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One dimensional assembly of Mn_6 Single Molecule Magnets linked by oligothiophene bridges

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Table S1. Crystal data and structure refinement for $[Mn_6(Et\text{-}Sao)_6(EtOH)_4(H_2O)_2(C_{10}H_4O_4S_2) \cdot EtOH]_n$.

Identification code	mhp042	
Empirical formula	C38 H49 Mn3 N3 O13 S	
Formula weight	952.68	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 12.5136(13) Å	α= 100.797(13)° .
	b = 13.188(2) Å	β= 93.295(11)° .
	c = 14.988(2) Å	γ = 110.925(11)° .
Volume	2248.5(6) $Å^3$	
Z	2	
Density (calculated)	1.407 Mg/m^3	
Absorption coefficient	0.938 mm^{-1}	
F(000)	986	
Crystal size	0.4 x 0.25 x 0.2 mm^3	
Theta range for data collection	3.18 to 30.00° .	
Index ranges	-17<=h<=17, -18<=k<=18, -20<=l<=21	
Reflections collected	40264	
Independent reflections	12652 [R(int) = 0.0366]	
Completeness to theta = 30.00°	96.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12652 / 0 / 536	
Goodness-of-fit on F^2	1.074	
Final R indices [I>2sigma(I)]	R1 = 0.0375, wR2 = 0.0950	
R indices (all data)	R1 = 0.0619, wR2 = 0.1007	
Largest diff. peak and hole	0.626 and -0.607 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[Mn_6(Et\text{-}Sao)_6(EtOH)_4(H_2O)_2(C_{10}H_4O_4S_2) \cdot EtOH]_n$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mn(1)	476(1)	5953(1)	956(1)	14(1)
Mn(2)	2777(1)	5531(1)	1707(1)	18(1)
Mn(3)	236(1)	3558(1)	1451(1)	17(1)
S(1)	342(1)	8451(1)	4641(1)	38(1)
O(1)	1151(1)	5049(1)	1427(1)	16(1)
O(2)	1565(1)	3214(1)	1768(1)	23(1)
O(3)	-743(1)	2087(1)	1420(1)	24(1)
O(4)	-985(1)	4661(1)	532(1)	16(1)
O(5)	-48(1)	6835(1)	295(1)	18(1)
O(6)	2989(1)	6892(1)	1307(1)	22(1)
O(7)	4399(1)	5962(1)	1942(1)	25(1)
O(8)	-159(1)	6574(1)	2155(1)	25(1)
O(9)	583(1)	6423(1)	3510(1)	34(1)
O(10)	2763(1)	4464(1)	317(1)	28(1)
O(11)	2711(1)	6368(1)	3172(1)	35(1)
O(12)	38(1)	4174(1)	2906(1)	30(1)
N(1)	2583(1)	4109(1)	2134(1)	20(1)
N(2)	-1164(1)	3858(1)	1070(1)	16(1)
N(3)	2039(1)	7194(1)	1252(1)	18(1)
C(1)	-1731(2)	1855(2)	1785(1)	23(1)
C(2)	-2076(2)	940(2)	2214(2)	35(1)
C(3)	-3066(2)	680(2)	2637(2)	45(1)
C(4)	-3758(2)	1305(2)	2639(2)	42(1)
C(5)	-3460(2)	2185(2)	2191(2)	34(1)
C(6)	-2458(2)	2473(2)	1752(1)	24(1)
C(7)	-2212(2)	3380(2)	1247(1)	20(1)
C(8)	-3168(2)	3748(2)	956(1)	27(1)
C(9)	-3132(2)	4791(2)	1640(2)	42(1)
C(10)	205(2)	7930(1)	678(1)	18(1)
C(11)	-632(2)	8371(2)	495(1)	24(1)

C(12)	−443(2)	9485(2)	855(1)	29(1)
C(13)	590(2)	10180(2)	1408(2)	31(1)
C(14)	1436(2)	9763(2)	1570(1)	28(1)
C(15)	1284(2)	8634(1)	1208(1)	21(1)
C(16)	2249(2)	8258(1)	1362(1)	21(1)
C(17)	3493(2)	9081(2)	1566(2)	29(1)
C(18)	3993(2)	9266(2)	685(2)	54(1)
C(19)	4940(2)	5789(2)	2669(1)	23(1)
C(20)	6026(2)	6596(2)	3083(2)	33(1)
C(21)	6656(2)	6444(2)	3797(2)	41(1)
C(22)	6219(2)	5476(2)	4137(2)	43(1)
C(23)	5148(2)	4670(2)	3742(2)	36(1)
C(24)	4478(2)	4797(2)	3009(1)	26(1)
C(25)	3355(2)	3889(2)	2606(1)	23(1)
C(26)	3095(2)	2707(2)	2723(2)	33(1)
C(27)	2340(3)	2396(2)	3466(2)	56(1)
C(28)	134(2)	6885(2)	3013(1)	23(1)
C(29)	−66(2)	7906(2)	3469(1)	25(1)
C(30)	−502(2)	8546(2)	3076(1)	35(1)
C(31)	−514(2)	9491(2)	3710(2)	43(1)
C(32)	−69(2)	9569(2)	4588(1)	31(1)
C(33)	−51(2)	3710(2)	3707(1)	39(1)
C(34A)	−1070(4)	3814(4)	4163(3)	58(1)
C(34B)	980(7)	4327(6)	4459(5)	54(2)
C(35A)	3553(7)	7575(7)	3555(5)	47(2)
C(36A)	3811(10)	7671(9)	4615(8)	97(3)
C(35B)	3488(5)	7320(5)	3757(4)	51(1)
C(36B)	3893(7)	7092(6)	4675(5)	100(2)
O(13)	4311(1)	3561(1)	−427(1)	48(1)
C(37)	3863(2)	2367(2)	−682(2)	59(1)
C(38)	3570(2)	1906(3)	154(3)	83(1)

Table S3. Bond lengths [Å] and angles [°] for $[Mn_6(Et\text{-}Sao)_6(EtOH)_4(H_2O)_2(C_{10}H_4O_4S_2)\cdot EtOH]_n$.

Mn(1)-O(1)	1.8970(12)
Mn(1)-O(5)	1.9156(12)
Mn(1)-O(4)	1.9718(12)
Mn(1)-N(3)	2.0106(15)
Mn(1)-O(8)	2.1470(13)
Mn(1)-O(4)#1	2.4271(13)
Mn(2)-O(7)	1.8936(12)
Mn(2)-O(1)	1.8967(12)
Mn(2)-O(6)	1.9322(13)
Mn(2)-N(1)	2.0327(15)
Mn(2)-O(10)	2.2795(14)
Mn(2)-O(11)	2.2869(15)
Mn(3)-O(3)	1.8787(13)
Mn(3)-O(1)	1.8977(12)
Mn(3)-O(2)	1.9302(12)
Mn(3)-N(2)	2.0045(15)
Mn(3)-O(12)	2.2409(14)
S(1)-C(29)	1.7390(19)
S(1)-C(32)	1.740(2)
O(2)-N(1)	1.3854(19)
O(3)-C(1)	1.339(2)
O(4)-N(2)	1.4112(17)
O(4)-Mn(1)#1	2.4271(13)
O(5)-C(10)	1.363(2)
O(6)-N(3)	1.3838(18)
O(7)-C(19)	1.347(2)
O(8)-C(28)	1.264(2)
O(9)-C(28)	1.267(2)
O(10)-H(10A)	0.8467
O(10)-H(10B)	0.8568
O(11)-C(35B)	1.381(6)
O(11)-C(35A)	1.538(8)
O(11)-H(110)	0.9144
O(12)-C(33)	1.439(2)

O(12)-H(120)	0.8337
N(1)-C(25)	1.310(2)
N(2)-C(7)	1.304(2)
N(3)-C(16)	1.307(2)
C(1)-C(2)	1.416(3)
C(1)-C(6)	1.427(3)
C(2)-C(3)	1.386(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.392(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.396(3)
C(4)-H(4)	0.9300
C(5)-C(6)	1.413(3)
C(5)-H(5)	0.9300
C(6)-C(7)	1.484(3)
C(7)-C(8)	1.512(2)
C(8)-C(9)	1.539(3)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(10)-C(11)	1.404(2)
C(10)-C(15)	1.422(2)
C(11)-C(12)	1.395(3)
C(11)-H(11)	0.9300
C(12)-C(13)	1.394(3)
C(12)-H(12)	0.9300
C(13)-C(14)	1.384(3)
C(13)-H(13)	0.9300
C(14)-C(15)	1.425(2)
C(14)-H(14)	0.9300
C(15)-C(16)	1.483(2)
C(16)-C(17)	1.519(2)
C(17)-C(18)	1.517(3)
C(17)-H(17A)	0.9700

C(17)-H(17B)	0.9700
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-C(20)	1.409(3)
C(19)-C(24)	1.432(3)
C(20)-C(21)	1.379(3)
C(20)-H(20)	0.9300
C(21)-C(22)	1.402(3)
C(21)-H(21)	0.9300
C(22)-C(23)	1.390(3)
C(22)-H(22)	0.9300
C(23)-C(24)	1.414(3)
C(23)-H(23)	0.9300
C(24)-C(25)	1.484(3)
C(25)-C(26)	1.521(3)
C(26)-C(27)	1.522(3)
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-C(29)	1.503(2)
C(29)-C(30)	1.355(3)
C(30)-C(31)	1.423(3)
C(30)-H(30)	0.9300
C(31)-C(32)	1.370(3)
C(31)-H(31)	0.9300
C(32)-C(32)#2	1.468(4)
C(33)-C(34A)	1.517(5)
C(33)-C(34B)	1.528(7)
C(33)-H(33A)	0.9700
C(33)-H(33B)	0.9700
C(33)-H(33C)	0.9700
C(33)-H(33D)	0.9700
C(34A)-H(33D)	0.5609

C(34A)-H(34A)	0.9600
C(34A)-H(34B)	0.9600
C(34A)-H(34C)	0.9600
C(34B)-H(34D)	0.9600
C(34B)-H(34E)	0.9600
C(34B)-H(34F)	0.9600
C(35A)-C(36A)	1.575(13)
C(35A)-H(35A)	0.9700
C(35A)-H(35B)	0.9700
C(36A)-H(36A)	0.9600
C(36A)-H(36B)	0.9600
C(36A)-H(36C)	0.9600
C(35B)-C(36B)	1.556(9)
C(35B)-H(35C)	0.9700
C(35B)-H(35D)	0.9700
C(36B)-H(36D)	0.9600
C(36B)-H(36E)	0.9600
C(36B)-H(36F)	0.9600
O(13)-C(37)	1.434(3)
O(13)-H(130)	0.8525
C(37)-C(38)	1.501(4)
C(37)-H(37A)	0.9700
C(37)-H(37B)	0.9700
C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600
C(38)-H(38C)	0.9600

O(1)-Mn(1)-O(5)	169.37(5)
O(1)-Mn(1)-O(4)	90.59(5)
O(5)-Mn(1)-O(4)	91.45(5)
O(1)-Mn(1)-N(3)	87.98(5)
O(5)-Mn(1)-N(3)	88.71(6)
O(4)-Mn(1)-N(3)	172.92(6)
O(1)-Mn(1)-O(8)	100.27(5)
O(5)-Mn(1)-O(8)	90.04(5)
O(4)-Mn(1)-O(8)	92.74(5)

N(3)-Mn(1)-O(8)	94.34(6)
O(1)-Mn(1)-O(4)#1	88.32(5)
O(5)-Mn(1)-O(4)#1	81.51(5)
O(4)-Mn(1)-O(4)#1	84.32(5)
N(3)-Mn(1)-O(4)#1	88.70(5)
O(8)-Mn(1)-O(4)#1	170.96(5)
O(7)-Mn(2)-O(1)	177.48(5)
O(7)-Mn(2)-O(6)	90.02(5)
O(1)-Mn(2)-O(6)	90.91(5)
O(7)-Mn(2)-N(1)	89.06(6)
O(1)-Mn(2)-N(1)	90.01(5)
O(6)-Mn(2)-N(1)	179.07(6)
O(7)-Mn(2)-O(10)	89.86(6)
O(1)-Mn(2)-O(10)	87.71(5)
O(6)-Mn(2)-O(10)	97.38(5)
N(1)-Mn(2)-O(10)	82.76(6)
O(7)-Mn(2)-O(11)	91.46(6)
O(1)-Mn(2)-O(11)	90.86(5)
O(6)-Mn(2)-O(11)	90.76(6)
N(1)-Mn(2)-O(11)	89.12(6)
O(10)-Mn(2)-O(11)	171.75(5)
O(3)-Mn(3)-O(1)	176.29(5)
O(3)-Mn(3)-O(2)	90.29(6)
O(1)-Mn(3)-O(2)	93.01(5)
O(3)-Mn(3)-N(2)	88.25(6)
O(1)-Mn(3)-N(2)	88.38(5)
O(2)-Mn(3)-N(2)	177.33(6)
O(3)-Mn(3)-O(12)	93.24(6)
O(1)-Mn(3)-O(12)	88.16(5)
O(2)-Mn(3)-O(12)	94.74(6)
N(2)-Mn(3)-O(12)	87.57(6)
C(29)-S(1)-C(32)	91.89(9)
Mn(2)-O(1)-Mn(1)	120.70(6)
Mn(2)-O(1)-Mn(3)	118.24(6)
Mn(1)-O(1)-Mn(3)	120.37(6)
N(1)-O(2)-Mn(3)	116.75(9)

C(1)-O(3)-Mn(3)	121.75(11)
N(2)-O(4)-Mn(1)	112.83(9)
N(2)-O(4)-Mn(1)#1	112.07(8)
Mn(1)-O(4)-Mn(1)#1	95.68(5)
C(10)-O(5)-Mn(1)	119.65(10)
N(3)-O(6)-Mn(2)	116.81(10)
C(19)-O(7)-Mn(2)	123.69(12)
C(28)-O(8)-Mn(1)	139.04(12)
Mn(2)-O(10)-H(10A)	137.2
Mn(2)-O(10)-H(10B)	116.8
H(10A)-O(10)-H(10B)	105.7
C(35B)-O(11)-C(35A)	18.0(4)
C(35B)-O(11)-Mn(2)	130.9(3)
C(35A)-O(11)-Mn(2)	118.1(3)
C(35B)-O(11)-H(110)	106.2
C(35A)-O(11)-H(110)	106.9
Mn(2)-O(11)-H(110)	114.2
C(33)-O(12)-Mn(3)	133.65(12)
C(33)-O(12)-H(120)	107.9
Mn(3)-O(12)-H(120)	116.5
C(25)-N(1)-O(2)	115.94(14)
C(25)-N(1)-Mn(2)	128.04(13)
O(2)-N(1)-Mn(2)	115.28(10)
C(7)-N(2)-O(4)	117.19(14)
C(7)-N(2)-Mn(3)	127.30(12)
O(4)-N(2)-Mn(3)	115.49(10)
C(16)-N(3)-O(6)	116.68(14)
C(16)-N(3)-Mn(1)	126.33(12)
O(6)-N(3)-Mn(1)	116.94(10)
O(3)-C(1)-C(2)	118.17(17)
O(3)-C(1)-C(6)	123.25(16)
C(2)-C(1)-C(6)	118.57(18)
C(3)-C(2)-C(1)	121.1(2)
C(3)-C(2)-H(2)	119.4
C(1)-C(2)-H(2)	119.4
C(2)-C(3)-C(4)	120.7(2)

C(2)-C(3)-H(3)	119.7
C(4)-C(3)-H(3)	119.7
C(3)-C(4)-C(5)	119.3(2)
C(3)-C(4)-H(4)	120.4
C(5)-C(4)-H(4)	120.4
C(4)-C(5)-C(6)	121.6(2)
C(4)-C(5)-H(5)	119.2
C(6)-C(5)-H(5)	119.2
C(5)-C(6)-C(1)	118.60(18)
C(5)-C(6)-C(7)	119.45(17)
C(1)-C(6)-C(7)	121.93(16)
N(2)-C(7)-C(6)	119.08(16)
N(2)-C(7)-C(8)	120.96(16)
C(6)-C(7)-C(8)	119.95(16)
C(7)-C(8)-C(9)	111.08(16)
C(7)-C(8)-H(8A)	109.4
C(9)-C(8)-H(8A)	109.4
C(7)-C(8)-H(8B)	109.4
C(9)-C(8)-H(8B)	109.4
H(8A)-C(8)-H(8B)	108.0
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
O(5)-C(10)-C(11)	117.25(15)
O(5)-C(10)-C(15)	122.86(15)
C(11)-C(10)-C(15)	119.83(15)
C(12)-C(11)-C(10)	121.15(17)
C(12)-C(11)-H(11)	119.4
C(10)-C(11)-H(11)	119.4
C(13)-C(12)-C(11)	119.93(17)
C(13)-C(12)-H(12)	120.0
C(11)-C(12)-H(12)	120.0
C(14)-C(13)-C(12)	119.44(17)

C(14)-C(13)-H(13)	120.3
C(12)-C(13)-H(13)	120.3
C(13)-C(14)-C(15)	122.44(17)
C(13)-C(14)-H(14)	118.8
C(15)-C(14)-H(14)	118.8
C(10)-C(15)-C(14)	117.13(16)
C(10)-C(15)-C(16)	123.09(15)
C(14)-C(15)-C(16)	119.73(16)
N(3)-C(16)-C(15)	119.70(15)
N(3)-C(16)-C(17)	119.17(16)
C(15)-C(16)-C(17)	120.93(15)
C(18)-C(17)-C(16)	110.78(18)
C(18)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17A)	109.5
C(18)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	108.1
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
O(7)-C(19)-C(20)	118.52(18)
O(7)-C(19)-C(24)	122.51(16)
C(20)-C(19)-C(24)	118.90(18)
C(21)-C(20)-C(19)	121.6(2)
C(21)-C(20)-H(20)	119.2
C(19)-C(20)-H(20)	119.2
C(20)-C(21)-C(22)	120.3(2)
C(20)-C(21)-H(21)	119.8
C(22)-C(21)-H(21)	119.8
C(23)-C(22)-C(21)	119.1(2)
C(23)-C(22)-H(22)	120.4
C(21)-C(22)-H(22)	120.4
C(22)-C(23)-C(24)	122.1(2)

C(22)-C(23)-H(23)	118.9
C(24)-C(23)-H(23)	118.9
C(23)-C(24)-C(19)	117.95(18)
C(23)-C(24)-C(25)	119.13(18)
C(19)-C(24)-C(25)	122.88(17)
N(1)-C(25)-C(24)	119.41(17)
N(1)-C(25)-C(26)	119.59(17)
C(24)-C(25)-C(26)	121.00(16)
C(25)-C(26)-C(27)	113.89(19)
C(25)-C(26)-H(26A)	108.8
C(27)-C(26)-H(26A)	108.8
C(25)-C(26)-H(26B)	108.8
C(27)-C(26)-H(26B)	108.8
H(26A)-C(26)-H(26B)	107.7
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
O(8)-C(28)-O(9)	126.09(17)
O(8)-C(28)-C(29)	115.79(17)
O(9)-C(28)-C(29)	118.12(16)
C(30)-C(29)-C(28)	128.26(17)
C(30)-C(29)-S(1)	111.09(14)
C(28)-C(29)-S(1)	120.58(14)
C(29)-C(30)-C(31)	113.30(18)
C(29)-C(30)-H(30)	123.4
C(31)-C(30)-H(30)	123.4
C(32)-C(31)-C(30)	113.25(19)
C(32)-C(31)-H(31)	123.4
C(30)-C(31)-H(31)	123.4
C(31)-C(32)-C(32)#2	128.5(2)
C(31)-C(32)-S(1)	110.46(14)
C(32)#2-C(32)-S(1)	121.0(2)
O(12)-C(33)-C(34A)	109.9(2)

O(12)-C(33)-C(34B)	113.9(3)
C(34A)-C(33)-C(34B)	104.0(4)
O(12)-C(33)-H(33A)	109.7
C(34A)-C(33)-H(33A)	109.7
C(34B)-C(33)-H(33A)	5.9
O(12)-C(33)-H(33B)	109.7
C(34A)-C(33)-H(33B)	109.7
C(34B)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	108.2
O(12)-C(33)-H(33C)	108.3
C(34A)-C(33)-H(33C)	112.2
C(34B)-C(33)-H(33C)	108.6
H(33A)-C(33)-H(33C)	107.0
H(33B)-C(33)-H(33C)	2.5
O(12)-C(33)-H(33D)	108.9
C(34A)-C(33)-H(33D)	5.8
C(34B)-C(33)-H(33D)	109.3
H(33A)-C(33)-H(33D)	115.0
H(33B)-C(33)-H(33D)	105.2
H(33C)-C(33)-H(33D)	107.7
C(33)-C(34A)-H(33D)	10.1
C(33)-C(34A)-H(34A)	109.5
H(33D)-C(34A)-H(34A)	116.2
C(33)-C(34A)-H(34B)	109.5
H(33D)-C(34A)-H(34B)	112.0
C(33)-C(34A)-H(34C)	109.5
H(33D)-C(34A)-H(34C)	99.7
C(33)-C(34B)-H(34D)	109.5
C(33)-C(34B)-H(34E)	109.5
H(34D)-C(34B)-H(34E)	109.5
C(33)-C(34B)-H(34F)	109.5
H(34D)-C(34B)-H(34F)	109.5
H(34E)-C(34B)-H(34F)	109.5
O(11)-C(35A)-C(36A)	105.0(6)
O(11)-C(35A)-H(35A)	110.7
C(36A)-C(35A)-H(35A)	110.7

O(11)-C(35A)-H(35B)	110.7
C(36A)-C(35A)-H(35B)	110.7
H(35A)-C(35A)-H(35B)	108.8
C(35A)-C(36A)-H(36A)	109.5
C(35A)-C(36A)-H(36B)	109.5
H(36A)-C(36A)-H(36B)	109.5
C(35A)-C(36A)-H(36C)	109.5
H(36A)-C(36A)-H(36C)	109.5
H(36B)-C(36A)-H(36C)	109.5
O(11)-C(35B)-C(36B)	112.5(5)
O(11)-C(35B)-H(35C)	109.1
C(36B)-C(35B)-H(35C)	109.1
O(11)-C(35B)-H(35D)	109.1
C(36B)-C(35B)-H(35D)	109.1
H(35C)-C(35B)-H(35D)	107.8
C(35B)-C(36B)-H(36D)	109.5
C(35B)-C(36B)-H(36E)	109.5
H(36D)-C(36B)-H(36E)	109.5
C(35B)-C(36B)-H(36F)	109.5
H(36D)-C(36B)-H(36F)	109.5
H(36E)-C(36B)-H(36F)	109.5
C(37)-O(13)-H(130)	106.2
O(13)-C(37)-C(38)	109.4(3)
O(13)-C(37)-H(37A)	109.8
C(38)-C(37)-H(37A)	109.8
O(13)-C(37)-H(37B)	109.8
C(38)-C(37)-H(37B)	109.8
H(37A)-C(37)-H(37B)	108.2
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z #2 -x,-y+2,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for mhp042. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(1)	16(1)	11(1)	15(1)	0(1)	1(1)	6(1)
Mn(2)	16(1)	16(1)	21(1)	3(1)	1(1)	8(1)
Mn(3)	17(1)	13(1)	21(1)	3(1)	2(1)	7(1)
S(1)	72(1)	33(1)	19(1)	-4(1)	-2(1)	37(1)
O(1)	16(1)	12(1)	20(1)	1(1)	1(1)	6(1)
O(2)	21(1)	16(1)	30(1)	2(1)	-3(1)	8(1)
O(3)	26(1)	14(1)	33(1)	6(1)	5(1)	7(1)
O(4)	20(1)	14(1)	16(1)	3(1)	1(1)	7(1)
O(5)	23(1)	12(1)	19(1)	-1(1)	-1(1)	8(1)
O(6)	16(1)	20(1)	33(1)	6(1)	3(1)	10(1)
O(7)	17(1)	27(1)	32(1)	9(1)	2(1)	9(1)
O(8)	32(1)	24(1)	19(1)	-4(1)	6(1)	14(1)
O(9)	53(1)	29(1)	25(1)	-1(1)	4(1)	26(1)
O(10)	31(1)	33(1)	23(1)	0(1)	2(1)	19(1)
O(11)	33(1)	38(1)	28(1)	-7(1)	0(1)	15(1)
O(12)	48(1)	22(1)	20(1)	4(1)	7(1)	15(1)
N(1)	19(1)	19(1)	22(1)	2(1)	2(1)	9(1)
N(2)	21(1)	12(1)	13(1)	1(1)	2(1)	5(1)
N(3)	17(1)	17(1)	21(1)	2(1)	0(1)	8(1)
C(1)	24(1)	19(1)	23(1)	3(1)	0(1)	4(1)
C(2)	40(1)	27(1)	39(1)	14(1)	7(1)	10(1)
C(3)	49(1)	36(1)	50(2)	26(1)	14(1)	7(1)
C(4)	33(1)	44(1)	46(1)	21(1)	14(1)	5(1)
C(5)	26(1)	39(1)	40(1)	16(1)	12(1)	11(1)
C(6)	23(1)	21(1)	23(1)	5(1)	3(1)	4(1)
C(7)	19(1)	21(1)	18(1)	2(1)	3(1)	8(1)
C(8)	19(1)	34(1)	31(1)	12(1)	7(1)	11(1)
C(9)	50(1)	53(1)	39(1)	13(1)	19(1)	36(1)
C(10)	26(1)	13(1)	17(1)	1(1)	4(1)	10(1)
C(11)	27(1)	19(1)	25(1)	-1(1)	-2(1)	12(1)
C(12)	36(1)	24(1)	31(1)	3(1)	0(1)	21(1)

C(13)	41(1)	15(1)	38(1)	0(1)	0(1)	16(1)
C(14)	30(1)	13(1)	37(1)	-2(1)	-2(1)	6(1)
C(15)	25(1)	15(1)	23(1)	3(1)	2(1)	9(1)
C(16)	22(1)	16(1)	21(1)	0(1)	1(1)	6(1)
C(17)	22(1)	17(1)	45(1)	2(1)	-1(1)	5(1)
C(18)	38(1)	53(2)	65(2)	24(1)	16(1)	4(1)
C(19)	20(1)	28(1)	22(1)	0(1)	1(1)	13(1)
C(20)	24(1)	34(1)	35(1)	1(1)	1(1)	9(1)
C(21)	27(1)	50(1)	32(1)	-5(1)	-6(1)	7(1)
C(22)	33(1)	62(2)	29(1)	8(1)	-9(1)	14(1)
C(23)	32(1)	46(1)	30(1)	12(1)	0(1)	15(1)
C(24)	24(1)	34(1)	22(1)	3(1)	1(1)	13(1)
C(25)	25(1)	25(1)	21(1)	5(1)	0(1)	13(1)
C(26)	35(1)	29(1)	37(1)	11(1)	-6(1)	14(1)
C(27)	75(2)	40(1)	43(2)	16(1)	6(1)	8(1)
C(28)	27(1)	18(1)	22(1)	-2(1)	7(1)	9(1)
C(29)	36(1)	23(1)	16(1)	-2(1)	7(1)	15(1)
C(30)	62(1)	36(1)	15(1)	-2(1)	2(1)	31(1)
C(31)	84(2)	40(1)	23(1)	2(1)	4(1)	47(1)
C(32)	52(1)	26(1)	20(1)	-2(1)	4(1)	25(1)
C(33)	57(1)	34(1)	23(1)	6(1)	2(1)	14(1)
C(34A)	58(3)	69(3)	26(2)	5(2)	17(2)	2(2)
C(34B)	77(5)	40(4)	38(4)	8(3)	-6(4)	16(4)
O(13)	50(1)	49(1)	60(1)	23(1)	27(1)	29(1)
C(37)	51(2)	53(2)	82(2)	21(2)	22(2)	23(1)
C(38)	39(2)	93(2)	131(3)	77(2)	8(2)	18(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for mhp042.

	x	y	z	U(eq)
H(10A)	3209	4184	59	42
H(10B)	2207	4342	-101	42
H(110)	1992	6341	3286	53
H(120)	205	4858	3079	44
H(2)	-1631	505	2212	42
H(3)	-3270	82	2922	54
H(4)	-4411	1138	2936	50
H(5)	-3932	2591	2182	41
H(8A)	-3909	3149	918	32
H(8B)	-3086	3908	353	32
H(9A)	-3188	4640	2242	62
H(9B)	-3767	4986	1457	62
H(9C)	-2418	5397	1649	62
H(11)	-1324	7912	128	29
H(12)	-1006	9764	726	34
H(13)	710	10917	1666	37
H(14)	2129	10238	1927	34
H(17A)	3524	9785	1929	35
H(17B)	3951	8799	1920	35
H(18A)	4032	8586	354	81
H(18B)	4754	9835	828	81
H(18C)	3508	9495	315	81
H(20)	6324	7246	2869	39
H(21)	7373	6987	4053	49
H(22)	6641	5375	4621	52
H(23)	4863	4027	3966	43
H(26A)	3818	2621	2869	39
H(26B)	2713	2192	2145	39
H(27A)	2741	2857	4051	83
H(27B)	2169	1629	3475	83

H(27C)	1633	2506	3340	83
H(30)	-767	8384	2453	42
H(31)	-795	10003	3544	52
H(33A)	654	4101	4135	47
H(33B)	-151	2932	3534	47
H(33C)	-119	2942	3522	47
H(33D)	-751	3710	3953	47
H(34A)	-1017	4572	4265	86
H(34B)	-1063	3597	4739	86
H(34C)	-1775	3339	3773	86
H(34D)	1684	4432	4197	81
H(34E)	939	3898	4916	81
H(34F)	966	5039	4736	81
H(35A)	3205	8097	3442	57
H(35B)	4257	7726	3275	57
H(36A)	3118	7259	4835	146
H(36B)	4083	8440	4930	146
H(36C)	4391	7374	4725	146
H(35C)	3132	7865	3888	61
H(35D)	4156	7633	3455	61
H(36D)	3233	6746	4961	150
H(36E)	4386	7783	5075	150
H(36F)	4311	6607	4554	150
H(130)	4708	3786	-844	71
H(37A)	4434	2116	-957	71
H(37B)	3177	2103	-1130	71
H(38A)	4258	2144	584	124
H(38B)	3247	1107	-19	124
H(38C)	3019	2171	431	124