)	6(1)	-2(1)
P(3)	16(1)	14(1)	26(1)	-1(1)	8(1)	-1(1)
P(2)	19(1)	13(1)	21(1)	0(1)	4(1)	1(1)
P(1)	20(1)	17(1)	20(1)	-4(1)	5(1)	-3(1)
Cl(2)	30(1)	26(1)	40(1)	12(1)	0(1)	-1(1)
Cl(3)	23(1)	32(1)	45(1)	1(1)	12(1)	-7(1)
Cl(1)	39(1)	24(1)	32(1)	-11(1)	9(1)	-4(1)
O(3)	28(1)	31(1)	23(1)	1(1)	2(1)	-1(1)
O(8)	28(1)	19(1)	25(1)	-3(1)	10(1)	-7(1)
O(5)	18(1)	23(1)	28(1)	-4(1)	4(1)	3(1)
O(9)	19(1)	16(1)	28(1)	0(1)	3(1)	-3(1)
O(2)	20(1)	19(1)	49(2)	2(1)	1(1)	-1(1)
O(7)	22(1)	14(1)	36(1)	-1(1)	10(1)	-2(1)
O(4)	22(1)	28(1)	31(1)	-11(1)	12(1)	-4(1)
O(1)	36(2)	26(1)	35(1)	-2(1)	19(1)	4(1)
O(6)	34(2)	19(1)	22(1)	0(1)	7(1)	0(1)
C(15)	25(2)	38(2)	57(3)	2(2)	3(2)	-3(2)
C(14)	14(2)	32(2)	37(2)	-2(2)	-1(2)	6(1)
C(4)	41(3)	16(2)	45(2)	9(2)	-4(2)	-8(2)
C(12)	30(2)	42(2)	39(2)	-10(2)	5(2)	3(2)
C(3)	41(2)	12(1)	58(3)	-6(2)	20(2)	-1(1)
C(16)	45(3)	37(2)	26(2)	-7(2)	9(2)	-1(2)
C(8)	41(3)	49(2)	43(2)	-12(2)	23(2)	12(2)
C(10)	48(3)	64(3)	26(2)	7(2)	5(2)	5(2)
C(5)	70(3)	19(2)	66(3)	-6(2)	46(3)	-20(2)
C(2)	68(3)	18(2)	42(2)	-5(2)	-3(2)	-17(2)
C(1)	24(2)	12(2)	126(4)	3(2)	5(3)	-9(1)
C(6)	55(3)	41(2)	94(4)	16(2)	-28(3)	4(2)
C(9)	61(3)	43(2)	66(3)	-25(2)	27(3)	3(2)
C(17)	62(3)	62(2)	38(2)	1(2)	25(2)	3(2)
C(13)	45(3)	104(4)	53(3)	-8(3)	31(2)	-7(3)
C(7)	39(3)	72(3)	63(3)	0(2)	-7(2)	17(2)
C(11)	24(1)	143(6)	70(4)	73(4)	68(5)	124(6)
C(101)	33(2)	31(2)	39(2)	-1(2)	7(2)	2(2)
C(102)	25(2)	38(2)	37(2)	-10(2)	9(2)	-6(2)
C(100)	30(2)	41(2)	35(2)	0(2)	2(2)	1(2)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zr	5000	5000	5000	20(1)
Co	7197(1)	5238(1)	7918(1)	22(1)
Cl	5466(1)	7789(1)	533(1)	37(1)
P(1)	7801(1)	6348(1)	6816(1)	24(1)
P(2)	5215(1)	5694(1)	7509(1)	23(1)
P(3)	6555(1)	3495(1)	6750(1)	22(1)
O(1)	6690(2)	6302(2)	5809(2)	28(1)
O(2)	4434(2)	5222(2)	6346(2)	27(1)
O(3)	5997(2)	3681(2)	5614(2)	25(1)

C(1)	8626(4)	6360(4)	9205(3)	45(1)
C(2)	7463(4)	5987(4)	9474(3)	42(1)
C(3)	7189(4)	4653(4)	9320(3)	41(1)
C(4)	8173(4)	4233(4)	8972(3)	46(1)
C(5)	9067(4)	5270(5)	8886(3)	49(1)
C(11)	9139(4)	5828(4)	6378(3)	40(1)
C(12)	9605(5)	6561(4)	5620(4)	64(1)
C(13)	8438(3)	8039(3)	7317(3)	32(1)
C(14)	7986(5)	8887(3)	6552(3)	50(1)
C(21)	5261(4)	7386(3)	7768(3)	36(1)
C(22)	4117(6)	7832(5)	7169(6)	92(2)
C(23)	4159(3)	5017(3)	8245(3)	32(1)
C(24)	2705(4)	4937(5)	7776(4)	55(1)
C(31)	7888(3)	2640(3)	6708(3)	31(1)
C(32)	7830(4)	1972(4)	5639(3)	41(1)
C(33)	5270(3)	2368(3)	6983(3)	33(1)
C(34)	4865(4)	1107(3)	6241(3)	46(1)
C(1S)	1799(6)	1021(8)	7527(4)	84(2)
Cl(1S)	1344(6)	1218(6)	6283(4)	100(2)
Cl(1T)	1188(6)	506(6)	6236(5)	107(2)
Cl(2S)	760(1)	1513(2)	8217(1)	81(1)
C(2S)	7086(4)	10688(4)	10023(3)	47(1)
Cl(3S)	8107(2)	11785(2)	11093(1)	106(1)
Cl(4S)	8112(6)	10632(7)	9219(5)	91(2)
Cl(4T)	7548(6)	10526(5)	8860(4)	79(2)

Bond lengths (Å) and angles (deg) for **5**.

Zr-O(1)	2.069(2)	P(3)-C(33)	1.817(3)
Zr-O(3)	2.072(2)	P(3)-C(31)	1.842(3)
Zr-O(2)	2.073(2)	C(1)-C(2)	1.404(6)
Zr-Cl	7.2495(9)	C(1)-C(5)	1.409(6)
Co-C(3)	2.095(3)	C(2)-C(3)	1.417(6)
Co-C(4)	2.096(3)	C(3)-C(4)	1.383(6)
Co-C(1)	2.098(4)	C(4)-C(5)	1.400(6)
Co-C(5)	2.099(4)	C(11)-C(12)	1.520(5)
Co-C(2)	2.102(3)	C(13)-C(14)	1.524(5)
Co-P(3)	2.2064(9)	C(21)-C(22)	1.486(6)
Co-P(1)	2.2065(9)	C(23)-C(24)	1.515(5)
Co-P(2)	2.2178(9)	C(31)-C(32)	1.525(5)
P(1)-O(1)	1.563(2)	C(33)-C(34)	1.527(5)
P(1)-C(11)	1.834(4)	C(1S)-Cl(1S)	1.695(7)
P(1)-C(13)	1.837(3)	C(1S)-Cl(1T)	1.698(8)
P(2)-O(2)	1.568(2)	C(1S)-Cl(2S)	1.738(6)
P(2)-C(21)	1.828(3)	C(2S)-Cl(4S)	1.745(8)
P(2)-C(23)	1.828(3)	C(2S)-Cl(3S)	1.753(5)
P(3)-O(3)	1.566(2)	C(2S)-Cl(4T)	1.774(8)

O(1)#1-Zr-O(3)	94.88(9)	O(1)-P(1)-C(11)	105.25(16)
O(1)-Zr-O(3)	85.12(8)	O(1)-P(1)-C(13)	104.20(14)
O(1)#1-Zr-O(3)#1	85.12(9)	C(11)-P(1)-C(13)	103.61(18)
O(1)-Zr-O(3)#1	94.88(9)	O(1)-P(1)-Co	114.78(9)
O(1)#1-Zr-O(2)	93.78(9)	C(11)-P(1)-Co	112.49(12)

O(1)-Zr-O(2)	86.22(9)	C(13)-P(1)-Co	115.32(12)
O(3)-Zr-O(2)	86.00(8)	O(2)-P(2)-C(21)	106.15(14)
O(3)#1-Zr-O(2)	94.00(8)	O(2)-P(2)-C(23)	105.82(15)
O(1)#1-Zr-O(2)#1	86.22(9)	C(21)-P(2)-C(23)	104.64(17)
O(1)-Zr-O(2)#1	93.78(9)	O(2)-P(2)-Co	113.67(9)
O(3)-Zr-O(2)#1	94.00(8)	C(21)-P(2)-Co	112.70(13)
O(3)#1-Zr-O(2)#1	86.00(8)	C(23)-P(2)-Co	113.11(12)
O(1)#1-Zr-Cl	93.32(6)	O(3)-P(3)-C(33)	105.08(15)
O(1)-Zr-Cl	86.68(6)	O(3)-P(3)-C(31)	104.71(14)
O(3)-Zr-Cl	128.29(6)	C(33)-P(3)-C(31)	105.20(16)
O(3)#1-Zr-Cl	51.71(6)	O(3)-P(3)-Co	115.27(9)
O(2)-Zr-Cl	144.12(6)	C(33)-P(3)-Co	112.76(12)
O(2)#1-Zr-Cl	35.88(6)	C(31)-P(3)-Co	112.89(12)
C(3)-Co-C(4)	38.52(16)	P(1)-O(1)-Zr	133.77(13)
C(3)-Co-C(1)	65.56(15)	P(2)-O(2)-Zr	133.19(13)
C(4)-Co-C(1)	65.16(16)	P(3)-O(3)-Zr	132.11(12)
C(3)-Co-C(5)	65.53(16)	C(2)-C(1)-C(5)	108.5(4)
C(4)-Co-C(5)	39.00(17)	C(2)-C(1)-Co	70.6(2)
C(1)-Co-C(5)	39.24(17)	C(5)-C(1)-Co	70.4(2)
C(3)-Co-C(2)	39.44(16)	C(1)-C(2)-C(3)	107.2(4)
C(4)-Co-C(2)	65.26(15)	C(1)-C(2)-Co	70.3(2)
C(1)-Co-C(2)	39.04(16)	C(3)-C(2)-Co	70.0(2)
C(5)-Co-C(2)	65.82(16)	C(4)-C(3)-C(2)	107.9(4)
C(3)-Co-P(3)	105.32(11)	C(4)-C(3)-Co	70.8(2)
C(4)-Co-P(3)	88.94(11)	C(2)-C(3)-Co	70.5(2)
C(1)-Co-P(3)	148.82(13)	C(3)-C(4)-C(5)	109.3(4)
C(5)-Co-P(3)	109.59(13)	C(3)-C(4)-Co	70.7(2)
C(2)-Co-P(3)	144.43(12)	C(5)-C(4)-Co	70.6(2)
C(3)-Co-P(1)	159.59(11)	C(4)-C(5)-C(1)	107.0(4)
C(4)-Co-P(1)	133.49(14)	C(4)-C(5)-Co	70.4(2)
C(1)-Co-P(1)	94.05(11)	C(1)-C(5)-Co	70.3(2)
C(5)-Co-P(1)	98.57(12)	C(12)-C(11)-P(1)	115.1(3)
C(2)-Co-P(1)	123.64(12)	C(14)-C(13)-P(1)	114.1(2)
P(3)-Co-P(1)	91.80(3)	C(22)-C(21)-P(2)	116.5(3)
C(3)-Co-P(2)	98.95(12)	C(24)-C(23)-P(2)	114.7(3)
C(4)-Co-P(2)	135.18(14)	C(32)-C(31)-P(3)	114.9(2)
C(1)-Co-P(2)	118.23(13)	C(34)-C(33)-P(3)	114.6(3)
C(5)-Co-P(2)	155.65(12)	Cl(1S)-C(1S)-Cl(2S)	112.4(4)
C(2)-Co-P(2)	90.18(11)	Cl(1T)-C(1S)-Cl(2S)	118.8(4)
P(3)-Co-P(2)	92.19(3)	Cl(4S)-C(2S)-Cl(3S)	101.0(3)
P(1)-Co-P(2)	91.27(3)	Cl(3S)-C(2S)-Cl(4T)	118.9(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1

Anisotropic displacement parameters ($Å^2 \times 10^3$) for **5**. 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
Zr	25(1)	21(1)	14(1)	3(1)	3(1)	5(1)
Co	25(1)	24(1)	16(1)	4(1)	3(1)	5(1)
Cl	39(1)	39(1)	32(1)	8(1)	11(1)	7(1)
P(1)	26(1)	23(1)	22(1)	4(1)	5(1)	2(1)

P(2)	27(1)	26(1)	17(1)	4(1)	7(1)	7(1)
P(3)	27(1)	22(1)	19(1)	5(1)	5(1)	6(1)
O(1)	32(1)	25(1)	20(1)	6(1)	1(1)	-2(1)
O(2)	26(1)	36(1)	19(1)	5(1)	6(1)	9(1)
O(3)	33(1)	24(1)	19(1)	4(1)	5(1)	10(1)
C(1)	50(2)	45(2)	23(2)	10(2)	-9(2)	-10(2)
C(2)	49(2)	57(2)	16(2)	0(2)	1(2)	22(2)
C(3)	42(2)	55(2)	21(2)	17(2)	2(2)	-3(2)
C(4)	67(3)	45(2)	22(2)	6(2)	-7(2)	26(2)
C(5)	30(2)	91(3)	24(2)	12(2)	-1(2)	19(2)
C(11)	36(2)	41(2)	48(2)	9(2)	21(2)	9(2)
C(12)	81(4)	50(3)	83(3)	18(2)	59(3)	14(2)
C(13)	34(2)	26(2)	29(2)	2(1)	1(1)	-2(1)
C(14)	68(3)	26(2)	46(2)	10(2)	7(2)	1(2)
C(21)	50(2)	29(2)	32(2)	5(1)	14(2)	13(2)
C(22)	70(4)	44(3)	159(6)	30(3)	12(4)	27(3)
C(23)	38(2)	38(2)	24(2)	6(1)	16(2)	8(2)
C(24)	31(2)	76(3)	66(3)	32(2)	21(2)	7(2)
C(31)	33(2)	30(2)	33(2)	11(1)	9(2)	13(1)
C(32)	49(2)	42(2)	39(2)	7(2)	18(2)	22(2)
C(33)	36(2)	28(2)	34(2)	7(1)	13(2)	1(1)
C(34)	53(2)	31(2)	54(2)	2(2)	21(2)	-1(2)
C(1S)	54(3)	145(6)	45(3)	5(3)	1(2)	31(4)
Cl(1S)	67(3)	193(6)	46(2)	45(3)	8(2)	39(4)
Cl(1T)	63(2)	162(5)	72(3)	-39(3)	19(2)	0(3)
Cl(2S)	51(1)	110(1)	65(1)	-16(1)	10(1)	6(1)
C(2S)	47(2)	45(2)	53(3)	13(2)	20(2)	8(2)
Cl(3S)	90(1)	101(1)	89(1)	-14(1)	-25(1)	17(1)
Cl(4S)	118(5)	72(2)	102(5)	-3(3)	79(4)	11(3)
Cl(4T)	140(5)	39(2)	74(3)	10(2)	61(3)	15(3)

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

	x	y	z	U(eq)
H(1)	9040	7195	9232	59(6)
H(2)	6961	6523	9713	59(6)
H(3)	6465	4144	9434	59(6)
H(4)	8232	3385	8817	59(6)
H(5)	9820	5244	8659	59(6)
H(11A)	9886	5892	6982	54(3)
H(11B)	8847	4937	6054	54(3)
H(12A)	8875	6505	5017	75(4)
H(12B)	10291	6207	5415	75(4)
H(12C)	9947	7437	5944	75(4)
H(13A)	8162	8270	7936	54(3)
H(13B)	9400	8197	7522	54(3)
H(14A)	8229	8649	5927	75(4)
H(14B)	8400	9758	6854	75(4)
H(14C)	7040	8793	6390	75(4)
H(21A)	5347	7636	8502	54(3)
H(21B)	6054	7828	7635	54(3)
H(22A)	4126	7759	6454	75(4)

H(22B)	4166	8705	7451	75(4)
H(22C)	3311	7321	7209	75(4)
H(23A)	4306	4167	8316	54(3)
H(23B)	4423	5526	8939	54(3)
H(24A)	2536	5778	7749	75(4)
H(24B)	2215	4535	8196	75(4)
H(24C)	2433	4445	7085	75(4)
H(31A)	8729	3239	6988	54(3)
H(31B)	7866	2014	7159	54(3)
H(32A)	7003	1372	5353	75(4)
H(32B)	8551	1530	5690	75(4)
H(32C)	7901	2588	5194	75(4)
H(33A)	5571	2211	7688	54(3)
H(33B)	4495	2745	6938	54(3)
H(34A)	4649	1255	5537	75(4)
H(34B)	4104	604	6358	75(4)
H(34C)	5584	662	6356	75(4)
H(1S)	1730(5)	1670(3)	7120(4)	54(3)
H(2S)	2690(2)	1230(4)	7890(3)	54(3)
H(3S)	6930(4)	9910(3)	10240(3)	54(3)
H(4S)	6300(3)	10980(4)	9820(3)	54(3)