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Supplementary Material

Two different barium(II) 2D coordination polymers constructed by pyrazine-2,3-dicarboxylate: synthesis, crystal structures and thermal decomposition to barium(II) carbonate nanoparticles

Masoumeh Tabatabaee[a]*, Boris-Marko Kukovec[b], Saeed Amjad[a], Masoud R. Shishebor[a]

[a]*Department of Chemistry, Yazd Branch, Islamic Azad University, Yazd, Iran*

[b]*Laboratory of General and Inorganic Chemistry, Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, HR-10000 Zagreb, Croatia*

[*]Corresponding author:

M. Tabatabaee

Department of Chemistry, Islamic Azad University, Yazd Branch, Yazd, Iran

E-mail: tabatabaee@iauyazd.ac.ir

Fax: +983518223313

Phone: +983518117582

X-ray Crystallographic Analysis

The X-ray diffraction data were corrected for Lorentz-polarization factor and scaled for the absorption effects by multi-scan using SORTAV [a] for **1** and SADABS [b] for **2**.

The structure of **1** was refined as a three-component twin (BASF instruction 0.24808 0.10272). The positions of the hydrogen atoms belonging to the Csp^2 carbon atoms were geometrically optimized applying the riding model (Csp^2–H, 0.95 Å, U_{iso}(H) = 1.2 U_{eq}(C)). The positions of hydrogen atoms belonging to the water molecules in **1** were also geometrically optimized applying the riding model (O–H, 0.84 Å, U_{iso}(H) = 1.5 U_{eq}(O)). The positions of hydrogen atoms belonging to the water molecules and to the carboxylic groups in **2** were found in the difference Fourier maps and O–H distances were restrained to the average value of 0.84 Å, using SHELXL-97 DFIX instruction. The isotropic U_{iso}(H) values for these H atoms were fixed at the same time (U_{iso}(H) = 1.2U_{eq}(O)).

The affirmation of the chosen space groups and the analysis of molecular geometry and hydrogen bonds were performed by PLATON [c].

[a] R. H. Blessing, ActaCrystallogr. A51 (1995) 33.

[b] G.M. Sheldrick, SADABS, University of Göttingen, Germany, 1996.

[c] A.L. Spek, J. Appl. Crystallogr. 36 (2003) 7.

Table S1. Selected bond angles (˚) for **1** and **2**.

1		**2**	
	Bond angles		
O6^{ii}–Ba1–O4	126.0(2)	O8^{vi}–Ba1–O4	153.20(6)
O6^{ii}–Ba1–O7^{iii}	66.9(2)	O8^{vi}–Ba1–O1	70.48(6)
O4–Ba1–O7^{iii}	166.3(2)	O4–Ba1–O1	135.68(6)
O6^{ii}–Ba1–O2^{i}	74.3(2)	O8^{vi}–Ba1–O3	88.43(6)
O4–Ba1–O2^{i}	125.5(2)	O4–Ba1–O3	72.64(6)
O7^{iii}–Ba1–O2^{i}	59.1(2)	O1–Ba1–O3	121.84(6)
O6^{ii}–Ba1–O2	139.8(2)	O8^{vi}–Ba1–O2	135.94(6)
O4–Ba1–O2	93.5(2)	O4–Ba1–O2	70.73(6)
O7^{iii}–Ba1–O2	74.7(2)	O1–Ba1–O2	65.59(6)
O2^{i}–Ba1–O2	76.54(9)	O3–Ba1–O2	117.28(6)
O6^{ii}–Ba1–O5^{ii}	64.0(2)	O8^{vi}–Ba1–O8^{v}	113.48(4)
O4–Ba1–O5^{ii}	75.3(2)	O4–Ba1–O8^{v}	71.86(5)
O7^{iii}–Ba1–O5^{ii}	117.6(2)	O1–Ba1–O8^{v}	101.92(6)
O2^{i}–Ba1–O5^{ii}	72.2(1)	O3–Ba1–O8^{v}	135.84(5)
O2–Ba1–O5^{ii}	130.2(1)	O2–Ba1–O8^{v}	73.69(5)
O6^{ii}–Ba1–O1	72.6(2)	O8^{vi}–Ba1–O10^{vii}	69.02(5)
O4–Ba1–O1	102.7(2)	O4–Ba1–O10^{vii}	85.33(5)
O7^{iii}–Ba1–O1	75.5(2)	O1–Ba1–O10^{vii}	138.96(6)
O2^{i}–Ba1–O1	131.4(2)	O3–Ba1–O10^{vii}	63.39(5)
O2–Ba1–O1	109.0(2)	O2–Ba1–O10^{vii}	153.43(5)
O5^{ii}–Ba1–O1	120.7(2)	O8^{v}–Ba1–O10^{vii}	88.29(5)
O6^{ii}–Ba1–O7^{iv}	136.2(2)	O8^{vi}–Ba1–O4^{v}	69.64(5)
O4–Ba1–O7^{iv}	70.0(2)	O4–Ba1–O4^{v}	114.81(4)
O7^{iii}–Ba1–O7^{iv}	97.5(1)	O1–Ba1–O4^{v}	79.81(6)
O2^{i}–Ba1–O7^{iv}	134.2(2)	O3–Ba1–O4^{v}	142.70(5)
O2–Ba1–O7^{iv}	58.6(2)	O2–Ba1–O4^{v}	98.96(5)
O5^{ii}–Ba1–O7^{iv}	144.8(2)	O8^{v}–Ba1–O4^{v}	44.67(5)
O1–Ba1–O7^{iv}	63.8(2)	O10^{vii}–Ba1–O4^{v}	80.37(5)
O6^{ii}–Ba1–O3	123.2(2)	O8^{vi}–Ba1–N1	94.01(6)
O4–Ba1–O3	62.8(2)	O4–Ba1–N1	90.46(6)
O7^{iii}–Ba1–O3	116.1(2)	O1–Ba1–N1	72.63(6)
O2^{i}–Ba1–O3	64.7(1)	O3–Ba1–N1	55.00(5)
O2–Ba1–O3	64.8(1)	O2–Ba1–N1	76.27(6)
O5^{ii}–Ba1–O3	67.1(2)	O8^{v}–Ba1–N1	148.80(6)
O1–Ba1–O3	162.5(2)	O10^{vii}–Ba1–N1	116.39(5)
O7^{iv}–Ba1–O3	100.5(2)	O4^{v}–Ba1–N1	151.52(5)
O6^{ii}–Ba1–N1	76.1(2)		
O4–Ba1–N1	55.7(2)		
O7^{iii}–Ba1–N1	131.7(2)		
O2^{i}–Ba1–N1	137.4(2)		
O2–Ba1–N1	142.3(2)		
O5^{ii}–Ba1–N1	67.5(2)		
O1–Ba1–N1	64.3(2)		
O7^{iv}–Ba1–N1	88.2(2)		
O3–Ba1–N1	109.7(2)		

Symmetry codes (i): x, -y+3/2, z+1/2; (ii): x, -y+1/2, z+1/2; (iii): x, y+1, z; (iv): x, -y+1/2, z-1/2; (v): –x+1, y-1/2, -z+1/2; (vi): x, y-1, z; (vii): –x+1, -y+1, -z.

Table S2. Hydrogen bond geometry for **1** and **2.**

D–H···A	*d*(D–H)/Å	*d*(H···A)/Å	*d*(D···A)/Å	∠(D–H···A)/°	Symmetry code on A
1					
O2–H21···O5	0.84	2.21	3.042(7)	173.8	-x+1, -y+1, -z
O2–H21···O4	0.84	2.43	2.976(7)	123.6	-x+1, -y+1, -z
O2–H22···O3	0.82	2.11	2.852(7)	149.9	-x+1, -y+1, -z
O3–H31···O4	0.84	1.98	2.776(7)	158.1	-x+1, -y+1, -z
O3–H31···O3	0.84	2.53	2.95(1)	111.6	-x+1, -y+1, -z
O3–H32···O5	0.83	2.04	2.829(8)	158.6	-x+1, y+1/2, -z+1/2
O1–H11···N2	0.85	2.24	2.984(8)	147.6	x, -y+1/2, z-1/2
O1–H12···O6	0.83	2.08	2.747(7)	137.3	x, y+1, z
2					
O9–H91···O3	0.85(2)	1.69(2)	2.505(3)	162(3)	-x+1, -y+1, -z
O7–H71···O12	0.82(2)	1.76(2)	2.546(3)	162(3)	x, y, z
O1–H11···O5	0.83(2)	2.02(2)	2.817(3)	160(3)	x, -y+1/2, z+1/2
O1–H12···O11	0.83(2)	2.09(2)	2.900(3)	165(3)	x, y-1, z
O2–H21···O10	0.83(2)	2.03(2)	2.853(3)	174(3)	x, -y+3/2, z+1/2
O2–H22···O5	0.84(2)	2.03(2)	2.868(3)	170(3)	x, -y+1/2, z+1/2
O11–H111···O2	0.84(2)	2.05(2)	2.857(3)	162(3)	x, y, z
O11–H112···N3	0.83(2)	1.96(2)	2.788(3)	171(4)	x, y, z
O12–H121···O11	0.83(2)	1.89(2)	2.717(3)	174(3)	x, -y+3/2, z-1/2
O12–H122···O6	0.83(2)	1.92(2)	2.751(3)	174(3)	-x, y+1/2, -z-1/2

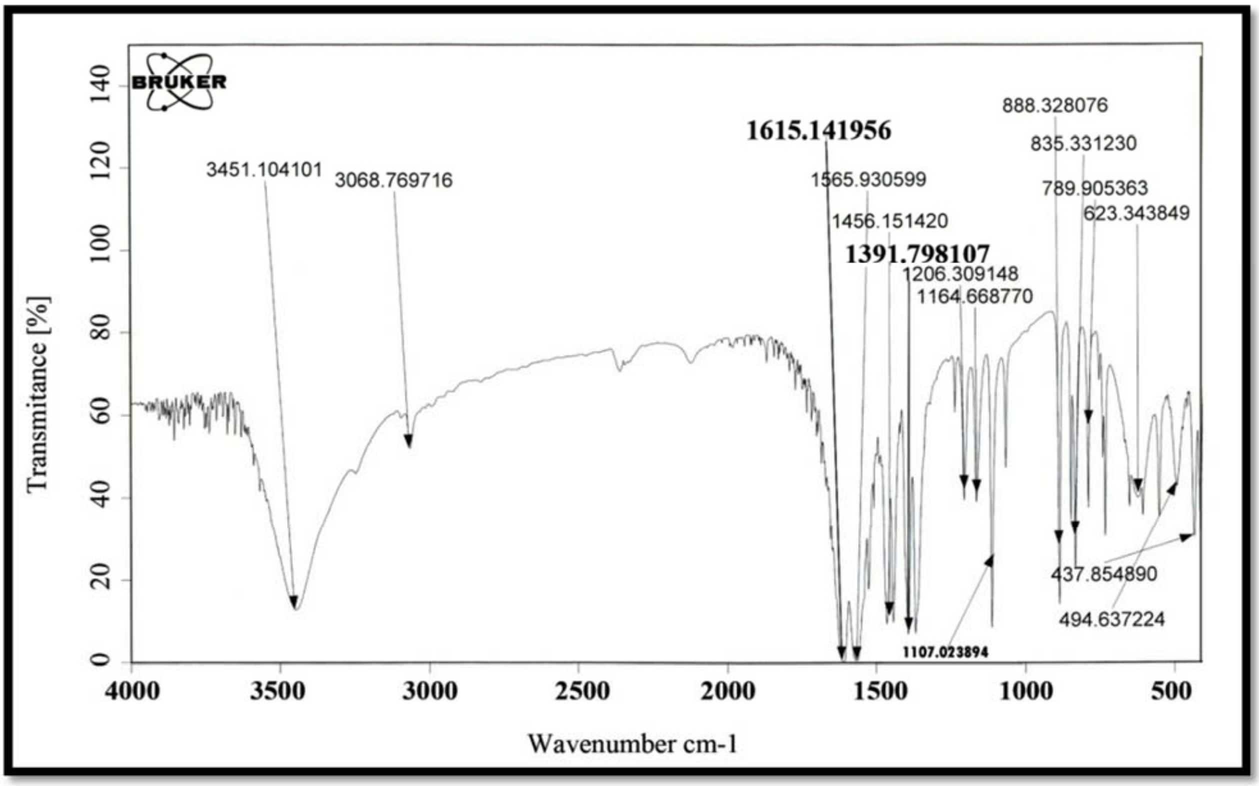

Fig. S1. FTIR spectrum of {[Ba(μ-H_2O)(H_2O)$_2$(μ-pyzdc)]}$_n$ (**1**)

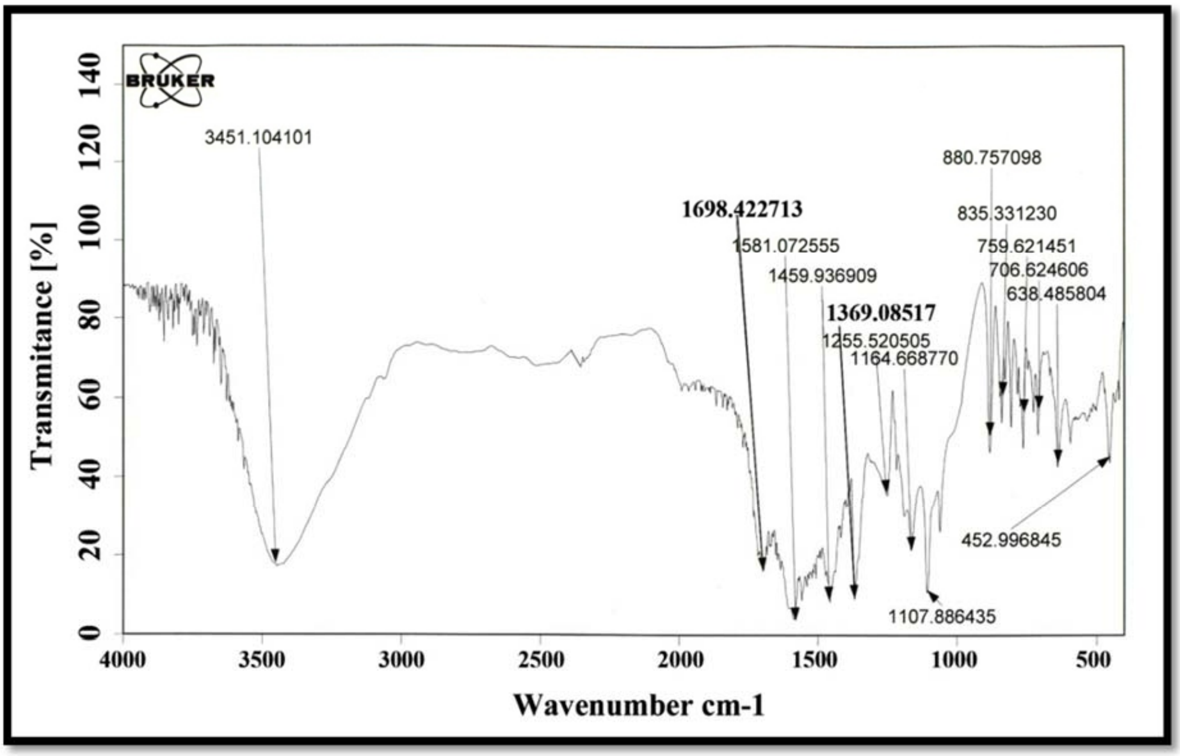

Fig. S2. FTIR spectrum of {[Ba(H_2O)$_2$(μ-Hpyzdc)(Hpyzdc)] · 2H_2O}$_n$ (**2**)

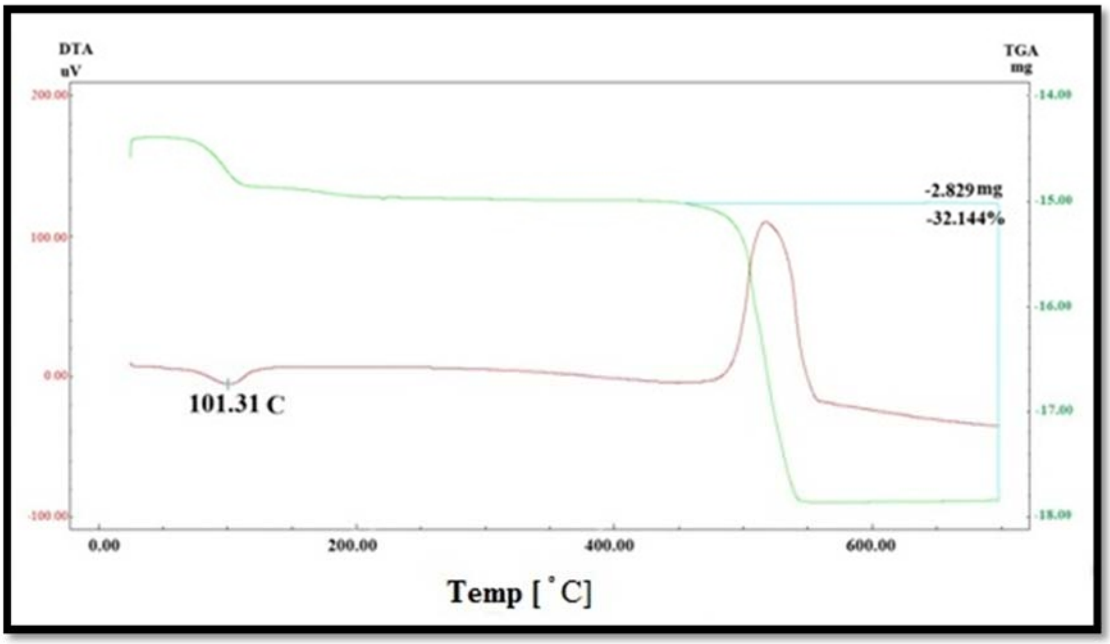

Fig. S3. TG/DTA curve of {[Ba(μ-H_2O)(H_2O)$_2$(μ-pyzdc)]}$_n$ (**1**)

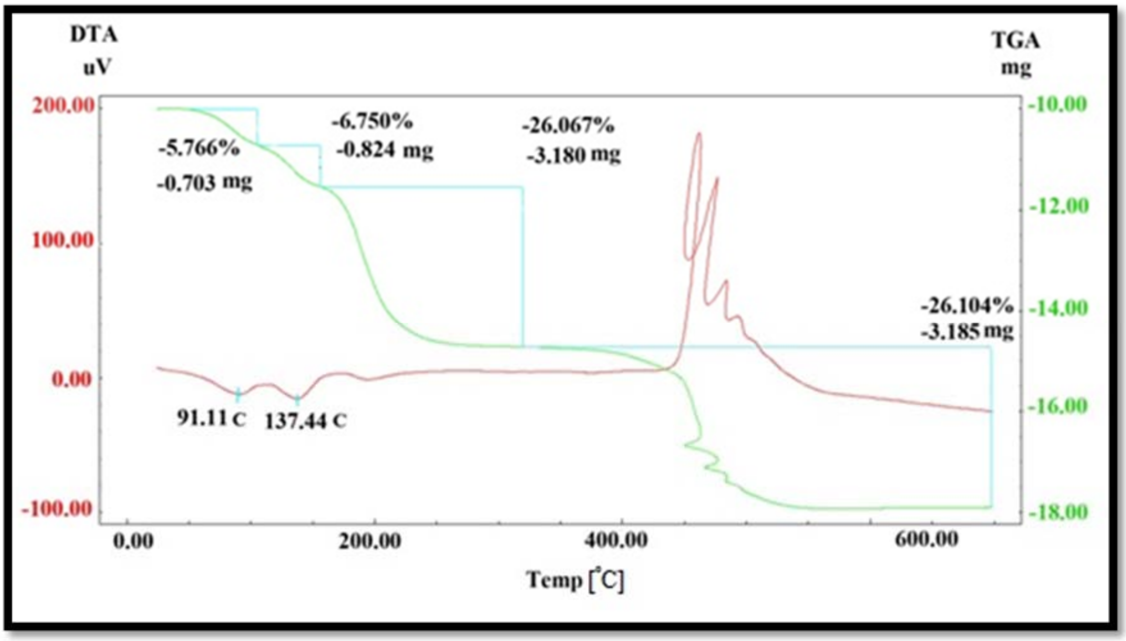

Fig. S4. TG/DTA curve of {[Ba(H_2O)$_2$(μ-Hpyzdc)(Hpyzdc)] · 2H_2O}$_n$ (**2**)