Table 1. Crystal data and structure refinement for complex 6.

$C_{32}H_{23}MnO_4PS$

Identification code	cd213	
Empirical formula	C32 H23 Mn O4 P S	
Formula weight	589.47	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P n a 21	
Unit cell dimensions	a = 23.588(4) Å	α= 90°.
	b = 9.1363(9) Å	β= 90°.
	c = 13.1639(10) Å	γ = 90°.
Volume	2836.9(6) $Å^3$	
Z	4	
Density (calculated)	1.380 Mg/m^3	
Absorption coefficient	0.631 mm^{-1}	
F(000)	1212	
Crystal size	0.48 x 0.44 x 0.33 mm^3	
Theta range for data collection	3.22 to 30.00°.	
Index ranges	-33<=h<=20, -12<=k<=12, -18<=l<=18	
Reflections collected	12347	
Independent reflections	7238 [R(int) = 0.0359]	
Completeness to theta = 30.00°	96.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.812 and 0.552	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7238 / 1 / 353	
Goodness-of-fit on F^2	1.014	
Final R indices [I>2sigma(I)]	R1 = 0.0416, wR2 = 0.0947	
R indices (all data)	R1 = 0.0594, wR2 = 0.1015	
Absolute structure parameter	0.037(15)	
Largest diff. peak and hole	0.505 and -0.565 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for cd213. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mn(1)	5337(1)	1277(1)	8518(1)	21(1)
P(1)	6806(1)	1844(1)	9017(1)	21(1)
S(1)	6160(1)	-1974(1)	7662(1)	54(1)
O(1)	4886(1)	4483(2)	7913(2)	30(1)
O(2)	5714(1)	-641(2)	10220(2)	45(1)
O(3)	4453(1)	2200(2)	9993(2)	51(1)
O(4)	4647(1)	-1092(2)	7595(2)	49(1)
C(1)	6037(1)	1056(2)	7412(2)	20(1)
C(2)	6175(1)	2110(2)	8175(2)	18(1)
C(3)	5796(1)	3311(2)	8347(2)	21(1)
C(24)	5994(1)	2411(3)	5698(2)	26(1)
C(4)	5295(1)	3436(3)	7748(2)	24(1)
C(5)	5171(1)	2350(3)	7012(2)	25(1)
C(6)	5663(1)	1556(3)	6505(2)	22(1)
C(7)	6399(1)	-281(3)	7283(2)	23(1)
C(8)	6950(1)	-402(3)	6854(2)	34(1)
C(9)	7143(1)	-1877(4)	6868(3)	43(1)
C(10)	6765(2)	-2830(3)	7272(3)	49(1)
C(11)	7361(1)	2764(2)	8259(2)	21(1)
C(12)	7903(1)	2871(3)	8699(2)	32(1)
C(13)	8344(1)	3563(3)	8189(3)	41(1)
C(14)	8264(1)	4131(3)	7232(3)	38(1)
C(15)	7735(1)	4032(3)	6773(2)	34(1)
C(16)	7286(1)	3339(3)	7280(2)	26(1)
C(17)	6664(1)	3280(3)	9972(2)	23(1)
C(18)	6828(1)	4746(3)	9860(2)	31(1)
C(19)	6665(1)	5807(3)	10585(3)	42(1)
C(20)	6347(2)	5379(4)	11423(3)	49(1)
C(21)	6189(2)	3944(4)	11555(2)	45(1)
C(22)	6349(1)	2882(3)	10830(2)	34(1)
C(23)	4966(1)	5473(3)	8753(2)	34(1)
C(30)	5592(1)	125(3)	9553(2)	29(1)
C(31)	4790(1)	1875(3)	9399(2)	31(1)
C(32)	4919(1)	-196(3)	7964(2)	30(1)

C(29)	6036(1)	3943(3)	5706(2)	29(1)
C(27)	6696(2)	3879(3)	4286(2)	44(1)
C(26)	6647(2)	2362(4)	4265(2)	47(1)
C(25)	6297(2)	1634(3)	4954(2)	38(1)
C(28)	6388(1)	4673(3)	5013(2)	36(1)

Table 3. Bond lengths [Å] and angles [°] for cd213.

Mn(1)-C(31)	1.819(3)
Mn(1)-C(32)	1.822(3)
Mn(1)-C(30)	1.824(3)
Mn(1)-C(3)	2.162(2)
Mn(1)-C(2)	2.164(2)
Mn(1)-C(1)	2.211(2)
Mn(1)-C(4)	2.220(3)
Mn(1)-C(5)	2.247(3)
P(1)-C(17)	1.848(3)
P(1)-C(11)	1.848(2)
P(1)-C(2)	1.872(2)
S(1)-C(10)	1.707(3)
S(1)-C(7)	1.720(2)
O(1)-C(4)	1.375(3)
O(1)-C(23)	1.441(3)
O(2)-C(30)	1.159(3)
O(3)-C(31)	1.153(3)
O(4)-C(32)	1.148(3)
C(1)-C(2)	1.428(3)
C(1)-C(7)	1.500(3)
C(1)-C(6)	1.553(3)
C(2)-C(3)	1.433(3)
C(3)-C(4)	1.425(3)
C(3)-H(3)	0.9500
C(24)-C(29)	1.403(4)
C(24)-C(25)	1.404(4)
C(24)-C(6)	1.533(3)
C(4)-C(5)	1.418(4)
C(5)-C(6)	1.523(4)
C(6)-H(6)	1.0000
C(7)-C(8)	1.421(4)
C(8)-C(9)	1.423(4)
C(8)-H(8)	0.9500
C(9)-C(10)	1.354(5)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
C(11)-C(16)	1.403(4)

C(11)-C(12)	1.406(3)
C(12)-C(13)	1.391(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.376(5)
C(13)-H(13)	0.9500
C(14)-C(15)	1.389(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.404(4)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(17)-C(22)	1.400(4)
C(17)-C(18)	1.402(4)
C(18)-C(19)	1.414(4)
C(18)-H(18)	0.9500
C(19)-C(20)	1.391(5)
C(19)-H(19)	0.9500
C(20)-C(21)	1.374(5)
C(20)-H(20)	0.9500
C(21)-C(22)	1.413(4)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(29)-C(28)	1.402(4)
C(29)-H(29)	0.9500
C(27)-C(26)	1.391(4)
C(27)-C(28)	1.403(4)
C(27)-H(27)	0.9500
C(26)-C(25)	1.395(4)
C(26)-H(26)	0.9500
C(25)-H(25)	0.9500
C(28)-H(28)	0.9500

C(31)-Mn(1)-C(32)	95.29(13)
C(31)-Mn(1)-C(30)	86.03(12)
C(32)-Mn(1)-C(30)	92.93(12)
C(31)-Mn(1)-C(3)	99.42(11)
C(32)-Mn(1)-C(3)	149.81(11)

C(30)-Mn(1)-C(3)	114.18(11)
C(31)-Mn(1)-C(2)	132.49(11)
C(32)-Mn(1)-C(2)	132.11(11)
C(30)-Mn(1)-C(2)	93.37(10)
C(3)-Mn(1)-C(2)	38.69(9)
C(31)-Mn(1)-C(1)	167.76(11)
C(32)-Mn(1)-C(1)	94.22(11)
C(30)-Mn(1)-C(1)	101.16(11)
C(3)-Mn(1)-C(1)	68.66(9)
C(2)-Mn(1)-C(1)	38.08(8)
C(31)-Mn(1)-C(4)	89.56(11)
C(32)-Mn(1)-C(4)	116.67(11)
C(30)-Mn(1)-C(4)	150.36(11)
C(3)-Mn(1)-C(4)	37.94(9)
C(2)-Mn(1)-C(4)	68.50(8)
C(1)-Mn(1)-C(4)	79.28(9)
C(31)-Mn(1)-C(5)	107.93(11)
C(32)-Mn(1)-C(5)	82.76(11)
C(30)-Mn(1)-C(5)	165.66(11)
C(3)-Mn(1)-C(5)	67.69(9)
C(2)-Mn(1)-C(5)	79.71(9)
C(1)-Mn(1)-C(5)	65.71(9)
C(4)-Mn(1)-C(5)	37.00(10)
C(17)-P(1)-C(11)	99.92(11)
C(17)-P(1)-C(2)	99.59(10)
C(11)-P(1)-C(2)	100.67(10)
C(10)-S(1)-C(7)	92.92(15)
C(4)-O(1)-C(23)	117.8(2)
C(2)-C(1)-C(7)	119.9(2)
C(2)-C(1)-C(6)	118.11(19)
C(7)-C(1)-C(6)	118.4(2)
C(2)-C(1)-Mn(1)	69.19(13)
C(7)-C(1)-Mn(1)	125.00(16)
C(6)-C(1)-Mn(1)	93.18(15)
C(1)-C(2)-C(3)	119.1(2)
C(1)-C(2)-P(1)	120.60(17)
C(3)-C(2)-P(1)	120.11(17)
C(1)-C(2)-Mn(1)	72.72(13)
C(3)-C(2)-Mn(1)	70.56(13)

P(1)-C(2)-Mn(1)	123.80(11)
C(4)-C(3)-C(2)	119.4(2)
C(4)-C(3)-Mn(1)	73.24(14)
C(2)-C(3)-Mn(1)	70.74(13)
C(4)-C(3)-H(3)	120.3
C(2)-C(3)-H(3)	120.3
Mn(1)-C(3)-H(3)	127.8
C(29)-C(24)-C(25)	118.3(2)
C(29)-C(24)-C(6)	122.6(2)
C(25)-C(24)-C(6)	119.0(2)
O(1)-C(4)-C(5)	116.8(2)
O(1)-C(4)-C(3)	123.3(2)
C(5)-C(4)-C(3)	119.5(2)
O(1)-C(4)-Mn(1)	125.28(17)
C(5)-C(4)-Mn(1)	72.52(15)
C(3)-C(4)-Mn(1)	68.82(14)
C(4)-C(5)-C(6)	118.4(2)
C(4)-C(5)-Mn(1)	70.48(14)
C(6)-C(5)-Mn(1)	92.64(15)
C(5)-C(6)-C(24)	116.7(2)
C(5)-C(6)-C(1)	103.66(19)
C(24)-C(6)-C(1)	113.1(2)
C(5)-C(6)-H(6)	107.6
C(24)-C(6)-H(6)	107.6
C(1)-C(6)-H(6)	107.6
C(8)-C(7)-C(1)	128.9(2)
C(8)-C(7)-S(1)	110.18(19)
C(1)-C(7)-S(1)	120.87(18)
C(7)-C(8)-C(9)	111.2(2)
C(7)-C(8)-H(8)	124.4
C(9)-C(8)-H(8)	124.4
C(10)-C(9)-C(8)	113.8(3)
C(10)-C(9)-H(9)	123.1
C(8)-C(9)-H(9)	123.1
C(9)-C(10)-S(1)	111.9(2)
C(9)-C(10)-H(10)	124.0
S(1)-C(10)-H(10)	124.0
C(16)-C(11)-C(12)	117.9(2)
C(16)-C(11)-P(1)	125.15(18)

C(12)-C(11)-P(1)	116.95(19)
C(13)-C(12)-C(11)	120.9(3)
C(13)-C(12)-H(12)	119.6
C(11)-C(12)-H(12)	119.6
C(14)-C(13)-C(12)	120.7(3)
C(14)-C(13)-H(13)	119.7
C(12)-C(13)-H(13)	119.7
C(13)-C(14)-C(15)	119.8(3)
C(13)-C(14)-H(14)	120.1
C(15)-C(14)-H(14)	120.1
C(14)-C(15)-C(16)	120.0(3)
C(14)-C(15)-H(15)	120.0
C(16)-C(15)-H(15)	120.0
C(11)-C(16)-C(15)	120.7(3)
C(11)-C(16)-H(16)	119.7
C(15)-C(16)-H(16)	119.7
C(22)-C(17)-C(18)	118.6(2)
C(22)-C(17)-P(1)	117.45(19)
C(18)-C(17)-P(1)	123.8(2)
C(17)-C(18)-C(19)	120.6(3)
C(17)-C(18)-H(18)	119.7
C(19)-C(18)-H(18)	119.7
C(20)-C(19)-C(18)	119.3(3)
C(20)-C(19)-H(19)	120.3
C(18)-C(19)-H(19)	120.3
C(21)-C(20)-C(19)	121.0(3)
C(21)-C(20)-H(20)	119.5
C(19)-C(20)-H(20)	119.5
C(20)-C(21)-C(22)	119.8(3)
C(20)-C(21)-H(21)	120.1
C(22)-C(21)-H(21)	120.1
C(17)-C(22)-C(21)	120.6(3)
C(17)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
O(1)-C(23)-H(23A)	109.5
O(1)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
O(1)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5

H(23B)-C(23)-H(23C)	109.5
O(2)-C(30)-Mn(1)	175.1(2)
O(3)-C(31)-Mn(1)	176.4(3)
O(4)-C(32)-Mn(1)	177.8(3)
C(28)-C(29)-C(24)	120.8(3)
C(28)-C(29)-H(29)	119.6
C(24)-C(29)-H(29)	119.6
C(26)-C(27)-C(28)	119.0(3)
C(26)-C(27)-H(27)	120.5
C(28)-C(27)-H(27)	120.5
C(27)-C(26)-C(25)	120.8(3)
C(27)-C(26)-H(26)	119.6
C(25)-C(26)-H(26)	119.6
C(26)-C(25)-C(24)	120.9(3)
C(26)-C(25)-H(25)	119.6
C(24)-C(25)-H(25)	119.6
C(29)-C(28)-C(27)	120.3(3)
C(29)-C(28)-H(28)	119.9
C(27)-C(28)-H(28)	119.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for cd213. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(1)	19(1)	23(1)	21(1)	1(1)	0(1)	-2(1)
P(1)	21(1)	21(1)	21(1)	2(1)	-3(1)	1(1)
S(1)	50(1)	27(1)	85(1)	12(1)	26(1)	5(1)
O(1)	28(1)	30(1)	33(1)	-2(1)	-5(1)	11(1)
O(2)	51(1)	49(1)	36(1)	18(1)	-6(1)	-5(1)
O(3)	48(1)	51(1)	53(2)	5(1)	24(1)	8(1)
O(4)	43(1)	41(1)	63(2)	-8(1)	-9(1)	-16(1)
C(1)	23(1)	21(1)	18(1)	-1(1)	3(1)	-4(1)
C(2)	18(1)	20(1)	17(1)	1(1)	0(1)	-3(1)
C(3)	23(1)	20(1)	20(1)	0(1)	-3(1)	-1(1)
C(24)	30(1)	32(1)	17(1)	1(1)	-5(1)	-3(1)
C(4)	23(1)	26(1)	22(1)	5(1)	0(1)	3(1)
C(5)	25(1)	28(1)	23(1)	2(1)	-4(1)	0(1)
C(6)	26(1)	23(1)	18(1)	-3(1)	-5(1)	-2(1)
C(7)	25(1)	22(1)	21(1)	0(1)	0(1)	0(1)
C(8)	38(2)	20(1)	44(2)	-5(1)	12(1)	1(1)
C(9)	36(2)	44(2)	49(2)	-9(2)	11(1)	9(1)
C(10)	61(2)	31(2)	55(2)	3(2)	11(2)	17(2)
C(11)	20(1)	20(1)	24(1)	-4(1)	-1(1)	1(1)
C(12)	23(1)	35(1)	37(2)	-6(1)	-3(1)	3(1)
C(13)	19(1)	48(2)	56(2)	-15(2)	-1(1)	-3(1)
C(14)	28(1)	31(1)	56(2)	-5(1)	15(1)	-8(1)
C(15)	40(2)	26(1)	37(2)	3(1)	11(1)	2(1)
C(16)	25(1)	23(1)	29(1)	-1(1)	0(1)	1(1)
C(17)	22(1)	29(1)	19(1)	-2(1)	-5(1)	1(1)
C(18)	30(1)	34(1)	29(2)	-4(1)	-2(1)	-3(1)
C(19)	47(2)	35(2)	44(2)	-15(1)	-2(2)	-7(1)
C(20)	45(2)	60(2)	42(2)	-32(2)	8(2)	-3(2)
C(21)	43(2)	65(2)	28(2)	-15(2)	9(1)	-7(2)
C(22)	36(2)	42(2)	24(1)	0(1)	-2(1)	-7(1)
C(23)	35(1)	28(1)	40(2)	-2(1)	4(1)	8(1)
C(30)	26(1)	34(1)	26(1)	6(1)	3(1)	-4(1)
C(31)	32(1)	30(1)	32(2)	3(1)	4(1)	1(1)
C(32)	27(1)	30(1)	34(2)	4(1)	1(1)	-2(1)

C(29)	33(1)	30(1)	24(1)	3(1)	-2(1)	1(1)
C(27)	50(2)	52(2)	30(2)	8(1)	8(1)	-10(2)
C(26)	65(2)	49(2)	28(2)	-7(1)	22(2)	-4(2)
C(25)	59(2)	31(1)	24(1)	-4(1)	6(1)	-6(1)
C(28)	43(2)	31(1)	33(2)	7(1)	0(1)	-5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for cd213.

	x	y	z	U(eq)
H(3)	5878	4018	8856	25
H(6)	5508	657	6173	27
H(8)	7161	397	6592	41
H(9)	7503	-2167	6618	51
H(10)	6829	-3853	7330	58
H(12)	7968	2466	9353	38
H(13)	8705	3645	8505	50
H(14)	8569	4590	6886	46
H(15)	7677	4434	6116	41
H(16)	6927	3258	6957	31
H(18)	7051	5028	9291	37
H(19)	6772	6802	10500	50
H(20)	6237	6089	11912	59
H(21)	5972	3666	12132	54
H(22)	6243	1889	10925	41
H(23A)	5011	4911	9382	51
H(23B)	4636	6117	8812	51
H(23C)	5307	6064	8637	51
H(29)	5823	4491	6186	35
H(27)	6935	4371	3816	53
H(26)	6853	1816	3776	57
H(25)	6264	599	4921	46
H(28)	6418	5710	5036	43

Table 6. Hydrogen bonds for cd213 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)