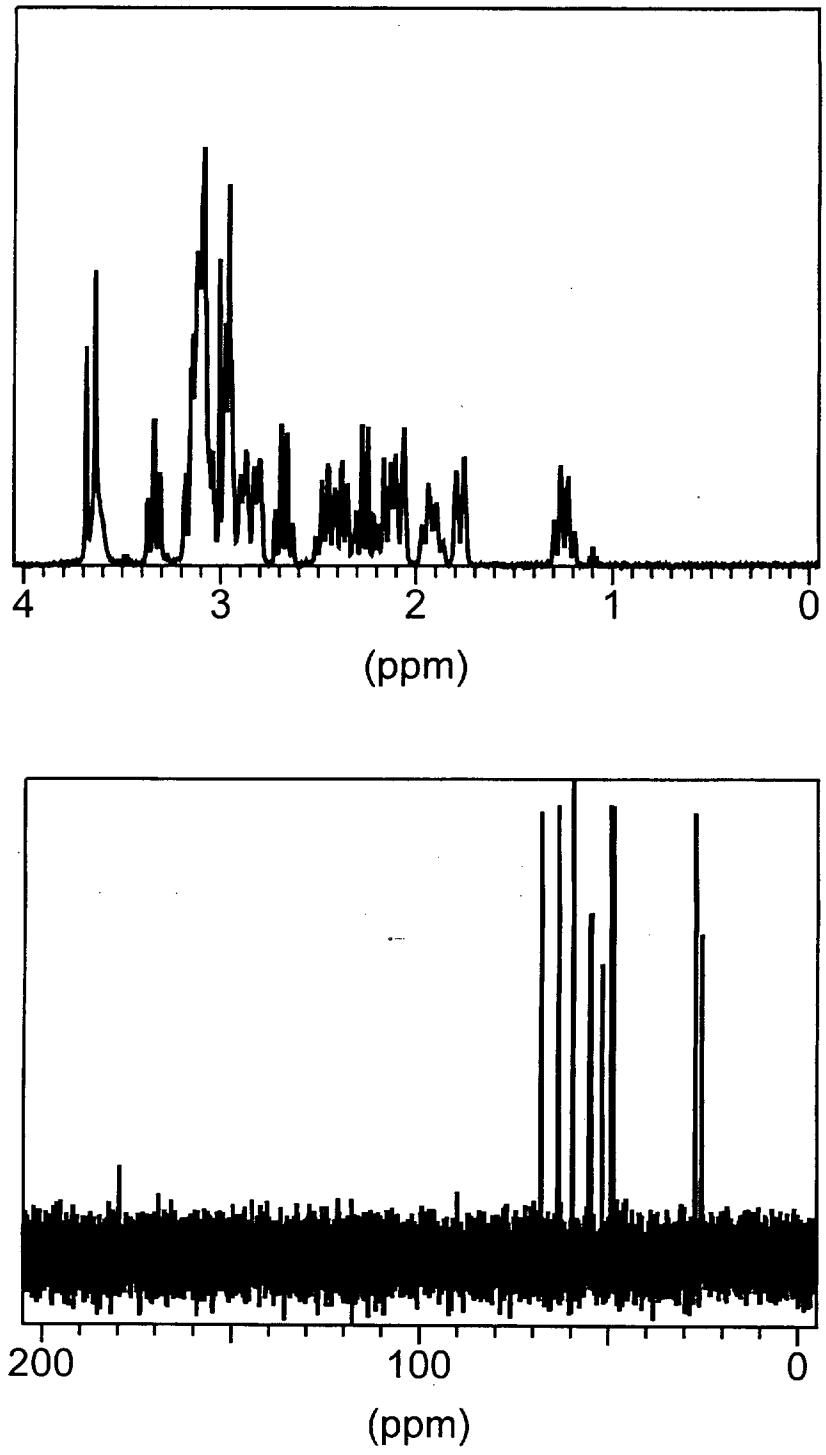

Figure S1. ^{1}H (top) and ^{13}C NMR (bottom) spectra of **2** recorded in D_2O (referenced to TMS). ^{13}C {H} signals: 180.0, 68.2, 63.7, 59.4, 55.1, 51.7, 49.9, 49.4, 49.2, 27.6, 26.0 (ppm).

Figure S2. Partial packing diagram of the monocation in crystals of **1**. Small open circles represent amine hydrogen atoms. Other hydrogen atoms have been eliminated.

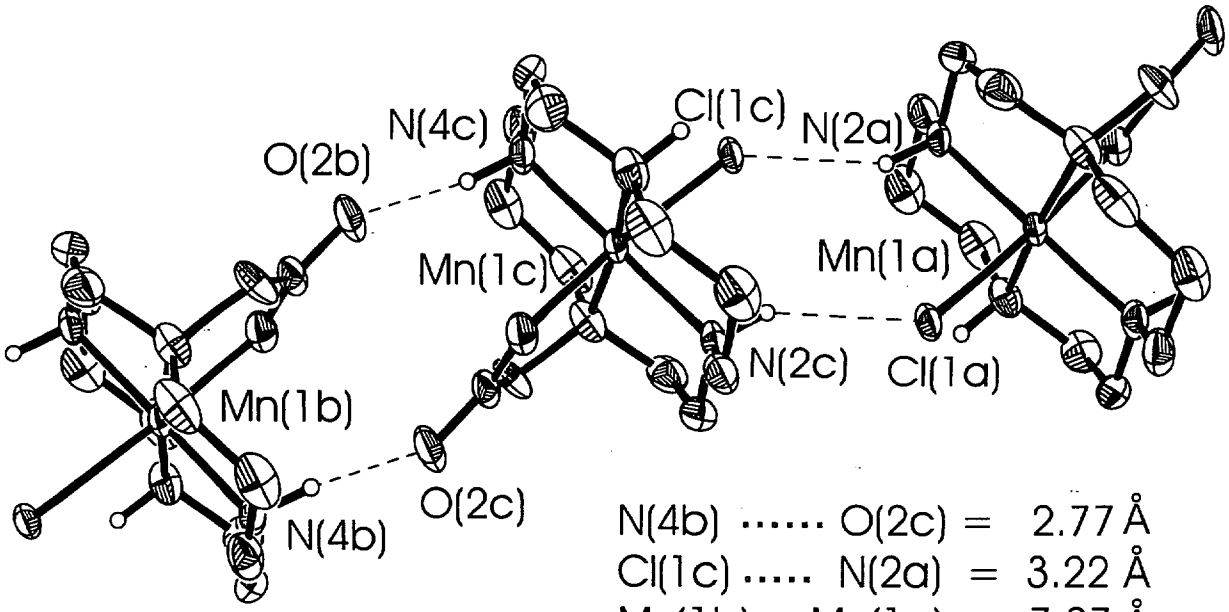

Table S1. Crystal data and structure refinement for 1.

Identification code	1
Empirical formula	C_{14} H_{28} Cl F_6 Mn N_5 O_2 P
Formula weight	533.77
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 7.965(1) Å alpha = 114.20(2) deg. b = 12.382(2) Å beta = 98.28(2) deg. c = 12.529(2) Å gamma = 94.28(2) deg.
Volume	1103.0(3) Å^3
Z	2
Density (calculated)	1.607 Mg/m^3
Absorption coefficient	0.863 mm^-1
F(000)	548
Crystal size	0.40 x 0.40 x 0.18 mm
Theta range for data collection	1.82 to 25.00 deg.
Index ranges	-11<=h<=11, -15<=k<=19, -17<=l<=19
Reflections collected	8206
Independent reflections	3738 [R(int) = 0.0456]
Absorption correction	SADABS, G.M. Sheldrick 1994
Max. and min. transmission	0.899 and 0.561
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3736 / 0 / 320
Goodness-of-fit on F^2	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0583, wR2 = 0.1511
R indices (all data)	R1 = 0.0783, wR2 = 0.1596
Largest diff. peak and hole	0.884 and -0.431 e.A^-3

Table S2. 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)
Mn(1)	9500(1)	7800(1)	7397(1)	21(1)
Cl(1)	7815(1)	9060(1)	8839(1)	27(1)
O(1)	11063(4)	6758(3)	6284(3)	30(1)
O(2)	12142(4)	5037(3)	5778(3)	46(1)
N(1)	9438(5)	6422(3)	7939(3)	33(1)
N(2)	11660(4)	8600(3)	8667(3)	29(1)
N(3)	9675(5)	9022(3)	6667(3)	33(1)
N(4)	7367(4)	6998(3)	6117(3)	29(1)
C(1)	10548(7)	7007(5)	9157(4)	44(1)
C(2)	12157(6)	7715(5)	9146(4)	42(1)
C(3)	13104(6)	9106(4)	8311(5)	40(1)
C(4)	12621(7)	10007(5)	7841(5)	49(1)
C(5)	11440(7)	9461(5)	6620(5)	45(1)
C(6)	8493(7)	8449(5)	5488(4)	43(1)
C(7)	6887(6)	7859(5)	5617(4)	41(1)
C(8)	5906(6)	6480(4)	6467(5)	39(1)
C(9)	6377(6)	5532(4)	6849(5)	43(1)
C(10)	7676(7)	5950(4)	7990(5)	41(1)
C(11)	10243(7)	5427(4)	7113(5)	40(1)
C(12)	11248(5)	5767(4)	6337(4)	33(1)
P(1)	7861(2)	12136(1)	7265(1)	42(1)
F(11)	9165(5)	11602(3)	7983(3)	65(1)
F(12)	6634(6)	12694(4)	6614(4)	101(2)
F(13)	8722(20)	13359(8)	8273(10)	77(3)
F(14)	9092(23)	12198(26)	6563(13)	211(13)
F(15)	7104(25)	10902(9)	6187(16)	120(5)
F(16)	6591(14)	11897(25)	7975(19)	142(7)
F(17)	8536(29)	11260(17)	6124(10)	115(6)
F(18)	6448(15)	11123(14)	7048(19)	106(4)
F(19)	7440(28)	13022(18)	8417(8)	130(7)
F(20)	9409(14)	12965(18)	7234(27)	174(10)
N(20)	13994(9)	5315(7)	8806(7)	62(2)
C(20)	13659(9)	4318(8)	8693(7)	49(2)
C(21)	13271(13)	3175(9)	8648(11)	68(3)
N(20X)	14949(32)	6254(24)	9700(23)	77(7)
C(20X)	15688(30)	6501(21)	10609(22)	46(5)
C(21X)	16690(44)	6961(33)	11934(30)	64(10)

Table S3. Bond lengths [Å] and angles [deg] for 1.

Mn(1)-N(4)	2.026(3)
Mn(1)-N(2)	2.034(3)
Mn(1)-N(3)	2.070(4)
Mn(1)-N(1)	2.079(4)
Mn(1)-O(1)	2.103(3)
Mn(1)-Cl(1)	2.4905(12)
O(1)-C(12)	1.275(6)
O(2)-C(12)	1.238(5)
N(1)-C(1)	1.498(6)
N(1)-C(10)	1.499(6)
N(1)-C(11)	1.504(6)
N(2)-C(3)	1.477(6)
N(2)-C(2)	1.501(6)
N(3)-C(6)	1.487(6)
N(3)-C(5)	1.487(6)
N(4)-C(7)	1.488(6)
N(4)-C(8)	1.491(6)
C(1)-C(2)	1.503(8)
C(3)-C(4)	1.510(8)
C(4)-C(5)	1.526(8)
C(6)-C(7)	1.487(7)
C(8)-C(9)	1.490(7)
C(9)-C(10)	1.507(7)
C(11)-C(12)	1.507(7)
P(1)-F(14)	1.425(13)
P(1)-F(19)	1.515(9)
P(1)-F(16)	1.527(10)
P(1)-F(18)	1.528(9)
P(1)-F(13)	1.544(9)
P(1)-F(12)	1.560(4)
P(1)-F(20)	1.560(10)
P(1)-F(15)	1.568(11)
P(1)-F(17)	1.596(10)
P(1)-F(11)	1.626(4)
N(20)-C(20)	1.188(10)
C(20)-C(21)	1.402(13)
N(20X)-C(20X)	1.11(3)
C(20X)-C(21X)	1.58(4)
N(4)-Mn(1)-N(2)	179.33(13)
N(4)-Mn(1)-N(3)	85.1(2)
N(2)-Mn(1)-N(3)	94.7(2)
N(4)-Mn(1)-N(1)	93.0(2)
N(2)-Mn(1)-N(1)	87.2(2)
N(3)-Mn(1)-N(1)	172.60(14)
N(4)-Mn(1)-O(1)	91.88(13)
N(2)-Mn(1)-O(1)	87.51(13)
N(3)-Mn(1)-O(1)	90.78(14)
N(1)-Mn(1)-O(1)	82.14(13)
N(4)-Mn(1)-Cl(1)	91.98(10)
N(2)-Mn(1)-Cl(1)	88.64(10)
N(3)-Mn(1)-Cl(1)	91.01(11)
N(1)-Mn(1)-Cl(1)	96.19(10)
O(1)-Mn(1)-Cl(1)	175.87(9)
C(12)-O(1)-Mn(1)	115.5(3)
C(1)-N(1)-C(10)	111.0(4)
C(1)-N(1)-C(11)	110.5(4)
C(10)-N(1)-C(11)	110.1(4)
C(1)-N(1)-Mn(1)	102.3(3)

C(10)-N(1)-Mn(1)	114.2(3)
C(11)-N(1)-Mn(1)	108.5(3)
C(3)-N(2)-C(2)	112.5(4)
C(3)-N(2)-Mn(1)	116.6(3)
C(2)-N(2)-Mn(1)	107.0(3)
C(6)-N(3)-C(5)	114.2(4)
C(6)-N(3)-Mn(1)	105.4(3)
C(5)-N(3)-Mn(1)	115.7(3)
C(7)-N(4)-C(8)	113.3(4)
C(7)-N(4)-Mn(1)	107.5(3)
C(8)-N(4)-Mn(1)	116.3(3)
N(1)-C(1)-C(2)	110.7(4)
N(2)-C(2)-C(1)	108.5(4)
N(2)-C(3)-C(4)	112.9(4)
C(3)-C(4)-C(5)	114.1(4)
N(3)-C(5)-C(4)	112.4(4)
N(3)-C(6)-C(7)	109.0(4)
C(6)-C(7)-N(4)	107.7(4)
C(9)-C(8)-N(4)	112.1(4)
C(8)-C(9)-C(10)	115.8(4)
N(1)-C(10)-C(9)	115.0(4)
N(1)-C(11)-C(12)	114.8(4)
O(2)-C(12)-O(1)	125.8(5)
O(2)-C(12)-C(11)	116.9(5)
O(1)-C(12)-C(11)	117.3(4)
F(14)-P(1)-F(16)	172.2(13)
F(19)-P(1)-F(18)	96.1(11)
F(14)-P(1)-F(13)	90.6(9)
F(16)-P(1)-F(13)	94.7(10)
F(14)-P(1)-F(12)	89.2(11)
F(19)-P(1)-F(12)	86.9(4)
F(16)-P(1)-F(12)	96.2(6)
F(18)-P(1)-F(12)	92.2(5)
F(13)-P(1)-F(12)	94.1(4)
F(19)-P(1)-F(20)	96.5(11)
F(18)-P(1)-F(20)	167.4(12)
F(12)-P(1)-F(20)	89.0(4)
F(14)-P(1)-F(15)	84.9(10)
F(16)-P(1)-F(15)	89.8(10)
F(13)-P(1)-F(15)	175.4(10)
F(12)-P(1)-F(15)	86.1(5)
F(19)-P(1)-F(17)	173.3(11)
F(18)-P(1)-F(17)	89.2(10)
F(12)-P(1)-F(17)	97.2(4)
F(20)-P(1)-F(17)	78.3(12)
F(14)-P(1)-F(11)	91.1(10)
F(19)-P(1)-F(11)	91.5(4)
F(16)-P(1)-F(11)	83.9(5)
F(18)-P(1)-F(11)	89.3(5)
F(13)-P(1)-F(11)	83.8(4)
F(12)-P(1)-F(11)	177.9(2)
F(20)-P(1)-F(11)	89.9(4)
F(15)-P(1)-F(11)	96.0(5)
F(17)-P(1)-F(11)	84.3(4)
N(20)-C(20)-C(21)	175.9(9)
N(20X)-C(20X)-C(21X)	175(3)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters (A^2 x 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
Mn(1)	24(1)	14(1)	19(1)	2(1)	5(1)	2(1)
Cl(1)	26(1)	21(1)	24(1)	-2(1)	7(1)	5(1)
O(1)	29(2)	25(2)	29(2)	4(1)	8(1)	0(1)
O(2)	32(2)	27(2)	51(2)	-12(2)	13(2)	2(2)
N(1)	44(2)	25(2)	35(2)	13(2)	19(2)	12(2)
N(2)	28(2)	23(2)	21(2)	-4(2)	4(1)	6(2)
N(3)	47(2)	24(2)	30(2)	12(2)	15(2)	6(2)
N(4)	27(2)	26(2)	21(2)	-2(2)	6(1)	2(2)
C(1)	61(3)	45(3)	34(3)	22(2)	14(2)	27(3)
C(2)	47(3)	38(3)	32(3)	7(2)	-2(2)	22(2)
C(3)	30(2)	28(3)	45(3)	-2(2)	9(2)	5(2)
C(4)	39(3)	32(3)	66(4)	12(3)	20(3)	-7(2)
C(5)	56(3)	33(3)	53(3)	21(3)	30(3)	4(2)
C(6)	63(3)	40(3)	33(3)	22(2)	9(2)	14(3)
C(7)	44(3)	41(3)	25(2)	4(2)	-7(2)	16(2)
C(8)	30(2)	29(3)	42(3)	-2(2)	11(2)	-4(2)
C(9)	42(3)	28(3)	53(3)	9(2)	25(2)	-4(2)
C(10)	60(3)	27(3)	53(3)	23(2)	37(3)	15(2)
C(11)	51(3)	19(3)	53(3)	12(2)	22(2)	18(2)
C(12)	20(2)	20(2)	37(3)	-7(2)	3(2)	-2(2)
P(1)	54(1)	31(1)	48(1)	20(1)	14(1)	10(1)
F(11)	86(2)	41(2)	61(2)	18(2)	1(2)	22(2)
F(12)	129(4)	63(3)	91(3)	33(2)	-46(3)	22(3)
F(13)	114(9)	35(4)	74(7)	26(4)	-22(6)	13(5)
F(14)	175(15)	295(26)	76(9)	-12(12)	89(10)	-68(16)
F(15)	166(14)	43(6)	118(11)	11(6)	-3(10)	11(8)
F(16)	60(6)	288(24)	137(12)	157(15)	18(8)	-14(10)
F(17)	203(16)	134(13)	47(6)	51(8)	57(8)	113(13)
F(18)	81(7)	115(11)	127(10)	80(10)	-22(8)	-43(7)
F(19)	181(14)	138(13)	41(5)	-5(7)	6(8)	133(12)
F(20)	68(6)	167(15)	369(28)	234(20)	-46(12)	-40(8)
N(20)	61(4)	71(6)	80(5)	51(5)	24(4)	23(4)
C(20)	38(4)	60(6)	54(5)	28(4)	9(3)	14(4)
C(21)	71(6)	50(6)	74(7)	18(5)	23(6)	-6(4)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 1.

	x	y	z	U(eq)
H(2)	11350(4)	9234(3)	9287(3)	34
H(3)	9219(5)	9685(3)	7139(3)	39
H(4)	7692(4)	6362(3)	5507(3)	34
H(1A)	10853(7)	6387(5)	9426(4)	52
H(1B)	9905(7)	7545(5)	9726(4)	52
H(2A)	12843(6)	8141(5)	9964(4)	50
H(2B)	12860(6)	7172(5)	8637(4)	50
H(3A)	13523(6)	8446(4)	7688(5)	48
H(3B)	14056(6)	9496(4)	9009(5)	48
H(4A)	13683(7)	10439(5)	7791(5)	58
H(4B)	12049(7)	10602(5)	8417(5)	58
H(5A)	11383(7)	10071(5)	6300(5)	54
H(5B)	11928(7)	8787(5)	6068(5)	54
H(6A)	9044(7)	7848(5)	4901(4)	51
H(6B)	8226(7)	9060(5)	5197(4)	51
H(7A)	6110(6)	7432(5)	4831(4)	50
H(7B)	6288(6)	8465(5)	6158(4)	50
H(8A)	5531(6)	7126(4)	7129(5)	47
H(8B)	4930(6)	6134(4)	5783(5)	47
H(9A)	6832(6)	4922(4)	6203(5)	51
H(9B)	5320(6)	5133(4)	6942(5)	51
H(10A)	7250(7)	6587(4)	8630(5)	50
H(10B)	7763(7)	5273(4)	8212(5)	50
H(11A)	9325(7)	4754(4)	6593(5)	48
H(11B)	11017(7)	5137(4)	7597(5)	48

Table S6. Crystal data and structure refinement for 2.

Identification code	2
Empirical formula	C_{12} H_{25} F_6 Mn N_5 O_2 P
Formula weight	471.28
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 8.684(1) Å alpha = 90 deg. b = 11.902(2) Å beta = 98.74(3) deg. c = 18.154(2) Å gamma = 90 deg.
Volume	1854.6(4) Å^3
Z	4
Density (calculated)	1.688 Mg/m^3
Absorption coefficient	0.875 mm^-1
F(000)	968
Crystal size	0.68 x 0.42 x 0.30 mm
Theta range for data collection	2.05 to 33.00 deg.
Index ranges	-13<=h<=11, -17<=k<=13, -24<=l<=28
Reflections collected	18830
Independent reflections	6419 [R(int) = 0.0225]
Absorption correction	SADABS, G.M. Sheldrick 1994
Max. and min. transmission	0.829 and 0.721
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6412 / 0 / 244
Goodness-of-fit on F^2	1.000
Final R indices [I>2sigma(I)]	R1 = 0.0350, wR2 = 0.0828
R indices (all data)	R1 = 0.0478, wR2 = 0.0878
Largest diff. peak and hole	0.603 and -0.305 e.A^-3

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 2. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mn(1)	2468(1)	1140(1)	2253(1)	13(1)
O(1)	1072(1)	-335(1)	2170(1)	16(1)
O(2)	-1169(1)	-1035(1)	1556(1)	25(1)
N(1)	1001(2)	1492(1)	1278(1)	19(1)
N(2)	3953(1)	251(1)	1713(1)	18(1)
N(3)	3642(1)	418(1)	3191(1)	16(1)
N(4)	747(1)	1799(1)	2778(1)	19(1)
N(5)	3415(2)	2234(1)	2269(1)	20(1)
C(1)	1842(2)	1895(1)	665(1)	27(1)
C(2)	3064(2)	1083(2)	457(1)	30(1)
C(3)	4438(2)	832(2)	1062(1)	26(1)
C(4)	5309(2)	-70(1)	2275(1)	22(1)
C(5)	4667(2)	-478(1)	2958(1)	21(1)
C(6)	2743(2)	5(1)	3770(1)	21(1)
C(7)	1680(2)	906(1)	4005(1)	25(1)
C(8)	284(2)	1182(1)	3422(1)	25(1)
C(9)	-622(2)	2058(1)	2204(1)	24(1)
C(10)	-24(2)	2410(1)	1502(1)	25(1)
C(11)	7(2)	498(1)	1021(1)	19(1)
C(12)	-61(2)	-369(1)	1633(1)	18(1)
P(1)	-3317(1)	2678(1)	-546(1)	18(1)
F(1)	-4731(1)	1896(1)	-910(1)	42(1)
F(2)	-3345(1)	3278(1)	-1338(1)	37(1)
F(3)	-1901(1)	3459(1)	-196(1)	30(1)
F(4)	-3295(1)	2075(1)	239(1)	40(1)
F(5)	-2091(1)	1773(1)	-770(1)	35(1)
F(6)	-4550(1)	3571(1)	-333(1)	33(1)

Table S8. Bond lengths [Å] and angles [deg] for 2.

Mn(1)-N(5)	1.5375(12)
Mn(1)-N(2)	2.0324(13)
Mn(1)-N(3)	2.0365(13)
Mn(1)-N(4)	2.0469(13)
Mn(1)-N(1)	2.0610(13)
Mn(1)-O(1)	2.1256(10)
O(1)-C(12)	1.276(2)
O(2)-C(12)	1.239(2)
N(1)-C(11)	1.497(2)
N(1)-C(1)	1.499(2)
N(1)-C(10)	1.504(2)
N(2)-C(4)	1.486(2)
N(2)-C(3)	1.484(2)
N(3)-C(6)	1.485(2)
N(3)-C(5)	1.491(2)
N(4)-C(8)	1.487(2)
N(4)-C(9)	1.489(2)
C(1)-C(2)	1.525(3)
C(2)-C(3)	1.523(2)
C(4)-C(5)	1.515(2)
C(6)-C(7)	1.517(2)
C(7)-C(8)	1.520(2)
C(9)-C(10)	1.507(2)
C(11)-C(12)	1.525(2)
P(1)-F(4)	1.5924(11)
P(1)-F(3)	1.5951(10)
P(1)-F(6)	1.5969(10)
P(1)-F(1)	1.6005(11)
P(1)-F(2)	1.6030(11)
P(1)-F(5)	1.6095(10)
N(5)-Mn(1)-N(2)	94.21(6)
N(5)-Mn(1)-N(3)	98.23(6)
N(2)-Mn(1)-N(3)	84.85(5)
N(5)-Mn(1)-N(4)	95.32(6)
N(2)-Mn(1)-N(4)	170.43(5)
N(3)-Mn(1)-N(4)	94.64(5)
N(5)-Mn(1)-N(1)	95.90(6)
N(2)-Mn(1)-N(1)	92.63(5)
N(3)-Mn(1)-N(1)	165.79(5)
N(4)-Mn(1)-N(1)	85.52(5)
N(5)-Mn(1)-O(1)	176.44(5)
N(2)-Mn(1)-O(1)	86.14(4)
N(3)-Mn(1)-O(1)	85.33(5)
N(4)-Mn(1)-O(1)	84.29(5)
N(1)-Mn(1)-O(1)	80.55(5)
C(12)-O(1)-Mn(1)	116.45(9)
C(11)-N(1)-C(1)	110.11(11)
C(11)-N(1)-C(10)	108.78(12)
C(1)-N(1)-C(10)	110.06(12)
C(11)-N(1)-Mn(1)	111.03(9)
C(1)-N(1)-Mn(1)	113.31(10)
C(10)-N(1)-Mn(1)	103.28(9)
C(4)-N(2)-C(3)	112.10(12)
C(4)-N(2)-Mn(1)	107.23(9)
C(3)-N(2)-Mn(1)	114.76(10)
C(6)-N(3)-C(5)	111.35(11)
C(6)-N(3)-Mn(1)	118.78(9)
C(5)-N(3)-Mn(1)	108.02(9)

C(8)-N(4)-C(9)	111.72(12)
C(8)-N(4)-Mn(1)	118.70(9)
C(9)-N(4)-Mn(1)	108.38(9)
N(1)-C(1)-C(2)	114.63(12)
C(3)-C(2)-C(1)	116.34(14)
N(2)-C(3)-C(2)	112.32(13)
N(2)-C(4)-C(5)	107.06(11)
N(3)-C(5)-C(4)	108.18(12)
N(3)-C(6)-C(7)	111.89(12)
C(6)-C(7)-C(8)	114.31(13)
N(4)-C(8)-C(7)	111.89(12)
N(4)-C(9)-C(10)	107.95(12)
N(1)-C(10)-C(9)	108.69(12)
N(1)-C(11)-C(12)	113.06(11)
O(2)-C(12)-O(1)	127.06(13)
O(2)-C(12)-C(11)	117.78(13)
O(1)-C(12)-C(11)	115.15(12)
F(4)-P(1)-F(3)	90.18(6)
F(4)-P(1)-F(6)	90.04(6)
F(3)-P(1)-F(6)	91.14(6)
F(4)-P(1)-F(1)	90.66(7)
F(3)-P(1)-F(1)	179.08(6)
F(6)-P(1)-F(1)	89.24(6)
F(4)-P(1)-F(2)	179.65(7)
F(3)-P(1)-F(2)	90.15(6)
F(6)-P(1)-F(2)	90.09(6)
F(1)-P(1)-F(2)	89.02(7)
F(4)-P(1)-F(5)	90.36(7)
F(3)-P(1)-F(5)	89.48(6)
F(6)-P(1)-F(5)	179.26(6)
F(1)-P(1)-F(5)	90.13(6)
F(2)-P(1)-F(5)	89.50(6)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters (A^2 x 10^3) for 2. 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
Mn(1)	15(1)	12(1)	12(1)	0(1)	1(1)	-1(1)
O(1)	18(1)	16(1)	15(1)	0(1)	0(1)	-1(1)
O(2)	21(1)	22(1)	30(1)	3(1)	-3(1)	-6(1)
N(1)	25(1)	16(1)	16(1)	2(1)	-1(1)	-1(1)
N(2)	19(1)	20(1)	17(1)	-3(1)	5(1)	-3(1)
N(3)	16(1)	17(1)	15(1)	0(1)	2(1)	-1(1)
N(4)	18(1)	18(1)	20(1)	-4(1)	2(1)	2(1)
N(5)	24(1)	17(1)	19(1)	0(1)	2(1)	-4(1)
C(1)	36(1)	26(1)	17(1)	7(1)	0(1)	-7(1)
C(2)	37(1)	37(1)	17(1)	1(1)	8(1)	-11(1)
C(3)	29(1)	31(1)	21(1)	-1(1)	12(1)	-8(1)
C(4)	16(1)	25(1)	26(1)	-3(1)	5(1)	2(1)
C(5)	19(1)	20(1)	24(1)	1(1)	0(1)	5(1)
C(6)	23(1)	23(1)	15(1)	3(1)	2(1)	-3(1)
C(7)	28(1)	32(1)	15(1)	-3(1)	7(1)	-2(1)
C(8)	22(1)	32(1)	23(1)	-3(1)	9(1)	0(1)
C(9)	20(1)	23(1)	28(1)	-6(1)	-2(1)	6(1)
C(10)	29(1)	16(1)	26(1)	0(1)	-7(1)	5(1)
C(11)	22(1)	18(1)	15(1)	0(1)	-3(1)	-2(1)
C(12)	19(1)	17(1)	17(1)	-1(1)	2(1)	1(1)
P(1)	16(1)	23(1)	15(1)	-1(1)	2(1)	1(1)
F(1)	26(1)	53(1)	46(1)	-24(1)	8(1)	-15(1)
F(2)	29(1)	62(1)	20(1)	14(1)	2(1)	10(1)
F(3)	25(1)	35(1)	28(1)	-7(1)	1(1)	-8(1)
F(4)	29(1)	59(1)	34(1)	23(1)	7(1)	1(1)
F(5)	28(1)	29(1)	52(1)	-7(1)	13(1)	7(1)
F(6)	27(1)	42(1)	32(1)	-9(1)	3(1)	13(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 2.

	x	y	z	U(eq)
H(2)	3447(1)	-408(1)	1539(1)	22
H(3)	4308(1)	970(1)	3420(1)	19
H(4)	1121(1)	2491(1)	2965(1)	23
H(1A)	2357(2)	2618(1)	818(1)	32
H(1B)	1066(2)	2040(1)	216(1)	32
H(2A)	2541(2)	364(2)	301(1)	36
H(2B)	3476(2)	1393(2)	20(1)	36
H(3A)	5198(2)	357(2)	851(1)	31
H(3B)	4963(2)	1546(2)	1230(1)	31
H(4A)	6000(2)	586(1)	2403(1)	27
H(4B)	5916(2)	-672(1)	2078(1)	27
H(5A)	4062(2)	-1178(1)	2841(1)	26
H(5B)	5531(2)	-638(1)	3366(1)	26
H(6A)	3477(2)	-246(1)	4211(1)	25
H(6B)	2109(2)	-651(1)	3574(1)	25
H(7A)	2296(2)	1599(1)	4126(1)	30
H(7B)	1300(2)	655(1)	4466(1)	30
H(8A)	-250(2)	476(1)	3243(1)	30
H(8B)	-461(2)	1645(1)	3652(1)	30
H(9A)	-1246(2)	2671(1)	2380(1)	29
H(9B)	-1294(2)	1386(1)	2107(1)	29
H(10A)	-908(2)	2543(1)	1098(1)	30
H(10B)	578(2)	3117(1)	1590(1)	30
H(11A)	423(2)	135(1)	601(1)	23
H(11B)	-1063(2)	759(1)	833(1)	23