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Table 4: Fractional parameters for complex 5b

Atom	x/a	y/b	z/c	U(eq)	U(iso)
Cr(1)	0.6050(2)	0.3247(1)	0.5515(1)	0.0545	
Mn(1)	0.7228(2)	0.0488(1)	0.7054(2)	0.0606	
Mn(2)	0.3290(2)	0.3739(1)	0.2306(1)	0.0592	
P(1)	0.8393(4)	0.0409(3)	0.8193(3)	0.0825	
P(2)	0.1878(3)	0.3793(3)	0.1522(3)	0.0780	
O(1)	0.5128(6)	0.1689(6)	0.4652(6)	0.0610	
O(3)	0.5705(7)	0.2840(5)	0.7312(6)	0.0559	
O(11)	0.844(1)	0.1068(9)	0.884(1)	0.1424	
O(12)	0.934(1)	0.048(1)	0.809(2)	0.1474	
O(13)	0.859(1)	-0.0314(9)	0.8750(9)	0.1281	
O(21)	0.137(1)	0.456(1)	0.128(1)	0.1430	
O(22)	0.160(1)	0.341(1)	0.0662(9)	0.1404	
O(23)	0.1215(8)	0.3371(9)	0.1906(8)	0.1016	
O(33)	0.6366(9)	0.4690(7)	0.4800(8)	0.0909	
O(34)	0.7763(9)	0.3478(7)	0.6915(9)	0.0979	
O(35)	0.708(1)	0.2476(8)	0.4564(9)	0.1051	
O(36)	0.5865(9)	-0.0092(7)	0.7729(9)	0.1049	
O(37)	0.7751(9)	-0.0987(8)	0.662(1)	0.1050	
O(38)	0.3546(9)	0.2279(8)	0.1653(9)	0.0981	
O(39)	0.3779(9)	0.4633(8)	0.1072(8)	0.0971	
C(1)	0.5097(9)	0.2307(7)	0.5120(8)	0.0435	
C(2)	0.5499(9)	0.2266(8)	0.6027(9)	0.0451	
C(3)	0.540(1)	0.2918(8)	0.6465(9)	0.0547	
C(4)	0.498(1)	0.3582(8)	0.6077(9)	0.0518	
C(5)	0.463(1)	0.3613(8)	0.5189(9)	0.0535	
C(6)	0.4652(9)	0.2976(7)	0.4688(9)	0.0428	
C(7)	0.5885(9)	0.1544(7)	0.6525(9)	0.0488	
C(8)	0.604(1)	0.0875(8)	0.6018(9)	0.0551	
C(9)	0.683(1)	0.084(1)	0.579(1)	0.0575	
C(10)	0.760(1)	0.124(1)	0.624(1)	0.0783	
C(11)	0.759(1)	0.1628(9)	0.697(1)	0.0729	
C(12)	0.680(1)	0.1637(8)	0.7182(9)	0.0537	
C(13)	0.423(1)	0.2983(8)	0.3739(8)	0.0510	
C(14)	0.325(1)	0.313(1)	0.3424(9)	0.0571	
C(15)	0.289(1)	0.386(1)	0.3403(9)	0.0608	
C(16)	0.343(1)	0.447(1)	0.3326(9)	0.0596	
C(17)	0.429(1)	0.434(1)	0.3288(9)	0.0626	
C(18)	0.461(1)	0.3598(9)	0.3319(8)	0.0542	
C(19)	0.430(1)	0.125(1)	0.439(1)	0.0696	
C(20)	0.571(1)	0.3495(9)	0.7811(9)	0.0671	
C(21)	0.894(3)	0.117(3)	0.977(3)		0.25(2)
C(22)	0.923(3)	0.183(3)	0.977(3)		0.25(2)
C(23)	0.991(5)	0.009(4)	0.798(4)		0.30(4)
C(24)	1.069(3)	-0.015(2)	0.817(2)		0.24(2)
C(25)	0.799(2)	-0.087(2)	0.884(2)		0.17(1)
C(26)	0.802(2)	-0.102(2)	0.962(2)		0.18(1)
C(27)	0.170(2)	0.523(2)	0.136(2)		0.17(1)
C(28)	0.139(3)	0.573(2)	0.074(3)		0.28(2)
C(29)	0.176(2)	0.337(2)	0.001(2)		0.20(1)
C(30)	0.114(2)	0.300(2)	-0.071(2)		0.20(1)
C(31)	0.035(2)	0.324(2)	0.154(2)		0.16(1)
C(32)	0.004(2)	0.268(2)	0.207(2)		0.15(1)
C(33)	0.623(1)	0.412(1)	0.507(1)	0.0570	
C(34)	0.708(1)	0.3371(9)	0.638(1)	0.0604	
C(35)	0.669(1)	0.278(1)	0.493(1)	0.0768	
C(36)	0.644(1)	0.0126(9)	0.751(1)	0.0622	
C(37)	0.753(1)	-0.040(1)	0.677(1)	0.0713	
C(38)	0.344(1)	0.288(1)	0.190(1)	0.0575	
C(39)	0.357(1)	0.428(1)	0.157(1)	0.0741	

Table 5. Anisotropic thermal parameters for complex 5b

Atom	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Cr(1)	0.064(2)	0.050(1)	0.057(2)	-0.006(1)	0.025(1)	-0.013(1)
Mn(1)	0.055(2)	0.058(2)	0.070(2)	-0.011(1)	0.017(1)	0.003(1)
Mn(2)	0.065(2)	0.063(2)	0.054(1)	-0.001(1)	0.023(1)	0.001(1)
P(1)	0.074(4)	0.067(3)	0.104(4)	-0.016(3)	0.003(3)	0.005(3)
P(2)	0.076(4)	0.101(4)	0.062(3)	-0.001(3)	0.018(3)	0.016(3)
O(1)	0.078(8)	0.054(6)	0.056(6)	-0.009(5)	0.022(6)	-0.005(6)
O(3)	0.083(8)	0.054(6)	0.046(6)	0.003(5)	0.030(6)	0.007(5)
O(11)	0.28(2)	0.12(1)	0.11(1)	-0.03(1)	-0.07(1)	0.07(1)
O(12)	0.07(1)	0.18(2)	0.27(2)	0.08(2)	-0.03(1)	-0.01(1)
O(13)	0.13(1)	0.14(1)	0.13(1)	0.05(1)	-0.03(1)	0.00(1)
O(21)	0.11(1)	0.14(1)	0.21(2)	0.06(1)	0.01(1)	0.01(1)
O(22)	0.10(1)	0.40(3)	0.08(1)	-0.08(2)	0.016(9)	0.02(2)
O(23)	0.051(8)	0.22(2)	0.09(1)	-0.01(1)	0.019(8)	-0.02(1)
O(33)	0.13(1)	0.082(9)	0.10(1)	0.004(8)	0.053(9)	-0.040(9)
O(34)	0.08(1)	0.12(1)	0.10(1)	-0.014(9)	0.015(8)	-0.039(9)
O(35)	0.13(1)	0.13(1)	0.13(1)	-0.05(1)	0.08(1)	-0.027(9)
O(36)	0.10(1)	0.10(1)	0.15(1)	0.021(9)	0.06(1)	-0.001(8)
O(37)	0.10(1)	0.10(1)	0.18(1)	-0.07(1)	0.03(1)	0.032(9)
O(38)	0.11(1)	0.09(1)	0.11(1)	-0.049(9)	0.034(9)	-0.005(9)
O(39)	0.13(1)	0.13(1)	0.078(9)	0.035(9)	0.051(9)	0.00(1)
C(1)	0.049(9)	0.045(9)	0.049(9)	-0.003(7)	0.027(7)	-0.002(7)
C(2)	0.06(1)	0.049(9)	0.053(9)	-0.001(8)	0.033(8)	-0.018(8)
C(3)	0.07(1)	0.05(1)	0.05(1)	-0.003(8)	0.025(8)	-0.013(8)
C(4)	0.08(1)	0.040(9)	0.053(9)	0.007(8)	0.028(8)	-0.005(8)
C(5)	0.07(1)	0.05(1)	0.06(1)	-0.018(8)	0.023(8)	-0.006(8)
C(6)	0.041(9)	0.045(9)	0.06(1)	-0.002(8)	0.031(8)	-0.009(7)
C(7)	0.055(9)	0.039(9)	0.054(9)	-0.003(7)	0.015(8)	0.005(7)
C(8)	0.06(1)	0.05(1)	0.054(9)	0.007(8)	0.016(8)	0.003(8)
C(9)	0.05(1)	0.08(1)	0.07(1)	0.00(1)	0.04(1)	0.01(1)
C(10)	0.08(1)	0.07(1)	0.08(1)	0.01(1)	0.03(1)	0.01(1)
C(11)	0.08(1)	0.05(1)	0.09(1)	0.01(1)	0.02(1)	-0.01(1)
C(12)	0.05(1)	0.05(1)	0.07(1)	0.002(8)	0.024(8)	-0.006(8)
C(13)	0.08(1)	0.06(1)	0.027(8)	-0.004(7)	0.016(8)	-0.000(8)
C(14)	0.06(1)	0.08(1)	0.04(1)	0.008(9)	0.020(8)	0.01(1)
C(15)	0.08(1)	0.12(2)	0.025(9)	-0.00(1)	0.013(9)	0.03(1)
C(16)	0.06(1)	0.08(1)	0.042(9)	-0.005(9)	0.021(9)	-0.00(1)
C(17)	0.09(1)	0.07(1)	0.04(1)	-0.004(9)	0.006(9)	-0.03(1)
C(18)	0.08(1)	0.06(1)	0.038(9)	-0.002(8)	0.023(8)	-0.020(9)
C(19)	0.07(1)	0.07(1)	0.09(1)	-0.02(1)	0.01(1)	-0.04(1)
C(20)	0.13(2)	0.06(1)	0.05(1)	-0.019(9)	0.03(1)	0.01(1)
C(33)	0.06(1)	0.08(1)	0.08(1)	-0.01(1)	0.05(1)	-0.02(1)
C(34)	0.05(1)	0.07(1)	0.09(1)	-0.008(9)	0.030(9)	-0.020(9)
C(35)	0.09(1)	0.06(1)	0.09(1)	-0.01(1)	0.04(1)	-0.02(1)
C(36)	0.07(1)	0.04(1)	0.10(1)	-0.01(1)	0.02(1)	0.022(9)
C(37)	0.05(1)	0.09(1)	0.09(1)	-0.03(1)	0.02(1)	-0.00(1)
C(38)	0.04(1)	0.10(1)	0.06(1)	-0.01(1)	0.025(9)	-0.02(1)
C(39)	0.09(1)	0.08(1)	0.06(1)	-0.01(1)	0.01(1)	0.01(1)

Table 6: Interatomic distances (Å) for complex 5b

Cr(1) - C(1)	2.21(1)	Cr(1) - C(2)	2.26(1)
Cr(1) - C(3)	2.26(1)	Cr(1) - C(4)	2.28(1)
Cr(1) - C(5)	2.23(2)	Cr(1) - C(6)	2.24(1)
Cr(1) - C(33)	1.80(2)	Cr(1) - C(34)	1.81(2)
Cr(1) - C(35)	1.83(2)		
Mn(1) - P(1)	2.183(6)	Mn(1) - C(8)	2.21(1)
Mn(1) - C(9)	2.12(2)	Mn(1) - C(10)	2.14(2)
Mn(1) - C(11)	2.14(2)	Mn(1) - C(12)	2.20(2)
Mn(1) - C(36)	1.79(2)	Mn(1) - C(37)	1.77(2)
Mn(2) - P(2)	2.184(5)	Mn(2) - C(14)	2.21(1)
Mn(2) - C(15)	2.17(1)	Mn(2) - C(16)	2.13(1)
Mn(2) - C(17)	2.16(2)	Mn(2) - C(18)	2.23(2)
Mn(2) - C(38)	1.74(2)	Mn(2) - C(39)	1.76(2)
P(1) - O(11)	1.59(2)	P(1) - O(12)	1.56(2)
P(1) - O(13)	1.57(2)	P(2) - O(21)	1.58(2)
P(2) - O(22)	1.54(2)	P(2) - O(23)	1.60(1)
O(1) - C(1)	1.37(1)	O(1) - C(19)	1.46(2)
O(3) - C(3)	1.36(2)	O(3) - C(20)	1.45(2)
O(11) - C(21)	1.52(4)	O(12) - C(23)	1.21(6)
O(13) - C(25)	1.42(3)	O(21) - C(27)	1.30(3)
O(22) - C(29)	1.22(4)	O(23) - C(31)	1.32(3)
O(33) - C(33)	1.17(2)	O(34) - C(34)	1.17(2)
O(35) - C(35)	1.15(2)	O(36) - C(36)	1.16(2)
O(37) - C(37)	1.16(2)	O(38) - C(38)	1.18(2)
O(39) - C(39)	1.18(2)	C(1) - C(2)	1.46(2)
C(1) - C(6)	1.45(2)	C(2) - C(3)	1.42(2)
C(2) - C(7)	1.55(2)	C(3) - C(4)	1.41(2)
C(4) - C(5)	1.42(2)	C(5) - C(6)	1.43(2)
C(6) - C(13)	1.52(2)	C(7) - C(8)	1.54(2)
C(7) - C(12)	1.51(2)	C(8) - C(9)	1.42(2)
C(9) - C(10)	1.39(2)	C(10) - C(11)	1.42(2)
C(11) - C(12)	1.41(2)	C(13) - C(14)	1.49(2)
C(13) - C(18)	1.54(2)	C(14) - C(15)	1.42(2)
C(15) - C(16)	1.43(2)	C(16) - C(17)	1.40(2)
C(17) - C(18)	1.42(2)	C(21) - C(22)	1.27(5)
C(23) - C(24)	1.24(6)	C(25) - C(26)	1.34(4)
C(27) - C(28)	1.33(4)	C(29) - C(30)	1.45(4)
C(31) - C(32)	1.53(3)		

Table 7: Bond angles (°) for complex 5b

C(1) - Cr(1) - C(2)	38.1(5)	C(1) - Cr(1) - C(3)	65.9(5)
C(2) - Cr(1) - C(3)	36.6(5)	C(1) - Cr(1) - C(4)	78.6(5)
C(2) - Cr(1) - C(4)	67.0(5)	C(3) - Cr(1) - C(4)	36.2(5)
C(1) - Cr(1) - C(5)	67.6(5)	C(2) - Cr(1) - C(5)	80.7(5)
C(3) - Cr(1) - C(5)	66.0(5)	C(4) - Cr(1) - C(5)	36.8(5)
C(1) - Cr(1) - C(6)	38.2(4)	C(2) - Cr(1) - C(6)	69.3(5)
C(3) - Cr(1) - C(6)	78.6(5)	C(4) - Cr(1) - C(6)	66.8(5)
C(5) - Cr(1) - C(6)	37.4(5)	C(1) - Cr(1) - C(33)	136.4(6)
C(2) - Cr(1) - C(33)	166.6(7)	C(3) - Cr(1) - C(33)	134.4(6)
C(4) - Cr(1) - C(33)	101.1(6)	C(5) - Cr(1) - C(33)	86.1(6)
C(1) - Cr(1) - C(34)	132.8(6)	C(2) - Cr(1) - C(34)	98.2(6)
C(3) - Cr(1) - C(34)	87.4(6)	C(4) - Cr(1) - C(34)	102.9(6)
C(5) - Cr(1) - C(34)	136.8(6)	C(1) - Cr(1) - C(35)	86.3(6)
C(2) - Cr(1) - C(35)	102.1(7)	C(3) - Cr(1) - C(35)	137.1(7)
C(4) - Cr(1) - C(35)	164.7(6)	C(5) - Cr(1) - C(35)	133.8(7)
C(6) - Cr(1) - C(33)	100.9(6)	C(6) - Cr(1) - C(34)	165.9(6)
C(33) - Cr(1) - C(34)	90.2(7)	C(6) - Cr(1) - C(35)	99.8(7)
C(33) - Cr(1) - C(35)	88.3(7)	C(34) - Cr(1) - C(35)	89.0(8)
P(1) - Mn(1) - C(8)	164.8(4)	P(1) - Mn(1) - C(9)	142.3(5)
C(8) - Mn(1) - C(9)	38.3(5)	P(1) - Mn(1) - C(10)	106.2(6)
C(8) - Mn(1) - C(10)	68.4(6)	C(9) - Mn(1) - C(10)	38.1(6)
P(1) - Mn(1) - C(11)	87.4(5)	C(8) - Mn(1) - C(11)	79.8(6)
C(9) - Mn(1) - C(11)	68.9(7)	C(10) - Mn(1) - C(11)	38.7(6)
P(1) - Mn(1) - C(12)	99.7(4)	C(8) - Mn(1) - C(12)	65.1(5)
C(9) - Mn(1) - C(12)	79.8(6)	C(10) - Mn(1) - C(12)	68.5(6)
C(11) - Mn(1) - C(12)	37.9(6)	P(1) - Mn(1) - C(36)	95.7(6)
C(8) - Mn(1) - C(36)	85.9(7)	C(9) - Mn(1) - C(36)	122.0(7)
C(10) - Mn(1) - C(36)	151.9(7)	C(11) - Mn(1) - C(36)	128.0(8)
P(1) - Mn(1) - C(37)	87.8(6)	C(8) - Mn(1) - C(37)	107.2(7)
C(9) - Mn(1) - C(37)	90.4(8)	C(10) - Mn(1) - C(37)	103.4(8)
C(11) - Mn(1) - C(37)	137.3(8)	C(12) - Mn(1) - C(36)	90.9(6)
C(12) - Mn(1) - C(37)	170.2(7)	C(36) - Mn(1) - C(37)	94.7(8)
P(2) - Mn(2) - C(14)	103.1(4)	P(2) - Mn(2) - C(15)	89.2(5)
C(14) - Mn(2) - C(15)	37.7(6)	P(2) - Mn(2) - C(16)	106.1(5)
C(14) - Mn(2) - C(16)	68.3(6)	C(15) - Mn(2) - C(16)	38.9(6)
P(2) - Mn(2) - C(17)	141.3(6)	C(14) - Mn(2) - C(17)	78.9(6)
C(15) - Mn(2) - C(17)	68.7(7)	C(16) - Mn(2) - C(17)	38.0(6)
P(2) - Mn(2) - C(18)	167.4(4)	C(14) - Mn(2) - C(18)	64.6(5)
C(15) - Mn(2) - C(18)	79.4(6)	C(16) - Mn(2) - C(18)	68.0(6)
C(17) - Mn(2) - C(18)	37.7(6)	P(2) - Mn(2) - C(38)	92.5(5)
C(14) - Mn(2) - C(38)	87.4(7)	C(15) - Mn(2) - C(38)	123.3(8)
C(16) - Mn(2) - C(38)	151.9(7)	C(17) - Mn(2) - C(38)	126.1(8)
P(2) - Mn(2) - C(39)	89.4(6)	C(14) - Mn(2) - C(39)	167.0(7)
C(15) - Mn(2) - C(39)	140.8(8)	C(16) - Mn(2) - C(39)	105.0(7)
C(17) - Mn(2) - C(39)	89.0(7)	C(18) - Mn(2) - C(38)	89.5(7)
C(18) - Mn(2) - C(39)	102.8(7)	C(38) - Mn(2) - C(39)	95.9(8)
Mn(1) - P(1) - O(11)	113.2(6)	Mn(1) - P(1) - O(12)	116.4(9)
O(11) - P(1) - O(12)	101.0(13)	Mn(1) - P(1) - O(13)	121.6(6)
O(11) - P(1) - O(13)	104.1(9)	O(12) - P(1) - O(13)	97.4(10)
Mn(2) - P(2) - O(21)	121.8(7)	Mn(2) - P(2) - O(22)	117.5(6)
O(21) - P(2) - O(22)	100.7(11)	Mn(2) - P(2) - O(23)	113.9(5)
O(21) - P(2) - O(23)	100.0(9)	O(22) - P(2) - O(23)	99.2(10)
C(1) - O(1) - C(19)	113.8(11)	C(3) - O(3) - C(20)	117.7(11)
P(1) - O(11) - C(21)	134.2(21)	P(1) - O(12) - C(23)	140.3(41)
P(1) - O(13) - C(25)	129.6(16)	P(2) - O(21) - C(27)	128.5(19)
P(2) - O(22) - C(29)	143.8(28)	P(2) - O(23) - C(31)	127.6(17)
Cr(1) - C(1) - O(1)	129.6(9)	Cr(1) - C(1) - C(2)	72.8(7)

Table 7. (cont.)

O(1) - C(1) - C(2)	118.9(12)	Cr(1) - C(1) - C(6)	72.1(7)
O(1) - C(1) - C(6)	118.4(11)	C(2) - C(1) - C(6)	122.7(12)
Cr(1) - C(2) - C(1)	69.1(7)	Cr(1) - C(2) - C(3)	71.7(8)
C(1) - C(2) - C(3)	115.2(13)	Cr(1) - C(2) - C(7)	136.4(9)
C(1) - C(2) - C(7)	124.7(12)	C(3) - C(2) - C(7)	119.4(12)
Cr(1) - C(3) - O(3)	134.1(10)	Cr(1) - C(3) - C(2)	71.7(8)
O(3) - C(3) - C(2)	113.9(13)	Cr(1) - C(3) - C(4)	72.7(8)
O(3) - C(3) - C(4)	121.7(13)	C(2) - C(3) - C(4)	124.3(14)
Cr(1) - C(4) - C(3)	71.1(9)	Cr(1) - C(4) - C(5)	69.6(8)
C(3) - C(4) - C(5)	119.0(13)	Cr(1) - C(5) - C(4)	73.6(9)
Cr(1) - C(5) - C(6)	71.8(8)	C(4) - C(5) - C(6)	121.2(14)
Cr(1) - C(6) - C(1)	69.7(7)	Cr(1) - C(6) - C(5)	70.8(8)
C(1) - C(6) - C(5)	117.4(13)	Cr(1) - C(6) - C(13)	130.7(10)
C(1) - C(6) - C(13)	120.4(12)	C(5) - C(6) - C(13)	122.2(13)
C(2) - C(7) - C(8)	116.7(11)	C(2) - C(7) - C(12)	114.5(12)
C(8) - C(7) - C(12)	101.7(11)	Mn(1) - C(8) - C(7)	92.9(8)
Mn(1) - C(8) - C(9)	67.4(9)	C(7) - C(8) - C(9)	120.0(13)
Mn(1) - C(9) - C(8)	74.3(9)	Mn(1) - C(9) - C(10)	71.8(10)
C(8) - C(9) - C(10)	120.8(16)	Mn(1) - C(10) - C(9)	70.1(10)
Mn(1) - C(10) - C(11)	70.6(10)	C(9) - C(10) - C(11)	118.1(17)
Mn(1) - C(11) - C(10)	70.7(10)	Mn(1) - C(11) - C(12)	73.3(10)
C(10) - C(11) - C(12)	119.5(16)	Mn(1) - C(12) - C(7)	94.2(9)
Mn(1) - C(12) - C(11)	68.8(9)	C(7) - C(12) - C(11)	121.4(14)
C(6) - C(13) - C(14)	114.6(12)	C(6) - C(13) - C(18)	113.4(12)
C(14) - C(13) - C(18)	103.1(13)	Mn(2) - C(14) - C(13)	93.9(9)
Mn(2) - C(14) - C(15)	69.7(9)	C(13) - C(14) - C(15)	122.2(15)
Mn(2) - C(15) - C(14)	72.6(9)	Mn(2) - C(15) - C(16)	68.9(9)
C(14) - C(15) - C(16)	117.5(16)	Mn(2) - C(16) - C(15)	72.3(9)
Mn(2) - C(16) - C(17)	72.4(9)	C(15) - C(16) - C(17)	119.8(16)
Mn(2) - C(17) - C(16)	69.6(9)	Mn(2) - C(17) - C(18)	73.7(9)
C(16) - C(17) - C(18)	119.7(16)	Mn(2) - C(18) - C(13)	91.9(9)
Mn(2) - C(18) - C(17)	68.7(9)	C(13) - C(18) - C(17)	120.1(14)
O(11) - C(21) - C(22)	100.4(40)	O(12) - C(23) - C(24)	152.2(73)
O(13) - C(25) - C(26)	116.2(28)	O(21) - C(27) - C(28)	119.8(33)
O(22) - C(29) - C(30)	120.5(34)	O(23) - C(31) - C(32)	108.9(24)
Cr(1) - C(33) - O(33)	178.7(15)	Cr(1) - C(34) - O(34)	176.7(15)
Cr(1) - C(35) - O(35)	178.1(16)	Mn(1) - C(36) - O(36)	173.7(17)
Mn(1) - C(37) - O(37)	176.9(17)	Mn(2) - C(38) - O(38)	177.0(16)
Mn(2) - C(39) - O(39)	178.2(17)		

Table 8: Hydrogen atoms fractional atomic coordinates for complex 5b

Atom	x/a	y/b	z/c	U(iso)
H(41)	0.4934	0.4023	0.6420	0.0567
H(51)	0.4356	0.4090	0.4910	0.0488
H(71)	0.5401	0.1441	0.6768	0.0485
H(81)	0.5589	0.0463	0.5847	0.0485
H(91)	0.6838	0.0532	0.5305	0.0548
H(101)	0.8139	0.1248	0.6062	0.0719
H(111)	0.8144	0.1893	0.7327	0.0797
H(121)	0.6850	0.1707	0.7780	0.0485
H(131)	0.4360	0.2463	0.3593	0.0514
H(141)	0.2824	0.2701	0.3219	0.0514
H(151)	0.2274	0.3939	0.3442	0.0609
H(161)	0.3199	0.4996	0.3300	0.0622
H(171)	0.4675	0.4770	0.3240	0.0572
H(181)	0.5079	0.3474	0.3066	0.0514
H(191)	0.4368	0.0811	0.4057	0.0758
H(192)	0.4169	0.1072	0.4901	0.0758
H(193)	0.3790	0.1570	0.4048	0.0758
H(201)	0.5946	0.3360	0.8417	0.0731
H(202)	0.6099	0.3888	0.7692	0.0731
H(203)	0.5081	0.3691	0.7669	0.0731

Table 9: Fractional parameters for complex 9

Atom	x/a	y/b	z/c	U(eq)	U(iso)
Cr (1)	0.3556 (2)	0.3018 (2)	0.0664 (1)	0.0393	
Mn (1)	0.1698 (2)	0.4871 (2)	0.2227 (1)	0.0424	
Mn (2)	0.3131 (2)	-0.0615 (2)	0.0793 (2)	0.0425	
Mn (3)	0.3354 (2)	0.4523 (2)	-0.1315 (2)	0.0554	
P (1)	0.0494 (4)	0.5107 (4)	0.2664 (3)	0.0614	
P (2)	0.2368 (4)	-0.1772 (3)	0.0780 (3)	0.0537	
P (3)	0.4528 (6)	0.5231 (6)	-0.1522 (3)	0.0979	
O (1)	0.2274 (8)	0.1903 (7)	0.1395 (4)		0.039 (3)
O (3)	0.2112 (8)	0.4568 (7)	0.0550 (5)		0.046 (3)
O (5)	0.2962 (8)	0.2113 (8)	-0.0380 (5)		0.052 (4)
O (11)	0.006 (1)	0.605 (1)	0.2535 (8)		0.116 (7)
O (12)	0.053 (1)	0.504 (1)	0.3275 (9)		0.123 (8)
O (13)	-0.035 (1)	0.453 (1)	0.2553 (7)		0.099 (6)
O (21)	0.181 (1)	-0.2028 (9)	0.1282 (6)		0.066 (4)
O (22)	0.2843 (9)	-0.2648 (9)	0.0715 (6)		0.073 (4)
O (23)	0.161 (1)	-0.1788 (9)	0.0366 (6)		0.070 (4)
O (31)	0.539 (2)	0.512 (1)	-0.1191 (9)		0.130 (8)
O (32)	0.485 (2)	0.551 (2)	-0.201 (1)		0.17 (1)
O (33)	0.449 (2)	0.631 (2)	-0.137 (1)		0.23 (1)
O (46)	0.511 (1)	0.234 (1)	0.0111 (7)		0.096 (6)
O (47)	0.458 (1)	0.4614 (9)	0.0779 (7)		0.076 (4)
O (48)	0.434 (1)	0.253 (1)	0.1662 (6)		0.084 (5)
O (49)	0.382 (1)	-0.076 (1)	-0.0227 (7)		0.098 (6)
O (50)	0.458 (1)	-0.158 (1)	0.1254 (6)		0.082 (5)
O (51)	0.258 (1)	0.616 (1)	0.2858 (6)		0.082 (5)
O (52)	0.228 (1)	0.347 (1)	0.2864 (7)		0.094 (6)
O (53)	0.274 (1)	0.470 (1)	-0.2343 (8)		0.106 (6)
O (54)	0.236 (1)	0.595 (1)	-0.0904 (8)		0.113 (7)
C (1)	0.236 (1)	0.237 (1)	0.0968 (7)	0.0311	
C (2)	0.222 (1)	0.327 (1)	0.0984 (6)	0.0336	
C (3)	0.231 (1)	0.373 (1)	0.0521 (7)	0.0336	
C (4)	0.258 (1)	0.335 (1)	0.0063 (7)	0.0435	
C (5)	0.272 (1)	0.249 (1)	0.0076 (7)	0.0378	
C (6)	0.265 (1)	0.195 (1)	0.0505 (8)	0.0396	
C (7)	0.207 (1)	0.366 (1)	0.1524 (7)	0.0301	
C (8)	0.264 (1)	0.439 (1)	0.1664 (7)	0.0400	
C (9)	0.246 (1)	0.522 (1)	0.1599 (8)	0.0478	
C (10)	0.159 (1)	0.547 (1)	0.1527 (8)	0.0483	
C (11)	0.094 (1)	0.486 (1)	0.1557 (8)	0.0444	
C (12)	0.114 (1)	0.402 (1)	0.1638 (8)	0.0415	
C (13)	0.290 (1)	0.101 (1)	0.0478 (7)	0.0396	
C (14)	0.359 (1)	0.072 (1)	0.0862 (8)	0.0414	
C (15)	0.337 (1)	0.041 (1)	0.1333 (8)	0.0411	
C (16)	0.253 (1)	0.005 (1)	0.1397 (9)	0.0503	
C (17)	0.195 (1)	0.003 (1)	0.0993 (8)	0.0477	
C (18)	0.218 (1)	0.037 (1)	0.0552 (8)	0.0455	
C (19)	0.275 (1)	0.395 (1)	-0.0378 (8)	0.0468	
C (20)	0.373 (2)	0.409 (1)	-0.0527 (9)	0.0621	
C (21)	0.411 (2)	0.362 (2)	-0.090 (1)	0.0640	
C (22)	0.365 (3)	0.322 (2)	-0.126 (1)	0.0820	
C (23)	0.274 (2)	0.334 (2)	-0.127 (1)	0.0691	
C (24)	0.235 (2)	0.377 (1)	-0.089 (1)	0.0601	
C (25)	0.138 (1)	0.178 (1)	0.1549 (8)		0.064 (6)
C (26)	0.127 (1)	0.476 (1)	0.0361 (8)		0.057 (6)
C (27)	0.223 (2)	0.171 (1)	-0.0639 (9)		0.074 (7)
C (28)	-0.083 (3)	0.633 (2)	0.263 (1)		0.13 (1)
C (29)	-0.072 (2)	0.727 (2)	0.264 (1)		0.11 (1)

Table 9 (cont)

Atom	x/a	y/b	z/c	U(eq)	U(iso)
C(30)	0.076(5)	0.541(5)	0.369(3)		0.30(4)
C(31)	0.029(2)	0.586(2)	0.404(1)		0.12(1)
C(32)	-0.042(2)	0.373(2)	0.271(1)		0.13(1)
C(33)	-0.128(3)	0.346(2)	0.276(1)		0.15(1)
C(34)	0.224(2)	-0.218(2)	0.175(1)		0.087(8)
C(35)	0.149(2)	-0.220(2)	0.218(1)		0.102(9)
C(36)	0.337(2)	-0.280(2)	0.027(1)		0.088(8)
C(37)	0.371(2)	-0.372(2)	0.031(1)		0.13(1)
C(38)	0.096(2)	-0.256(2)	0.037(1)		0.12(1)
C(39)	0.084(3)	-0.270(2)	-0.017(1)		0.15(1)
C(40)	0.629(4)	0.557(3)	-0.128(2)		0.20(2)
C(41)	0.667(3)	0.572(3)	-0.088(2)		0.16(2)
C(42)	0.511(2)	0.461(2)	-0.223(1)		0.12(1)
C(43)	0.508(2)	0.480(2)	-0.288(1)		0.14(1)
C(44)	0.396(3)	0.686(3)	-0.166(2)		0.17(2)
C(45)	0.402(3)	0.758(3)	-0.123(2)		0.20(2)
C(46)	0.449(1)	0.262(1)	0.0342(8)		0.058(6)
C(47)	0.414(1)	0.400(1)	0.0730(8)		0.054(5)
C(48)	0.405(1)	0.272(1)	0.1271(8)		0.058(6)
C(49)	0.354(2)	-0.071(1)	0.0194(9)		0.064(6)
C(50)	0.397(2)	-0.120(1)	0.1061(9)		0.064(6)
C(51)	0.219(2)	0.564(1)	0.2621(9)		0.065(6)
C(52)	0.203(1)	0.404(1)	0.2633(9)		0.060(6)
C(53)	0.301(2)	0.464(2)	-0.189(1)		0.079(7)
C(54)	0.283(2)	0.537(2)	-0.108(1)		0.076(7)

Table 10. Anisotropic thermal parameters for complex 9

Atom	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Cr(1)	0.036(2)	0.040(2)	0.043(2)	0.002(2)	0.005(2)	0.002(1)
Mn(1)	0.040(2)	0.044(2)	0.046(2)	-0.008(2)	-0.001(2)	-0.001(1)
Mn(2)	0.042(2)	0.037(1)	0.050(2)	-0.003(1)	0.004(2)	0.000(1)
Mn(3)	0.069(2)	0.064(2)	0.041(2)	0.011(2)	0.008(2)	0.010(2)
P(1)	0.052(4)	0.082(4)	0.063(4)	-0.027(4)	0.002(3)	-0.004(3)
P(2)	0.053(3)	0.044(3)	0.067(4)	0.002(3)	0.006(4)	-0.004(2)
P(3)	0.096(6)	0.137(8)	0.095(6)	0.056(6)	0.003(5)	-0.008(6)
C(1)	0.04(1)	0.025(9)	0.05(1)	0.008(9)	0.013(9)	-0.008(8)
C(2)	0.04(1)	0.04(1)	0.021(9)	0.002(8)	-0.003(8)	0.003(9)
C(3)	0.04(1)	0.03(1)	0.04(1)	-0.000(8)	-0.006(9)	0.000(8)
C(4)	0.04(1)	0.05(1)	0.05(1)	-0.01(1)	-0.00(1)	0.01(1)
C(5)	0.04(1)	0.03(1)	0.04(1)	-0.01(1)	0.01(1)	0.002(9)
C(6)	0.03(1)	0.04(1)	0.07(1)	-0.01(1)	0.00(1)	0.006(9)
C(7)	0.019(9)	0.05(1)	0.03(1)	-0.005(9)	0.001(8)	0.005(8)
C(8)	0.04(1)	0.05(1)	0.04(1)	-0.01(1)	0.001(9)	-0.01(1)
C(9)	0.06(1)	0.05(1)	0.04(1)	-0.01(1)	-0.00(1)	-0.01(1)
C(10)	0.06(2)	0.04(1)	0.05(1)	-0.00(1)	0.00(1)	0.01(1)
C(11)	0.05(1)	0.05(1)	0.06(1)	-0.00(1)	-0.01(1)	0.03(1)
C(12)	0.04(1)	0.05(1)	0.06(1)	-0.00(1)	0.02(1)	0.01(1)
C(13)	0.05(1)	0.03(1)	0.04(1)	-0.005(9)	0.01(1)	-0.01(1)
C(14)	0.03(1)	0.04(1)	0.08(1)	-0.02(1)	0.01(1)	0.001(9)
C(15)	0.05(1)	0.03(1)	0.06(1)	-0.02(1)	0.02(1)	-0.01(1)
C(16)	0.06(1)	0.03(1)	0.08(2)	0.00(1)	0.01(1)	0.01(1)
C(17)	0.03(1)	0.05(1)	0.06(1)	-0.00(1)	-0.00(1)	0.00(1)
C(18)	0.08(2)	0.03(1)	0.05(1)	-0.006(9)	0.00(1)	-0.01(1)
C(19)	0.04(1)	0.06(1)	0.05(1)	0.02(1)	0.01(1)	0.00(1)
C(20)	0.09(2)	0.06(2)	0.05(1)	0.00(1)	-0.02(1)	0.00(1)
C(21)	0.06(2)	0.07(2)	0.08(2)	0.03(2)	0.02(1)	0.01(1)
C(22)	0.21(4)	0.05(2)	0.07(2)	0.00(1)	0.05(3)	-0.01(2)
C(23)	0.11(2)	0.10(2)	0.05(2)	0.02(2)	-0.02(2)	-0.05(2)
C(24)	0.06(2)	0.07(2)	0.06(2)	0.01(1)	0.01(1)	0.01(1)

Table 11 Interatomic distances (Å) for complex 9

Cr(1) - C(1)	2.24(2)	Cr(1) - C(2)	2.22(2)
Cr(1) - C(3)	2.23(2)	Cr(1) - C(4)	2.23(2)
Cr(1) - C(5)	2.16(2)	Cr(1) - C(6)	2.22(2)
Cr(1) - C(46)	1.77(2)	Cr(1) - C(47)	1.80(2)
Cr(1) - C(48)	1.82(2)		
Mn(1) - P(1)	2.188(7)	Mn(1) - C(8)	2.20(2)
Mn(1) - C(9)	2.09(2)	Mn(1) - C(10)	2.08(2)
Mn(1) - C(11)	2.10(2)	Mn(1) - C(12)	2.22(2)
Mn(1) - C(51)	1.76(2)	Mn(1) - C(52)	1.77(2)
Mn(2) - P(2)	2.170(6)	Mn(2) - C(14)	2.23(2)
Mn(2) - C(15)	2.19(2)	Mn(2) - C(16)	2.11(2)
Mn(2) - C(17)	2.13(2)	Mn(2) - C(18)	2.22(2)
Mn(2) - C(49)	1.69(2)	Mn(2) - C(50)	1.73(2)
Mn(3) - P(3)	2.17(1)	Mn(3) - C(20)	2.25(2)
Mn(3) - C(21)	2.13(2)	Mn(3) - C(22)	2.11(3)
Mn(3) - C(23)	2.10(3)	Mn(3) - C(24)	2.23(2)
Mn(3) - C(53)	1.61(3)	Mn(3) - C(54)	1.68(3)
P(1) - O(11)	1.66(2)	P(1) - O(12)	1.61(2)
P(1) - O(13)	1.60(2)	P(2) - O(21)	1.62(2)
P(2) - O(22)	1.57(1)	P(2) - O(23)	1.58(2)
P(3) - O(31)	1.58(2)	P(3) - O(32)	1.43(3)
P(3) - O(33)	1.75(4)	O(1) - C(1)	1.35(2)
O(1) - C(25)	1.42(2)	O(3) - C(3)	1.36(2)
O(3) - C(26)	1.41(2)	O(5) - C(5)	1.38(2)
O(5) - C(27)	1.46(3)	O(11) - C(28)	1.45(4)
O(12) - C(30)	1.29(8)	O(13) - C(32)	1.34(4)
O(21) - C(34)	1.42(3)	O(22) - C(36)	1.45(3)
O(23) - C(38)	1.57(4)	O(31) - C(40)	1.57(5)
O(32) - C(42)	1.59(4)	O(33) - C(44)	1.41(5)
O(46) - C(46)	1.20(2)	O(47) - C(47)	1.18(2)
O(48) - C(48)	1.16(2)	O(49) - C(49)	1.19(3)
O(50) - C(50)	1.21(2)	O(51) - C(51)	1.19(2)
O(52) - C(52)	1.15(3)	O(53) - C(53)	1.26(3)
O(54) - C(54)	1.25(3)	C(1) - C(2)	1.43(2)
C(1) - C(6)	1.46(2)	C(2) - C(3)	1.43(2)
C(2) - C(7)	1.57(2)	C(3) - C(4)	1.41(2)
C(4) - C(5)	1.38(3)	C(4) - C(19)	1.52(3)
C(5) - C(6)	1.42(3)	C(6) - C(13)	1.53(3)
C(7) - C(8)	1.50(2)	C(7) - C(12)	1.55(2)
C(8) - C(9)	1.35(3)	C(9) - C(10)	1.39(3)
C(10) - C(11)	1.39(3)	C(11) - C(12)	1.38(3)
C(13) - C(14)	1.52(3)	C(13) - C(18)	1.51(3)
C(14) - C(15)	1.37(3)	C(15) - C(16)	1.41(3)
C(16) - C(17)	1.38(3)	C(17) - C(18)	1.32(3)
C(19) - C(20)	1.55(3)	C(19) - C(24)	1.50(3)
C(20) - C(21)	1.36(3)	C(21) - C(22)	1.34(4)
C(22) - C(23)	1.39(4)	C(23) - C(24)	1.35(4)
C(28) - C(29)	1.50(4)	C(30) - C(31)	1.36(8)
C(32) - C(33)	1.38(4)	C(34) - C(35)	1.59(4)
C(36) - C(37)	1.55(4)	C(38) - C(39)	1.44(4)
C(40) - C(41)	1.22(6)	C(44) - C(45)	1.60(6)

Table 12: Bond angles (°) for complex 9

C(1) - Cr(1) - C(2)	37.5(6)	C(1) - Cr(1) - C(3)	66.8(6)
C(2) - Cr(1) - C(3)	37.4(6)	C(1) - Cr(1) - C(4)	79.6(7)
C(2) - Cr(1) - C(4)	67.8(6)	C(3) - Cr(1) - C(4)	36.8(6)
C(1) - Cr(1) - C(5)	66.6(7)	C(2) - Cr(1) - C(5)	79.0(6)
C(3) - Cr(1) - C(5)	65.5(6)	C(4) - Cr(1) - C(5)	36.7(7)
C(1) - Cr(1) - C(6)	38.1(6)	C(2) - Cr(1) - C(6)	69.1(6)
C(3) - Cr(1) - C(6)	80.4(6)	C(4) - Cr(1) - C(6)	68.7(7)
C(5) - Cr(1) - C(6)	37.8(7)	C(1) - Cr(1) - C(46)	131.5(8)
C(2) - Cr(1) - C(46)	166.9(8)	C(3) - Cr(1) - C(46)	141.1(8)
C(4) - Cr(1) - C(46)	106.2(9)	C(5) - Cr(1) - C(46)	89.4(8)
C(1) - Cr(1) - C(47)	139.5(8)	C(2) - Cr(1) - C(47)	104.7(8)
C(3) - Cr(1) - C(47)	89.2(8)	C(4) - Cr(1) - C(47)	100.7(8)
C(5) - Cr(1) - C(47)	133.5(9)	C(1) - Cr(1) - C(48)	84.5(8)
C(2) - Cr(1) - C(48)	95.0(8)	C(3) - Cr(1) - C(48)	128.6(8)
C(4) - Cr(1) - C(48)	162.5(9)	C(5) - Cr(1) - C(48)	139.8(8)
C(6) - Cr(1) - C(46)	98.0(8)	C(6) - Cr(1) - C(47)	169.0(8)
C(46) - Cr(1) - C(47)	87.8(9)	C(6) - Cr(1) - C(48)	102.8(8)
C(46) - Cr(1) - C(48)	89.9(10)	C(47) - Cr(1) - C(48)	86.6(9)
P(1) - Mn(1) - C(8)	163.1(5)	P(1) - Mn(1) - C(9)	146.0(6)
C(8) - Mn(1) - C(9)	36.8(7)	P(1) - Mn(1) - C(10)	108.6(6)
C(8) - Mn(1) - C(10)	67.3(7)	C(9) - Mn(1) - C(10)	38.9(8)
P(1) - Mn(1) - C(11)	89.0(6)	C(8) - Mn(1) - C(11)	77.9(7)
C(9) - Mn(1) - C(11)	69.0(8)	C(10) - Mn(1) - C(11)	38.7(8)
P(1) - Mn(1) - C(12)	98.7(5)	C(8) - Mn(1) - C(12)	64.4(7)
C(9) - Mn(1) - C(12)	79.6(7)	C(10) - Mn(1) - C(12)	68.4(7)
C(11) - Mn(1) - C(12)	37.2(7)	P(1) - Mn(1) - C(51)	85.9(8)
C(8) - Mn(1) - C(51)	110.9(9)	C(9) - Mn(1) - C(51)	92.6(9)
C(10) - Mn(1) - C(51)	103.6(9)	C(11) - Mn(1) - C(51)	136.7(9)
P(1) - Mn(1) - C(52)	92.8(8)	C(8) - Mn(1) - C(52)	87.9(9)
C(9) - Mn(1) - C(52)	121.2(10)	C(10) - Mn(1) - C(52)	153.8(9)
C(11) - Mn(1) - C(52)	130.6(9)	C(12) - Mn(1) - C(51)	171.6(9)
C(12) - Mn(1) - C(52)	94.1(9)	C(51) - Mn(1) - C(52)	92.5(10)
P(2) - Mn(2) - C(14)	165.4(5)	P(2) - Mn(2) - C(15)	136.6(6)
C(14) - Mn(2) - C(15)	36.1(7)	P(2) - Mn(2) - C(16)	101.6(6)
C(14) - Mn(2) - C(16)	66.5(7)	C(15) - Mn(2) - C(16)	38.2(7)
P(2) - Mn(2) - C(17)	87.8(5)	C(14) - Mn(2) - C(17)	77.6(7)
C(15) - Mn(2) - C(17)	67.7(8)	C(16) - Mn(2) - C(17)	37.9(7)
P(2) - Mn(2) - C(18)	104.1(5)	C(14) - Mn(2) - C(18)	63.9(7)
C(15) - Mn(2) - C(18)	76.6(7)	C(16) - Mn(2) - C(18)	65.2(8)
C(17) - Mn(2) - C(18)	35.3(7)	P(2) - Mn(2) - C(49)	95.9(8)
C(14) - Mn(2) - C(49)	92.8(9)	C(15) - Mn(2) - C(49)	127.5(9)
C(16) - Mn(2) - C(49)	153.9(9)	C(17) - Mn(2) - C(49)	125.2(10)
P(2) - Mn(2) - C(50)	86.9(7)	C(14) - Mn(2) - C(50)	104.2(9)
C(15) - Mn(2) - C(50)	90.8(9)	C(16) - Mn(2) - C(50)	106.4(10)
C(17) - Mn(2) - C(50)	141.2(10)	C(18) - Mn(2) - C(49)	92.0(9)
C(18) - Mn(2) - C(50)	167.1(9)	C(49) - Mn(2) - C(50)	93.6(11)
P(3) - Mn(3) - C(20)	100.4(7)	P(3) - Mn(3) - C(21)	92.0(7)
C(20) - Mn(3) - C(21)	35.9(9)	P(3) - Mn(3) - C(22)	110.1(12)
C(20) - Mn(3) - C(22)	65.9(11)	C(21) - Mn(3) - C(22)	36.8(11)
P(3) - Mn(3) - C(23)	147.0(11)	C(20) - Mn(3) - C(23)	77.6(9)
C(21) - Mn(3) - C(23)	66.9(10)	C(22) - Mn(3) - C(23)	38.6(12)
P(3) - Mn(3) - C(24)	163.5(7)	C(20) - Mn(3) - C(24)	63.2(9)
C(21) - Mn(3) - C(24)	75.5(8)	C(22) - Mn(3) - C(24)	66.0(11)
C(23) - Mn(3) - C(24)	36.1(10)	P(3) - Mn(3) - C(53)	88.5(9)
C(20) - Mn(3) - C(53)	168.1(11)	C(21) - Mn(3) - C(53)	136.9(13)
C(22) - Mn(3) - C(53)	103.8(13)	C(23) - Mn(3) - C(53)	90.6(11)
P(3) - Mn(3) - C(54)	93.7(9)	C(20) - Mn(3) - C(54)	91.3(11)
C(21) - Mn(3) - C(54)	126.9(12)	C(22) - Mn(3) - C(54)	149.1(12)

C (23) - Mn (3) - C (54)	119.2 (14)	C (24) - Mn (3) - C (53)	108.0 (11)
C (24) - Mn (3) - C (54)	85.5 (10)	C (53) - Mn (3) - C (54)	96.0 (13)
Mn (1) - P (1) - O (11)	112.1 (8)	Mn (1) - P (1) - O (12)	118.9 (9)
O (11) - P (1) - O (12)	105.8 (12)	Mn (1) - P (1) - O (13)	118.4 (7)
O (11) - P (1) - O (13)	99.1 (11)	O (12) - P (1) - O (13)	100.0 (12)
Mn (2) - P (2) - O (21)	118.7 (6)	Mn (2) - P (2) - O (22)	120.3 (6)
O (21) - P (2) - O (22)	96.2 (8)	Mn (2) - P (2) - O (23)	114.2 (6)
O (21) - P (2) - O (23)	100.1 (8)	O (22) - P (2) - O (23)	104.1 (8)
Mn (3) - P (3) - O (31)	118.6 (9)	Mn (3) - P (3) - O (32)	131.1 (12)
O (31) - P (3) - O (32)	104.5 (15)	Mn (3) - P (3) - O (33)	114.9 (13)
O (31) - P (3) - O (33)	90.9 (16)	O (32) - P (3) - O (33)	84.7 (17)
C (1) - O (1) - C (25)	113.3 (14)	C (3) - O (3) - C (26)	113.4 (14)
C (5) - O (5) - C (27)	113.3 (15)	P (1) - O (11) - C (28)	128.0 (21)
P (1) - O (12) - C (30)	145.6 (41)	P (1) - O (13) - C (32)	123.3 (22)
P (2) - O (21) - C (34)	120.3 (15)	P (2) - O (22) - C (36)	119.3 (15)
P (2) - O (23) - C (38)	117.8 (16)	P (3) - O (31) - C (40)	126.1 (27)
P (3) - O (32) - C (42)	97.4 (21)	P (3) - O (33) - C (44)	120.6 (33)
Cr (1) - C (1) - O (1)	128.5 (12)	Cr (1) - C (1) - C (2)	70.9 (9)
O (1) - C (1) - C (2)	120.4 (15)	Cr (1) - C (1) - C (6)	70.5 (10)
O (1) - C (1) - C (6)	117.7 (14)	C (2) - C (1) - C (6)	121.7 (16)
Cr (1) - C (2) - C (1)	71.7 (10)	Cr (1) - C (2) - C (3)	71.5 (10)
C (1) - C (2) - C (3)	118.3 (15)	Cr (1) - C (2) - C (7)	123.2 (11)
C (1) - C (2) - C (7)	116.3 (15)	C (3) - C (2) - C (7)	125.2 (15)
Cr (1) - C (3) - O (3)	132.5 (12)	Cr (1) - C (3) - C (2)	71.0 (10)
O (3) - C (3) - C (2)	115.8 (15)	Cr (1) - C (3) - C (4)	71.4 (11)
O (3) - C (3) - C (4)	122.2 (16)	C (2) - C (3) - C (4)	122.0 (15)
Cr (1) - C (4) - C (3)	71.8 (11)	Cr (1) - C (4) - C (5)	69.1 (11)
C (3) - C (4) - C (5)	116.8 (17)	Cr (1) - C (4) - C (19)	125.0 (13)
C (3) - C (4) - C (19)	115.4 (16)	C (5) - C (4) - C (19)	127.6 (18)
Cr (1) - C (5) - O (5)	129.2 (13)	Cr (1) - C (5) - C (4)	74.2 (11)
O (5) - C (5) - C (4)	116.4 (17)	Cr (1) - C (5) - C (6)	73.5 (11)
O (5) - C (5) - C (6)	116.6 (16)	C (4) - C (5) - C (6)	127.0 (17)
Cr (1) - C (6) - C (1)	71.3 (10)	Cr (1) - C (6) - C (5)	68.7 (11)
C (1) - C (6) - C (5)	114.1 (15)	Cr (1) - C (6) - C (13)	126.1 (12)
C (1) - C (6) - C (13)	124.2 (17)	C (5) - C (6) - C (13)	121.6 (17)
C (2) - C (7) - C (8)	116.3 (15)	C (2) - C (7) - C (12)	117.3 (15)
C (8) - C (7) - C (12)	101.2 (14)	Mn (1) - C (8) - C (7)	93.0 (11)
Mn (1) - C (8) - C (9)	67.2 (12)	C (7) - C (8) - C (9)	126.8 (18)
Mn (1) - C (9) - C (8)	76.0 (12)	Mn (1) - C (9) - C (10)	70.2 (12)
C (8) - C (9) - C (10)	119.6 (18)	Mn (1) - C (10) - C (9)	70.9 (12)
Mn (1) - C (10) - C (11)	71.7 (12)	C (9) - C (10) - C (11)	117.8 (17)
Mn (1) - C (11) - C (10)	69.6 (12)	Mn (1) - C (11) - C (12)	75.9 (12)
C (10) - C (11) - C (12)	121.5 (18)	Mn (1) - C (12) - C (7)	90.9 (11)
Mn (1) - C (12) - C (11)	66.9 (11)	C (7) - C (12) - C (11)	122.0 (17)
C (6) - C (13) - C (14)	116.0 (15)	C (6) - C (13) - C (18)	117.8 (16)
C (14) - C (13) - C (18)	101.6 (15)	Mn (2) - C (14) - C (13)	91.5 (11)
Mn (2) - C (14) - C (15)	70.3 (10)	C (13) - C (14) - C (15)	122.7 (17)
Mn (2) - C (15) - C (14)	73.6 (11)	Mn (2) - C (15) - C (16)	68.1 (11)
C (14) - C (15) - C (16)	118.2 (20)	Mn (2) - C (16) - C (15)	73.8 (11)
Mn (2) - C (16) - C (17)	71.8 (12)	C (15) - C (16) - C (17)	119.6 (20)
Mn (2) - C (17) - C (16)	70.4 (11)	Mn (2) - C (17) - C (18)	75.8 (13)
C (16) - C (17) - C (18)	119.8 (19)	Mn (2) - C (18) - C (13)	92.3 (13)
Mn (2) - C (18) - C (17)	68.9 (13)	C (13) - C (18) - C (17)	125.4 (18)
C (4) - C (19) - C (20)	116.4 (17)	C (4) - C (19) - C (24)	119.4 (18)
C (20) - C (19) - C (24)	100.8 (17)	Mn (3) - C (20) - C (19)	92.0 (13)
Mn (3) - C (20) - C (21)	67.2 (13)	C (19) - C (20) - C (21)	120.8 (22)
Mn (3) - C (21) - C (20)	76.9 (14)	Mn (3) - C (21) - C (22)	70.8 (17)
C (20) - C (21) - C (22)	123.6 (26)	Mn (3) - C (22) - C (21)	72.5 (15)
Mn (3) - C (22) - C (23)	70.3 (18)	C (21) - C (22) - C (23)	117.4 (28)
Mn (3) - C (23) - C (22)	71.1 (16)	Mn (3) - C (23) - C (24)	77.2 (17)
C (22) - C (23) - C (24)	119.5 (27)	Mn (3) - C (24) - C (19)	94.0 (14)
Mn (3) - C (24) - C (23)	66.8 (14)	C (19) - C (24) - C (23)	125.6 (23)
O (11) - C (28) - C (29)	102.4 (29)	O (12) - C (30) - C (31)	131.0 (64)

O(13) - C(32) - C(33)	113.5(32)	O(21) - C(34) - C(35)	106.5(21)
O(22) - C(36) - C(37)	106.2(22)	O(23) - C(38) - C(39)	101.6(28)
O(31) - C(40) - C(41)	111.9(49)	O(33) - C(44) - C(45)	92.2(37)
Cr(1) - C(46) - O(46)	177.4(20)	Cr(1) - C(47) - O(47)	174.5(17)
Cr(1) - C(48) - O(48)	177.9(20)	Mn(2) - C(49) - O(49)	178.4(22)
Mn(2) - C(50) - O(50)	177.6(20)	Mn(1) - C(51) - O(51)	174.6(21)
Mn(1) - C(52) - O(52)	174.5(21)	Mn(3) - C(53) - O(53)	178.4(23)
Mn(3) - C(54) - O(54)	172.8(23)		

Table 13: Hydrogen atoms parameters for complex 9

Atom	x/a	y/b	z/c	U(iso)
H(71)	0.2223	0.3125	0.1718	0.09(1)
H(81)	0.3226	0.4261	0.1847	0.09(1)
H(91)	0.2961	0.5646	0.1602	0.09(1)
H(101)	0.1444	0.6088	0.1434	0.09(1)
H(111)	0.0288	0.5037	0.1531	0.09(1)
H(121)	0.0663	0.3630	0.1773	0.09(1)
H(131)	0.3159	0.1039	0.0111	0.09(1)
H(141)	0.4235	0.0734	0.0784	0.09(1)
H(151)	0.3800	0.0479	0.1628	0.09(1)
H(161)	0.2358	-0.0185	0.1748	0.09(1)
H(171)	0.1345	-0.0218	0.1057	0.09(1)
H(181)	0.1841	0.0154	0.0244	0.09(1)
H(191)	0.2450	0.4460	-0.0189	0.09(1)
H(201)	0.4118	0.4523	-0.0349	0.09(1)
H(211)	0.4785	0.3570	-0.0900	0.09(1)
H(221)	0.3974	0.2863	-0.1545	0.09(1)
H(231)	0.2386	0.3075	-0.1568	0.09(1)
H(241)	0.1735	0.4001	-0.0951	0.09(1)
H(251)	0.1341	0.1449	0.1866	0.09(1)
H(252)	0.1095	0.2361	0.1614	0.09(1)
H(253)	0.1038	0.1504	0.1270	0.09(1)
H(261)	0.1145	0.5386	0.0394	0.09(1)
H(262)	0.1205	0.4601	-0.0007	0.09(1)
H(263)	0.0802	0.4451	0.0562	0.09(1)
H(271)	0.2411	0.1435	-0.0970	0.09(1)
H(272)	0.1739	0.2130	-0.0725	0.09(1)
H(273)	0.1939	0.1251	-0.0422	0.09(1)