Electronic Supplementary Material for CrystEngComm

Electronic Supplementary Information for

Structural and Chemical Complexity in Multicomponent Inorganic-Organic Framework Materials

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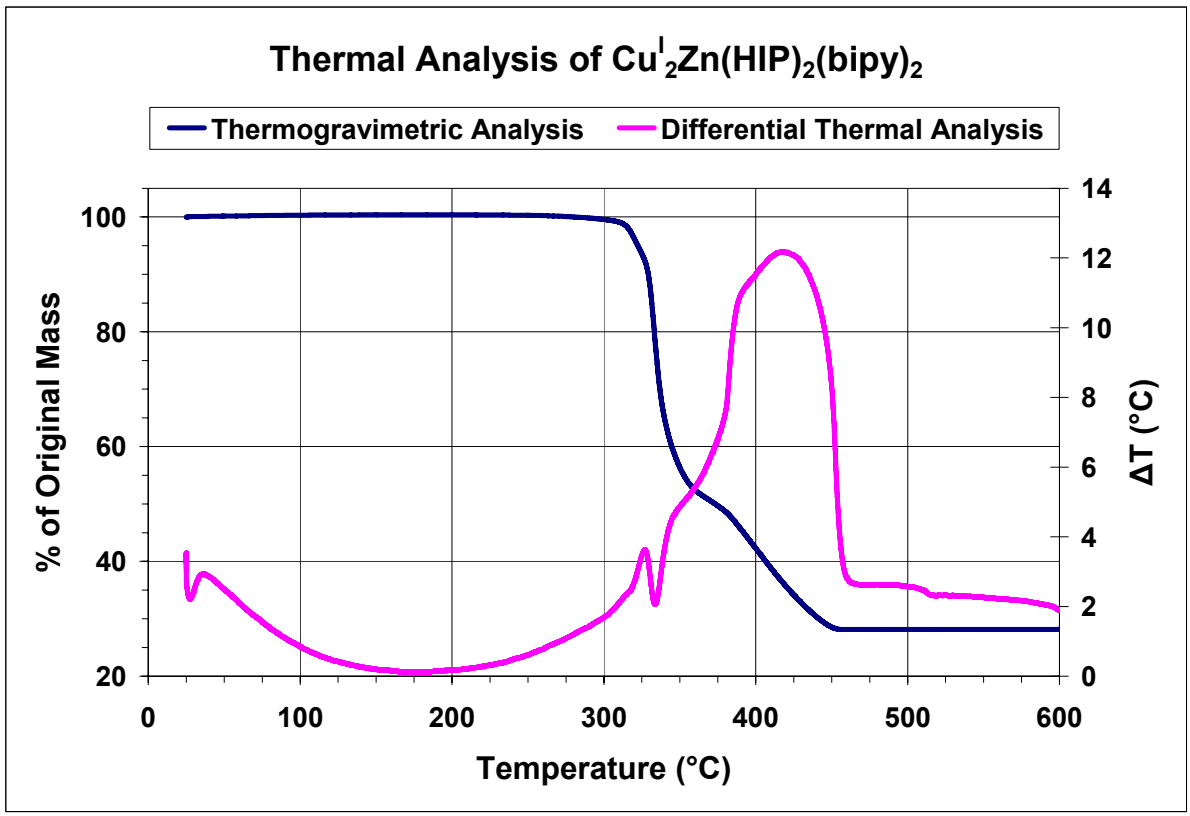
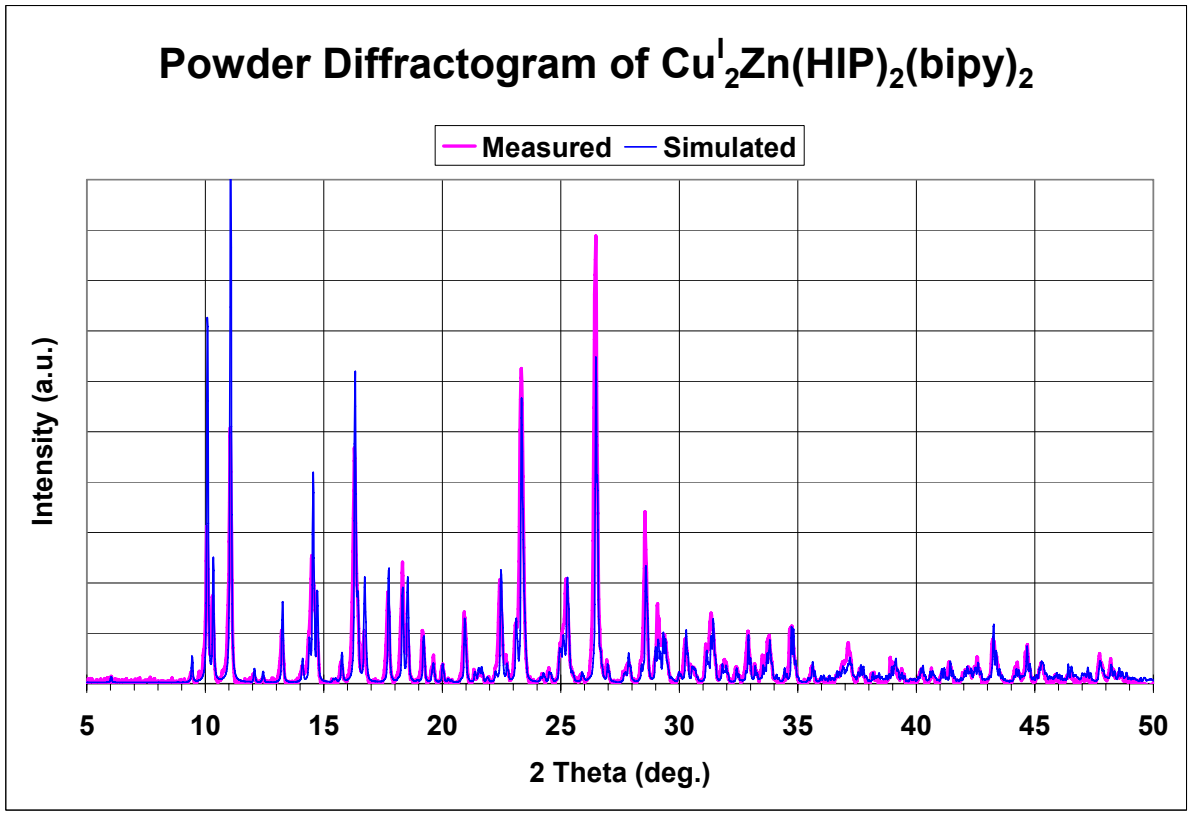
including powder diffractogram for compound **III**, thermal analysis data for compound **III**, and crystallographic data tables.


Thermal Analysis of Cu$^{I}_{2}$Zn(HIP)$_2$(bipy)$_2$
Thermogravimetric Analysis
Differential Thermal Analysis
% of Original Mass
ΔT (°C)
Temperature (°C)
100
80
60
40
20
14
12
10
8
6
4
2
0
0
100
200
300
400
500
600


Powder Diffractogram of Cu$^{I}_{2}$Zn(HIP)$_2$(bipy)$_2$
Measured
Simulated
Intensity (a.u.)
2 Theta (deg.)
5
10
15
20
25
30
35
40
45
50

Crystallographic Data for $Cu^{II}Zn(HIP)_2(bipy)(H_2O) \cdot 1.5\ H_2O$:

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Cu^{II}Zn(HIP)_2(bipy)(H_2O) \cdot 1.5\ H_2O$:

	x	y	z	U_{eq}
Cu(1)	4950(1)	2304(1)	1755(1)	32(1)
Zn(1)	2617(1)	11153(1)	561(1)	34(1)
O(1)	7001(4)	2541(3)	1879(2)	33(1)
O(2)	6046(4)	907(3)	1946(2)	38(1)
O(3)	12434(4)	2592(4)	2518(2)	48(1)
O(4)	13175(4)	1609(3)	1772(2)	35(1)
O(5)	10040(4)	-1818(3)	2086(2)	35(1)
O(6)	-298(4)	10725(3)	581(2)	39(1)
O(7)	1138(4)	12163(3)	678(2)	36(1)
O(8)	-5484(4)	11756(3)	676(2)	30(1)
O(9)	-6073(4)	13139(4)	47(2)	43(1)
O(10)	-1710(4)	15559(3)	274(2)	43(1)
O(11)	2311(5)	10828(4)	-323(2)	43(1)
O(12)	6757(7)	2412(5)	3884(3)	72(2)
N(1)	4437(5)	3859(4)	1542(2)	26(1)
N(2)	2944(5)	9558(4)	816(2)	30(1)
C(1)	9961(6)	-671(5)	2070(3)	23(2)
C(2)	8670(6)	-190(5)	2022(3)	30(2)
C(3)	8544(6)	963(5)	2015(3)	25(2)
C(4)	9706(6)	1633(5)	2063(3)	27(2)
C(5)	11008(6)	1138(5)	2099(3)	22(2)
C(6)	11111(6)	-19(5)	2089(3)	30(2)
C(7)	7134(7)	1506(6)	1944(3)	30(2)
C(8)	12299(6)	1847(5)	2136(3)	27(2)
C(11)	5415(7)	4651(5)	1572(3)	30(2)
C(12)	3163(7)	4208(5)	1364(3)	33(2)
C(13)	5159(6)	5752(5)	1442(3)	32(2)
C(14)	2820(7)	5302(5)	1223(3)	36(2)
C(15)	3837(6)	6115(5)	1259(3)	26(2)
C(16)	3519(6)	7314(5)	1114(3)	28(2)

C(17)	4568(7)	8095(5)	1086(3)	43(2)
C(18)	2185(6)	7690(5)	989(3)	29(2)
C(19)	4257(7)	9183(5)	941(3)	46(2)
C(20)	1933(6)	8794(5)	842(3)	29(2)
C(21)	-2044(6)	14454(5)	346(3)	27(2)
C(22)	-971(6)	13689(5)	456(3)	29(2)
C(23)	-1260(6)	12582(5)	543(3)	24(2)
C(24)	-2637(6)	12220(5)	517(3)	27(2)
C(25)	-3707(6)	12951(5)	397(3)	23(2)
C(26)	-3394(6)	14077(5)	305(3)	29(2)
C(27)	-85(7)	11758(5)	608(3)	26(2)
C(28)	-5201(6)	12605(6)	362(3)	28(2)
O(13)	-476(17)	5117(13)	1838(7)	161(8)

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

Bond lengths [Å] and angles [°] for $Cu^{II}Zn(HIP)_2(bipy)(H_2O) \cdot 1.5\ H_2O$:

Cu(1)-O(4)#1	1.911(4)	O(7)-C(27)	1.274(6)
Cu(1)-N(1)	1.968(5)	O(8)-C(28)	1.284(7)
Cu(1)-O(1)	1.999(4)	O(8)-Zn(1)#1	1.968(4)
Cu(1)-O(2)	2.001(4)	O(9)-C(28)	1.231(7)
Cu(1)-C(7)	2.321(6)	O(10)-C(21)	1.371(6)
Zn(1)-O(7)	1.909(4)	O(10)-H(10)	0.8200
Zn(1)-O(8)#2	1.968(4)	O(11)-H(11B)	0.817(18)
Zn(1)-N(2)	2.004(5)	O(11)-H(11A)	0.826(18)
Zn(1)-O(11)	2.040(5)	O(12)-H(12A)	0.82(2)
O(1)-C(7)	1.248(7)	O(12)-H(12B)	0.82(2)
O(2)-C(7)	1.273(7)	N(1)-C(12)	1.327(7)
O(3)-C(8)	1.242(7)	N(1)-C(11)	1.335(7)
O(4)-C(8)	1.272(7)	N(2)-C(20)	1.343(7)
O(4)-Cu(1)#2	1.911(4)	N(2)-C(19)	1.351(7)
O(5)-C(1)	1.369(6)	C(1)-C(6)	1.355(8)
O(5)-H(5)	0.8200	C(1)-C(2)	1.370(8)
O(6)-C(27)	1.250(6)	C(2)-C(3)	1.380(8)

C(2)-H(2)	0.9300	---	
C(3)-C(4)	1.375(7)	O(4)#1-Cu(1)-N(1)	102.01(18)
C(3)-C(7)	1.505(8)	O(4)#1-Cu(1)-O(1)	160.22(17)
C(4)-C(5)	1.386(7)	N(1)-Cu(1)-O(1)	97.19(18)
C(4)-H(4)	0.9300	O(4)#1-Cu(1)-O(2)	95.36(17)
C(5)-C(6)	1.384(8)	N(1)-Cu(1)-O(2)	162.57(19)
C(5)-C(8)	1.504(8)	O(1)-Cu(1)-O(2)	65.65(16)
C(6)-H(6)	0.9300	O(4)#1-Cu(1)-C(7)	128.5(2)
C(11)-C(13)	1.363(8)	N(1)-Cu(1)-C(7)	129.5(2)
C(11)-H(11)	0.9300	O(1)-Cu(1)-C(7)	32.51(18)
C(12)-C(14)	1.376(8)	O(2)-Cu(1)-C(7)	33.22(18)
C(12)-H(12)	0.9300	O(7)-Zn(1)-O(8)#2	117.02(17)
C(13)-C(15)	1.377(8)	O(7)-Zn(1)-N(2)	131.16(19)
C(13)-H(13)	0.9300	O(8)#2-Zn(1)-N(2)	100.88(19)
C(14)-C(15)	1.379(8)	O(7)-Zn(1)-O(11)	102.53(19)
C(14)-H(14)	0.9300	O(8)#2-Zn(1)-O(11)	104.21(18)
C(15)-C(16)	1.493(8)	N(2)-Zn(1)-O(11)	96.25(19)
C(16)-C(18)	1.371(8)	C(7)-O(1)-Cu(1)	88.1(4)
C(16)-C(17)	1.383(8)	C(7)-O(2)-Cu(1)	87.3(4)
C(17)-C(19)	1.365(8)	C(8)-O(4)-Cu(1)#2	125.0(4)
C(17)-H(17)	0.9300	C(1)-O(5)-H(5)	109.5
C(18)-C(20)	1.374(8)	C(27)-O(7)-Zn(1)	116.3(4)
C(18)-H(18)	0.9300	C(28)-O(8)-Zn(1)#1	117.5(4)
C(19)-H(19)	0.9300	C(21)-O(10)-H(10)	109.5
C(20)-H(20)	0.9300	Zn(1)-O(11)-H(11B)	115(2)
C(21)-C(26)	1.376(7)	Zn(1)-O(11)-H(11A)	114(2)
C(21)-C(22)	1.387(8)	H(11B)-O(11)-H(11A)	109(3)
C(22)-C(23)	1.368(7)	H(12A)-O(12)-H(12B)	109(4)
C(22)-H(22)	0.9300	C(12)-N(1)-C(11)	115.3(5)
C(23)-C(24)	1.397(7)	C(12)-N(1)-Cu(1)	125.1(4)
C(23)-C(27)	1.499(8)	C(11)-N(1)-Cu(1)	119.6(4)
C(24)-C(25)	1.361(7)	C(20)-N(2)-C(19)	116.1(5)
C(24)-H(24)	0.9300	C(20)-N(2)-Zn(1)	124.1(4)
C(25)-C(26)	1.397(8)	C(19)-N(2)-Zn(1)	119.6(4)
C(25)-C(28)	1.498(8)	C(6)-C(1)-O(5)	121.9(5)
C(26)-H(26)	0.9300	C(6)-C(1)-C(2)	120.1(6)

O(5)-C(1)-C(2)	117.9(5)	C(15)-C(14)-H(14)	120.1
C(1)-C(2)-C(3)	119.8(6)	C(13)-C(15)-C(14)	115.7(6)
C(1)-C(2)-H(2)	120.1	C(13)-C(15)-C(16)	122.3(5)
C(3)-C(2)-H(2)	120.1	C(14)-C(15)-C(16)	122.0(5)
C(4)-C(3)-C(2)	120.5(6)	C(18)-C(16)-C(17)	116.8(6)
C(4)-C(3)-C(7)	119.0(6)	C(18)-C(16)-C(15)	121.9(6)
C(2)-C(3)-C(7)	120.5(6)	C(17)-C(16)-C(15)	121.2(5)
C(3)-C(4)-C(5)	119.3(6)	C(19)-C(17)-C(16)	120.4(6)
C(3)-C(4)-H(4)	120.3	C(19)-C(17)-H(17)	119.8
C(5)-C(4)-H(4)	120.3	C(16)-C(17)-H(17)	119.8
C(6)-C(5)-C(4)	119.3(5)	C(16)-C(18)-C(20)	120.4(6)
C(6)-C(5)-C(8)	120.0(5)	C(16)-C(18)-H(18)	119.8
C(4)-C(5)-C(8)	120.7(6)	C(20)-C(18)-H(18)	119.8
C(1)-C(6)-C(5)	120.8(6)	N(2)-C(19)-C(17)	123.1(6)
C(1)-C(6)-H(6)	119.6	N(2)-C(19)-H(19)	118.4
C(5)-C(6)-H(6)	119.6	C(17)-C(19)-H(19)	118.4
O(1)-C(7)-O(2)	118.7(6)	N(2)-C(20)-C(18)	123.2(6)
O(1)-C(7)-C(3)	121.3(6)	N(2)-C(20)-H(20)	118.4
O(2)-C(7)-C(3)	120.0(6)	C(18)-C(20)-H(20)	118.4
O(1)-C(7)-Cu(1)	59.4(3)	O(10)-C(21)-C(26)	122.6(5)
O(2)-C(7)-Cu(1)	59.4(3)	O(10)-C(21)-C(22)	118.2(5)
C(3)-C(7)-Cu(1)	175.5(5)	C(26)-C(21)-C(22)	119.1(6)
O(3)-C(8)-O(4)	125.7(6)	C(23)-C(22)-C(21)	120.1(5)
O(3)-C(8)-C(5)	118.2(6)	C(23)-C(22)-H(22)	120.0
O(4)-C(8)-C(5)	116.1(6)	C(21)-C(22)-H(22)	120.0
N(1)-C(11)-C(13)	123.9(6)	C(22)-C(23)-C(24)	120.0(5)
N(1)-C(11)-H(11)	118.1	C(22)-C(23)-C(27)	118.9(5)
C(13)-C(11)-H(11)	118.1	C(24)-C(23)-C(27)	120.9(5)
N(1)-C(12)-C(14)	124.3(6)	C(25)-C(24)-C(23)	121.0(6)
N(1)-C(12)-H(12)	117.8	C(25)-C(24)-H(24)	119.5
C(14)-C(12)-H(12)	117.8	C(23)-C(24)-H(24)	119.5
C(11)-C(13)-C(15)	120.8(6)	C(24)-C(25)-C(26)	118.3(5)
C(11)-C(13)-H(13)	119.6	C(24)-C(25)-C(28)	123.1(6)
C(15)-C(13)-H(13)	119.6	C(26)-C(25)-C(28)	118.6(5)
C(12)-C(14)-C(15)	119.9(6)	C(21)-C(26)-C(25)	121.5(6)
C(12)-C(14)-H(14)	120.1	C(21)-C(26)-H(26)	119.3

C(25)-C(26)-H(26)	119.3	O(9)-C(28)-O(8)	124.1(6)
O(6)-C(27)-O(7)	121.8(6)	O(9)-C(28)-C(25)	119.6(6)
O(6)-C(27)-C(23)	121.4(6)	O(8)-C(28)-C(25)	116.3(6)
O(7)-C(27)-C(23)	116.8(5)		

Symmetry transformations used to generate equivalent atoms:

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

Anisotropic displacement parameters ($Å^2 \times 10^3$) for $Cu^{II}Zn(HIP)_2(bipy)(H_2O) \cdot 1.5\ H_2O$:

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	19(1)	24(1)	54(1)	8(1)	3(1)	1(1)
Zn(1)	20(1)	22(1)	60(1)	4(1)	1(1)	2(1)
O(1)	28(3)	27(3)	45(3)	2(2)	4(2)	8(2)
O(2)	19(2)	25(3)	69(4)	4(2)	-2(2)	-1(2)
O(3)	35(3)	49(3)	63(4)	-27(3)	13(3)	-17(2)
O(4)	21(3)	31(3)	52(3)	2(2)	5(2)	-3(2)
O(5)	24(3)	24(3)	56(3)	5(2)	-2(3)	5(2)
O(6)	31(3)	22(3)	64(4)	-5(2)	-3(2)	5(2)
O(7)	21(3)	30(3)	57(3)	-2(2)	0(2)	-5(2)
O(8)	23(2)	30(3)	38(3)	10(2)	2(2)	-7(2)
O(9)	22(3)	48(3)	57(4)	17(3)	-7(2)	4(2)
O(10)	36(3)	22(3)	68(4)	19(2)	-1(3)	1(2)
O(11)	39(3)	28(3)	60(4)	10(3)	-3(3)	-7(2)
O(12)	88(5)	49(4)	71(5)	7(3)	-29(4)	1(3)
N(1)	20(3)	25(3)	33(3)	3(3)	0(3)	-2(3)
N(2)	21(3)	35(3)	34(4)	-6(3)	3(3)	6(3)
C(1)	21(4)	15(3)	33(4)	4(3)	6(3)	-3(3)
C(2)	23(4)	25(4)	43(5)	4(3)	2(3)	-4(3)
C(3)	15(3)	30(4)	31(4)	1(3)	4(3)	-1(3)
C(4)	17(3)	30(4)	33(4)	3(3)	2(3)	5(3)
C(5)	14(3)	24(4)	27(4)	2(3)	1(3)	-1(3)
C(6)	20(4)	34(4)	35(5)	-1(3)	-2(3)	6(3)

C(7)	24(4)	31(4)	35(5)	-5(4)	1(3)	3(3)
C(8)	21(4)	25(4)	34(5)	4(3)	1(3)	3(3)
C(11)	26(4)	26(4)	38(5)	7(3)	4(3)	4(3)
C(12)	32(4)	16(4)	50(5)	0(3)	-1(4)	-2(3)
C(13)	20(4)	20(4)	53(5)	-4(3)	-3(3)	-3(3)
C(14)	29(4)	20(4)	56(5)	10(4)	-9(4)	2(3)
C(15)	30(4)	23(4)	26(4)	8(3)	3(3)	-5(3)
C(16)	23(4)	29(4)	29(4)	3(3)	-4(3)	3(3)
C(17)	30(4)	18(4)	81(6)	11(4)	-1(4)	5(3)
C(18)	25(4)	21(4)	41(5)	0(3)	4(3)	-2(3)
C(19)	28(4)	29(4)	81(6)	10(4)	-2(4)	-1(3)
C(20)	20(4)	24(4)	43(5)	6(4)	1(3)	0(3)
C(21)	15(3)	20(4)	46(5)	3(3)	7(3)	-2(3)
C(22)	16(3)	18(4)	52(5)	3(3)	-1(3)	-1(3)
C(23)	19(3)	28(4)	24(4)	4(3)	6(3)	5(3)
C(24)	28(4)	20(3)	33(4)	4(3)	2(3)	-2(3)
C(25)	18(3)	22(4)	30(4)	-1(3)	6(3)	-1(3)
C(26)	18(4)	33(4)	37(5)	8(3)	5(3)	6(3)
C(27)	27(4)	25(4)	25(4)	-6(3)	-5(3)	3(3)
C(28)	18(3)	31(4)	36(5)	-8(4)	4(3)	-2(3)
O(13)	232(19)	133(13)	137(15)	-98(11)	118(14)	-46(12)

(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 $Cu^{II}Zn(HIP)_2(bipy)(H_2O) \cdot 1.5\ H_2O$:

	x	y	z	U_{eq}
H(5)	10857	-2010	2134	52
H(10)	-2351	15876	79	64
H(11B)	1680(50)	10390(40)	-418(11)	62(19)
H(11A)	2220(60)	11400(20)	-530(10)	62(19)
H(12A)	6500(90)	1830(50)	4030(40)	140(30)

H(12B)	6200(80)	2590(70)	3610(30)	140(30)
H(2)	7880	-638	1994	36
H(4)	9620	2409	2072	32
H(6)	11981	-353	2095	36
H(11)	6326	4440	1688	36
H(12)	2455	3677	1332	40
H(13)	5887	6264	1478	38
H(14)	1904	5492	1105	43
H(17)	5489	7878	1167	52
H(18)	1446	7195	1004	35
H(19)	4983	9690	927	56
H(20)	1017	9023	757	35
H(22)	-54	13929	470	35
H(24)	-2826	11468	582	32
H(26)	-4114	14583	213	35

Hydrogen bond parameters for $Cu^{II}Zn(HIP)_2(bipy)(H_2O) \cdot 1.5\ H_2O$:

D-H...A	d (D-H)	d (H...A)	d (D...A)	< (DHA)
O(5)-H(5)...O(3)#3	0.82	1.83	2.619(6)	162.1
O(10)-H(10)...O(9)#4	0.82	1.92	2.691(6)	155.4
O(11)-H(11B)...O(6)#5	0.817(18)	1.896(19)	2.710(6)	174(5)
O(11)-H(11A)...O(12)#6	0.826(18)	1.97(2)	2.786(7)	170(4)
O(12)-H(12A)...O(10)#7	0.82(2)	2.19(4)	2.926(7)	150(8)
O(12)-H(12B)...O(5)#8	0.82(2)	2.01(2)	2.828(7)	174(8)

Symmetry transformations used to generate equivalent atoms: #1 x-1,y,z #2 x+1,y,z #3 -x+5/2,y-1/2,-z+1/2 #4 -x-1,-y+3,-z #5 -x,-y+2,-z #6 x-1/2,-y+3/2,z-1/2 #7 -x+1/2,y-3/2,-z+1/2 #8 -x+3/2,y+1/2,-z+1/2

Crystallographic Data for $Cu^{I}_2Zn_2(HIP)_2(bipy)_2(ox)(H_2O)_2$:

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Cu^{I}_2Zn_2(HIP)_2(bipy)_2(ox)(H_2O)_2$:

	x	y	z	U_{eq}
Zn(1)	4972(2)	1648(1)	4678(2)	47(1)
Cu(1)	5873(2)	748(1)	8576(2)	52(1)
O(5)	-896(9)	911(6)	5161(9)	56(3)
O(2)	2157(9)	2321(7)	2276(10)	58(3)
O(8)	4825(8)	2412(7)	3170(8)	47(3)
O(6)	4936(9)	-591(6)	6298(10)	47(3)
O(3)	-2780(9)	3175(7)	587(9)	59(3)
O(4)	-4040(9)	2522(5)	1305(8)	40(3)
O(7)	5072(9)	754(6)	6118(10)	50(3)
O(1)	3022(10)	1745(6)	4257(10)	64(3)
N(1)	7690(10)	734(8)	8740(11)	46(3)
N(2)	4204(11)	725(7)	8741(12)	39(3)
C(8)	-2876(15)	2680(10)	1374(15)	44(4)
C(17)	1667(12)	728(8)	8793(13)	28(3)
C(18)	2768(13)	1090(8)	9785(14)	39(4)
C(16)	1845(13)	408(9)	7738(14)	48(5)
C(1)	-411(13)	2322(7)	2344(12)	29(4)
C(6)	-1710(14)	2248(8)	2301(15)	39(4)
C(2)	704(13)	1960(8)	3316(13)	30(4)
C(19)	4026(13)	1067(8)	9693(15)	43(4)
C(3)	530(13)	1508(8)	4240(13)	38(4)
C(12)	10262(13)	713(9)	8782(13)	36(4)
C(10)	8049(14)	191(9)	8058(14)	44(4)
C(14)	8611(13)	1260(8)	9468(13)	35(4)
C(20)	4994(14)	55(14)	5728(16)	59(5)
C(5)	-1835(13)	1778(8)	3276(13)	30(4)
C(4)	-776(14)	1373(8)	4183(15)	43(4)
C(7)	2024(16)	2021(10)	3230(18)	51(5)
C(13)	9888(14)	1283(8)	9508(13)	41(4)

C(15)	3140(15)	416(9)	7747(14)	55(5)
C(11)	9313(12)	148(8)	8028(13)	40(4)

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

Bond lengths [Å] and angles [°] for $Cu^{I}_2Zn_2(HIP)_2(bipy)_2(ox)(H_2O)_2$:

Zn(1)-O(1)	1.980(9)	C(17)-C(16)	1.368(16)
Zn(1)-O(8)	2.050(9)	C(17)-C(18)	1.385(16)
Zn(1)-O(6)#1	2.078(9)	C(17)-C(12)#4	1.522(16)
Zn(1)-O(7)	2.144(10)	C(18)-C(19)	1.413(16)
Zn(1)-O(4)#2	2.167(9)	C(18)-H(18)	0.9300
Zn(1)-O(3)#2	2.246(9)	C(16)-C(15)	1.404(17)
Zn(1)-C(8)#2	2.573(17)	C(16)-H(16)	0.9300
Cu(1)-N(2)	1.897(10)	C(1)-C(2)	1.383(15)
Cu(1)-N(1)	1.908(10)	C(1)-C(6)	1.398(15)
O(5)-C(4)	1.375(15)	C(1)-H(1)	0.9300
O(5)-H(5)	0.8200	C(6)-C(5)	1.384(16)
O(2)-C(7)	1.230(16)	C(2)-C(3)	1.343(15)
O(8)-H(8A)	0.80(2)	C(2)-C(7)	1.481(18)
O(8)-H(8B)	0.808(18)	C(19)-H(19)	0.9300
O(6)-C(20)	1.26(2)	C(3)-C(4)	1.413(16)
O(6)-Zn(1)#1	2.078(9)	C(3)-H(3)	0.9300
O(3)-C(8)	1.231(15)	C(12)-C(11)	1.386(17)
O(3)-Zn(1)#3	2.246(9)	C(12)-C(13)	1.405(16)
O(4)-C(8)	1.264(15)	C(12)-C(17)#5	1.522(16)
O(4)-Zn(1)#3	2.167(9)	C(10)-C(11)	1.390(16)
O(7)-C(20)	1.22(2)	C(10)-H(10)	0.9300
O(1)-C(7)	1.291(16)	C(14)-C(13)	1.370(16)
N(1)-C(14)	1.320(15)	C(14)-H(14)	0.9300
N(1)-C(10)	1.331(15)	C(20)-C(20)#1	1.63(3)
N(2)-C(19)	1.280(15)	C(5)-C(4)	1.353(16)
N(2)-C(15)	1.328(15)	C(5)-H(5A)	0.9300
C(8)-C(6)	1.449(18)	C(13)-H(13)	0.9300
C(8)-Zn(1)#3	2.573(17)	C(15)-H(15)	0.9300

C(11)-H(11)	0.9300	C(19)-N(2)-C(15)	118.6(12)
---		C(19)-N(2)-Cu(1)	123.1(11)
O(1)-Zn(1)-O(8)	92.4(4)	C(15)-N(2)-Cu(1)	117.9(10)
O(1)-Zn(1)-O(6)#1	102.8(4)	O(3)-C(8)-O(4)	118.0(15)
O(8)-Zn(1)-O(6)#1	95.5(4)	O(3)-C(8)-C(6)	121.8(14)
O(1)-Zn(1)-O(7)	87.3(4)	O(4)-C(8)-C(6)	120.2(15)
O(8)-Zn(1)-O(7)	174.4(4)	O(3)-C(8)-Zn(1)#3	60.8(8)
O(6)#1-Zn(1)-O(7)	79.2(4)	O(4)-C(8)-Zn(1)#3	57.2(8)
O(1)-Zn(1)-O(4)#2	105.1(4)	C(6)-C(8)-Zn(1)#3	176.0(11)
O(8)-Zn(1)-O(4)#2	97.8(4)	C(16)-C(17)-C(18)	117.8(12)
O(6)#1-Zn(1)-O(4)#2	148.4(4)	C(16)-C(17)-C(12)#4	118.8(13)
O(7)-Zn(1)-O(4)#2	87.6(4)	C(18)-C(17)-C(12)#4	123.3(13)
O(1)-Zn(1)-O(3)#2	163.0(4)	C(17)-C(18)-C(19)	118.4(13)
O(8)-Zn(1)-O(3)#2	89.5(3)	C(17)-C(18)-H(18)	120.8
O(6)#1-Zn(1)-O(3)#2	93.8(4)	C(19)-C(18)-H(18)	120.8
O(7)-Zn(1)-O(3)#2	92.5(4)	C(17)-C(16)-C(15)	119.0(13)
O(4)#2-Zn(1)-O(3)#2	57.9(3)	C(17)-C(16)-H(16)	120.5
O(1)-Zn(1)-C(8)#2	134.5(5)	C(15)-C(16)-H(16)	120.5
O(8)-Zn(1)-C(8)#2	94.2(4)	C(2)-C(1)-C(6)	122.5(13)
O(6)#1-Zn(1)-C(8)#2	121.2(5)	C(2)-C(1)-H(1)	118.8
O(7)-Zn(1)-C(8)#2	90.0(4)	C(6)-C(1)-H(1)	118.8
O(4)#2-Zn(1)-C(8)#2	29.4(4)	C(5)-C(6)-C(1)	116.5(13)
O(3)#2-Zn(1)-C(8)#2	28.6(3)	C(5)-C(6)-C(8)	119.5(12)
N(2)-Cu(1)-N(1)	169.8(5)	C(1)-C(6)-C(8)	123.8(14)
C(4)-O(5)-H(5)	109.5	C(3)-C(2)-C(1)	118.8(12)
Zn(1)-O(8)-H(8A)	146(9)	C(3)-C(2)-C(7)	122.1(13)
Zn(1)-O(8)-H(8B)	97(6)	C(1)-C(2)-C(7)	118.8(13)
H(8A)-O(8)-H(8B)	106(4)	N(2)-C(19)-C(18)	123.5(13)
C(20)-O(6)-Zn(1)#1	115.3(12)	N(2)-C(19)-H(19)	118.3
C(8)-O(3)-Zn(1)#3	90.6(9)	C(18)-C(19)-H(19)	118.3
C(8)-O(4)-Zn(1)#3	93.4(10)	C(2)-C(3)-C(4)	120.6(13)
C(20)-O(7)-Zn(1)	114.2(12)	C(2)-C(3)-H(3)	119.7
C(7)-O(1)-Zn(1)	131.8(10)	C(4)-C(3)-H(3)	119.7
C(14)-N(1)-C(10)	117.7(11)	C(11)-C(12)-C(13)	118.5(12)
C(14)-N(1)-Cu(1)	123.1(10)	C(11)-C(12)-C(17)#5	120.7(13)
C(10)-N(1)-Cu(1)	119.2(10)	C(13)-C(12)-C(17)#5	120.8(13)

N(1)-C(10)-C(11)	124.9(13)	O(5)-C(4)-C(3)	118.2(13)
N(1)-C(10)-H(10)	117.5	O(2)-C(7)-O(1)	123.2(14)
C(11)-C(10)-H(10)	117.5	O(2)-C(7)-C(2)	122.9(15)
N(1)-C(14)-C(13)	122.8(13)	O(1)-C(7)-C(2)	113.8(15)
N(1)-C(14)-H(14)	118.6	C(14)-C(13)-C(12)	119.4(13)
C(13)-C(14)-H(14)	118.6	C(14)-C(13)-H(13)	120.3
O(7)-C(20)-O(6)	129.3(17)	C(12)-C(13)-H(13)	120.3
O(7)-C(20)-C(20)#1	115(2)	N(2)-C(15)-C(16)	122.5(14)
O(6)-C(20)-C(20)#1	115(2)	N(2)-C(15)-H(15)	118.7
C(4)-C(5)-C(6)	122.1(13)	C(16)-C(15)-H(15)	118.7
C(4)-C(5)-H(5A)	119.0	C(12)-C(11)-C(10)	116.7(13)
C(6)-C(5)-H(5A)	119.0	C(12)-C(11)-H(11)	121.7
C(5)-C(4)-O(5)	122.2(13)	C(10)-C(11)-H(11)	121.7
C(5)-C(4)-C(3)	119.1(14)		

Symmetry transformations used to generate equivalent atoms:

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

Anisotropic displacement parameters ($Å^2 \times 10^3$) for $Cu^I_2Zn_2(HIP)_2(bipy)_2(ox)(H_2O)_2$:

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	31(1)	57(1)	52(1)	-6(1)	15(1)	-2(1)
Cu(1)	29(1)	65(1)	69(1)	-1(1)	28(1)	-1(1)
O(5)	65(7)	64(8)	63(7)	19(6)	52(6)	14(6)
O(2)	26(6)	91(9)	58(8)	15(7)	20(6)	14(6)
O(8)	26(6)	69(7)	50(7)	11(6)	19(5)	3(6)
O(6)	50(6)	29(7)	58(7)	1(6)	19(6)	0(6)
O(3)	42(7)	88(10)	45(7)	17(7)	16(6)	14(6)
O(4)	26(6)	48(6)	36(6)	-1(5)	1(5)	2(5)
O(7)	52(7)	49(7)	53(8)	1(7)	26(6)	-9(6)
O(1)	33(7)	89(9)	72(8)	16(8)	25(6)	0(6)
N(1)	18(7)	80(10)	44(8)	-8(8)	18(7)	-8(7)
N(2)	32(5)	50(6)	41(6)	-2(5)	21(5)	15(5)

C(8)	33(11)	62(13)	38(12)	-19(10)	16(10)	-10(9)
C(17)	35(9)	21(8)	30(9)	13(8)	15(8)	6(7)
C(18)	32(9)	42(10)	43(10)	-31(8)	16(8)	-10(7)
C(16)	26(9)	78(13)	40(11)	-22(9)	13(8)	-16(8)
C(1)	37(9)	24(9)	27(9)	-9(7)	16(8)	-3(7)
C(6)	28(9)	38(11)	63(12)	-7(9)	29(9)	10(8)
C(2)	26(9)	42(10)	24(9)	9(8)	12(8)	8(7)
C(19)	33(9)	34(10)	68(12)	-2(9)	25(9)	-16(7)
C(3)	31(6)	42(7)	41(7)	-4(6)	16(5)	18(5)
C(12)	31(6)	41(7)	34(6)	7(6)	13(5)	10(6)
C(10)	36(6)	41(7)	53(7)	5(6)	16(6)	-8(5)
C(14)	26(9)	43(10)	45(11)	-1(8)	26(9)	-1(7)
C(20)	20(9)	94(16)	49(14)	-4(14)	1(10)	-6(12)
C(5)	26(6)	30(7)	37(6)	-4(6)	17(5)	10(5)
C(4)	40(10)	34(10)	61(12)	-3(9)	27(9)	6(8)
C(7)	31(11)	61(13)	53(14)	-3(11)	9(11)	4(9)
C(13)	40(10)	37(10)	32(9)	5(8)	-1(8)	-13(8)
C(15)	52(11)	78(13)	33(11)	-7(9)	16(10)	-5(10)
C(11)	18(8)	46(11)	49(11)	-3(9)	6(8)	5(7)

(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 $Cu^I_2Zn_2(HIP)_2(bipy)_2(ox)(H_2O)_2$:

	x	y	z	U_{eq}
H(5)	-1583	1041	5247	83
H(8A)	5070(80)	2510(80)	2590(70)	47
H(8B)	4013(17)	2450(60)	2840(90)	47
H(18)	2682	1343	10495	47
H(16)	1119	189	7025	58
H(1)	-292	2626	1694	34
H(19)	4763	1312	10358	52

H(3)	1276	1282	4923	45
H(10)	7406	-188	7566	53
H(14)	8384	1631	9974	42
H(5A)	-2674	1739	3310	36
H(13)	10501	1673	10013	50
H(15)	3257	197	7030	66
H(11)	9511	-239	7527	48

Hydrogen bond parameters for $Cu^{I}_{2}Zn_{2}(HIP)_{2}(bipy)_{2}(ox)(H_{2}O)_{2}$:

D-H...A	d (D-H)	d (H...A)	d (D...A)	< (DHA)
O(5)-H(5)...O(3)#6	0.82	1.98	2.738(13)	153.6
O(8)-H(8A)...O(4)#5	0.80(2)	2.03(3)	2.817(12)	167(12)
O(8)-H(8B)...O(2)	0.808(18)	1.862(18)	2.655(12)	167(9)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z+1 #2 x+1,-y+1/2,z+1/2 #3 x-1,-y+1/2,z-1/2 #4 x-1,y,z #5 x+1,y,z #6 x,-y+1/2,z+1/2

Crystallographic Data for $Cu^{I}_{2}Zn(HIP)_2(bipy)_2$:

Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Cu^{I}_{2}Zn(HIP)_2(bipy)_2$:

	x	y	z	U_{eq}
Cu(1)	9736(1)	-552(1)	6530(1)	50(1)
Cu(2)	5412(1)	874(1)	8400(1)	44(1)
Zn(1)	7428(1)	-127(1)	7562(1)	25(1)
O(1)	12881(2)	3026(3)	8639(2)	42(1)
O(2)	11826(2)	3624(2)	7726(2)	39(1)
O(3)	9122(2)	974(3)	7127(2)	42(1)
O(4)	8408(2)	721(2)	8155(2)	36(1)
O(5)	10840(2)	1139(3)	10354(2)	48(1)
O(6)	2595(2)	3630(3)	5952(2)	60(1)
O(7)	3566(2)	4231(2)	6917(2)	33(1)
O(8)	6257(2)	1732(2)	7592(2)	37(1)
O(9)	6702(2)	643(2)	6702(2)	33(1)
O(10)	4531(2)	1375(3)	4364(2)	47(1)
N(1)	9004(2)	-358(3)	5564(2)	39(1)
N(2)	4370(2)	497(3)	7685(2)	35(1)
N(3)	6184(2)	1242(3)	9322(2)	38(1)
N(4)	10602(2)	-1024(3)	7362(2)	37(1)
C(1)	12107(3)	3010(3)	8285(2)	28(1)
C(2)	11399(2)	2237(3)	8539(2)	27(1)
C(3)	10625(3)	1930(3)	8058(2)	28(1)
C(4)	9920(2)	1391(3)	8350(2)	28(1)
C(5)	9082(3)	1017(3)	7831(2)	29(1)
C(6)	9992(3)	1154(3)	9129(2)	32(1)
C(7)	10795(3)	1409(3)	9593(2)	33(1)
C(8)	11494(3)	1938(3)	9304(2)	30(1)
C(11)	6193(2)	1387(3)	6926(2)	27(1)
C(12)	5444(3)	1837(3)	6344(2)	28(1)
C(13)	4833(3)	2607(3)	6568(2)	30(1)
C(14)	4094(2)	2945(3)	6055(2)	27(1)

C(15)	3358(3)	3648(3)	6318(2)	29(1)
C(16)	3990(3)	2542(3)	5313(2)	32(1)
C(17)	4607(3)	1793(3)	5087(2)	32(1)
C(18)	5327(3)	1424(3)	5608(2)	31(1)
C(21)	8223(3)	213(4)	5533(2)	46(1)
C(22)	7577(3)	224(4)	4903(2)	46(1)
C(23)	7708(3)	-354(3)	4246(2)	33(1)
C(24)	8524(3)	-928(4)	4280(2)	39(1)
C(25)	9142(3)	-910(4)	4931(2)	41(1)
C(26)	4438(3)	-175(3)	7098(2)	35(1)
C(27)	3773(3)	-258(4)	6479(2)	35(1)
C(28)	2995(3)	382(3)	6431(2)	32(1)
C(29)	2919(3)	1074(4)	7047(2)	41(1)
C(30)	3606(3)	1091(4)	7659(2)	42(1)
C(31)	7028(3)	1608(4)	9301(2)	45(1)
C(32)	7668(3)	1692(4)	9944(2)	42(1)
C(33)	7440(3)	1371(3)	10649(2)	33(1)
C(34)	6550(3)	1025(4)	10671(2)	43(1)
C(35)	5953(3)	983(4)	10011(3)	45(1)
C(36)	11493(3)	-1213(4)	7304(2)	40(1)
C(37)	12141(3)	-1370(4)	7923(2)	38(1)
C(38)	11884(3)	-1350(3)	8655(2)	33(1)
C(39)	10960(3)	-1235(3)	8708(2)	37(1)
C(40)	10354(3)	-1085(3)	8059(2)	38(1)

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

Bond lengths [Å] and angles [°] for $Cu^{I}_{2}Zn(HIP)_2(bipy)_2$:

Cu(1)-N(4)	1.911(3)	Cu(2)-O(8)	2.269(3)
Cu(1)-N(1)	1.916(3)	Zn(1)-O(4)	1.968(3)
Cu(1)-O(3)	2.373(3)	Zn(1)-O(9)	1.981(3)
Cu(2)-N(2)	1.918(3)	Zn(1)-O(2)#1	1.983(3)
Cu(2)-N(3)	1.919(3)	Zn(1)-O(7)#2	1.991(3)

O(1)-C(1)	1.231(4)	C(13)-C(14)	1.389(5)
O(2)-C(1)	1.266(5)	C(13)-H(13)	0.9300
O(2)-Zn(1)#3	1.983(3)	C(14)-C(16)	1.391(5)
O(3)-C(5)	1.256(5)	C(14)-C(15)	1.503(5)
O(4)-C(5)	1.264(5)	C(16)-C(17)	1.384(5)
O(5)-C(7)	1.378(4)	C(16)-H(16)	0.9300
O(5)-H(5)	0.8200	C(17)-C(18)	1.390(5)
O(6)-C(15)	1.226(5)	C(18)-H(18)	0.9300
O(7)-C(15)	1.280(4)	C(21)-C(22)	1.372(6)
O(7)-Zn(1)#4	1.991(3)	C(21)-H(21)	0.9300
O(8)-C(11)	1.242(4)	C(22)-C(23)	1.392(6)
O(9)-C(11)	1.272(5)	C(22)-H(22)	0.9300
O(10)-C(17)	1.367(4)	C(23)-C(24)	1.387(6)
O(10)-H(10)	0.8200	C(23)-C(28)#5	1.481(5)
N(1)-C(21)	1.342(6)	C(24)-C(25)	1.375(6)
N(1)-C(25)	1.343(6)	C(24)-H(24)	0.9300
N(2)-C(26)	1.335(5)	C(25)-H(25)	0.9300
N(2)-C(30)	1.337(5)	C(26)-C(27)	1.377(5)
N(3)-C(31)	1.330(5)	C(26)-H(26)	0.9300
N(3)-C(35)	1.344(6)	C(27)-C(28)	1.382(6)
N(4)-C(40)	1.331(5)	C(27)-H(27)	0.9300
N(4)-C(36)	1.353(6)	C(28)-C(29)	1.393(6)
C(1)-C(2)	1.517(5)	C(28)-C(23)#5	1.481(5)
C(2)-C(3)	1.386(5)	C(29)-C(30)	1.386(5)
C(2)-C(8)	1.390(5)	C(29)-H(29)	0.9300
C(3)-C(4)	1.386(5)	C(30)-H(30)	0.9300
C(3)-H(3)	0.9300	C(31)-C(32)	1.387(5)
C(4)-C(6)	1.397(5)	C(31)-H(31)	0.9300
C(4)-C(5)	1.514(5)	C(32)-C(33)	1.388(6)
C(6)-C(7)	1.388(5)	C(32)-H(32)	0.9300
C(6)-H(6)	0.9300	C(33)-C(34)	1.387(6)
C(7)-C(8)	1.371(5)	C(33)-C(38)#6	1.483(5)
C(8)-H(8)	0.9300	C(34)-C(35)	1.371(6)
C(11)-C(12)	1.514(5)	C(34)-H(34)	0.9300
C(12)-C(18)	1.385(5)	C(35)-H(35)	0.9300
C(12)-C(13)	1.394(5)	C(36)-C(37)	1.372(5)

C(36)-H(36)	0.9300	C(31)-N(3)-Cu(2)	120.8(3)
C(37)-C(38)	1.394(6)	C(35)-N(3)-Cu(2)	121.5(3)
C(37)-H(37)	0.9300	C(40)-N(4)-C(36)	116.5(3)
C(38)-C(39)	1.387(6)	C(40)-N(4)-Cu(1)	119.4(3)
C(38)-C(33)#6	1.483(5)	C(36)-N(4)-Cu(1)	123.7(3)
C(39)-C(40)	1.375(5)	O(1)-C(1)-O(2)	125.3(4)
C(39)-H(39)	0.9300	O(1)-C(1)-C(2)	119.4(3)
C(40)-H(40)	0.9300	O(2)-C(1)-C(2)	115.3(3)
----------	----------	C(3)-C(2)-C(8)	119.9(3)
N(4)-Cu(1)-N(1)	165.82(16)	C(3)-C(2)-C(1)	122.2(3)
N(4)-Cu(1)-O(3)	98.65(13)	C(8)-C(2)-C(1)	117.5(3)
N(1)-Cu(1)-O(3)	95.47(14)	C(2)-C(3)-C(4)	120.0(3)
N(2)-Cu(2)-N(3)	162.81(15)	C(2)-C(3)-H(3)	120.0
N(2)-Cu(2)-O(8)	98.94(12)	C(4)-C(3)-H(3)	120.0
N(3)-Cu(2)-O(8)	96.41(13)	C(3)-C(4)-C(6)	119.9(3)
O(4)-Zn(1)-O(9)	116.76(12)	C(3)-C(4)-C(5)	120.9(3)
O(4)-Zn(1)-O(2)#1	98.26(12)	C(6)-C(4)-C(5)	119.2(3)
O(9)-Zn(1)-O(2)#1	115.49(11)	O(3)-C(5)-O(4)	125.3(3)
O(4)-Zn(1)-O(7)#2	119.72(11)	O(3)-C(5)-C(4)	118.3(4)
O(9)-Zn(1)-O(7)#2	100.44(11)	O(4)-C(5)-C(4)	116.3(3)
O(2)#1-Zn(1)-O(7)#2	106.58(12)	C(7)-C(6)-C(4)	119.2(4)
C(1)-O(2)-Zn(1)#3	121.0(2)	C(7)-C(6)-H(6)	120.4
C(5)-O(3)-Cu(1)	122.9(3)	C(4)-C(6)-H(6)	120.4
C(5)-O(4)-Zn(1)	118.5(2)	C(8)-C(7)-O(5)	122.1(3)
C(7)-O(5)-H(5)	109.5	C(8)-C(7)-C(6)	120.8(4)
C(15)-O(7)-Zn(1)#4	119.2(2)	O(5)-C(7)-C(6)	117.1(3)
C(11)-O(8)-Cu(2)	117.3(2)	C(7)-C(8)-C(2)	119.9(3)
C(11)-O(9)-Zn(1)	112.4(2)	C(7)-C(8)-H(8)	120.0
C(17)-O(10)-H(10)	109.5	C(2)-C(8)-H(8)	120.0
C(21)-N(1)-C(25)	116.6(4)	O(8)-C(11)-O(9)	124.0(3)
C(21)-N(1)-Cu(1)	118.9(3)	O(8)-C(11)-C(12)	118.8(3)
C(25)-N(1)-Cu(1)	123.6(3)	O(9)-C(11)-C(12)	117.1(3)
C(26)-N(2)-C(30)	116.9(3)	C(18)-C(12)-C(13)	120.2(3)
C(26)-N(2)-Cu(2)	121.7(3)	C(18)-C(12)-C(11)	120.0(3)
C(30)-N(2)-Cu(2)	119.7(3)	C(13)-C(12)-C(11)	119.6(3)
C(31)-N(3)-C(35)	116.9(4)	C(14)-C(13)-C(12)	119.9(3)

C(14)-C(13)-H(13)	120.1	C(26)-C(27)-H(27)	119.6
C(12)-C(13)-H(13)	120.1	C(28)-C(27)-H(27)	119.6
C(13)-C(14)-C(16)	119.6(3)	C(27)-C(28)-C(29)	116.2(4)
C(13)-C(14)-C(15)	120.4(3)	C(27)-C(28)-C(23)#5	121.9(4)
C(16)-C(14)-C(15)	119.6(3)	C(29)-C(28)-C(23)#5	121.8(4)
O(6)-C(15)-O(7)	123.6(4)	C(30)-C(29)-C(28)	119.6(4)
O(6)-C(15)-C(14)	118.7(3)	C(30)-C(29)-H(29)	120.2
O(7)-C(15)-C(14)	117.7(3)	C(28)-C(29)-H(29)	120.2
C(17)-C(16)-C(14)	120.5(3)	N(2)-C(30)-C(29)	123.4(4)
C(17)-C(16)-H(16)	119.8	N(2)-C(30)-H(30)	118.3
C(14)-C(16)-H(16)	119.8	C(29)-C(30)-H(30)	118.3
O(10)-C(17)-C(16)	122.5(3)	N(3)-C(31)-C(32)	123.1(4)
O(10)-C(17)-C(18)	117.6(3)	N(3)-C(31)-H(31)	118.5
C(16)-C(17)-C(18)	119.9(3)	C(32)-C(31)-H(31)	118.5
C(12)-C(18)-C(17)	119.9(4)	C(31)-C(32)-C(33)	119.8(4)
C(12)-C(18)-H(18)	120.0	C(31)-C(32)-H(32)	120.1
C(17)-C(18)-H(18)	120.0	C(33)-C(32)-H(32)	120.1
N(1)-C(21)-C(22)	122.9(4)	C(34)-C(33)-C(32)	116.8(4)
N(1)-C(21)-H(21)	118.5	C(34)-C(33)-C(38)#6	120.8(4)
C(22)-C(21)-H(21)	118.5	C(32)-C(33)-C(38)#6	122.3(4)
C(21)-C(22)-C(23)	121.0(4)	C(35)-C(34)-C(33)	119.9(4)
C(21)-C(22)-H(22)	119.5	C(35)-C(34)-H(34)	120.1
C(23)-C(22)-H(22)	119.5	C(33)-C(34)-H(34)	120.1
C(24)-C(23)-C(22)	115.5(4)	N(3)-C(35)-C(34)	123.5(4)
C(24)-C(23)-C(28)#5	122.6(4)	N(3)-C(35)-H(35)	118.3
C(22)-C(23)-C(28)#5	121.8(4)	C(34)-C(35)-H(35)	118.3
C(25)-C(24)-C(23)	120.6(4)	N(4)-C(36)-C(37)	123.3(4)
C(25)-C(24)-H(24)	119.7	N(4)-C(36)-H(36)	118.3
C(23)-C(24)-H(24)	119.7	C(37)-C(36)-H(36)	118.3
N(1)-C(25)-C(24)	123.3(4)	C(36)-C(37)-C(38)	119.5(4)
N(1)-C(25)-H(25)	118.3	C(36)-C(37)-H(37)	120.3
C(24)-C(25)-H(25)	118.3	C(38)-C(37)-H(37)	120.3
N(2)-C(26)-C(27)	123.0(4)	C(39)-C(38)-C(37)	116.9(4)
N(2)-C(26)-H(26)	118.5	C(39)-C(38)-C(33)#6	120.7(4)
C(27)-C(26)-H(26)	118.5	C(37)-C(38)-C(33)#6	122.3(4)
C(26)-C(27)-C(28)	120.8(4)	C(40)-C(39)-C(38)	119.9(4)

C(40)-C(39)-H(39)	120.0	N(4)-C(40)-H(40)	118.3
C(38)-C(39)-H(39)	120.0	C(39)-C(40)-H(40)	118.3
N(4)-C(40)-C(39)	123.5(4)		

Symmetry transformations used to generate equivalent atoms:

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

Anisotropic displacement parameters ($Å^2 \times 10^3$) for $Cu^I_2Zn(HIP)_2(bipy)_2$:

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	42(1)	67(1)	35(1)	14(1)	-18(1)	-9(1)
Cu(2)	33(1)	64(1)	31(1)	-6(1)	-12(1)	-1(1)
Zn(1)	18(1)	32(1)	25(1)	0(1)	-3(1)	1(1)
O(1)	25(2)	58(2)	38(2)	6(1)	-6(1)	-14(1)
O(2)	30(2)	43(2)	41(2)	12(1)	-4(1)	-11(1)
O(3)	34(2)	56(2)	33(2)	3(1)	-7(1)	-8(1)
O(4)	21(1)	46(2)	37(2)	-6(1)	-5(1)	-6(1)
O(5)	32(2)	79(2)	32(2)	13(2)	-2(1)	-15(2)
O(6)	30(2)	94(3)	51(2)	-30(2)	-13(2)	24(2)
O(7)	23(1)	40(2)	36(2)	-6(1)	2(1)	3(1)
O(8)	34(2)	48(2)	28(1)	-3(1)	-7(1)	2(1)
O(9)	22(1)	43(2)	33(1)	3(1)	-5(1)	11(1)
O(10)	37(2)	72(2)	30(2)	-17(2)	-9(1)	23(2)
N(1)	34(2)	56(2)	25(2)	10(2)	-5(2)	-8(2)
N(2)	28(2)	50(2)	24(2)	1(2)	-7(1)	-3(2)
N(3)	30(2)	50(2)	31(2)	-7(2)	-6(2)	7(2)
N(4)	34(2)	41(2)	33(2)	3(2)	-13(2)	-5(2)
C(1)	24(2)	32(2)	29(2)	-9(2)	1(2)	-6(2)
C(2)	23(2)	30(2)	28(2)	-2(2)	4(2)	-3(2)
C(3)	27(2)	28(2)	27(2)	0(2)	-1(2)	-1(2)
C(4)	21(2)	29(2)	33(2)	1(2)	-6(2)	-1(2)
C(5)	25(2)	27(2)	33(2)	0(2)	-7(2)	-3(2)

C(6)	26(2)	38(2)	32(2)	4(2)	0(2)	-5(2)
C(7)	30(2)	40(2)	28(2)	4(2)	-3(2)	-7(2)
C(8)	20(2)	40(2)	27(2)	-2(2)	-3(2)	-4(2)
C(11)	20(2)	28(2)	30(2)	5(2)	-5(2)	-1(2)
C(12)	23(2)	29(2)	30(2)	6(2)	-2(2)	4(2)
C(13)	27(2)	36(2)	24(2)	-2(2)	-3(2)	2(2)
C(14)	24(2)	28(2)	30(2)	-1(2)	0(2)	1(2)
C(15)	26(2)	34(2)	25(2)	1(2)	0(2)	2(2)
C(16)	25(2)	42(2)	27(2)	0(2)	-5(2)	9(2)
C(17)	29(2)	41(2)	24(2)	0(2)	-2(2)	8(2)
C(18)	24(2)	36(2)	31(2)	-2(2)	0(2)	8(2)
C(21)	40(3)	71(3)	25(2)	-2(2)	-3(2)	3(2)
C(22)	28(2)	76(3)	33(2)	-11(2)	-4(2)	9(2)
C(23)	30(2)	41(2)	27(2)	5(2)	-3(2)	-4(2)
C(24)	34(2)	52(3)	29(2)	1(2)	-2(2)	3(2)
C(25)	30(2)	50(3)	41(2)	8(2)	-5(2)	4(2)
C(26)	30(2)	41(2)	34(2)	2(2)	-2(2)	6(2)
C(27)	30(2)	44(2)	28(2)	-1(2)	-6(2)	1(2)
C(28)	27(2)	40(2)	29(2)	9(2)	-3(2)	-3(2)
C(29)	34(2)	56(3)	32(2)	-6(2)	-5(2)	11(2)
C(30)	32(2)	61(3)	29(2)	-12(2)	-5(2)	5(2)
C(31)	35(2)	70(3)	28(2)	2(2)	-2(2)	0(2)
C(32)	30(2)	64(3)	29(2)	1(2)	-2(2)	-3(2)
C(33)	28(2)	40(2)	30(2)	-3(2)	-2(2)	5(2)
C(34)	32(2)	66(3)	28(2)	-1(2)	0(2)	-2(2)
C(35)	29(2)	60(3)	44(3)	-3(2)	0(2)	-2(2)
C(36)	42(3)	50(3)	26(2)	2(2)	-2(2)	-2(2)
C(37)	28(2)	54(3)	30(2)	5(2)	-1(2)	1(2)
C(38)	31(2)	37(2)	28(2)	2(2)	-5(2)	3(2)
C(39)	35(2)	43(2)	30(2)	2(2)	-4(2)	3(2)
C(40)	31(2)	42(2)	37(2)	2(2)	-6(2)	1(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 $Cu^I_2Zn(HIP)_2(bipy)_2$:

	x	y	z	U_{eq}
H(5)	11371	1180	10555	72
H(10)	4065	1609	4116	71
H(3)	10579	2087	7540	33
H(6)	9508	829	9334	38
H(8)	12031	2097	9619	36
H(13)	4919	2894	7060	36
H(16)	3502	2777	4966	39
H(18)	5729	901	5463	37
H(21)	8115	618	5959	55
H(22)	7043	623	4914	56
H(24)	8653	-1328	3859	46
H(25)	9683	-1300	4933	50
H(26)	4958	-608	7107	42
H(27)	3848	-749	6090	42
H(29)	2410	1523	7048	50
H(30)	3532	1538	8073	50
H(31)	7197	1818	8833	54
H(32)	8249	1962	9903	50
H(34)	6359	822	11132	51
H(35)	5356	763	10042	53
H(36)	11675	-1237	6820	48
H(37)	12747	-1490	7855	46
H(39)	10752	-1259	9182	44
H(40)	9737	-1022	8109	45

Hydrogen bond parameters for $Cu^{I}_{2}Zn(HIP)_2(bipy)_2$:

D-H...A	d (D-H)	d (H...A)	d (D...A)	< (DHA)
O(5)-H(5)...O(6)#7	0.82	1.87	2.688(4)	175.0
O(10)-H(10)...O(1)#8	0.82	1.90	2.707(4)	170.0

Symmetry transformations used to generate equivalent atoms: #1 -x+2,y-1/2,-z+3/2 #2 -x+1,y-1/2,-z+3/2 #3 -x+2,y+1/2,-z+3/2 #4 -x+1,y+1/2,-z+3/2 #5 -x+1,-y,-z+1 #6 -x+2,-y,-z+2 #7 x+1,-y+1/2,z+1/2 #8 x-1,-y+1/2,z-1/2