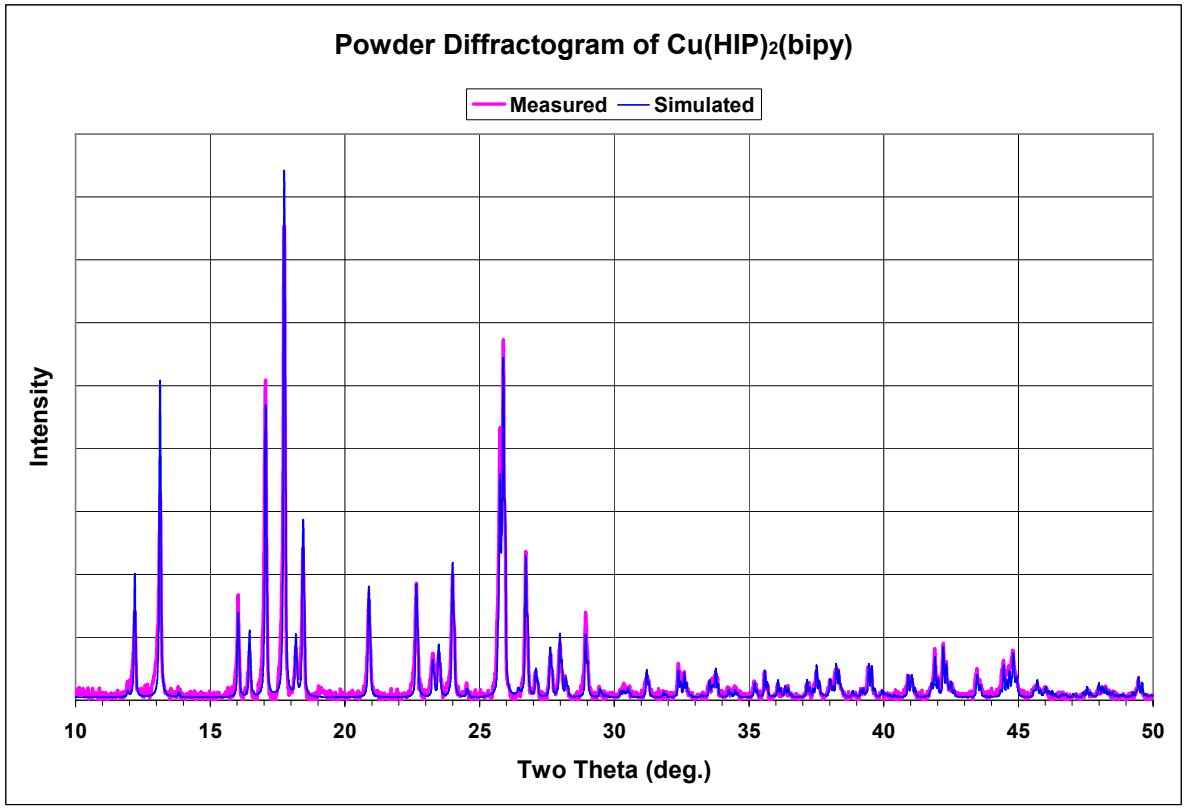

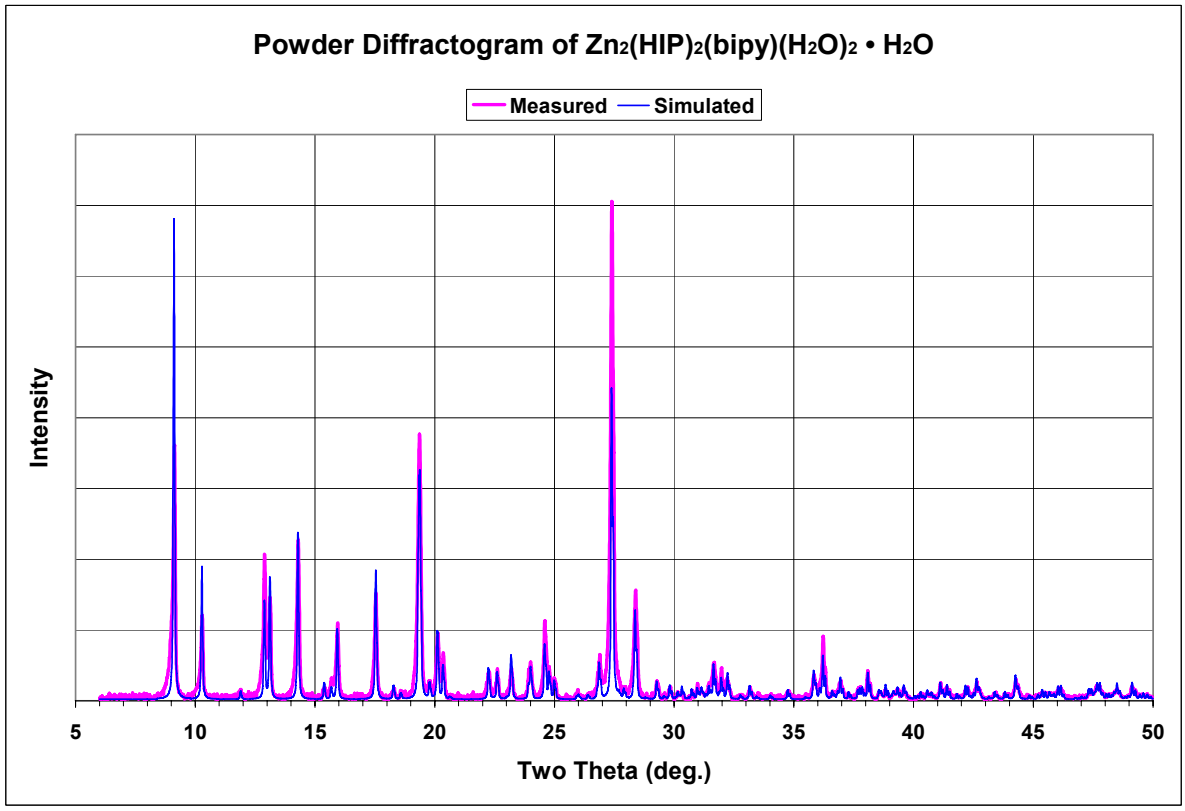

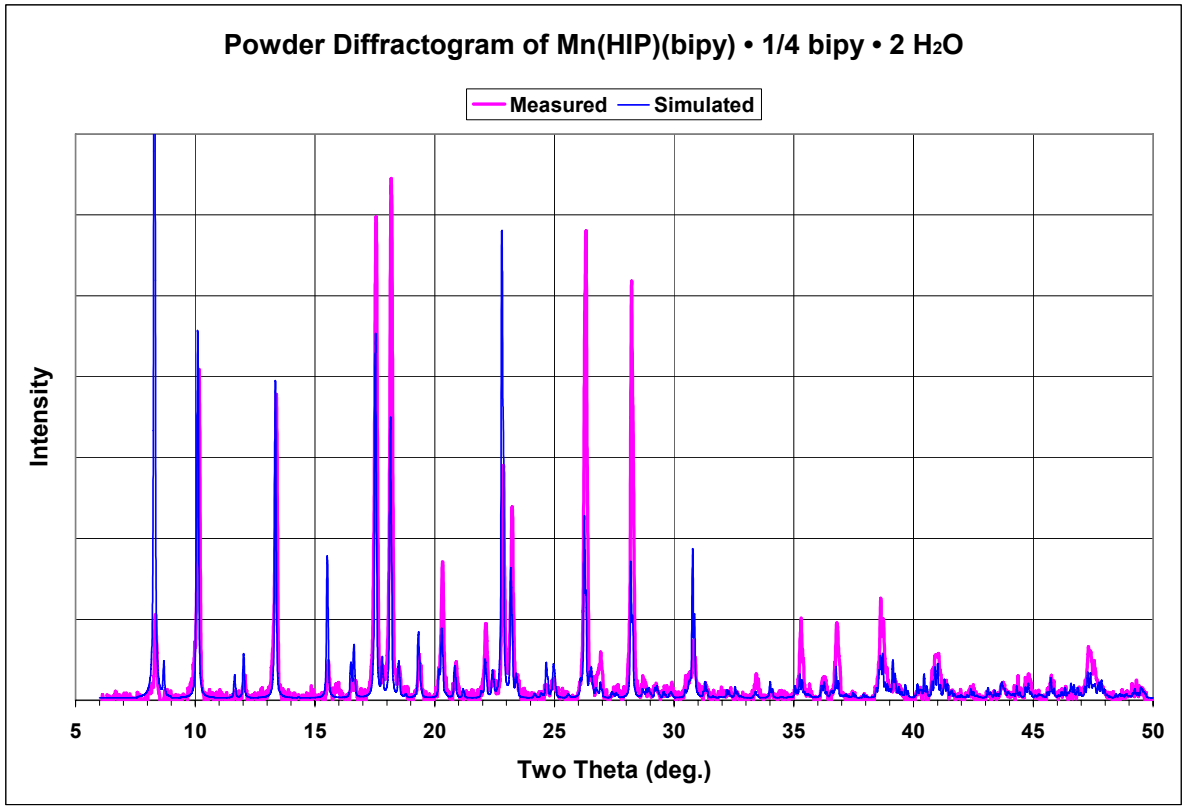

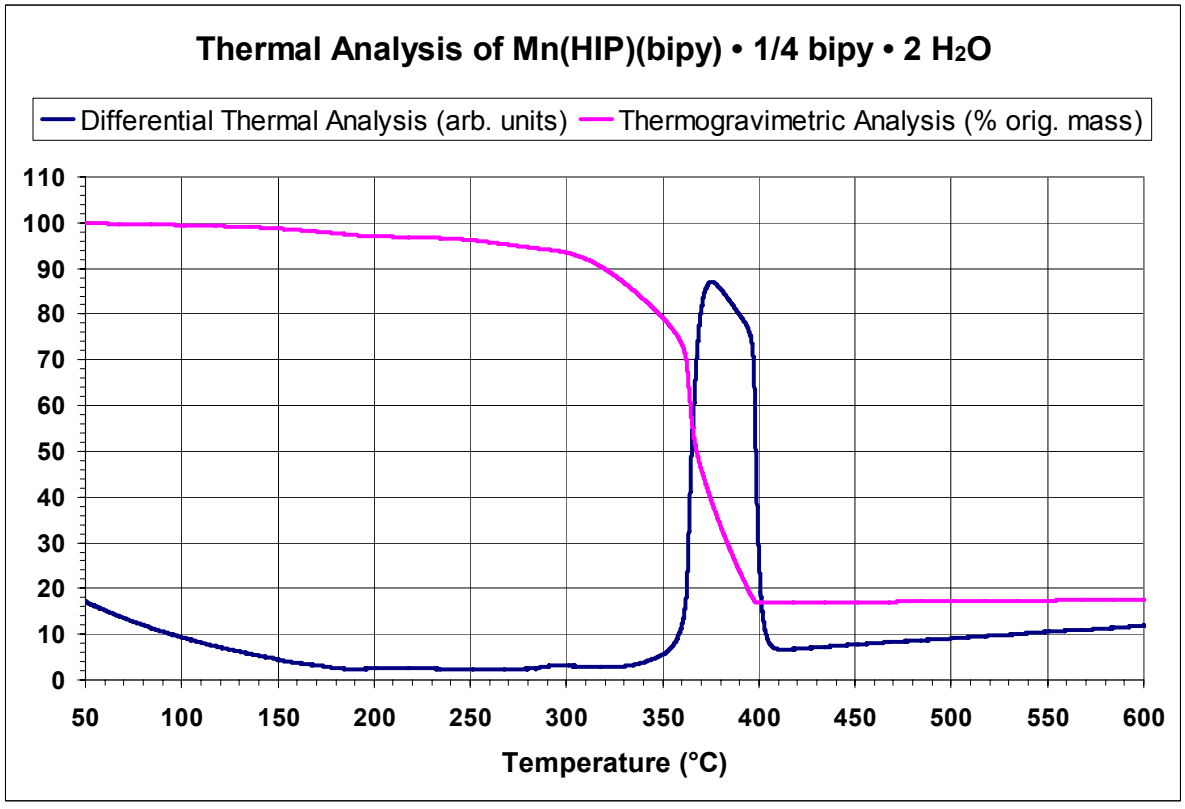

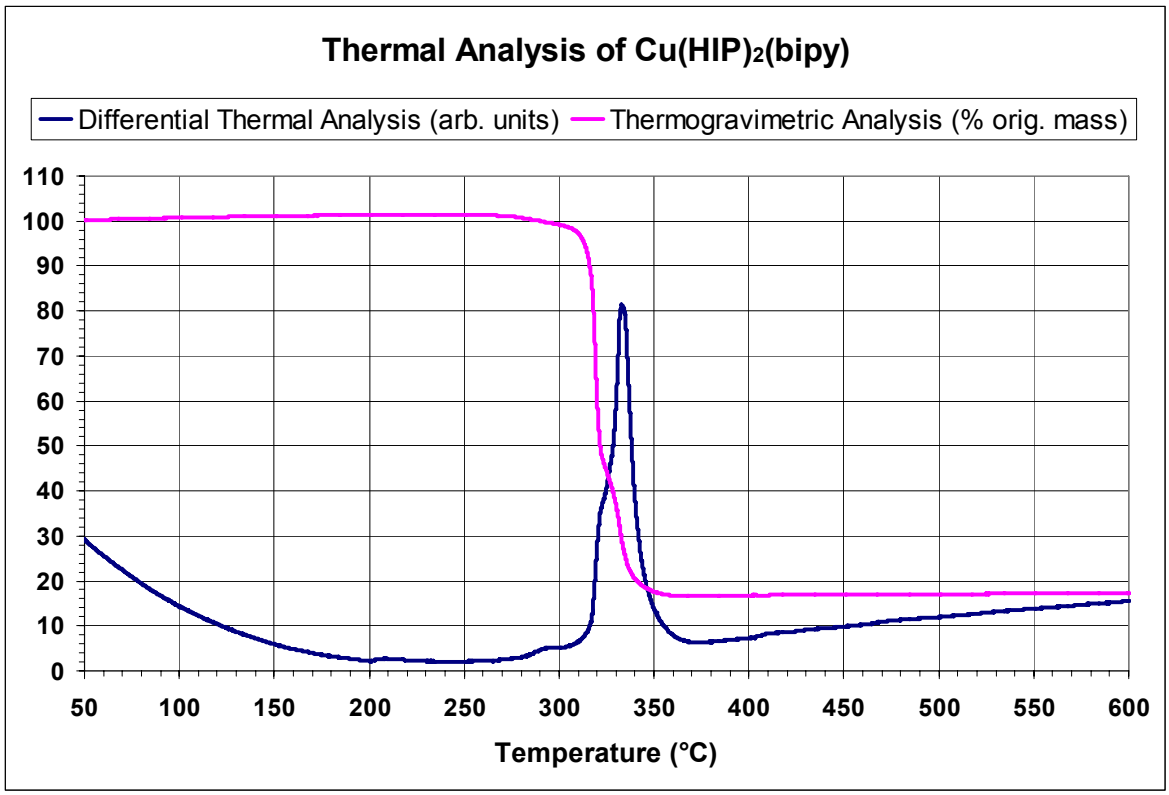

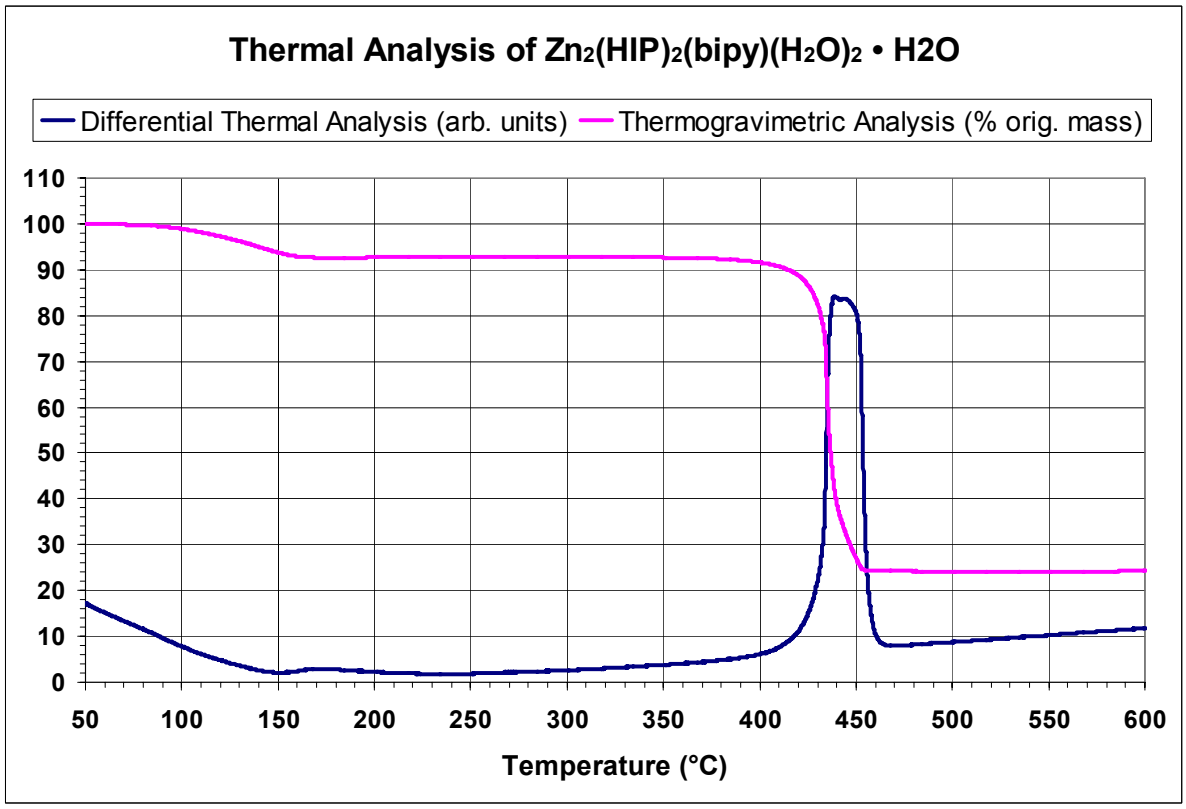

Crystallographic data for Mn(HIP)(bipy) · 3 H_2O, **I**:

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **I**.

	x	y	z	U(eq)
Mn(1)	3826(1)	6534(1)	8332(1)	30(1)
N(1)	3854(4)	8500(2)	8285(2)	43(1)
N(2)	3953(3)	4595(2)	8303(2)	34(1)
O(1)	1574(3)	6275(3)	8277(2)	56(1)
O(2)	2902(3)	6712(3)	9476(2)	57(1)
O(3)	-3424(3)	6544(2)	7995(2)	44(1)
O(4)	-4195(2)	6562(2)	9150(2)	40(1)
C(3)	3875(4)	10907(3)	8291(2)	34(1)
C(6)	3100(4)	4005(3)	7703(3)	44(1)
C(7)	3048(4)	2815(3)	7677(3)	44(1)
C(8)	3911(4)	2184(3)	8292(2)	36(1)
C(9)	4794(4)	2796(3)	8911(3)	42(1)
C(10)	4785(4)	3974(3)	8896(2)	39(1)
C(11)	551(4)	6530(4)	9432(3)	45(1)
C(15)	-1842(4)	6525(3)	9308(2)	41(1)
C(16)	-752(4)	6535(3)	8932(2)	35(1)
C(17)	1751(4)	6513(3)	9040(3)	36(1)
C(18)	-3252(4)	6546(3)	8776(2)	29(1)
C(12A)	758(8)	6296(5)	10312(6)	42(2)
C(14A)	-1615(8)	6258(5)	10178(5)	39(2)
C(13A)	-330(7)	6192(6)	10682(4)	40(1)
O(5A)	-49(5)	6018(5)	11539(3)	61(1)
OWA	-103(16)	8801(13)	12035(11)	131(8)
C(12B)	762(15)	6905(10)	10262(10)	42(2)
C(14B)	-1604(13)	6898(9)	10150(9)	39(2)
C(13B)	-304(11)	6997(10)	10633(7)	40(1)
O(5B)	-82(8)	7233(8)	11500(5)	61(1)
OWB	0	5368(10)	12500	72(4)
C(4A)	5048(9)	10285(7)	8674(6)	50(2)
C(5A)	5013(10)	9105(8)	8651(6)	53(2)

C(2A)	2747(9)	10289(7)	7948(6)	56(2)
C(1A)	2773(10)	9109(7)	7968(6)	56(3)
C(4B)	4422(11)	10269(9)	8975(8)	50(2)
C(5B)	4376(13)	9094(11)	8923(9)	53(2)
C(2B)	3311(10)	10332(9)	7551(8)	56(2)
C(1B)	3315(12)	9106(9)	7551(9)	56(3)
OW1	-155(17)	10701(19)	11973(12)	282(14)
OW2	-154(16)	9795(10)	11377(17)	234(12)
OW3	-100(70)	9910(50)	10720(30)	480(40)
OW4	-1840(30)	10560(40)	9730(20)	450(20)
OW5	820(40)	10648(17)	10230(40)	370(20)

(U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor)

Bond lengths [Å] and angles [°] for **I**:

Mn(1)-O(3)#1	2.101(3)
Mn(1)-O(4)#2	2.142(3)
Mn(1)-N(2)	2.261(3)
Mn(1)-O(2)	2.277(3)
Mn(1)-N(1)	2.290(3)
Mn(1)-O(1)	2.291(3)
Mn(1)-C(17)	2.626(4)
N(1)-C(5B)	1.258(14)
N(1)-C(1A)	1.309(9)
N(1)-C(5A)	1.384(10)
N(1)-C(1B)	1.385(13)
N(2)-C(6)	1.338(4)
N(2)-C(10)	1.339(4)
O(1)-C(17)	1.243(5)
O(2)-C(17)	1.242(5)
O(3)-C(18)	1.242(4)
O(3)-Mn(1)#1	2.101(3)
O(4)-C(18)	1.249(4)
O(4)-Mn(1)#3	2.142(3)

C(3)-C(4B)	1.347(12)
C(3)-C(2A)	1.360(9)
C(3)-C(2B)	1.380(12)
C(3)-C(4A)	1.412(9)
C(3)-C(8)#4	1.487(5)
C(6)-C(7)	1.386(5)
C(6)-H(6)	0.9300
C(7)-C(8)	1.380(5)
C(7)-H(7)	0.9300
C(8)-C(9)	1.382(5)
C(8)-C(3)#5	1.487(5)
C(9)-C(10)	1.372(5)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-C(16)	1.386(5)
C(11)-C(12B)	1.387(17)
C(11)-C(12A)	1.423(10)
C(11)-C(17)	1.502(6)
C(15)-C(16)	1.384(5)
C(15)-C(14B)	1.403(15)
C(15)-C(14A)	1.413(9)
C(15)-C(18)	1.494(5)
C(16)-H(16)	0.9300
C(12A)-C(13A)	1.382(11)
C(12A)-H(12A)	0.9300
C(14A)-C(13A)	1.376(10)
C(14A)-H(14A)	0.9300
C(13A)-O(5A)	1.371(8)
O(5A)-H(5A)	0.8200
OWA-OWA#6	1.48(4)
OWA-OW2	1.57(3)
C(12B)-C(13B)	1.361(19)
C(12B)-H(12B)	0.9300
C(14B)-C(13B)	1.379(17)
C(14B)-H(14B)	0.9300
C(13B)-O(5B)	1.403(13)

O(5B)-H(5B)	0.8200
C(4A)-C(5A)	1.374(12)
C(4A)-H(4A)	0.9300
C(5A)-H(5A1)	0.9300
C(2A)-C(1A)	1.375(11)
C(2A)-H(2A)	0.9300
C(1A)-H(1A)	0.9300
C(4B)-C(5B)	1.370(15)
C(4B)-H(4B)	0.9300
C(5B)-H(5B1)	0.9300
C(2B)-C(1B)	1.427(15)
C(2B)-H(2B)	0.9300
C(1B)-H(1B)	0.9300
OW1-OW2	1.43(3)
OW1-OW1#6	1.67(4)
OW2-OW3	1.09(4)
OW3-OW5	1.61(4)
OW3-OW5#7	1.67(6)
OW4-OW5#7	1.74(5)
OW5-OW3#7	1.67(6)
OW5-OW4#7	1.74(5)

O(3)#1-Mn(1)-O(4)#2	124.75(11)
O(3)#1-Mn(1)-N(2)	89.01(10)
O(4)#2-Mn(1)-N(2)	88.73(10)
O(3)#1-Mn(1)-O(2)	144.90(11)
O(4)#2-Mn(1)-O(2)	89.86(10)
N(2)-Mn(1)-O(2)	98.28(11)
O(3)#1-Mn(1)-N(1)	87.75(11)
O(4)#2-Mn(1)-N(1)	89.35(11)
N(2)-Mn(1)-N(1)	174.39(12)
O(2)-Mn(1)-N(1)	86.98(12)
O(3)#1-Mn(1)-O(1)	90.22(11)
O(4)#2-Mn(1)-O(1)	144.54(11)
N(2)-Mn(1)-O(1)	85.96(11)
O(2)-Mn(1)-O(1)	56.45(10)

N(1)-Mn(1)-O(1)	98.63(12)
O(3)#1-Mn(1)-C(17)	117.63(12)
O(4)#2-Mn(1)-C(17)	117.61(12)
N(2)-Mn(1)-C(17)	93.16(11)
O(2)-Mn(1)-C(17)	28.22(11)
N(1)-Mn(1)-C(17)	92.39(12)
O(1)-Mn(1)-C(17)	28.25(11)
C(5B)-N(1)-C(1A)	100.6(7)
C(5B)-N(1)-C(5A)	37.8(6)
C(1A)-N(1)-C(5A)	116.7(6)
C(5B)-N(1)-C(1B)	116.0(8)
C(1A)-N(1)-C(1B)	42.0(5)
C(5A)-N(1)-C(1B)	103.9(7)
C(5B)-N(1)-Mn(1)	121.8(6)
C(1A)-N(1)-Mn(1)	122.5(5)
C(5A)-N(1)-Mn(1)	120.6(4)
C(1B)-N(1)-Mn(1)	122.1(5)
C(6)-N(2)-C(10)	116.4(3)
C(6)-N(2)-Mn(1)	119.8(2)
C(10)-N(2)-Mn(1)	123.6(2)
C(17)-O(1)-Mn(1)	91.0(2)
C(17)-O(2)-Mn(1)	91.7(2)
C(18)-O(3)-Mn(1)#1	177.0(3)
C(18)-O(4)-Mn(1)#3	114.6(2)
C(4B)-C(3)-C(2A)	101.3(7)
C(4B)-C(3)-C(2B)	117.5(7)
C(2A)-C(3)-C(2B)	40.9(5)
C(4B)-C(3)-C(4A)	37.5(5)
C(2A)-C(3)-C(4A)	117.2(5)
C(2B)-C(3)-C(4A)	105.9(6)
C(4B)-C(3)-C(8)#4	123.0(6)
C(2A)-C(3)-C(8)#4	123.2(5)
C(2B)-C(3)-C(8)#4	119.4(6)
C(4A)-C(3)-C(8)#4	119.6(5)
N(2)-C(6)-C(7)	123.3(3)
N(2)-C(6)-H(6)	118.3

C(7)-C(6)-H(6)	118.3
C(8)-C(7)-C(6)	119.8(4)
C(8)-C(7)-H(7)	120.1
C(6)-C(7)-H(7)	120.1
C(7)-C(8)-C(9)	116.8(3)
C(7)-C(8)-C(3)#5	121.3(4)
C(9)-C(8)-C(3)#5	121.8(4)
C(10)-C(9)-C(8)	120.1(3)
C(10)-C(9)-H(9)	119.9
C(8)-C(9)-H(9)	119.9
N(2)-C(10)-C(9)	123.6(4)
N(2)-C(10)-H(10)	118.2
C(9)-C(10)-H(10)	118.2
C(16)-C(11)-C(12B)	118.8(7)
C(16)-C(11)-C(12A)	119.4(5)
C(12B)-C(11)-C(12A)	29.4(5)
C(16)-C(11)-C(17)	120.9(4)
C(12B)-C(11)-C(17)	117.3(7)
C(12A)-C(11)-C(17)	118.5(5)
C(16)-C(15)-C(14B)	116.9(6)
C(16)-C(15)-C(14A)	118.7(4)
C(14B)-C(15)-C(14A)	30.8(4)
C(16)-C(15)-C(18)	120.3(3)
C(14B)-C(15)-C(18)	119.1(6)
C(14A)-C(15)-C(18)	119.8(5)
C(15)-C(16)-C(11)	119.8(4)
C(15)-C(16)-H(16)	120.1
C(11)-C(16)-H(16)	120.1
O(2)-C(17)-O(1)	120.7(4)
O(2)-C(17)-C(11)	120.5(4)
O(1)-C(17)-C(11)	118.8(3)
O(2)-C(17)-Mn(1)	60.1(2)
O(1)-C(17)-Mn(1)	60.7(2)
C(11)-C(17)-Mn(1)	178.4(3)
O(3)-C(18)-O(4)	123.7(3)
O(3)-C(18)-C(15)	118.8(3)

O(4)-C(18)-C(15)	117.5(3)
C(13A)-C(12A)-C(11)	120.4(7)
C(13A)-C(12A)-H(12A)	119.8
C(11)-C(12A)-H(12A)	119.8
C(13A)-C(14A)-C(15)	121.5(7)
C(13A)-C(14A)-H(14A)	119.2
C(15)-C(14A)-H(14A)	119.2
O(5A)-C(13A)-C(14A)	124.1(7)
O(5A)-C(13A)-C(12A)	117.1(6)
C(14A)-C(13A)-C(12A)	118.8(7)
C(13A)-O(5A)-H(5A)	109.5
OWA#6-OWA-OW2	132.3(9)
C(13B)-C(12B)-C(11)	119.7(12)
C(13B)-C(12B)-H(12B)	120.2
C(11)-C(12B)-H(12B)	120.2
C(13B)-C(14B)-C(15)	120.6(11)
C(13B)-C(14B)-H(14B)	119.7
C(15)-C(14B)-H(14B)	119.7
C(12B)-C(13B)-C(14B)	119.9(12)
C(12B)-C(13B)-O(5B)	120.0(11)
C(14B)-C(13B)-O(5B)	120.0(11)
C(13B)-O(5B)-H(5B)	109.5
C(5A)-C(4A)-C(3)	119.1(8)
C(5A)-C(4A)-H(4A)	120.4
C(3)-C(4A)-H(4A)	120.4
C(4A)-C(5A)-N(1)	122.3(8)
C(4A)-C(5A)-H(5A1)	118.9
N(1)-C(5A)-H(5A1)	118.9
C(3)-C(2A)-C(1A)	120.6(8)
C(3)-C(2A)-H(2A)	119.7
C(1A)-C(2A)-H(2A)	119.7
N(1)-C(1A)-C(2A)	124.1(8)
N(1)-C(1A)-H(1A)	118.0
C(2A)-C(1A)-H(1A)	118.0
C(3)-C(4B)-C(5B)	119.8(11)
C(3)-C(4B)-H(4B)	120.1

C(5B)-C(4B)-H(4B)	120.1
N(1)-C(5B)-C(4B)	127.0(12)
N(1)-C(5B)-H(5B1)	116.5
C(4B)-C(5B)-H(5B1)	116.5
C(3)-C(2B)-C(1B)	119.0(11)
C(3)-C(2B)-H(2B)	120.5
C(1B)-C(2B)-H(2B)	120.5
N(1)-C(1B)-C(2B)	120.6(11)
N(1)-C(1B)-H(1B)	119.7
C(2B)-C(1B)-H(1B)	119.7
OW2-OW1-OW1#6	131.7(13)
OW3-OW2-OW1	126(4)
OW3-OW2-OWA	139(3)
OW1-OW2-OWA	95(2)
OW2-OW3-OW5	136(7)
OW2-OW3-OW5#7	138(7)
OW5-OW3-OW5#7	86(2)
OW3-OW5-OW3#7	94(2)
OW3-OW5-OW4#7	87(2)
OW3#7-OW5-OW4#7	82(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2 #2 x+1,y,z #3 x-1,y,z #4 x,y+1,z
#5 x,y-1,z #6 -x,y,-z+5/2 #7 -x,-y+2,-z+2

Anisotropic displacement parameters ($Å^2 \times 10^3$) for **I**:

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(1)	24(1)	26(1)	39(1)	0(1)	6(1)	-1(1)
N(1)	48(2)	28(2)	53(2)	1(2)	9(2)	0(2)
N(2)	31(2)	29(2)	42(2)	-1(2)	4(2)	-2(1)
O(1)	29(2)	98(3)	43(2)	-6(2)	10(1)	2(2)
O(2)	23(2)	95(2)	53(2)	-14(2)	7(1)	-8(2)
O(3)	37(2)	53(2)	38(2)	-1(1)	1(1)	5(1)
O(4)	24(1)	49(2)	46(2)	-1(1)	8(1)	-2(1)

C(3)	36(2)	29(2)	38(2)	-3(2)	8(2)	2(2)
C(6)	43(3)	34(2)	46(3)	8(2)	-6(2)	2(2)
C(7)	45(3)	32(2)	46(3)	-3(2)	-5(2)	-5(2)
C(8)	40(2)	26(2)	43(2)	-1(2)	14(2)	2(2)
C(9)	43(3)	31(2)	47(3)	6(2)	-1(2)	4(2)
C(10)	39(2)	37(2)	36(2)	0(2)	1(2)	-2(2)
C(11)	25(2)	68(3)	42(2)	-3(2)	8(2)	-4(2)
C(15)	27(2)	64(3)	31(2)	-3(2)	6(2)	0(2)
C(16)	27(2)	45(2)	32(2)	-2(2)	6(2)	2(2)
C(17)	29(2)	42(2)	40(2)	3(2)	13(2)	1(2)
C(18)	25(2)	21(2)	38(2)	-1(2)	4(2)	-1(2)
C(12A)	27(3)	51(5)	45(3)	-1(5)	0(2)	-1(4)
C(14A)	29(3)	47(4)	43(3)	3(5)	12(2)	2(4)
C(13A)	33(3)	58(4)	28(3)	-1(4)	7(2)	-6(4)
O(5A)	36(2)	109(3)	37(2)	4(3)	7(2)	1(3)
OWA	52(8)	79(9)	240(20)	-35(10)	-12(15)	-13(8)
C(12B)	27(3)	51(5)	45(3)	-1(5)	0(2)	-1(4)
C(14B)	29(3)	47(4)	43(3)	3(5)	12(2)	2(4)
C(13B)	33(3)	58(4)	28(3)	-1(4)	7(2)	-6(4)
O(5B)	36(2)	109(3)	37(2)	4(3)	7(2)	1(3)
OWB	79(9)	67(8)	74(9)	0	25(7)	0
C(4A)	45(5)	37(3)	66(6)	-14(4)	6(3)	-6(4)
C(5A)	54(7)	33(3)	63(6)	1(4)	-3(4)	5(4)
C(2A)	30(5)	39(3)	90(7)	0(4)	-2(3)	-1(4)
C(1A)	44(6)	27(3)	86(8)	-3(4)	-9(4)	0(4)
C(4B)	45(5)	37(3)	66(6)	-14(4)	6(3)	-6(4)
C(5B)	54(7)	33(3)	63(6)	1(4)	-3(4)	5(4)
C(2B)	30(5)	39(3)	90(7)	0(4)	-2(3)	-1(4)
C(1B)	44(6)	27(3)	86(8)	-3(4)	-9(4)	0(4)
OW1	129(13)	300(20)	370(40)	160(20)	-40(20)	-38(16)
OW2	167(13)	58(7)	450(30)	-86(13)	5(17)	9(8)
OW3	750(80)	460(50)	420(50)	0(40)	500(60)	70(50)
OW4	340(40)	600(60)	380(40)	-70(40)	10(40)	-210(40)
OW5	460(40)	138(14)	580(60)	-10(20)	260(40)	92(19)

(The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$)

Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **I**:

	x	y	z	U(eq)
H(6)	2512	4413	7281	52
H(7)	2433	2443	7247	52
H(9)	5395	2407	9338	50
H(10)	5391	4362	9321	46
H(16)	-893	6545	8346	41
H(12A)	1632	6212	10640	51
H(14A)	-2351	6124	10414	47
H(5A)	-758	5961	11695	92
H(12B)	1627	7092	10564	51
H(14B)	-2330	7081	10385	47
H(5B)	731	7291	11703	92
H(4A)	5834	10668	8938	60
H(5A1)	5794	8698	8890	63
H(2A)	1950	10669	7698	67
H(1A)	1974	8718	7742	68
H(4B)	4831	10625	9482	60
H(5B1)	4773	8693	9412	63
H(2B)	2935	10737	7060	67
H(1B)	2953	8710	7053	68

Crystallographic data for Mn(HIP)(bipy) · ¼ bipy · 2 H_2O, **II**:

Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for **II**.

	x	y	z	U(eq)
Mn(1)	4648(1)	3474(1)	4233(1)	32(1)
N(1)	6606(4)	3521(5)	4208(3)	42(1)
C(1)	7413(5)	3102(7)	4792(4)	52(2)
C(2)	8584(5)	3065(7)	4801(4)	52(2)
C(3)	8989(5)	3493(5)	4181(3)	40(1)
C(4)	8170(6)	3979(9)	3579(4)	72(2)
C(5)	7000(6)	3953(9)	3608(4)	70(2)
N(2)	2684(4)	3551(4)	4219(3)	40(1)
C(10)	1888(6)	3550(8)	3569(4)	61(2)
C(9)	713(6)	3534(8)	3524(4)	65(2)
C(8)	271(5)	3522(5)	4183(3)	40(1)
C(7)	1099(6)	3476(6)	4874(4)	51(2)
C(6)	2265(5)	3506(6)	4861(4)	47(1)
O(1)	4561(4)	1296(4)	4289(2)	48(1)
O(2)	4300(4)	2167(4)	3153(2)	49(1)
O(3)	4904(4)	-3596(4)	4563(2)	48(1)
O(4)	4433(4)	-4826(3)	3529(2)	45(1)
O(5)	3566(6)	-1741(5)	1353(3)	90(2)
C(11)	4232(6)	-175(5)	3235(3)	42(1)
C(12)	3923(6)	-302(6)	2447(3)	51(2)
C(13)	3843(7)	-1547(6)	2122(3)	58(2)
C(14)	4046(6)	-2640(5)	2579(3)	49(2)
C(15)	4337(5)	-2525(5)	3370(3)	35(1)
C(16)	4421(5)	-1271(5)	3699(3)	36(1)
C(17)	4362(5)	1180(5)	3572(3)	37(1)
C(18)	4571(5)	-3737(5)	3862(3)	34(1)
N(3)	7332(12)	-450(15)	4117(7)	99(6)
C(21)	7570(12)	-268(14)	4886(8)	57(4)
C(22)	8654(11)	-72(11)	5264(6)	51(3)
C(23)	9427(8)	-15(11)	4838(7)	73(5)

C(24)	9289(11)	-108(14)	4076(7)	60(3)
C(25)	8124(10)	-359(13)	3710(7)	39(3)
OW1	7568(10)	-250(9)	5372(6)	65(3)
OW2	7877(11)	-870(30)	2698(10)	200(11)
OW3	6698(14)	358(19)	2626(11)	142(6)
OW4	7640(30)	-410(30)	3589(12)	227(14)

(U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor)

Bond lengths [Å] and angles [°] for **II**:

Mn(1)-O(3)#1	2.111(4)
Mn(1)-O(4)#2	2.124(4)
Mn(1)-O(1)	2.222(4)
Mn(1)-N(2)	2.292(5)
Mn(1)-N(1)	2.299(5)
Mn(1)-O(2)	2.311(4)
Mn(1)-C(17)	2.607(5)
N(1)-C(1)	1.321(7)
N(1)-C(5)	1.331(7)
C(1)-C(2)	1.367(8)
C(1)-H(1)	0.9300
C(2)-C(3)	1.368(8)
C(2)-H(2)	0.9300
C(3)-C(4)	1.372(8)
C(3)-C(8)#3	1.499(8)
C(4)-C(5)	1.381(9)
C(4)-H(4)	0.9300
C(5)-H(5)	0.9300
N(2)-C(10)	1.327(8)
N(2)-C(6)	1.344(7)
C(10)-C(9)	1.359(10)
C(10)-H(10)	0.9300
C(9)-C(8)	1.385(9)
C(9)-H(9)	0.9300

C(8)-C(7)	1.401(9)
C(8)-C(3)#4	1.499(8)
C(7)-C(6)	1.368(9)
C(7)-H(7)	0.9300
C(6)-H(6)	0.9300
O(1)-C(17)	1.260(6)
O(2)-C(17)	1.246(7)
O(3)-C(18)	1.241(7)
O(3)-Mn(1)#1	2.111(4)
O(4)-C(18)	1.252(6)
O(4)-Mn(1)#5	2.124(4)
O(5)-C(13)	1.360(7)
O(5)-H(5A)	0.8200
C(11)-C(16)	1.380(7)
C(11)-C(12)	1.386(8)
C(11)-C(17)	1.500(7)
C(12)-C(13)	1.390(8)
C(12)-H(12)	0.9300
C(13)-C(14)	1.371(8)
C(14)-C(15)	1.389(8)
C(14)-H(14)	0.9300
C(15)-C(16)	1.399(7)
C(15)-C(18)	1.506(7)
C(16)-H(16)	0.9300
N(3)-C(25)	1.299(14)
N(3)-C(21)	1.359(13)
C(21)-C(22)	1.318(15)
C(21)-H(21)	0.9300
C(22)-C(23)	1.303(14)
C(22)-H(22)	0.9300
C(23)-C(23)#6	1.342(17)
C(23)-C(24)	1.343(14)
C(24)-C(25)	1.403(14)
C(24)-H(24)	0.9300
C(25)-H(25)	0.9300
OW2-OW2#7	1.01(2)

OW2-OW3#7	1.50(2)
OW2-OW4	1.74(3)
OW3-OW2#7	1.50(2)

O(3)#1-Mn(1)-O(4)#2	122.03(15)
O(3)#1-Mn(1)-O(1)	90.98(14)
O(4)#2-Mn(1)-O(1)	146.96(15)
O(3)#1-Mn(1)-N(2)	92.21(17)
O(4)#2-Mn(1)-N(2)	88.53(16)
O(1)-Mn(1)-N(2)	88.83(16)
O(3)#1-Mn(1)-N(1)	89.31(17)
O(4)#2-Mn(1)-N(1)	87.91(17)
O(1)-Mn(1)-N(1)	94.40(17)
N(2)-Mn(1)-N(1)	176.41(17)
O(3)#1-Mn(1)-O(2)	148.19(14)
O(4)#2-Mn(1)-O(2)	89.69(14)
O(1)-Mn(1)-O(2)	57.42(14)
N(2)-Mn(1)-O(2)	90.80(16)
N(1)-Mn(1)-O(2)	89.62(17)
O(3)#1-Mn(1)-C(17)	119.78(16)
O(4)#2-Mn(1)-C(17)	118.19(16)
O(1)-Mn(1)-C(17)	28.86(15)
N(2)-Mn(1)-C(17)	89.72(17)
N(1)-Mn(1)-C(17)	92.35(17)
O(2)-Mn(1)-C(17)	28.55(15)
C(1)-N(1)-C(5)	115.7(5)
C(1)-N(1)-Mn(1)	121.6(4)
C(5)-N(1)-Mn(1)	122.7(4)
N(1)-C(1)-C(2)	124.3(6)
N(1)-C(1)-H(1)	117.9
C(2)-C(1)-H(1)	117.9
C(1)-C(2)-C(3)	120.0(5)
C(1)-C(2)-H(2)	120.0
C(3)-C(2)-H(2)	120.0
C(2)-C(3)-C(4)	116.7(5)
C(2)-C(3)-C(8)#3	121.6(5)

C(4)-C(3)-C(8)#3	121.5(5)
C(3)-C(4)-C(5)	119.6(6)
C(3)-C(4)-H(4)	120.2
C(5)-C(4)-H(4)	120.2
N(1)-C(5)-C(4)	123.6(6)
N(1)-C(5)-H(5)	118.2
C(4)-C(5)-H(5)	118.2
C(10)-N(2)-C(6)	115.9(5)
C(10)-N(2)-Mn(1)	121.5(4)
C(6)-N(2)-Mn(1)	122.5(4)
N(2)-C(10)-C(9)	124.2(6)
N(2)-C(10)-H(10)	117.9
C(9)-C(10)-H(10)	117.9
C(10)-C(9)-C(8)	120.4(6)
C(10)-C(9)-H(9)	119.8
C(8)-C(9)-H(9)	119.8
C(9)-C(8)-C(7)	116.1(5)
C(9)-C(8)-C(3)#4	123.6(5)
C(7)-C(8)-C(3)#4	120.2(5)
C(6)-C(7)-C(8)	119.2(6)
C(6)-C(7)-H(7)	120.4
C(8)-C(7)-H(7)	120.4
N(2)-C(6)-C(7)	124.2(6)
N(2)-C(6)-H(6)	117.9
C(7)-C(6)-H(6)	117.9
C(17)-O(1)-Mn(1)	92.8(3)
C(17)-O(2)-Mn(1)	89.0(3)
C(18)-O(3)-Mn(1)#1	174.9(4)
C(18)-O(4)-Mn(1)#5	116.8(4)
C(13)-O(5)-H(5A)	109.5
C(16)-C(11)-C(12)	120.7(5)
C(16)-C(11)-C(17)	120.8(5)
C(12)-C(11)-C(17)	118.5(5)
C(11)-C(12)-C(13)	119.5(5)
C(11)-C(12)-H(12)	120.3
C(13)-C(12)-H(12)	120.3

O(5)-C(13)-C(14)	117.5(5)
O(5)-C(13)-C(12)	122.5(5)
C(14)-C(13)-C(12)	120.1(5)
C(13)-C(14)-C(15)	120.9(5)
C(13)-C(14)-H(14)	119.5
C(15)-C(14)-H(14)	119.5
C(14)-C(15)-C(16)	119.0(5)
C(14)-C(15)-C(18)	120.1(5)
C(16)-C(15)-C(18)	120.9(5)
C(11)-C(16)-C(15)	119.8(5)
C(11)-C(16)-H(16)	120.1
C(15)-C(16)-H(16)	120.1
O(2)-C(17)-O(1)	120.8(5)
O(2)-C(17)-C(11)	120.7(5)
O(1)-C(17)-C(11)	118.5(5)
O(2)-C(17)-Mn(1)	62.4(3)
O(1)-C(17)-Mn(1)	58.4(3)
C(11)-C(17)-Mn(1)	176.7(4)
O(3)-C(18)-O(4)	124.3(5)
O(3)-C(18)-C(15)	118.4(5)
O(4)-C(18)-C(15)	117.2(5)
C(25)-N(3)-C(21)	122.9(12)
C(22)-C(21)-N(3)	120.5(12)
C(22)-C(21)-H(21)	119.7
N(3)-C(21)-H(21)	119.7
C(23)-C(22)-C(21)	114.6(10)
C(23)-C(22)-H(22)	122.7
C(21)-C(22)-H(22)	122.7
C(22)-C(23)-C(23)#6	120.1(15)
C(22)-C(23)-C(24)	130.1(10)
C(23)#6-C(23)-C(24)	109.4(14)
C(23)-C(24)-C(25)	112.4(11)
C(23)-C(24)-H(24)	123.8
C(25)-C(24)-H(24)	123.8
N(3)-C(25)-C(24)	119.2(11)
N(3)-C(25)-H(25)	120.4

C(24)-C(25)-H(25)	120.4
OW2#7-OW2-OW3#7	92.3(15)
OW2#7-OW2-OW4	111(2)
OW3#7-OW2-OW4	105(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1 #2 x,y+1,z #3 x+1,y,z #4 x-1,y,z
#5 x,y-1,z #6 -x+2,-y,-z+1 #7 -x+3/2,y,-z+1/2

Anisotropic displacement parameters ($Å^2 \times 10^3$) for **II**:

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(1)	36(1)	27(1)	32(1)	0(1)	7(1)	1(1)
N(1)	34(2)	52(3)	40(3)	0(2)	7(2)	-1(2)
C(1)	46(4)	64(4)	49(4)	22(3)	14(3)	8(3)
C(2)	39(3)	68(4)	46(4)	22(3)	5(3)	7(3)
C(3)	38(3)	44(3)	36(3)	-4(2)	6(2)	1(2)
C(4)	45(4)	134(7)	37(3)	25(4)	12(3)	8(4)
C(5)	42(4)	133(7)	34(3)	21(4)	4(3)	13(4)
N(2)	37(3)	42(3)	41(3)	-1(2)	10(2)	0(2)
C(10)	47(4)	104(6)	34(3)	4(3)	13(3)	6(4)
C(9)	47(4)	112(6)	34(3)	-6(4)	5(3)	5(4)
C(8)	34(3)	44(3)	41(3)	-2(2)	6(2)	1(2)
C(7)	49(4)	67(4)	38(3)	4(3)	13(3)	-6(3)
C(6)	40(3)	61(4)	40(3)	3(3)	6(3)	2(3)
O(1)	77(3)	31(2)	36(2)	-4(2)	13(2)	-1(2)
O(2)	81(3)	26(2)	40(2)	2(2)	12(2)	-2(2)
O(3)	63(3)	43(2)	34(2)	7(2)	5(2)	8(2)
O(4)	60(3)	27(2)	47(2)	2(2)	8(2)	-2(2)
O(5)	192(7)	44(3)	27(2)	-1(2)	10(3)	-6(3)
C(11)	60(4)	29(3)	36(3)	-1(2)	12(3)	-3(2)
C(12)	83(5)	34(3)	34(3)	3(2)	7(3)	-4(3)
C(13)	111(6)	36(3)	25(3)	2(2)	9(3)	-4(3)
C(14)	82(4)	29(3)	34(3)	-4(2)	6(3)	-4(3)
C(15)	42(3)	30(3)	32(3)	4(2)	7(2)	-3(2)

C(16)	49(3)	30(3)	29(3)	-3(2)	6(2)	-1(2)
C(17)	44(3)	30(3)	36(3)	-2(2)	6(2)	-2(2)
C(18)	31(3)	35(3)	38(3)	2(2)	9(2)	2(2)
N(3)	86(11)	80(10)	104(13)	36(9)	-38(10)	-27(8)
C(21)	71(10)	63(9)	43(8)	-12(7)	21(8)	-13(7)
C(22)	85(10)	45(7)	25(6)	-12(5)	19(7)	-6(6)
C(23)	113(14)	51(8)	47(9)	-9(7)	3(9)	-6(9)
C(24)	56(8)	74(9)	52(8)	-10(7)	19(6)	6(7)
C(25)	31(6)	52(6)	23(6)	-15(5)	-19(5)	16(6)
OW1	95(8)	59(6)	43(6)	-22(5)	21(6)	-30(5)
OW2	49(8)	400(30)	135(14)	183(17)	-16(7)	0(11)
OW3	112(12)	137(14)	169(16)	-13(12)	13(12)	32(10)
OW4	250(30)	340(30)	95(15)	-44(17)	47(17)	-200(20)

(The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$)

Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **II**:

	x	y	z	U(eq)
H(1)	7168	2814	5225	63
H(2)	9107	2749	5230	62
H(4)	8403	4324	3154	86
H(5)	6457	4253	3185	84
H(10)	2152	3561	3114	73
H(9)	202	3530	3048	78
H(7)	859	3425	5336	61
H(6)	2801	3495	5327	57
H(5A)	3451	-1029	1135	135
H(12)	3770	440	2139	61
H(14)	3987	-3470	2357	59
H(16)	4603	-1178	4227	43
H(21)	6964	-283	5148	69

H(22)	8851	19	5793	61
H(24)	9898	-16	3820	71
H(25)	7922	-459	3182	47

Crystallographic data for Ni(HIP)(bipy)(H_2O), **III**:

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **III**.

	x	y	z	U(eq)
Ni(1)	9764(1)	5838(1)	1033(1)	26(1)
C(3)	9835(5)	10210(5)	986(2)	40(1)
O(2)	3722(3)	4655(3)	3626(1)	37(1)
N(2)	9750(4)	3988(4)	1036(2)	36(1)
O(1)	11072(4)	6388(4)	1674(2)	43(1)
O(5)	8064(3)	5108(3)	1480(1)	35(1)
O(3)	4770(3)	3446(3)	3656(1)	33(1)
C(7)	10969(5)	2751(5)	987(4)	72(2)
N(1)	9858(4)	7733(3)	998(2)	34(1)
C(17)	4392(4)	4178(4)	3393(2)	30(1)
C(12)	4118(5)	4850(5)	2471(2)	35(1)
C(9)	8592(5)	1566(5)	1010(5)	83(2)
O(6)	3795(4)	5416(5)	1600(2)	56(1)
C(13)	4543(5)	5132(5)	1942(2)	39(1)
C(15)	6494(5)	4848(5)	2150(2)	32(1)
O(4)	8676(4)	5020(5)	2312(2)	57(1)
C(11)	4862(5)	4530(5)	2832(2)	33(1)
C(2)	11019(6)	10172(5)	980(5)	88(3)
C(5)	8686(5)	7766(5)	983(3)	62(2)
C(4)	8636(5)	8960(5)	984(4)	62(2)
C(10)	8607(5)	2789(5)	1024(4)	74(2)
C(14)	5720(5)	5103(5)	1788(2)	38(1)
C(18)	7851(5)	4973(5)	1969(2)	36(1)
C(8)	9783(5)	1502(5)	992(3)	44(1)
C(16)	6037(5)	4533(5)	2674(2)	35(1)
C(6)	10900(6)	3969(5)	1015(4)	73(2)
C(1)	10976(6)	8921(6)	989(4)	73(2)

(U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor)

Bond lengths [Å] and angles [°] for **III**:

Ni(1)-O(5)	2.000(3)
Ni(1)-O(1)	2.050(4)
Ni(1)-N(2)	2.068(3)
Ni(1)-O(3)#1	2.071(3)
Ni(1)-N(1)	2.077(3)
Ni(1)-O(2)#1	2.181(3)
Ni(1)-C(17)#1	2.451(5)
C(3)-C(2)	1.351(7)
C(3)-C(4)	1.375(7)
C(3)-C(8)#2	1.480(6)
O(2)-C(17)	1.262(5)
O(2)-Ni(1)#3	2.181(3)
N(2)-C(6)	1.302(7)
N(2)-C(10)	1.316(6)
O(1)-HW1	0.77(3)
O(1)-HW2	0.77(3)
O(5)-C(18)	1.240(6)
O(3)-C(17)	1.278(6)
O(3)-Ni(1)#3	2.071(3)
C(7)-C(8)	1.368(7)
C(7)-C(6)	1.409(7)
C(7)-H(7)	0.9300
N(1)-C(1)	1.296(7)
N(1)-C(5)	1.335(6)
C(17)-C(11)	1.483(7)
C(17)-Ni(1)#3	2.451(5)
C(12)-C(13)	1.390(7)
C(12)-C(11)	1.393(6)
C(12)-H(12)	0.9300
C(9)-C(10)	1.364(7)
C(9)-C(8)	1.375(7)
C(9)-H(9)	0.9300
O(6)-C(13)	1.345(6)

O(6)-H(21)	0.78(3)
C(13)-C(14)	1.392(7)
C(15)-C(14)	1.381(7)
C(15)-C(16)	1.388(7)
C(15)-C(18)	1.527(7)
O(4)-C(18)	1.245(6)
C(11)-C(16)	1.376(6)
C(2)-C(1)	1.380(7)
C(2)-H(2)	0.9300
C(5)-C(4)	1.368(7)
C(5)-H(5)	0.9300
C(4)-H(4)	0.9300
C(10)-H(10)	0.9300
C(14)-H(14)	0.9300
C(8)-C(3)#4	1.480(6)
C(16)-H(16)	0.9300
C(6)-H(6)	0.9300
C(1)-H(1)	0.9300

O(5)-Ni(1)-O(1)	94.48(15)
O(5)-Ni(1)-N(2)	93.41(16)
O(1)-Ni(1)-N(2)	86.78(17)
O(5)-Ni(1)-O(3)#1	93.52(13)
O(1)-Ni(1)-O(3)#1	170.69(15)
N(2)-Ni(1)-O(3)#1	88.00(16)
O(5)-Ni(1)-N(1)	89.63(14)
O(1)-Ni(1)-N(1)	93.62(17)
N(2)-Ni(1)-N(1)	176.89(18)
O(3)#1-Ni(1)-N(1)	91.18(16)
O(5)-Ni(1)-O(2)#1	155.67(13)
O(1)-Ni(1)-O(2)#1	109.75(14)
N(2)-Ni(1)-O(2)#1	86.11(17)
O(3)#1-Ni(1)-O(2)#1	62.15(12)
N(1)-Ni(1)-O(2)#1	90.86(15)
O(5)-Ni(1)-C(17)#1	124.80(14)
O(1)-Ni(1)-C(17)#1	139.99(15)

N(2)-Ni(1)-C(17)#1	83.90(18)
O(3)#1-Ni(1)-C(17)#1	31.43(13)
N(1)-Ni(1)-C(17)#1	93.85(16)
O(2)#1-Ni(1)-C(17)#1	30.93(13)
C(2)-C(3)-C(4)	116.3(4)
C(2)-C(3)-C(8)#2	123.5(4)
C(4)-C(3)-C(8)#2	120.1(4)
C(17)-O(2)-Ni(1)#3	86.4(3)
C(6)-N(2)-C(10)	116.7(4)
C(6)-N(2)-Ni(1)	120.4(3)
C(10)-N(2)-Ni(1)	122.7(3)
Ni(1)-O(1)-HW1	110(4)
Ni(1)-O(1)-HW2	131(4)
HW1-O(1)-HW2	119(6)
C(18)-O(5)-Ni(1)	133.4(3)
C(17)-O(3)-Ni(1)#3	90.9(3)
C(8)-C(7)-C(6)	119.8(5)
C(8)-C(7)-H(7)	120.1
C(6)-C(7)-H(7)	120.1
C(1)-N(1)-C(5)	115.6(4)
C(1)-N(1)-Ni(1)	125.5(3)
C(5)-N(1)-Ni(1)	118.9(3)
O(2)-C(17)-O(3)	119.7(4)
O(2)-C(17)-C(11)	122.1(4)
O(3)-C(17)-C(11)	118.0(4)
O(2)-C(17)-Ni(1)#3	62.7(2)
O(3)-C(17)-Ni(1)#3	57.6(2)
C(11)-C(17)-Ni(1)#3	167.2(3)
C(13)-C(12)-C(11)	119.7(4)
C(13)-C(12)-H(12)	120.2
C(11)-C(12)-H(12)	120.2
C(10)-C(9)-C(8)	122.0(5)
C(10)-C(9)-H(9)	119.0
C(8)-C(9)-H(9)	119.0
C(13)-O(6)-H(21)	112(4)
O(6)-C(13)-C(12)	118.5(5)

O(6)-C(13)-C(14)	122.8(5)
C(12)-C(13)-C(14)	118.7(4)
C(14)-C(15)-C(16)	118.8(4)
C(14)-C(15)-C(18)	119.2(4)
C(16)-C(15)-C(18)	122.0(4)
C(16)-C(11)-C(12)	120.7(5)
C(16)-C(11)-C(17)	119.1(4)
C(12)-C(11)-C(17)	120.3(4)
C(3)-C(2)-C(1)	119.8(5)
C(3)-C(2)-H(2)	120.1
C(1)-C(2)-H(2)	120.1
N(1)-C(5)-C(4)	123.4(5)
N(1)-C(5)-H(5)	118.3
C(4)-C(5)-H(5)	118.3
C(5)-C(4)-C(3)	120.1(4)
C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0
N(2)-C(10)-C(9)	123.0(5)
N(2)-C(10)-H(10)	118.5
C(9)-C(10)-H(10)	118.5
C(15)-C(14)-C(13)	121.7(4)
C(15)-C(14)-H(14)	119.2
C(13)-C(14)-H(14)	119.2
O(5)-C(18)-O(4)	125.6(5)
O(5)-C(18)-C(15)	115.3(4)
O(4)-C(18)-C(15)	119.0(4)
C(7)-C(8)-C(9)	114.8(4)
C(7)-C(8)-C(3)#4	120.6(4)
C(9)-C(8)-C(3)#4	124.6(4)
C(11)-C(16)-C(15)	120.3(4)
C(11)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
N(2)-C(6)-C(7)	123.6(5)
N(2)-C(6)-H(6)	118.2
C(7)-C(6)-H(6)	118.2
N(1)-C(1)-C(2)	124.7(5)

N(1)-C(1)-H(1)	117.6
C(2)-C(1)-H(1)	117.6

Symmetry transformations used to generate equivalent atoms:

#1 -x+y+1,-x+1,z-1/3 #2 x,y+1,z #3 -y+1,x-y,z+1/3
#4 x,y-1,z

Anisotropic displacement parameters ($Å^2 \times 10^3$) for **III**:

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	31(1)	25(1)	24(1)	-3(1)	-2(1)	16(1)
C(3)	42(3)	27(2)	52(3)	-7(2)	-4(2)	19(2)
O(2)	43(2)	44(2)	30(2)	5(1)	5(1)	27(2)
N(2)	32(2)	26(2)	49(2)	-8(2)	-8(2)	15(2)
O(1)	39(2)	40(2)	40(2)	-1(2)	-9(2)	12(2)
O(5)	41(2)	44(2)	24(2)	4(1)	5(1)	23(2)
O(3)	44(2)	37(2)	23(2)	2(1)	2(1)	24(2)
C(7)	37(3)	31(3)	158(7)	-7(4)	-14(4)	27(2)
N(1)	39(2)	32(2)	39(2)	2(2)	1(2)	23(2)
C(17)	34(2)	28(2)	24(2)	-1(2)	1(2)	14(2)
C(12)	34(2)	38(3)	33(3)	6(2)	3(2)	19(2)
C(9)	33(3)	25(2)	187(8)	-4(4)	-8(4)	12(2)
O(6)	52(2)	89(3)	37(2)	24(2)	5(2)	43(2)
C(13)	42(3)	45(3)	33(3)	6(2)	0(2)	23(2)
C(15)	34(2)	39(2)	25(2)	2(2)	2(2)	20(2)
O(4)	47(2)	101(3)	33(2)	11(2)	4(2)	44(2)
C(11)	33(2)	30(2)	34(3)	2(2)	-1(2)	13(2)
C(2)	29(3)	21(2)	207(10)	-2(4)	0(4)	7(2)
C(5)	37(3)	29(2)	119(6)	-7(3)	-7(3)	16(2)
C(4)	32(3)	35(3)	122(6)	-1(4)	-2(3)	20(2)
C(10)	36(3)	35(3)	156(7)	-3(4)	1(4)	21(2)
C(14)	40(3)	49(3)	26(3)	7(2)	4(2)	22(2)
C(18)	37(2)	41(3)	29(3)	2(2)	0(2)	20(2)
C(8)	36(2)	30(2)	71(4)	-3(3)	-5(3)	20(2)
C(16)	39(2)	44(2)	27(2)	6(2)	1(2)	25(2)

C(6)	38(3)	31(3)	155(7)	-11(4)	-15(4)	21(2)
C(1)	42(3)	41(3)	147(7)	-6(4)	-1(4)	28(2)

(The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$)

Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **III**:

	x	y	z	U(eq)
H(7)	11818	2796	965	86
H(12)	3341	4874	2584	42
H(9)	7750	751	1013	99
H(2)	11861	10986	971	106
H(5)	7860	6935	972	74
H(4)	7791	8925	984	74
H(10)	7771	2774	1025	89
H(14)	5992	5259	1432	46
H(16)	6528	4322	2919	42
H(6)	11721	4806	1018	88
H(1)	11810	8931	989	88
H(21)	4170(50)	5700(50)	1329(16)	37(16)
HW1	10650(50)	6110(50)	1934(18)	36(11)
HW2	11860(30)	6710(50)	1690(20)	36(11)

Hydrogen bond parameters for **III**:

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(6)-H(21)...O(4)#5	0.78(3)	1.92(4)	2.692(6)	178(6)
O(1)-HW1...O(4)	0.77(3)	2.14(4)	2.829(6)	148(6)
O(1)-HW2...O(3)#6	0.77(3)	2.16(5)	2.734(5)	131(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x+y+1,-x+1,z-1/3 #2 x,y+1,z #3 -y+1,x-y,z+1/3
#4 x,y-1,z #5 y,-x+y+1,z-1/6 #6 y+1,-x+y+1,z-1/6

Crystallographic data for $Cu(HIP)_2(bipy)$, **IV**:

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **IV**.

	x	y	z	U(eq)
Cu(1)	0	2555(1)	2500	26(1)
O(1)	4010(3)	419(3)	489(1)	49(1)
O(2)	3415(3)	171(3)	-565(1)	48(1)
O(3)	809(2)	2469(2)	1711(1)	29(1)
O(4)	-1328(3)	2426(2)	1293(1)	36(1)
O(5)	-1134(4)	1767(4)	-1107(2)	65(1)
N(1)	0	744(3)	2500	28(1)
N(2)	0	4364(3)	2500	26(1)
C(1)	-482(5)	4996(3)	1976(2)	44(1)
C(2)	-495(4)	6238(3)	1957(2)	43(1)
C(3)	0	6888(4)	2500	28(1)
C(4)	0	-1764(4)	2500	26(1)
C(5)	-1151(4)	-1116(3)	2275(2)	35(1)
C(6)	-1111(4)	122(3)	2289(2)	35(1)
C(7)	-303(4)	1669(4)	-535(2)	40(1)
C(8)	-630(4)	2064(4)	45(2)	37(1)
C(9)	268(4)	1927(3)	610(2)	29(1)
C(10)	1500(4)	1414(3)	593(2)	31(1)
C(11)	1830(4)	1019(3)	11(2)	30(1)
C(12)	931(4)	1137(4)	-549(2)	37(1)
C(13)	3179(4)	506(3)	3(2)	34(1)
C(14)	-129(4)	2315(3)	1239(2)	28(1)

(U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor)

Bond lengths [Å] and angles [°] for **IV**:

Cu(1)-O(3)	1.965(2)
Cu(1)-O(3)#1	1.965(2)

Cu(1)-N(2)	2.000(4)
Cu(1)-N(1)	2.001(4)
O(1)-C(13)	1.221(5)
O(2)-C(13)	1.309(4)
O(2)-H(2A)	0.82(5)
O(3)-C(14)	1.274(4)
O(4)-C(14)	1.242(4)
O(5)-C(7)	1.360(5)
O(5)-H(5)	0.79(6)
N(1)-C(6)	1.333(4)
N(1)-C(6)#1	1.333(4)
N(2)-C(1)#1	1.332(4)
N(2)-C(1)	1.332(4)
C(1)-C(2)	1.373(5)
C(1)-H(1)	0.9300
C(2)-C(3)	1.376(5)
C(2)-H(2)	0.9300
C(3)-C(2)#1	1.376(5)
C(3)-C(4)#2	1.489(6)
C(4)-C(5)#1	1.386(4)
C(4)-C(5)	1.386(4)
C(4)-C(3)#3	1.489(6)
C(5)-C(6)	1.368(5)
C(5)-H(5A)	0.9300
C(6)-H(6)	0.9300
C(7)-C(8)	1.384(6)
C(7)-C(12)	1.385(6)
C(8)-C(9)	1.388(5)
C(8)-H(8)	0.9300
C(9)-C(10)	1.375(5)
C(9)-C(14)	1.505(5)
C(10)-C(11)	1.391(5)
C(10)-H(10)	0.9300
C(11)-C(12)	1.377(5)
C(11)-C(13)	1.480(5)
C(12)-H(12)	0.9300

O(3)-Cu(1)-O(3)#1	174.50(13)
O(3)-Cu(1)-N(2)	92.75(7)
O(3)#1-Cu(1)-N(2)	92.75(7)
O(3)-Cu(1)-N(1)	87.25(7)
O(3)#1-Cu(1)-N(1)	87.25(7)
N(2)-Cu(1)-N(1)	180.000(1)
C(13)-O(2)-H(2A)	104(3)
C(14)-O(3)-Cu(1)	107.9(2)
C(7)-O(5)-H(5)	114(4)
C(6)-N(1)-C(6)#1	117.9(4)
C(6)-N(1)-Cu(1)	121.1(2)
C(6)#1-N(1)-Cu(1)	121.1(2)
C(1)#1-N(2)-C(1)	116.8(4)
C(1)#1-N(2)-Cu(1)	121.6(2)
C(1)-N(2)-Cu(1)	121.6(2)
N(2)-C(1)-C(2)	123.2(4)
N(2)-C(1)-H(1)	118.4
C(2)-C(1)-H(1)	118.4
C(1)-C(2)-C(3)	119.8(4)
C(1)-C(2)-H(2)	120.1
C(3)-C(2)-H(2)	120.1
C(2)-C(3)-C(2)#1	117.0(5)
C(2)-C(3)-C(4)#2	121.5(2)
C(2)#1-C(3)-C(4)#2	121.5(2)
C(5)#1-C(4)-C(5)	117.8(4)
C(5)#1-C(4)-C(3)#3	121.1(2)
C(5)-C(4)-C(3)#3	121.1(2)
C(6)-C(5)-C(4)	119.2(4)
C(6)-C(5)-H(5A)	120.4
C(4)-C(5)-H(5A)	120.4
N(1)-C(6)-C(5)	122.9(4)
N(1)-C(6)-H(6)	118.5
C(5)-C(6)-H(6)	118.5
O(5)-C(7)-C(8)	123.7(4)
O(5)-C(7)-C(12)	116.7(4)

C(8)-C(7)-C(12)	119.6(4)
C(7)-C(8)-C(9)	120.4(4)
C(7)-C(8)-H(8)	119.8
C(9)-C(8)-H(8)	119.8
C(10)-C(9)-C(8)	119.8(4)
C(10)-C(9)-C(14)	120.6(3)
C(8)-C(9)-C(14)	119.6(3)
C(9)-C(10)-C(11)	119.7(4)
C(9)-C(10)-H(10)	120.1
C(11)-C(10)-H(10)	120.1
C(12)-C(11)-C(10)	120.5(4)
C(12)-C(11)-C(13)	120.9(3)
C(10)-C(11)-C(13)	118.6(3)
C(11)-C(12)-C(7)	119.9(4)
C(11)-C(12)-H(12)	120.0
C(7)-C(12)-H(12)	120.0
O(1)-C(13)-O(2)	122.9(4)
O(1)-C(13)-C(11)	122.4(3)
O(2)-C(13)-C(11)	114.8(3)
O(4)-C(14)-O(3)	122.3(3)
O(4)-C(14)-C(9)	120.6(3)
O(3)-C(14)-C(9)	117.1(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2 #2 x,y+1,z #3 x,y-1,z

Anisotropic displacement parameters ($Å^2 \times 10^3$) for **IV**:

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	33(1)	20(1)	24(1)	0	6(1)	0
O(1)	41(2)	79(2)	28(2)	-2(2)	4(1)	20(2)
O(2)	39(2)	74(2)	32(2)	-12(2)	7(1)	15(2)
O(3)	33(1)	30(1)	24(1)	-3(1)	7(1)	0(1)
O(4)	30(2)	43(2)	36(2)	-2(1)	11(1)	6(1)
O(5)	41(2)	123(3)	30(2)	-5(2)	0(2)	25(2)

N(1)	34(3)	24(2)	27(2)	0	7(2)	0
N(2)	42(3)	20(2)	19(2)	0	9(2)	0
C(1)	69(3)	26(2)	32(2)	-4(2)	-8(2)	-1(2)
C(2)	67(3)	24(2)	33(2)	5(2)	-7(2)	1(2)
C(3)	34(3)	24(2)	27(3)	0	5(2)	0
C(4)	39(3)	22(2)	17(3)	0	5(2)	0
C(5)	39(2)	26(2)	39(2)	0(2)	1(2)	-4(2)
C(6)	34(2)	31(2)	38(2)	4(2)	1(2)	7(2)
C(7)	36(2)	51(2)	30(2)	-4(2)	-3(2)	3(2)
C(8)	29(2)	51(2)	32(2)	0(2)	7(2)	4(2)
C(9)	29(2)	26(2)	31(2)	-1(2)	6(2)	-1(2)
C(10)	34(2)	32(2)	26(2)	0(2)	2(2)	1(2)
C(11)	30(2)	36(2)	26(2)	-1(2)	9(2)	1(2)
C(12)	36(2)	53(2)	21(2)	-4(2)	8(2)	0(2)
C(13)	37(2)	39(2)	27(2)	-3(2)	7(2)	3(2)
C(14)	33(2)	24(2)	27(2)	3(1)	8(2)	0(2)

(The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$)

Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **IV**:

	x	y	z	U(eq)
H(2A)	4190(50)	-70(40)	-500(20)	50(15)
H(5)	-1830(60)	2060(50)	-1080(30)	77(19)
H(1)	-825	4575	1604	53
H(2)	-839	6639	1579	51
H(5A)	-1942	-1517	2115	42
H(6)	-1894	548	2146	42
H(8)	-1458	2423	56	45
H(10)	2111	1331	970	37
H(12)	1152	859	-936	44

Hydrogen bond parameters for **IV**:

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2A)...O(1)#4	0.82(5)	1.86(5)	2.667(4)	168(5)
O(5)-H(5)...O(4)#5	0.79(6)	1.93(6)	2.688(4)	161(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2 #2 x,y+1,z #3 x,y-1,z #4 -x+1,-y,-z
#5 -x-1/2,-y+1/2,-z

Crystallographic data for $Zn_2(HIP)_2(bipy)(H_2O)_2 \cdot H_2O$, **V**:

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **V**.

	x	y	z	U(eq)
Zn(1)	9576(1)	6808(1)	10323(1)	40(1)
N(1)	8025(4)	6177(3)	8348(3)	31(1)
O(3)	18461(4)	14829(3)	10836(2)	36(1)
O(4)	11971(4)	9759(3)	9942(3)	38(1)
O(5)	12216(4)	8238(3)	11280(3)	37(1)
O(2)	19261(4)	16059(3)	13051(3)	48(1)
O(1)	17713(4)	11471(3)	15245(3)	44(1)
O(6)	7951(5)	7936(4)	11165(3)	48(1)
O(7)	9193(18)	9411(12)	13952(9)	105(4)
C(8)	12847(5)	9530(4)	10950(3)	27(1)
C(6)	15692(5)	12173(4)	11508(3)	26(1)
C(2)	7091(6)	6734(4)	6230(4)	35(1)
C(10)	17062(5)	11756(4)	14027(3)	31(1)
C(9)	15426(5)	10570(4)	13122(3)	30(1)
C(7)	14716(5)	10783(4)	11869(3)	27(1)
C(3)	5649(5)	5246(4)	5702(3)	29(1)
C(13)	18427(5)	14871(4)	12106(3)	29(1)
C(12)	17328(5)	13359(4)	12434(3)	27(1)
C(11)	17994(5)	13141(4)	13698(3)	31(1)
C(1)	8245(6)	7156(4)	7554(4)	35(1)
C(4)	5442(7)	4233(5)	6542(4)	48(1)
C(5)	6624(7)	4735(5)	7843(4)	50(1)

(U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor)

Bond lengths [Å] and angles [°] for **V**:

Zn(1)-O(5)	1.920(2)
Zn(1)-O(3)#1	1.962(2)

Zn(1)-N(1)	2.034(3)
Zn(1)-O(6)	2.072(3)
N(1)-C(1)	1.322(5)
N(1)-C(5)	1.335(5)
O(3)-C(13)	1.280(4)
O(3)-Zn(1)#2	1.962(2)
O(4)-C(8)	1.241(4)
O(5)-C(8)	1.274(4)
O(2)-C(13)	1.230(4)
O(1)-C(10)	1.380(4)
O(1)-H(3)	0.82(5)
O(6)-HWA	0.78(2)
O(6)-HWB	0.78(2)
O(7)-HWC	0.80(2)
O(7)-HWD	0.80(2)
C(8)-C(7)	1.500(4)
C(6)-C(12)	1.390(5)
C(6)-C(7)	1.398(5)
C(6)-H(6)	0.92(3)
C(2)-C(3)	1.376(5)
C(2)-C(1)	1.395(5)
C(2)-H(2)	0.93(3)
C(10)-C(11)	1.373(5)
C(10)-C(9)	1.381(5)
C(9)-C(7)	1.392(5)
C(9)-H(9)	0.93(3)
C(3)-C(4)	1.384(5)
C(3)-C(3)#3	1.496(7)
C(13)-C(12)	1.495(5)
C(12)-C(11)	1.394(5)
C(11)-H(11)	0.92(3)
C(1)-H(1)	0.93(4)
C(4)-C(5)	1.376(6)
C(4)-H(4)	0.93(4)
C(5)-H(5)	0.93(4)

O(5)-Zn(1)-O(3)#1	117.03(11)
O(5)-Zn(1)-N(1)	134.68(11)
O(3)#1-Zn(1)-N(1)	100.40(11)
O(5)-Zn(1)-O(6)	100.57(12)
O(3)#1-Zn(1)-O(6)	101.15(12)
N(1)-Zn(1)-O(6)	95.96(12)
C(1)-N(1)-C(5)	117.6(3)
C(1)-N(1)-Zn(1)	123.2(2)
C(5)-N(1)-Zn(1)	119.1(2)
C(13)-O(3)-Zn(1)#2	118.1(2)
C(8)-O(5)-Zn(1)	114.8(2)
C(10)-O(1)-H(3)	113(4)
Zn(1)-O(6)-HWA	111(5)
Zn(1)-O(6)-HWB	107(5)
HWA-O(6)-HWB	111(6)
HWC-O(7)-HWD	109(4)
O(4)-C(8)-O(5)	122.7(3)
O(4)-C(8)-C(7)	121.4(3)
O(5)-C(8)-C(7)	115.9(3)
C(12)-C(6)-C(7)	119.4(3)
C(12)-C(6)-H(6)	118(3)
C(7)-C(6)-H(6)	123(3)
C(3)-C(2)-C(1)	120.0(3)
C(3)-C(2)-H(2)	126(3)
C(1)-C(2)-H(2)	114(3)
C(11)-C(10)-O(1)	122.4(3)
C(11)-C(10)-C(9)	120.5(3)
O(1)-C(10)-C(9)	117.1(3)
C(10)-C(9)-C(7)	119.7(3)
C(10)-C(9)-H(9)	121(2)
C(7)-C(9)-H(9)	119(2)
C(9)-C(7)-C(6)	120.2(3)
C(9)-C(7)-C(8)	118.9(3)
C(6)-C(7)-C(8)	120.9(3)
C(2)-C(3)-C(4)	116.6(3)
C(2)-C(3)-C(3)#3	121.7(4)

C(4)-C(3)-C(3)#3	121.6(4)
O(2)-C(13)-O(3)	124.2(3)
O(2)-C(13)-C(12)	119.2(3)
O(3)-C(13)-C(12)	116.6(3)
C(6)-C(12)-C(11)	119.8(3)
C(6)-C(12)-C(13)	121.8(3)
C(11)-C(12)-C(13)	118.5(3)
C(10)-C(11)-C(12)	120.4(3)
C(10)-C(11)-H(11)	113(2)
C(12)-C(11)-H(11)	127(2)
N(1)-C(1)-C(2)	122.7(3)
N(1)-C(1)-H(1)	118(3)
C(2)-C(1)-H(1)	119(3)
C(5)-C(4)-C(3)	120.2(4)
C(5)-C(4)-H(4)	117(3)
C(3)-C(4)-H(4)	123(3)
N(1)-C(5)-C(4)	122.9(4)
N(1)-C(5)-H(5)	119(3)
C(4)-C(5)-H(5)	118(3)

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y-1,z #2 x+1,y+1,z #3 -x+1,-y+1,-z+1

Anisotropic displacement parameters ($Å^2 \times 10^3$) for **V**:

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	38(1)	27(1)	33(1)	13(1)	-12(1)	-5(1)
N(1)	29(2)	30(2)	25(1)	7(1)	-4(1)	7(1)
O(3)	43(2)	28(1)	28(1)	14(1)	2(1)	4(1)
O(4)	35(1)	30(1)	36(1)	9(1)	-6(1)	4(1)
O(5)	34(1)	23(1)	38(1)	10(1)	-4(1)	-2(1)
O(2)	55(2)	28(1)	35(1)	4(1)	2(1)	-6(1)
O(1)	51(2)	32(2)	29(1)	12(1)	-9(1)	0(1)
O(6)	53(2)	45(2)	41(2)	18(1)	3(1)	15(2)
O(7)	144(9)	119(8)	57(5)	-19(5)	-25(6)	93(8)

C(8)	25(2)	24(2)	24(2)	3(1)	1(1)	2(1)
C(6)	26(2)	23(2)	23(2)	7(1)	2(1)	5(1)
C(2)	36(2)	34(2)	29(2)	16(2)	-1(2)	7(2)
C(10)	34(2)	28(2)	25(2)	9(1)	1(1)	6(2)
C(9)	33(2)	26(2)	27(2)	12(1)	3(1)	5(2)
C(7)	26(2)	23(2)	26(2)	4(1)	3(1)	6(1)
C(3)	26(2)	31(2)	26(2)	6(1)	0(1)	10(1)
C(13)	25(2)	23(2)	30(2)	6(1)	-1(1)	2(1)
C(12)	26(2)	24(2)	25(2)	8(1)	5(1)	4(1)
C(11)	31(2)	28(2)	23(2)	5(1)	-1(1)	4(2)
C(1)	35(2)	31(2)	31(2)	10(2)	0(2)	6(2)
C(4)	51(3)	28(2)	41(2)	10(2)	-16(2)	-3(2)
C(5)	52(3)	34(2)	44(2)	17(2)	-16(2)	0(2)

(The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$)

Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **V**:

	x	y	z	U(eq)
HWC	10360(50)	9670(110)	13990(130)	80(30)
HWD	9030(130)	10050(90)	14490(90)	80(30)
HWA	8370(80)	8280(60)	11960(20)	82(14)
H(1)	9200(60)	8160(40)	7910(50)	55(7)
H(6)	15280(60)	12350(40)	10690(30)	33(6)
H(11)	19040(50)	13850(40)	14390(30)	33(6)
H(2)	7390(70)	7530(50)	5780(40)	55(7)
H(9)	14770(50)	9640(30)	13350(40)	33(6)
H(4)	4580(60)	3190(40)	6260(50)	55(7)
HWB	8040(90)	8600(50)	10790(60)	82(14)
H(3)	18500(80)	12260(60)	15810(50)	62(16)
H(5)	6550(70)	4000(50)	8340(40)	55(7)

Hydrogen bond parameters for **V**:

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(6)-HWA...O(7)	0.78(2)	2.00(2)	2.772(9)	170(6)
O(6)-HWB...O(4)#4	0.78(2)	1.87(2)	2.645(4)	172(6)
O(1)-H(3)...O(2)#5	0.82(5)	1.87(5)	2.675(4)	167(5)
O(7)-HWD...O(1)#6	0.80(2)	2.06(4)	2.817(9)	158(10)

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y-1,z #2 x+1,y+1,z #3 -x+1,-y+1,-z+1
#4 -x+2,-y+2,-z+2 #5 -x+4,-y+3,-z+3 #6 x-1,y,z