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Supporting Information

Structural and Functional Studies on Ternary Coordination Polymers from 5-Bromoisophthalate and Imidazole based Flexible Linker

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This supporting information file contains following data:

1. **Fig. S1** FTIR spectra of **CP1**-**CP3**
2. **Fig. S2** TGA plots for **CP1**-**CP3**
3. **Fig. S3** Experimental and simulated PXRD patterns for pristine **CP1**-**CP3**
4. **Fig. S4** Time dependent absorbance recorded for **blank** and **CP1** catalyzed experiments for metanil yellow (MY) photodegradation using dilute H_2O_2
5. **Fig. S5** Experimental and simulated PXRD patterns for **CP1**-**CP3** recovered after photocatalysis experiments
6. **Fig. S6** Emission spectra of **CP2** and **CP3**
7. **Table S1** Selected bond length and bond angle for **CP1-CP3**

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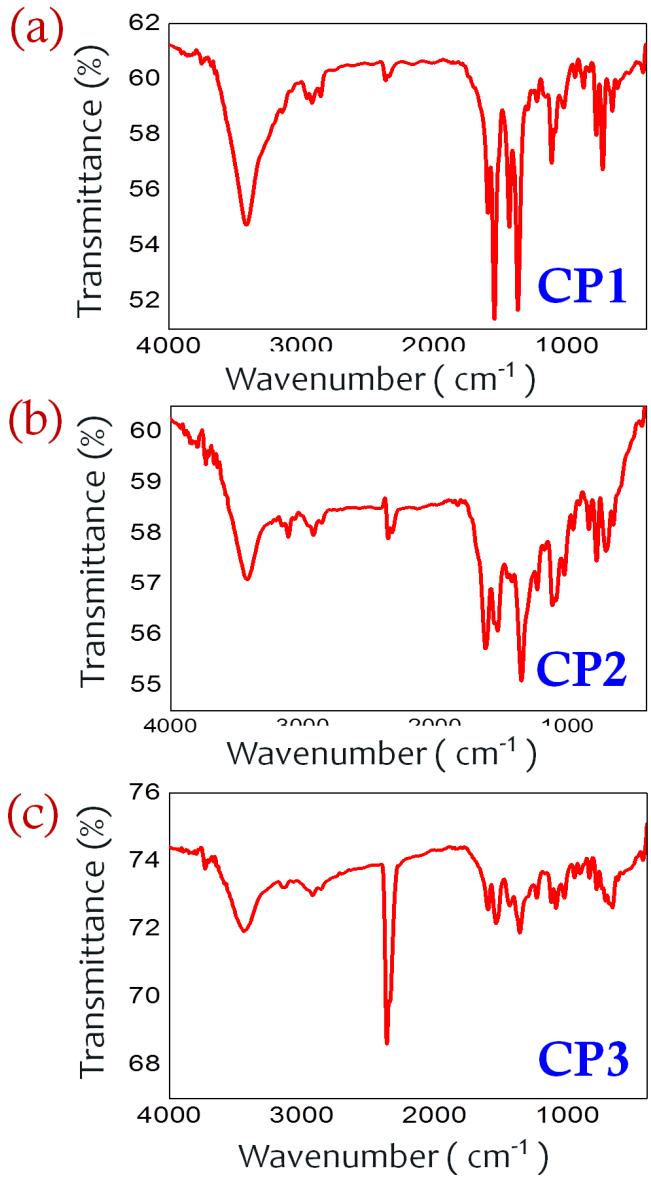
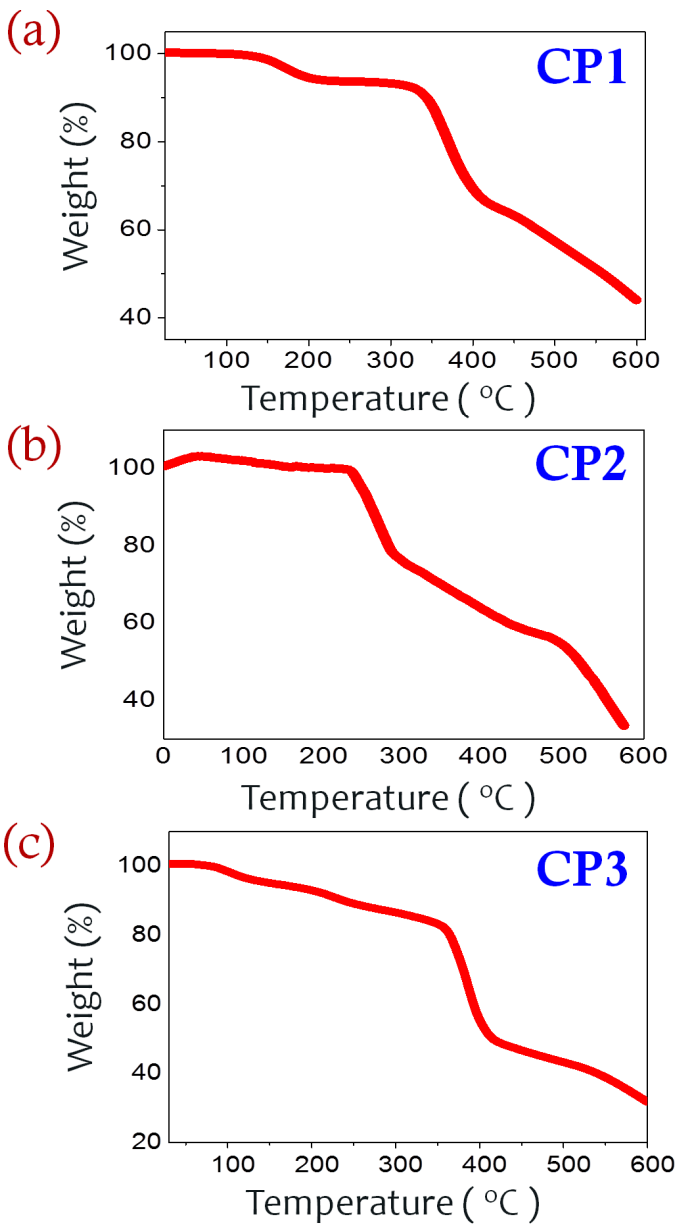
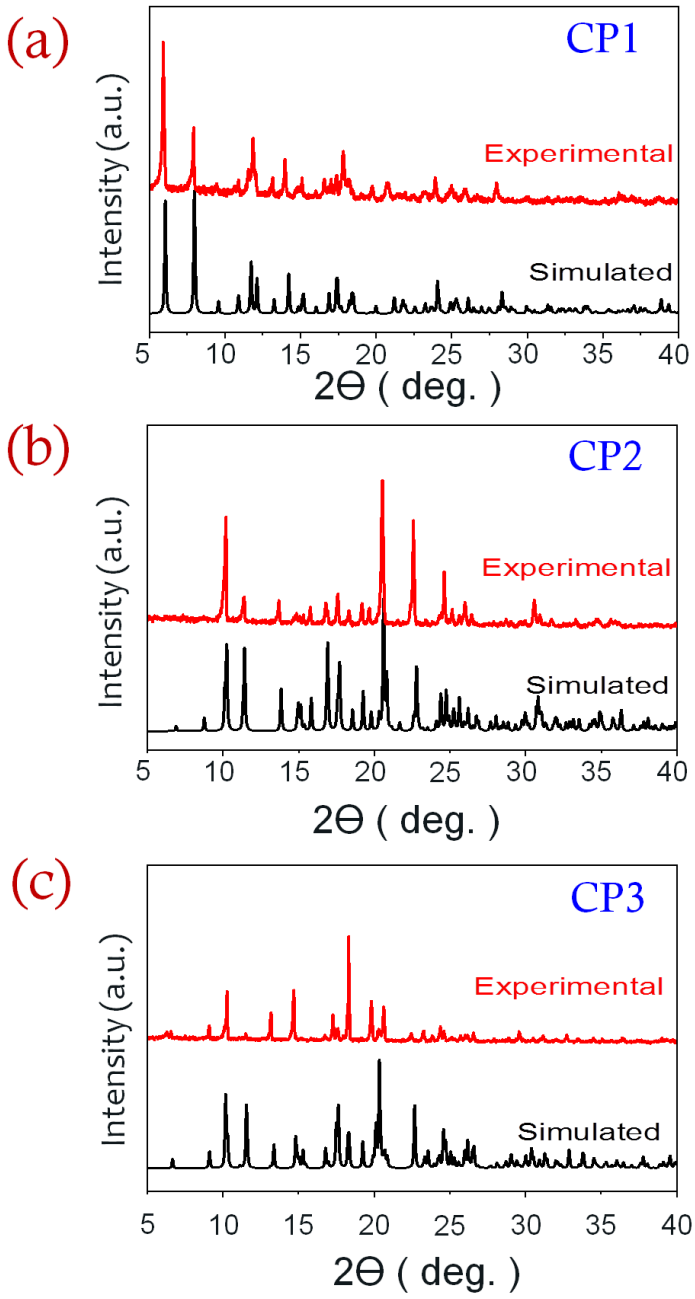
S1. FTIR of CP1-CP3 recorded for compounds dispersed in KBr pellets.



S2. TGA plots for compounds CP1-CP3.



S3. Simulated and experimental PXRD of CP1-CP3.



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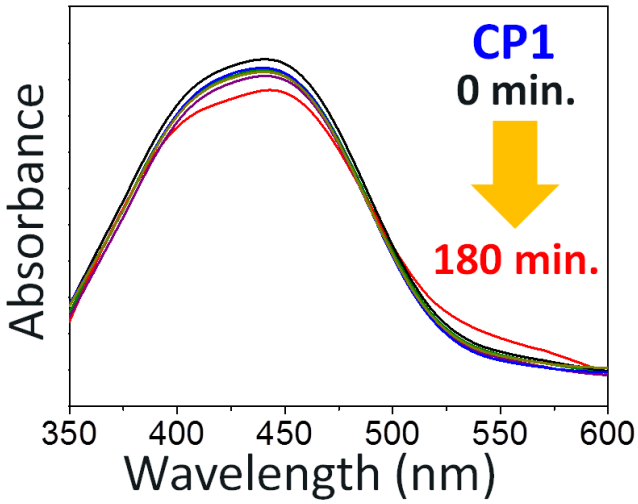
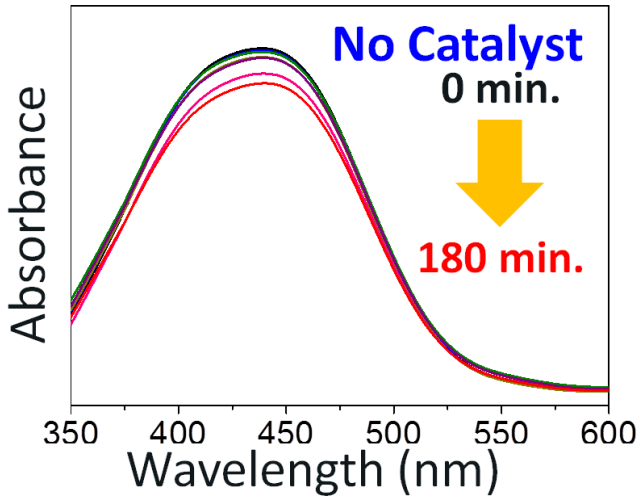
S4. Time dependent absorbance change recorded for the photoctalysis experiments using CP1 (top) and control experiment (bottom) for the metanil yellow (MY) photodegradation using dilute H_2O_2. Apparently, CP1 does not show much effect on the reaction.





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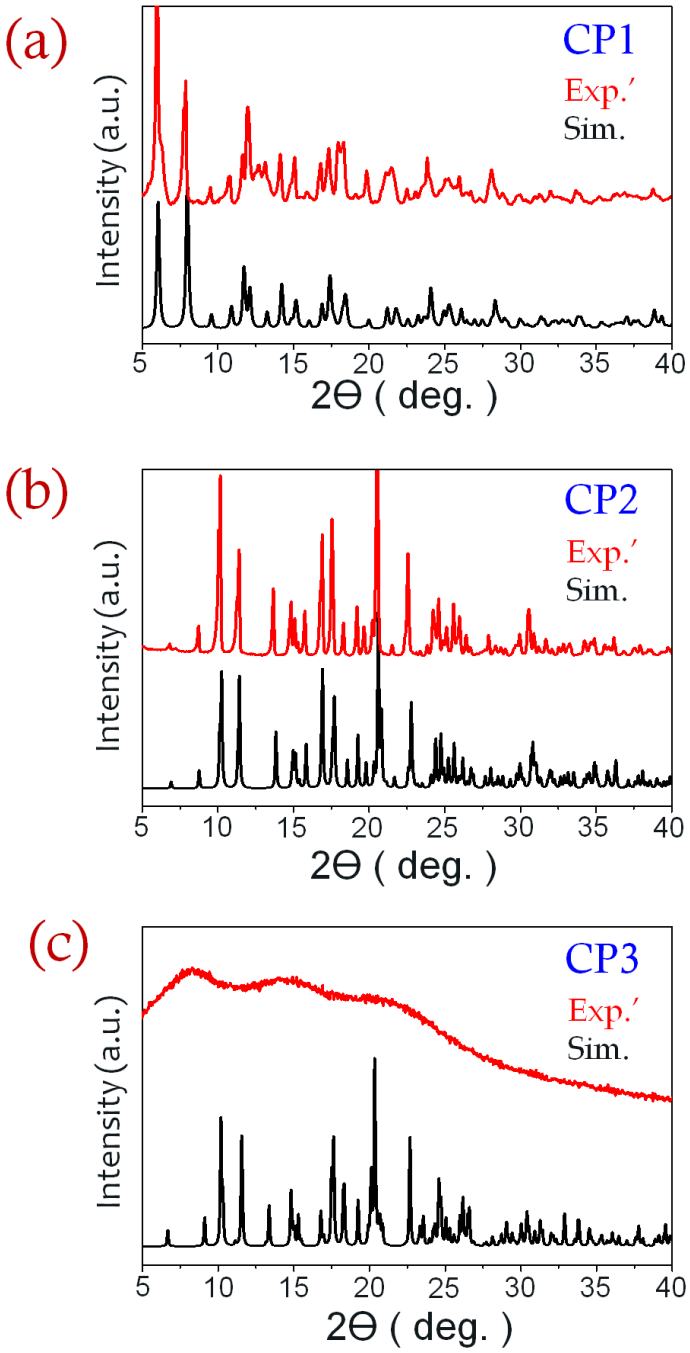
S5. PXRD profiles (Exp.') for the CPs recovered after photocatalysis reactions. Patterns simulated using single crystal data (Sim.) are also presented for Comparison.



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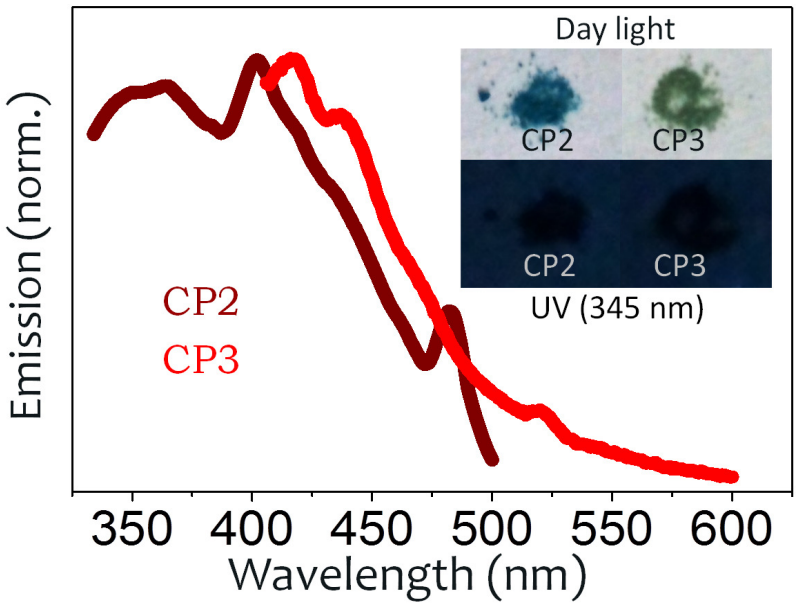
S6. Emission spectra of CP2 and CP3 (Inset comprises of digital photographs captured in day light and UV irradiation for CP2 and CP3).



Moderate intensity emission bands at 364 nm (λ_{ex} 290 nm) for **CP2** and at 416 nm (λ_{ex} 379 nm) for **CP3** were observed. In solid state, geometrical proximity and rigidity of organic linkers can create favourable conformations for intra-ligand charge transfer processes resulting in good emission behaviour of CPs comprising open shell configuration metal nodes such as Cu(II) and Ni(II). Chen and other groups have underlined the complexity of MOF fluorescence in the recent articles and have established that the specific MOF/CP topologies and the rigid structural motifs may result in significant emissive behaviour regardless to the employed metal nodes.[1]

1. (a) Y. Cui, Y. Yue, G. Qian and B. Chen, *Chem. Rev.*, 2012, **112**, 1126; (b) J. J. Perry IV, P. L. Feng, S. T. Meek, K. Leong, F. P. Doty and M. D. Allendorf, *J. Mater. Chem.*, 2012, **22**, 10235; (c) C. C. Wang, W. Z. Lin, W. T. Huang, M. J. Ko, G. H. Lee, M. L. Ho, C. W. Lin, C. W. Shih and P. T. Chou, *Chem. Commun.*, 2008, 1299; (d) N. Zhao, K. Wang, W. Li, Y. Bian, C. Sun, Z. Chang and H. Fan, *Solid State Sci.*, 2011, **13**, 1948; (e) M. Barwiolek, E. Szlyk, T. M. Muzioła and T. Lis, *Dalton Trans.*, 2011, **40**, 11012.

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Table S1. Selected bond length and bond angle for CP1-CP3

CP1			
Cd(1)-N(1)	2.247(9)	Cd(2)-O(4)#2	2.371(7)
Cd(1)-O(9)	2.304(8)	Cd(2)-O(3)#2	2.376(7)
Cd(1)-O(1)	2.328(7)	Cd(2)-O(6)	2.399(7)
Cd(1)-O(5)	2.369(7)	Cd(2)-O(5)	2.470(7)
Cd(1)-O(8)#1	2.450(7)	N(4)-Cd(2)#3	2.272(9)
Cd(1)-O(7)#1	2.452(7)	O(3)-Cd(2)#4	2.376(7)
Cd(1)-O(2)	2.486(6)	O(4)-Cd(2)#4	2.371(7)
Cd(2)-N(4)#1	2.272(9)	O(7)-Cd(2)#3	2.331(6)
Cd(2)-O(10)	2.299(7)	O(7)-Cd(1)#3	2.452(7)
Cd(2)-O(7)#1	2.331(7)	O(8)-Cd(1)#3	2.450(7)
N(1)-Cd(1)-O(9)	89.5(3)	O(3)#2-Cd(2)-O(6)	158.1(3)
N(1)-Cd(1)-O(1)	96.3(3)	N(4)#1-Cd(2)-O(5)	90.0(3)
O(9)-Cd(1)-O(1)	84.7(3)	O(10)-Cd(2)-O(5)	137.3(2)
N(1)-Cd(1)-O(5)	168.8(3)	O(7)#1-Cd(2)-O(5)	74.8(2)
O(9)-Cd(1)-O(5)	88.1(2)	O(4)#2-Cd(2)-O(5)	90.0(2)
O(1)-Cd(1)-O(5)	94.4(3)	O(3)#2-Cd(2)-O(5)	142.4(2)
N(1)-Cd(1)-O(8)#1	82.0(3)	O(6)-Cd(2)-O(5)	53.6(2)
O(9)-Cd(1)-O(8)#1	136.6(2)	N(4)#1-Cd(2)-C(8)#2	99.0(3)
O(1)-Cd(1)-O(8)#1	138.4(2)	O(10)-Cd(2)-C(8)#2	105.8(3)
O(5)-Cd(1)-O(8)#1	92.3(2)	O(7)#1-Cd(2)-C(8)#2	82.4(3)
N(1)-Cd(1)-O(7)#1	94.4(3)	O(4)#2-Cd(2)-C(8)#2	27.6(3)
O(9)-Cd(1)-O(7)#1	85.2(2)	O(3)#2-Cd(2)-C(8)#2	27.5(3)
O(1)-Cd(1)-O(7)#1	165.2(3)	O(6)-Cd(2)-C(8)#2	167.9(3)
O(5)-Cd(1)-O(7)#1	74.5(2)	O(5)-Cd(2)-C(8)#2	116.6(3)
O(8)#1-Cd(1)-O(7)#1	53.6(2)	C(30)-N(4)-Cd(2)#3	126.3(7)
N(1)-Cd(1)-O(2)	97.4(3)	C(29)-N(4)-Cd(2)#3	127.4(8)
O(9)-Cd(1)-O(2)	138.3(3)	C(1)-O(1)-Cd(1)	95.3(6)
O(1)-Cd(1)-O(2)	53.8(2)	C(1)-O(2)-Cd(1)	88.3(6)
O(5)-Cd(1)-O(2)	91.6(2)	C(8)-O(3)-Cd(2)#4	91.6(6)
O(8)#1-Cd(1)-O(2)	85.0(2)	C(8)-O(4)-Cd(2)#4	91.7(6)
O(7)#1-Cd(1)-O(2)	134.6(2)	C(9)-O(5)-Cd(1)	115.0(6)
N(1)-Cd(1)-C(1)	98.4(3)	C(9)-O(5)-Cd(2)	89.8(6)
O(9)-Cd(1)-C(1)	111.5(3)	Cd(1)-O(5)-Cd(2)	102.8(3)
O(1)-Cd(1)-C(1)	27.0(3)	C(9)-O(6)-Cd(2)	93.6(6)
O(5)-Cd(1)-C(1)	92.6(3)	C(16)-O(7)-Cd(2)#3	120.1(6)

O(8)#1-Cd(1)-C(1)	111.8(3)	C(16)-O(7)-Cd(1)#3	92.4(6)
O(7)#1-Cd(1)-C(1)	158.9(3)	Cd(2)#3-O(7)-Cd(1)#3	104.6(3)
O(2)-Cd(1)-C(1)	26.8(3)	C(16)-O(8)-Cd(1)#3	92.4(6)
N(4)#1-Cd(2)-O(10)	88.3(3)	Cd(1)-O(9)-H(9C)	107(8)
N(4)#1-Cd(2)-O(7)#1	163.4(3)	Cd(1)-O(9)-H(9D)	97(8)
O(10)-Cd(2)-O(7)#1	107.4(3)	Cd(2)-O(10)-H(10C)	103(6)
N(4)#1-Cd(2)-O(4)#2	92.4(3)	Cd(2)-O(10)-H(10D)	146(7)
O(10)-Cd(2)-O(4)#2	132.7(2)	O(2)-C(1)-O(1)	122.5(10)
O(7)#1-Cd(2)-O(4)#2	81.2(2)	O(2)-C(1)-Cd(1)	64.9(5)
N(4)#1-Cd(2)-O(3)#2	103.7(3)	O(1)-C(1)-Cd(1)	57.7(5)
O(10)-Cd(2)-O(3)#2	78.8(2)	C(2)-C(1)-Cd(1)	174.6(7)
O(7)#1-Cd(2)-O(3)#2	85.2(2)	O(3)-C(8)-O(4)	121.5(9)
O(4)#2-Cd(2)-O(3)#2	55.1(2)	O(3)-C(8)-Cd(2)#4	60.9(5)
N(4)#1-Cd(2)-O(6)	88.6(3)	O(4)-C(8)-Cd(2)#4	60.6(5)
O(10)-Cd(2)-O(6)	83.7(2)	C(6)-C(8)-Cd(2)#4	179.1(7)
O(7)#1-Cd(2)-O(6)	87.6(2)	O(6)-C(9)-O(5)	122.7(9)
O(4)#2-Cd(2)-O(6)	143.6(2)		
Symmetry transformation: #1 -x,y+1/2,-z+1/2 ; #2 x,y+1,z ; #3 -x,y-1/2, -z+1/2; #4 x,y-1,z			

CP2

Cu(1)-N(1)	1.957(3)	Cu(1)-O(5)	2.221(3)
Cu(1)-N(4)#1	1.968(3)	N(4)-Cu(1)#3	1.968(3)
Cu(1)-O(1)	1.988(3)	O(3)-Cu(1)#4	2.053(3)
Cu(1)-O(3)#2	2.053(3)		
N(1)-Cu(1)-N(4)#1	178.22(13)	C(11)-N(1)-Cu(1)	127.9(3)
N(1)-Cu(1)-O(1)	91.03(12)	C(9)-N(1)-Cu(1)	126.0(3)
N(4)#1-Cu(1)-O(1)	88.51(12)	C(22)-N(4)-Cu(1)#3	127.6(3)
N(1)-Cu(1)-O(3)#2	90.38(12)	C(21)-N(4)-Cu(1)#3	126.7(3)
N(4)#1-Cu(1)-O(3)#2	91.09(12)	C(1)-O(1)-Cu(1)	121.1(3)
O(1)-Cu(1)-O(3)#2	139.15(11)	C(8)-O(3)-Cu(1)#4	127.8(3)
N(1)-Cu(1)-O(5)	85.82(13)	Cu(1)-O(5)-H(5C)	89(3)
N(4)#1-Cu(1)-O(5)	93.08(13)	Cu(1)-O(5)-H(5D)	127(4)
O(1)-Cu(1)-O(5)	127.10(11)	O(2)-C(1)-O(1)	126.4(4)
O(3)#2-Cu(1)-O(5)	93.72(11)	O(4)-C(8)-O(3)	127.0(4)
Symmetry transformation: #1 x-1,y+1,z; #2 x,y-1,z; #3 x+1,y-1,z; #4 x,y+1,z			

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CP3			
Ni(1)-N(4)#1	2.024(5)	Ni(1)-O(2)	2.119(4)
Ni(1)-N(1)	2.033(5)	Ni(1)-O(1)	2.235(4)
Ni(1)-O(5)	2.063(4)	O(4)-Ni(1)#3	2.070(4)
Ni(1)-O(4)#2	2.070(4)	N(4)-Ni(1)#4	2.024(5)
N(4)#1-Ni(1)-N(1)	176.9(2)	O(4)#2-Ni(1)-O(1)	167.45(16)
N(4)#1-Ni(1)-O(5)	88.41(19)	O(2)-Ni(1)-O(1)	60.69(15)
N(1)-Ni(1)-O(5)	94.5(2)	C(1)-O(1)-Ni(1)	85.8(3)
N(4)#1-Ni(1)-O(4)#2	89.94(18)	C(1)-O(2)-Ni(1)	91.7(4)
N(1)-Ni(1)-O(4)#2	90.75(18)	C(8)-O(4)-Ni(1)#3	127.2(4)
O(5)-Ni(1)-O(4)#2	92.72(17)	Ni(1)-O(5)-H(5C)	94(5)
N(4)#1-Ni(1)-O(2)	88.78(18)	Ni(1)-O(5)-H(5D)	136(6)
N(1)-Ni(1)-O(2)	88.16(18)	C(11)-N(1)-Ni(1)	128.7(4)
O(5)-Ni(1)-O(2)	160.22(16)	C(9)-N(1)-Ni(1)	127.5(4)
O(4)#2-Ni(1)-O(2)	106.85(16)	C(22)-N(4)-Ni(1)#4	126.7(4)
N(4)#1-Ni(1)-O(1)	88.35(18)	C(21)-N(4)-Ni(1)#4	128.4(4)
N(1)-Ni(1)-O(1)	90.33(17)	O(2)-C(1)-O(1)	121.6(5)
O(5)-Ni(1)-O(1)	99.66(16)	O(3)-C(8)-O(4)	126.4(6)
Symmetry transformation: #1 x-1,y+1,z; #2 x,y+1,z; #3 x,y-1,z; #4 x+1,y-1,z			