Supporting Information

A Series of Transition-metal Coordination Complexes Assembled from 3-Nitrophthalic Acid and Thiabendazole: Synthesis, Structure and Properties

Wen-Jia Xu, Qi-Jun Xue,† Peng Liang, Ling-Yu Zhang, Yan-Feng Huang, and Yu Feng*

College of Chemistry and Chemical Engineering, Guangxi University for Nationalities, Nanning 530006, P.R. China
**E-mail: fengyu19871212@126.com*
†*College of pharmacy, Liaoning University, Shenyang 110036, P.R. China*
Received September 3, 2013, Accepted October 28, 2013

Table S1 Experimental data for complexes

Identification code	**1**	**2**	**3**	**4**
Empiricalf formula	$C_{36}H_{26}Cd_2N_8O_{16}S_2$	$C_{36}H_{18}N_8O_{12}S_2Zn_2$	$C_{18}H_{11}N_4O_8SZn_2$	$C_{36}H_{22}Co_2N_8O_{14}S_2$
Formula weight	1115.57	949.44	574.11	972.60
Temperature(k)	296(2)	296(2)	296(2)	296(2)
Crystal system	Triclinic	Triclinic	Triclinic	Monoclinic
Sspace group	P-1	P-1	P-1	P2(1)/c
a (Å)	8.142 (2)	7.668(3)	7.954(2)	7.5577(9)
b (Å)	10.755(2)	9.585(3)	10.975(3)	14.561 (2)
c (Å)	12.302(3)	12.538(4)	11.537(3)	16.154(2)
Volume ($Å^3$)	1006.6(4)	898.4(5)	978.0(4)	1771.2(4)
Z	1	1	2	2
Absorption coefficient (mm^{-1})	1.245	1.531	2.619	1.143
Theta range for data collection	1.70 to 25.00	1.63 to 25.00	1.78 to 25.00	1.89 to 25.00
Reflections collected	5504	4763	5276	9338
Data/restraints/ parameters	3501 / 0 / 289	3112 / 6 / 271	3401 / 0 / 298	3106 / 0 / 280
Goodness-of-fit on F^2	1.136	1.130	1.115	1.050
Final R1 and wR2 [I>2σ(I)]	R1 = 0.0278, wR2 = 0.0714	R1 = 0.0300, wR2 = 0.0837	R1 = 0.0372, wR2 = 0.1138	R1 = 0.0314, wR2 = 0.0871
R1 and wR2 indices (all data)	R1 = 0.0314, wR2 = 0.0782	R1 = 0.0328, wR2 = 0.0855	R1 = 0.0446, wR2 = 0.1243	R1 = 0.0332, wR2 = 0.0885

Bull. Korean Chem. Soc. **2012**, Vol. 33, No. #. 1
http://dx.doi.org/10.5012/bkcs.2012.33.#.XXX

Table S2 Selected bond lengths (Å) and angles (°) for complexes

Complex **1**			
Cd(1)-O(2)	2.261(2)	Cd(1)-N(3)	2.270(3)
Cd(1)-O(7)	2.325(3)	Cd(1)-N(2)	2.359(3)
Cd(1)-O(4)#1	2.372(3)	Cd(1)-O(3)#1	2.468(3)
O(3)-Cd(1)#1	2.468(3)	O(4)-Cd(1)#1	2.372(2)
O(2)-Cd(1)-N(3)	120.3(2)	O(2)-Cd(1)-O(7)	80.75(9)
N(3)-Cd(1)-O(7)	98.9(2)	O(2)-Cd(1)-N(2)	100.3(2)
N(3)-Cd(1)-N(2)	73.2 (2)	O(7)-Cd(1)-N(2)	171.5(2)
O(2)-Cd(1)-O(4)#1	138.72(9)	N(3)-Cd(1)-O(4)#1	100.0(2)
O(7)-Cd(1)-O(4)#1	84.57(9)	N(2)-Cd(1)-O(4)#1	99.8(2)
O(2)-Cd(1)-O(3)#1	94.47(8)	N(3)-Cd(1)-O(3)#1	139.10(9)
O(7)-Cd(1)-O(3)#1	108.03(9)	N(2)-Cd(1)-O(3)#1	80.38(9)
O(4)#1-Cd(1)-O(3)#1	54.23(8)		
Complex **2**			
Zn(1)-O(2)	1.985(2)	Zn(1)-O(5)#1	1.991(2)
Zn(1)-N(1)	2.044(2)	Zn(1)-N(3)	2.150(2)
Zn(1)-O(5)	2.196(2)	O(5)-Zn(1)#1	1.991(2)
O(2)-Zn(1)-O(5)#1	103.11(9)	O(2)-Zn(1)-N(1)	97.83(9)
O(5)#1-Zn(1)-N(1)	122.09(9)	O(2)-Zn(1)-N(3)	150.62(9)
O(5)#1-Zn(1)-N(3)	103.27(9)	N(1)-Zn(1)-N(3)	78.75(9)
O(2)-Zn(1)-O(5)	84.26(9)	O(5)#1-Zn(1)-O(5)	77.14(8)
N(1)-Zn(1)-O(5)	159.07(9)	N(3)-Zn(1)-O(5)	89.20(9)
Complex **3**			
Zn(1)-O(7)	1.924(3)	Zn(1)-O(4)	1.961(3)
Zn(1)-O(2)#1	1.984(3)	Zn(1)-N(2)#2	1.989(3)
Zn(2)-O(8)	1.956(3)	Zn(2)-O(7)	1.981(3)
Zn(2)-N(3)	2.063(3)	Zn(2)-N(4)	2.117(4)
Zn(2)-O(1)#1	2.251(3)	O(1)-Zn(2)#1	2.251(3)
O(2)-Zn(1)#1	1.984(3)	N(2)-Zn(1)#2	1.989(3)
O(7)-Zn(1)-O(4)	112.8 (2)	O(7)-Zn(1)-O(2)#1	105.6 (2)
O(4)-Zn(1)-O(2)#1	105.6 (2)	O(7)-Zn(1)-N(2)#2	115.9(2)
O(4)-Zn(1)-N(2)#2	107.9(2)	O(2)#1-Zn(1)-N(2)#2	108.4(2)
O(8)-Zn(2)-O(7)	110.5(2)	O(8)-Zn(2)-N(3)	106.3(2)
O(7)-Zn(2)-N(3)	100.2 (2)	O(8)-Zn(2)-N(4)	123.4(2)
O(7)-Zn(2)-N(4)	124.3 (2)	N(3)-Zn(2)-N(4)	78.4(2)
O(8)-Zn(2)-O(1)#1	82.7 (2)	O(7)-Zn(2)-O(1)#1	88.0(2)
N(3)-Zn(2)-O(1)#1	164.5(2)	N(4)-Zn(2)-O(1)#1	86.1(2)
Complex **4**			
O(7)-Co(1)#1	2.381 (2)	O(6)-Co(1)#2	2.099 (2)
O(1)-Co(1)	2.095(2)	Co(1)-O(5)	2.075(2)
Co(1)-N(4)	2.095(2)	Co(1)-O(6)#2	2.099 (2)
Co(1)-N(3)	2.149(2)	Co(1)-O(7)#3	2.382(2)
O(5)-Co(1)-N(4)	100.32(7)	O(5)-Co(1)-O(1)	94.03(6)
N(4)-Co(1)-O(1)	165.53(7)	O(5)-Co(1)-O(6)#2	88.42(6)
N(4)-Co(1)-O(6)#2	92.19(6)	O(1)-Co(1)-O(6)#2	90.04(6)
O(5)-Co(1)-N(3)	98.17(6)	N(4)-Co(1)-N(3)	79.27(7)
O(1)-Co(1)-N(3)	96.96(7)	O(6)#2-Co(1)-N(3)	170.00(7)
O(5)-Co(1)-O(7)#3	174.56(6)	N(4)-Co(1)-O(7)#3	80.04(7)
O(1)-Co(1)-O(7)#3	85.85(6)	O(6)#2-Co(1)-O(7)#3	86.14(6)
N(3)-Co(1)-O(7)#3	87.24(6)		

Table S3 Hydrogen-bond geometry (Å) and angles (°) for complexes

D-H···A	D-H	H···A	D···A	D-H···A	Symmetry codes
Complex **1**					
O7-H7A···O8	0.85	1.93	2.741(4)	159	-x+1, -y+1, -z+1
O7-H7B···O3	0.85	1.93	2.740(4)	159	
O7-H7B···O2	0.85	2.49	2.971	117	
O8-H8A···O4	0.85	2.29	2.826(4)	121	-x, -y+1, -z+1
O8-H8B···O4	0.85	2.55	2.826(4)	100	
C10-H10···O1	0.93	2.39	3.223(5)	148	
Complex **2**					
C7-H7···O1	0.93	2.48	3.296(4)	146	
C13-H13···O3	0.93	2.45	3.358(4)	164	
Complex **3**					
O8-H8A···O3	0.85	1.83	2.678(5)	179	-x+2, -y+2, -z+1
O8-H8B···O4	0.85	1.89	2.736(4)	179	x+1, y, z
C3-H3···O1	0.93	2.42	2.746(6)	100	
C9-H9···O2	0.93	2.52	3.232(5)	134	
C17-H17···O6	0.93	2.53	3.141(6)	123	
C17-H17···O7	0.93	2.43	3.202(5)	140	
C18-H18···O5	0.93	2.38	3.113(6)	135	
Complex **4**					
O1-H1B···O5	0.85	2.23	3.050	163	
O1-H1C···O6	0.85	2.48	2.966	117	-x, -y+2, -z
O1-H1C···O7	0.85	1.82	2.668	177	-x, -y+2, -z
C3-H3···O2	0.93	2.36	2.675(3)	100	
C17-H17···O3	0.93	2.40	2.997(3)	122	
C17-H17···O4	0.93	2.57	3.404(3)	149	
C18-H18···O5	0.93	2.36	3.275(3)	170	

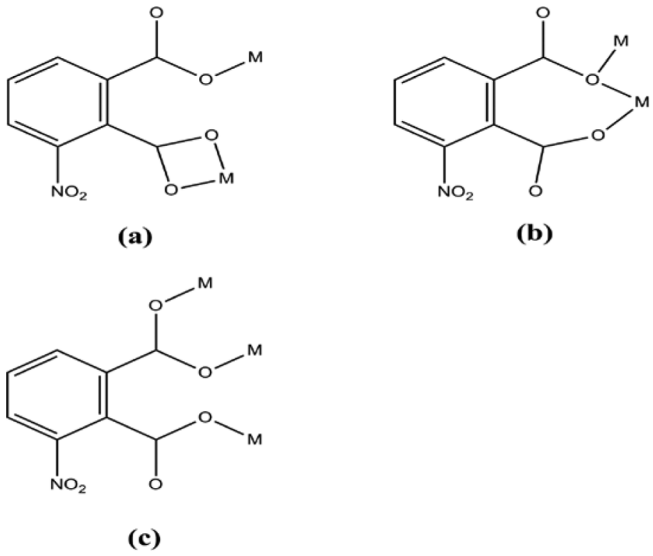

Figure S1. Coordination modes of the 3-NPA^{2-} anion, a in **1**; b in **2**; c in **3** and **4**.

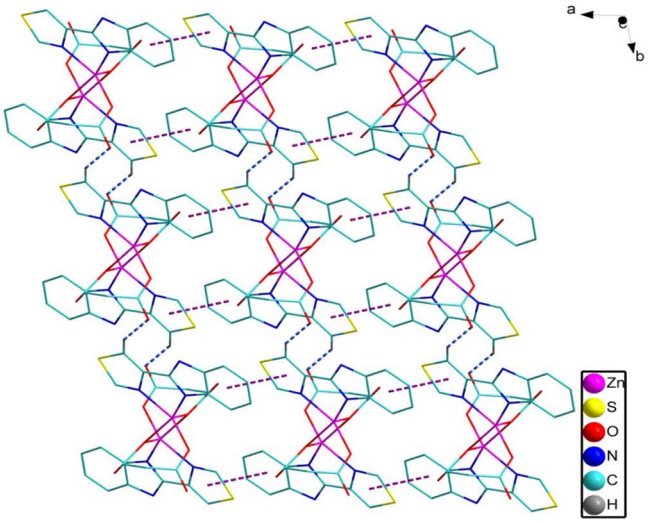

Figure S2. Infinite 2D networks of **2** connected by O-H···O hydrogen bonds and ð-ð stacking interactions. Unnecessary atoms are omitted for clarity.