

A Three-Component 1D/2D → 2D Interpenetrated Coordination Network: Structure and Gas Adsorption Studies

Jin-Xiang Chen,^{A,D} Ni-Ni Ding,^B Ming Chen,^A Wen-Hua Chen,^A David J. Young,^B

Wen-Hua Zhang,^{B,D,E} and T. S. Andy Hor^{B,C,D}

^ASchool of Pharmaceutical Sciences, Southern Medical University, Guangzhou 510515, P. R.

China.

^BInstitute of Materials Research and Engineering (IMRE), A*STAR, 3 Research Link, 117602,

Singapore.

^CDepartment of Chemistry, National University of Singapore, 3 Science Drive 3, 117543,

Singapore.

^DCorresponding author. E-mail: jxchen@smu.edu.cn; zhangw@imre.a-star.edu.sg;

andyhor@nus.edu.sg

^EPresent Address: College of Chemistry, Chemical Engineering and Materials Science, Soochow

University, Suzhou 215123, P. R. China. Email: whzhang@suda.edu.cn

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Table S1. Selected bond distances (Å) and angles (°) for complex **1**·25H₂O.

Cd(1)-N(2)#1	2.363(6)	Cd(1)-N(2)#2	2.363(6)
Cd(1)-O(3)#3	2.431(6)	Cd(1)-O(3)	2.431(6)
Cd(1)-O(1)#3	2.485(7)	Cd(1)-O(1)	2.485(7)
Cd(1)-O(2)	2.570(8)	Cd(1)-O(2)#3	2.570(7)
Cd(2)-O(5)	2.238(7)	Cd(2)-O(8)	2.299(6)
Cd(2)-N(4)#4	2.307(6)	Cd(2)-O(7)	2.457(6)
Cd(2)-Br(1)	2.5838(13)	Cd(2)-O(6)	2.625(7)
N(2)#1-Cd(1)-N(2)#2	147.3(3)	N(2)#1-Cd(1)-O(3)#3	130.6(2)
N(2)#2-Cd(1)-O(3)#3	81.4(2)	N(2)#1-Cd(1)-O(3)	81.4(2)
N(2)#2-Cd(1)-O(3)	130.6(2)	O(3)#3-Cd(1)-O(3)	53.8(3)
N(2)#1-Cd(1)-O(1)#3	79.8(2)	N(2)#2-Cd(1)-O(1)#3	102.9(2)
O(3)#3-Cd(1)-O(1)#3	81.0(2)	O(3)-Cd(1)-O(1)#3	90.7(2)
N(2)#1-Cd(1)-O(1)	102.9(2)	N(2)#2-Cd(1)-O(1)	79.8(2)
O(3)#3-Cd(1)-O(1)	90.7(2)	O(3)-Cd(1)-O(1)	81.0(2)
O(1)#3-Cd(1)-O(1)	170.7(3)	N(2)#1-Cd(1)-O(2)	80.9(2)
N(2)#2-Cd(1)-O(2)	75.3(2)	O(3)#3-Cd(1)-O(2)	138.77(19)
O(3)-Cd(1)-O(2)	123.7(2)	O(1)#3-Cd(1)-O(2)	137.0(2)
O(1)-Cd(1)-O(2)	52.2(2)	N(2)#1-Cd(1)-O(2)#3	75.3(2)
N(2)#2-Cd(1)-O(2)#3	80.9(2)	O(3)#3-Cd(1)-O(2)#3	123.7(2)
O(3)-Cd(1)-O(2)#3	138.8(2)	O(1)#3-Cd(1)-O(2)#3	52.2(2)
O(1)-Cd(1)-O(2)#3	137.0(2)	O(2)-Cd(1)-O(2)#3	85.8(3)
O(5)-Cd(2)-O(8)	98.4(3)	O(5)-Cd(2)-N(4)#4	126.0(3)
O(8)-Cd(2)-N(4)#4	85.9(2)	O(5)-Cd(2)-O(7)	79.5(3)
O(8)-Cd(2)-O(7)	54.6(2)	N(4)#4-Cd(2)-O(7)	137.6(2)
O(5)-Cd(2)-Br(1)	127.6(2)	O(8)-Cd(2)-Br(1)	116.09(17)
N(4)#4-Cd(2)-Br(1)	96.06(17)	O(7)-Cd(2)-Br(1)	89.47(17)
O(5)-Cd(2)-O(6)	52.8(2)	O(8)-Cd(2)-O(6)	121.3(3)
N(4)#4-Cd(2)-O(6)	79.0(2)	O(7)-Cd(2)-O(6)	132.0(2)
Br(1)-Cd(2)-O(6)	121.7(2)		

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

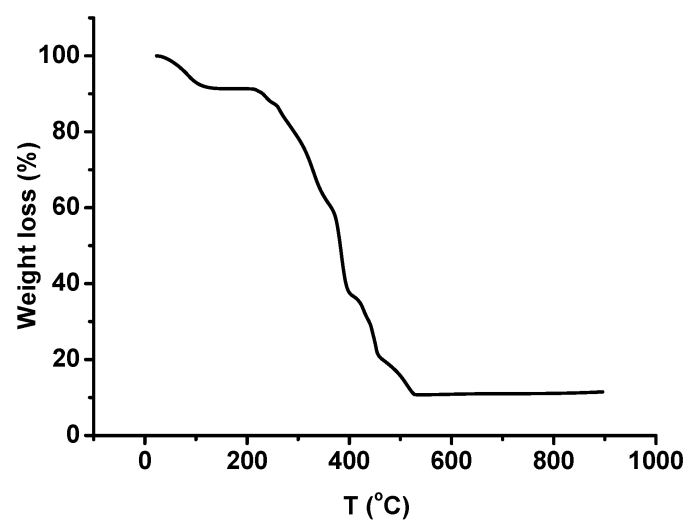


Figure S1. TGA plots of complex 1·10H₂O.

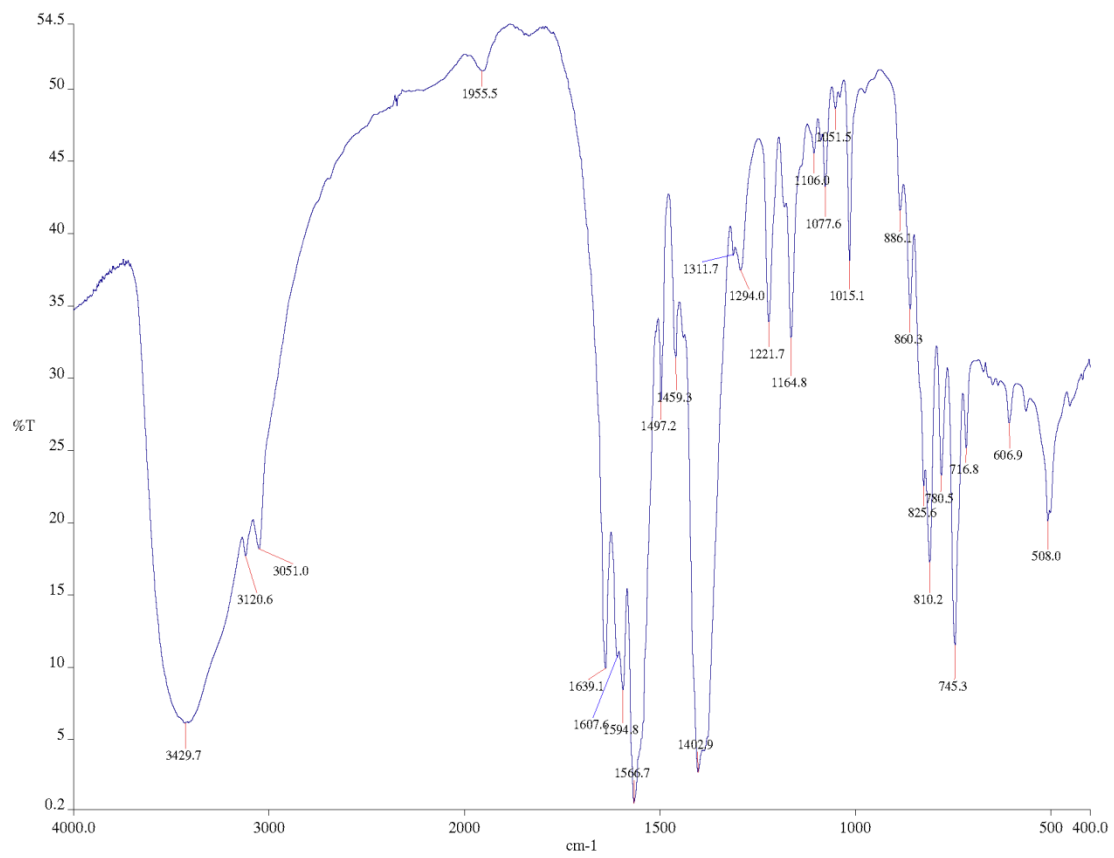


Figure S2. IR spectrum of complex 1·10H₂O.