Syntheses, Structures, and Magnetic Properties of One-dimensional Coordination Polymers Based on N-Succinopyridine Ligand

Li-Zhen Cai,^{a,b} Ming-Sheng Wang,^a Shuai-Hua Wang,^a Pei-Xin Li,^a Guo-Cong Guo,^{a,*} and Jin-Shun Huang^a

a State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China b Key Laboratory of Coal to Ethylene Glycol and Its Related Technology, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China

1	
Cu(1)-O(1)	1.940(2)
Cu(1)-O(3)#1	1.946(2)
Cu(1)-O(2W)	1.956(3)
Cu(1)-O(1W)	1.976(3)
Cu(1)-O(3)#2	2.296(3)
Cu(1)-Cu(1)#3	3.3178(10)
Cu(1)-Cu(1)#4	6.3994(13)
Cu(1)-Cu(1)#2	7.2505(9)
O(1)-Cu(1)-O(3)#1	176.08(11)
O(1)-Cu(1)-O(2W)	87.52(12)
O(3)#1-Cu(1)-O(2W)	89.51(11)
O(1)-Cu(1)-O(1W)	92.69(11)
O(3)#1-Cu(1)-O(1W)	90.71(11)
O(2W)-Cu(1)-O(1W)	169.38(12)
O(1)-Cu(1)-O(3)#2	100.62(10)
O(3)#1-Cu(1)-O(3)#2	77.38(10)
O(2W)-Cu(1)-O(3)#2	99.93(11)
O(1W)-Cu(1)-O(3)#2	90.48(11)
2	
Pr(1)-O(1)	2.413(2)
Pr(1)-O(3)#1	2.425(3)
Pr(1)-O(4)#2	2.476(3)
Pr(1)-O(3W)	2.476(3)
Pr(1)-O(2W)	2.510(3)
Pr(1)-O(4W)	2.539(3)
Pr(1)-O(1W)	2.566(3)

Table S1. Selected bond lengths (Å) and angles (°) for 1-5.

* Author to whom correspondence should be addressed. E-mail: gcguo@fjirsm.ac.cn (G.-C.Guo).

Pr(1)-O(1)#3	2.566(3)
Pr(1)-O(2)#3	2.696(3)
Pr(1)-Pr(1)#3	4.0302(5)
Pr(1)-Pr(1)#4	7.181(3)
O(1)-Pr(1)-O(3)#1	74.91(9)
O(1)-Pr(1)-O(4)#2	72.47(9)
O(3)#1-Pr(1)-O(4)#2	137.20(8)
O(1)-Pr(1)-O(3W)	148.62(10)
O(3)#1-Pr(1)-O(3W)	83.57(10)
O(4)#2-Pr(1)-O(3W)	136.31(9)
O(1)-Pr(1)-O(2W)	86.00(11)
O(3)#1-Pr(1)-O(2W)	138.16(10)
O(4)#2-Pr(1)-O(2W)	65.64(10)
O(3W)-Pr(1)-O(2W)	95.54(12)
O(1)-Pr(1)-O(4W)	139.85(9)
O(3)#1-Pr(1)-O(4W)	138.92(9)
O(4)#2-Pr(1)-O(4W)	67.38(9)
O(3W)-Pr(1)-O(4W)	70.14(9)
O(2W)-Pr(1)-O(4W)	77.13(10)
O(1)-Pr(1)-O(1W)	80.66(9)
O(3)#1-Pr(1)-O(1W)	71.79(10)
O(4)#2-Pr(1)-O(1W)	127.71(9)
O(3W)-Pr(1)-O(1W)	70.95(10)
O(2W)- $Pr(1)$ - $O(1W)$	68.54(10)
O(4W)- $Pr(1)$ - $O(1W)$	124.18(9)
O(1)-Pr(1)-O(1)#3	71.93(9)
O(3)#1-Pr(1)-O(1)#3	73.52(9)
O(4)#2-Pr(1)-O(1)#3	70.54(8)
O(3W)-Pr(1)-O(1)#3	123.55(10)
O(2W)-Pr(1)-O(1)#3	135.13(10)
O(4W)-Pr(1)-O(1)#3	94.95(9)
O(1W)-Pr(1)-O(1)#3	140.19(9)
O(1)-Pr(1)-O(2)#3	118.82(8)
O(3)#1-Pr(1)-O(2)#3	74.38(9)
O(4)#2-Pr(1)-O(2)#3	98.10(9)
O(3W)-Pr(1)-O(2)#3	75.42(10)
O(2W)-Pr(1)-O(2)#3	145.94(10)
O(4W)-Pr(1)-O(2)#3	68.88(9)
O(1W)-Pr(1)-O(2)#3	134.18(9)
O(1)#3-Pr(1)-O(2)#3	49.09(8)
3	
Eu(1)-O(4W)	2.389(3)
Eu(1)-O(5W)	2.434(3)
Eu(1)-O(1W)	2.437(3)

Eu(1)-O(1)	2.452(3)
Eu(1)-O(2W)	2.455(4)
Eu(1)-O(3W)	2.455(3)
Eu(1)-O(4)#1	2.479(3)
Eu(1)-O(3)#1	2.496(3)
Eu(1)-O(2)	2.607(3)
O(4W)-Eu(1)-O(5W)	72.41(10)
O(4W)-Eu(1)-O(1W)	139.93(11)
O(5W)-Eu(1)-O(1W)	143.60(10)
O(4W)-Eu(1)-O(1)	77.58(10)
O(5W)-Eu(1)-O(1)	76.03(10)
O(1W)-Eu(1)-O(1)	93.25(11)
O(4W)-Eu(1)-O(3W)	81.28(10)
O(5W)-Eu(1)-O(3W)	140.60(11)
O(1W)-Eu(1)-O(3W)	73.22(11)
O(1)-Eu(1)-O(3W)	126.57(12)
O(4W)-Eu(1)-O(2W)	136.59(10)
O(5W)-Eu(1)-O(2W)	68.74(10)
O(1W)-Eu(1)-O(2W)	74.90(11)
O(1)-Eu(1)-O(2W)	75.01(10)
O(3W)-Eu(1)-O(2W)	142.07(10)
O(4W)-Eu(1)-O(4)#1	124.61(10)
O(5W)-Eu(1)-O(4)#1	90.18(10)
O(1W)-Eu(1)-O(4)#1	81.69(11)
O(1)-Eu(1)-O(4)#1	149.35(10)
O(3W)-Eu(1)-O(4)#1	81.05(12)
O(2W)-Eu(1)-O(4)#1	74.48(10)
O(4W)-Eu(1)-O(3)#1	72.36(10)
O(5W)-Eu(1)-O(3)#1	71.55(10)
O(1W)-Eu(1)-O(3)#1	125.80(11)
O(1)-Eu(1)-O(3)#1	140.94(11)
O(3W)-Eu(1)-O(3)#1	72.83(12)
O(2W)-Eu(1)-O(3)#1	111.51(10)
O(4)#1-Eu(1)-O(3)#1	52.28(10)
O(4W)-Eu(1)-O(2)	74.12(10)
O(5W)-Eu(1)-O(2)	122.31(10)
O(1W)-Eu(1)-O(2)	69.96(11)
O(1)-Eu(1)-O(2)	51.61(10)
O(3W)-Eu(1)-O(2)	75.56(12)
O(2W)-Eu(1)-O(2)	111.74(10)
O(4)#1-Eu(1)-O(2)	147.31(10)
O(3)#1-Eu(1)-O(2)	136.60(10)
4	
Gd(1)-O(4W)	2.369(2)

Gd(1)-O(1W)	2.418(3)
Gd(1)-O(2W)	2.421(4)
Gd(1)-O(5W)	2.426(2)
Gd(1)-O(3W)	2.444(3)
Gd(1)-O(1)	2.450(2)
Gd(1)-O(3)#1	2.465(2)
Gd(1)-O(4)#1	2.490(2)
Gd(1)-O(2)	2.588(2)
O(4W)-Gd(1)-O(1W)	139.25(10)
O(4W)-Gd(1)-O(2W)	81.43(10)
O(1W)-Gd(1)-O(2W)	72.51(11)
O(4W)-Gd(1)-O(5W)	73.19(9)
O(1W)-Gd(1)-O(5W)	143.73(9)
O(2W)-Gd(1)-O(5W)	140.83(10)
O(4W)-Gd(1)-O(3W)	136.55(9)
O(1W)-Gd(1)-O(3W)	75.21(10)
O(2W)-Gd(1)-O(3W)	142.01(10)
O(5W)-Gd(1)-O(3W)	68.53(9)
O(4W)-Gd(1)-O(1)	77.32(9)
O(1W)-Gd(1)-O(1)	93.53(10)
O(2W)-Gd(1)-O(1)	126.61(10)
O(5W)-Gd(1)-O(1)	76.45(8)
O(3W)-Gd(1)-O(1)	74.48(8)
O(4W)-Gd(1)-O(3)#1	125.10(8)
O(1W)-Gd(1)-O(3)#1	81.54(9)
O(2W)-Gd(1)-O(3)#1	80.95(10)
O(5W)-Gd(1)-O(3)#1	89.68(8)
O(3W)-Gd(1)-O(3)#1	74.96(8)
O(1)-Gd(1)-O(3)#1	149.30(8)
O(4W)-Gd(1)-O(4)#1	73.01(8)
O(1W)-Gd(1)-O(4)#1	125.36(9)
O(2W)-Gd(1)-O(4)#1	72.99(10)
O(5W)-Gd(1)-O(4)#1	71.34(8)
O(3W)-Gd(1)-O(4)#1	111.85(9)
O(1)-Gd(1)-O(4)#1	141.11(9)
O(3)#1-Gd(1)-O(4)#1	52.13(8)
O(4W)-Gd(1)-O(2)	73.41(9)
O(1W)-Gd(1)-O(2)	70.12(9)
O(2W)-Gd(1)-O(2)	75.58(10)
O(5W)-Gd(1)-O(2)	122.69(8)
O(3W)-Gd(1)-O(2)	111.35(8)
O(1)-Gd(1)-O(2)	51.56(8)
O(3)#1-Gd(1)-O(2)	147.43(8)
O(4)#1-Gd(1)-O(2)	136.64(8)

5	
Er(1)-O(2)	2.2902(17)
Er(1)-O(4)#1	2.2953(14)
Er(1)-O(3W)	2.303(2)
Er(1)-O(1W)	2.3041(17)
Er(1)-O(2W)	2.344(2)
Er(1)-O(4W)	2.3560(19)
Er(1)-O(3)#2	2.4364(17)
Er(1)-O(4)#2	2.5002(15)
Er(1)-C(4)#2	2.847(2)
Er(1)-Er(1)#3	3.9922(8)
Er(1)-Er(1)#1	8.4239(19)
O(2)-Er(1)-O(4)#1	85.17(5)
O(2)-Er(1)-O(3W)	75.49(6)
O(2)-Er(1)-O(1W)	81.02(5)
O(2)-Er(1)-O(2W)	70.68(7)
O(2)-Er(1)-O(4W)	138.82(6)
O(2)-Er(1)-O(3)#2	144.69(6)
O(2)-Er(1)-O(4)#2	135.55(6)
O(4)#1-Er(1)-O(3W)	97.08(7)
O(4)#1-Er(1)-O(1W)	164.27(6)
O(4)#1-Er(1)-O(2W)	87.74(6)
O(4)#1-Er(1)-O(4W)	83.84(6)
O(4)#1-Er(1)-O(3)#2	119.08(5)
O(4)#1-Er(1)-O(4)#2	67.36(6)
O(3)#2-Er(1)-O(4)#2	52.39(5)
O(1W)-Er(1)-O(2W)	80.61(7)
O(1W)-Er(1)-O(4W)	101.68(7)
O(1W)-Er(1)-O(3)#2	76.64(5)
O(1W)-Er(1)-O(4)#2	128.23(5)
O(2W)-Er(1)-O(3)#2	130.59(6)
O(2W)-Er(1)-O(4W)	69.34(7)
O(2W)-Er(1)-O(4)#2	137.74(6)
O(3W)-Er(1)-O(1W)	86.76(8)
O(3W)-Er(1)-O(2W)	145.28(7)
O(3W)-Er(1)-O(3)#2	76.27(6)
O(3W)-Er(1)-O(4W)	145.29(6)
O(3W)-Er(1)-O(4)#2	74.17(6)
O(4W)-Er(1)-O(4)#2	74.29(6)
O(4W)-Er(1)-O(3)#2	73.19(6)

Symmetry codes for 1: #1 x-1,y,z; #2 -x+1,-y+2,-z+1; #3 -x,-y+2,-z+1;#4 -x+1,-y+1,-z+1;#5 x+1,y,z; for 2: #1 x+1,y,z; #2 -x,-y,-z-1; #3 -x+1,-y,-z-1; #4 x-1,y,z; for 3: #1 x,-y+3/2,z+1/2; #2 x,-y+3/2,z-1/2; #3 x,-y+1/2,z+1/2; #4 x,-y+1/2,z+1/2; #4 x,-y+1/2,z+1/2; #4 x,-y+1/2,z+1/2; #4 x,-y+1/2,z+1/2; #4 x,-y+1/2,z+1/2; #4 x,-y+3/2,z+1/2; #3 x,y,z+1; #4 x,y,z-1; for 5: #1 -x+1,-y+1,-z; #2 x,y-1,z; #3 -x+1,-y,-z; #4 x,y+1,z

D-H	HA	DA	<(DHA)	D-HA
1				
0.848(10)	2.198(12)	3.041(4)	173(5)	O1W-H1WBCl1
0.847(10)	1.863(15)	2.701(4)	170(5)	O1W-H1WAO2_\$1
0.846(10)	2.250(14)	3.091(3)	173(5)	O2W-H2WACl1_\$2
0.846(11)	1.821(18)	2.648(6)	165(6)	O2W-H2WBO3W
0.850(11)	2.294(12)	3.144(5)	178(7)	O3W-H3WACl1_\$3
0.849(11)	1.93(2)	2.754(7)	163(7)	O3W-H3WBO4W_\$4
0.849(11)	2.31(5)	2.961(5)	134(6)	O4W-H4WBO2_\$5
0.850(11)	1.895(19)	2.726(6)	166(7)	O4W-H4WAO4
2				
0.843(10)	2.295(11)	3.136(3)	176(4)	O1W-H1WACl2_\$1
0.845(10)	2.299(19)	3.101(3)	159(4)	O2W-H2WACl2_\$1
0.849(10)	2.211(12)	3.054(3)	172(4)	O3W-H3WBCl1_\$1
0.852(10)	2.311(13)	3.139(3)	164(3)	O4W-H4WBCl1_\$1
0.841(10)	2.36(2)	3.144(3)	156(4)	O1W-H1WBCl2_\$2
0.849(10)	2.36(2)	3.161(3)	158(4)	O3W-H3WACl2_\$4
0.854(10)	2.325(16)	3.154(3)	164(4)	O4W-H4WACl1_\$5
3				
0.848(7)	2.62(2)	3.079(3)	115.1(18)	O5W-H5WBCl2_\$2
0.847(7)	2.856(18)	3.295(3)	114.2(15)	O2W-H2WBCl1_\$2
0.848(8)	1.894(10)	2.716(4)	162.6(19)	O6W-H6WBO1_\$5
0.848(8)	2.295(9)	3.112(4)	161.6(13)	O1W-H1WBCl2
0.847(8)	1.826(9)	2.669(4)	173.3(19)	O4W-H4WAO6W
4				
0.851(10)	2.267(12)	3.098(3)	165(2)	O6W-H6WACl2_\$1
0.849(10)	1.878(12)	2.723(4)	174(3)	O6W-H6WBO1_\$2
0.846(10)	2.446(12)	3.276(3)	167(2)	O3W-H3WACl2_\$2
0.849(10)	1.955(13)	2.776(3)	162(3)	O5W-H5WAO3_\$3
0.848(10)	2.247(14)	3.068(3)	163(2)	O5W-H5WBCl1_\$4
0.846(10)	1.820(10)	2.663(3)	174(3)	O4W-H4WAO6W_\$4
0.849(10)	2.270(13)	3.085(3)	161(2)	O4W-H4WBCl1_\$5
0.847(10)	2.000(12)	2.832(3)	167(2)	O3W-H3WBO4_\$6
0.852(10)	2.288(12)	3.113(3)	163(2)	O1W-H1WBCl1_\$6
5				
0.851(6)	2.297(7)	3.1448(19)	174(3)	O1W-H1WBCl1_\$1
0.850(7)	2.307(11)	3.103(2)	156.0(17)	O2W-H2WBCl2
0.845(7)	2.159(9)	2.853(4)	139.3(7)	O3W-H3WAO5W_\$3
0.850(7)	1.745(6)	2.573(3)	164.1(14)	O3W-H3WBO1
0.850(7)	2.465(13)	2.812(3)	105.3(12)	O3W-H3WBO2
0.846(5)	2.242(7)	3.076(2)	168.5(14)	O4W-H4WBCl2_\$4
0.857(6)	2.309(8)	3.102(3)	153.9(14)	O5W-H5WBCl1

 Table S2. Specified hydrogen bonds for 1-5 (with esds except fixed and riding H).

Symmetry codes for 1: \$1 -x+1, -y+1, -z+1; \$2 -x, -y+2, -z+1; \$3 x, y, z+1; \$4 x-1, y+1, z; \$5 x+1, y, z; for

2: \$1 -x+2, -y, -z; \$2 x-1, y, z; \$3 -x, -y, -z-1; \$4 -x+3, -y, -z; \$5 x-1, y-1, z-1; for **3**: \$1 -x, -y+2, -z; \$2 -x, y-1/2, -z+1/2; \$3 x, y-1, z; \$4 x, -y+5/2, z-1/2; \$5 -x, -y+1, -z; for **4**: \$1 x, y+1, z; \$2 -x, y+1/2, -z+1/2; \$3 -x, -y+1, -z+1; \$4 x, -y+3/2, z+1/2; \$5 -x, -y+1, -z+1; \$6 -x, -y+2, -z+1; for **5**: \$1 -x+2, y+1/2, -z+/2; \$2 x, y+1, z; \$3 -x+2, -y, -z; \$4 -x+1, y-1/2, -z+1/2.



Figure S1. PXRD patterns of 1-5.

IR spectra of 1–5 (Figure S2) show a strong, broad band at 3055–3600 cm⁻¹, assignable to v(OH) of lattice water molecules, in agreement with participation in hydrogen bonds. The strong absorption at 1488 cm⁻¹ and ~1415 cm⁻¹ is attributed to $v_{(CN)}$ and $\delta_{(CH2)}$, respectively. Characteristic peaks of the coordinated COO⁻ at 1614 cm⁻¹ for 1, 1656 and 1583 cm⁻¹ for 2, 1637, 1606 and 1552 cm⁻¹ for 3 or 4, and 1633 and 1587 cm⁻¹ for 5 are attributed to $v_{as}(COO^-)$, while those at 1385 cm⁻¹ for 1, 1388 and 1374 cm⁻¹ for 2, 1384 and 1343 cm⁻¹ for 3 or 4, 1445 and 1374 cm⁻¹ for 5 are ascribed to $v_s(COO^-)$. Deacon and Phillips¹ have proved that the difference Δ between the asymmetrical and symmetrical stretching frequencies of the coordinated carboxylate group, $v_{as}(COO^-)$ and $v_s(COO^-)$, are closely related to carboxylate coordination modes. The different Δ values of 229 cm⁻¹ for 1, 239 cm⁻¹ for 2, 215 cm⁻¹ for 3 and 4, 200 cm⁻¹ for 5 indicate the presence of various coordination modes in 1–5, as confirmed by the single-crystal analysis.





Figure S3. Optical diffuse reflectance spectra for 1–5.



Figure S4. View of the hydrogen bonding 2-D framework of 1 along the *b* axis.



Figure S5. View of the hydrogen bonding 3-D framework of 1 along the *a* axis.



Figure S6. View of the hydrogen bonding 3-D framework of 2 along the *a* axis.



Figure S7. View of the hydrogen bonding 2-D framework of 4 along the *a* axis.



Figure S8. View of the hydrogen bonding 2-D framework of **5** along the *a* axis.



Figure S9. View of the hydrogen bonding 3-D framework of 5 along the *b* axis.

¹ G. B. Deacon and R. J. Phillips, *Coord. Chem. Rev.*, 1980, **33**, 227.