New Polynuclear Coordination Compounds Based on 2–(Carboxyphenyl)iminodiacetate Anion: Synthesis and X-rays Crystal Structures

1) Infrared spectra of compounds **1-4** in KBr mulls.

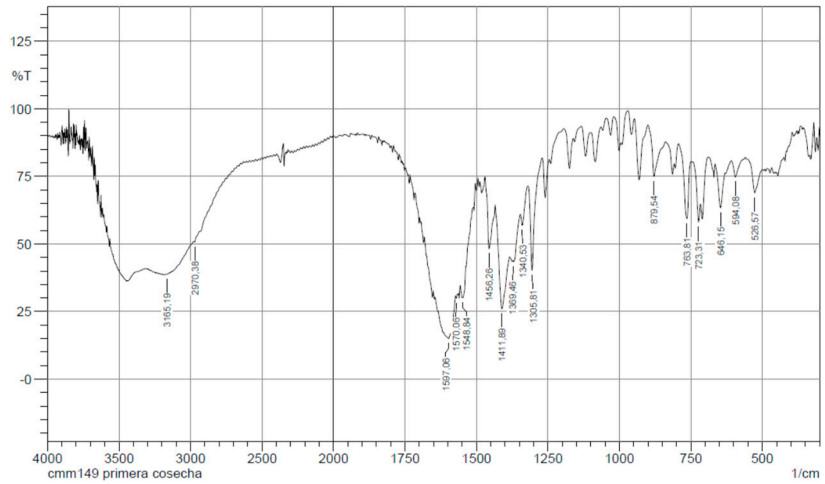

Figure S1. FT-IR spectrum of compound **1.**

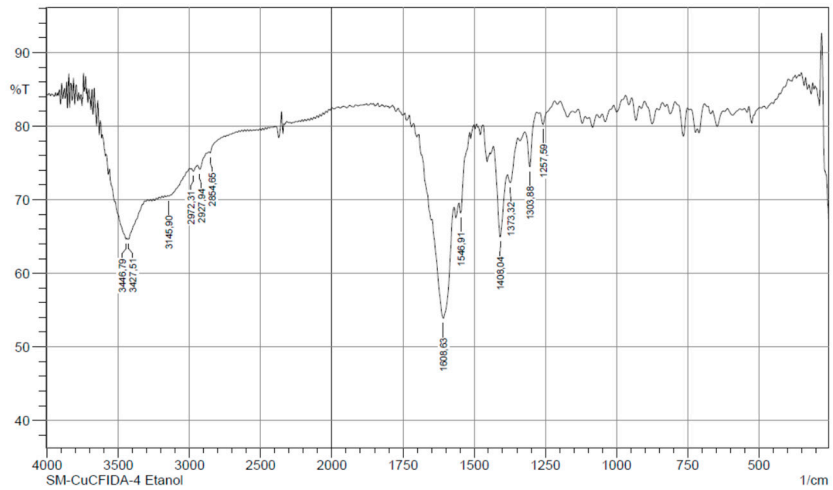

Figure S2. FT-IR spectrum of compound **2**.

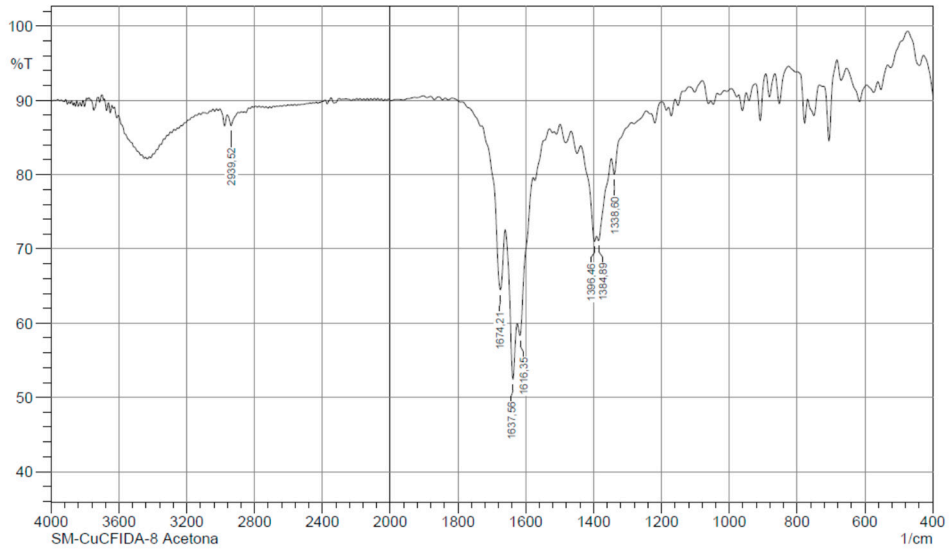

Figure S3. FT-IR of compound **3**.

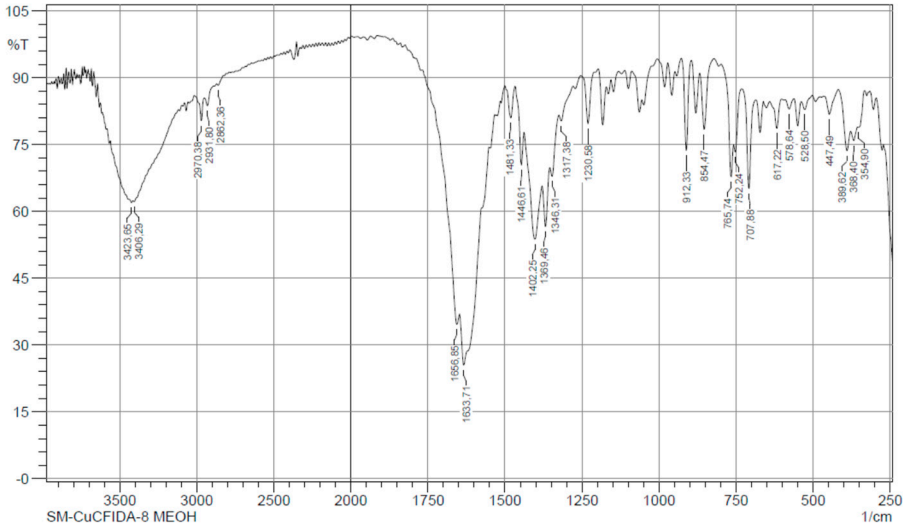

Figure S4. FT-IR of compound **4**.

2) Thermogravimetric analysis of compounds **1** and **4**.

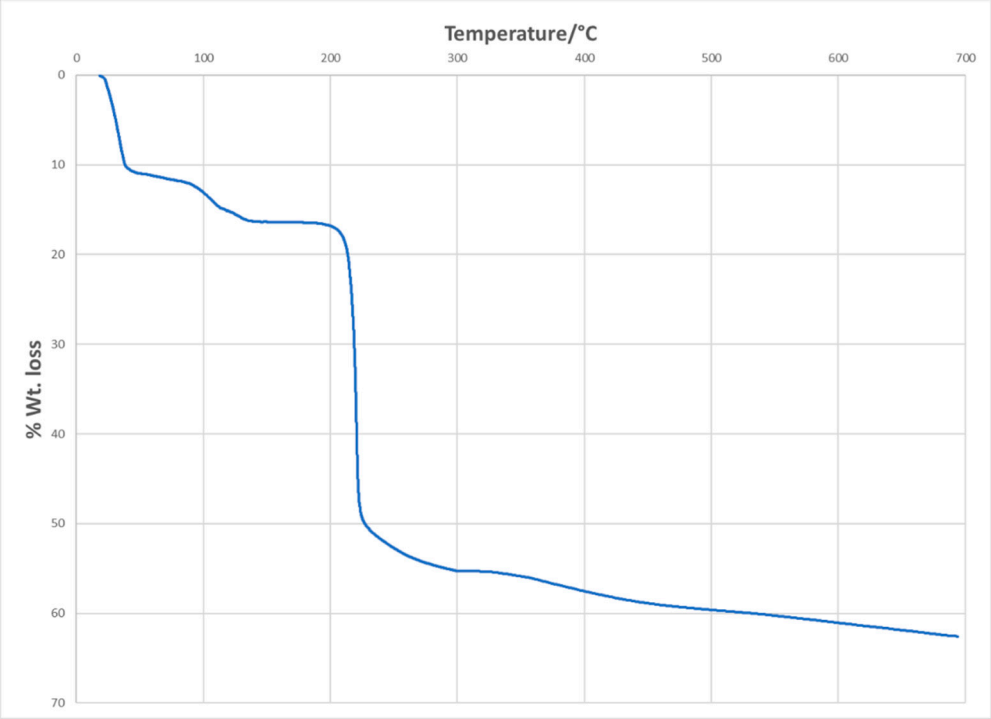

Figure S5. TGA of compound **1**.

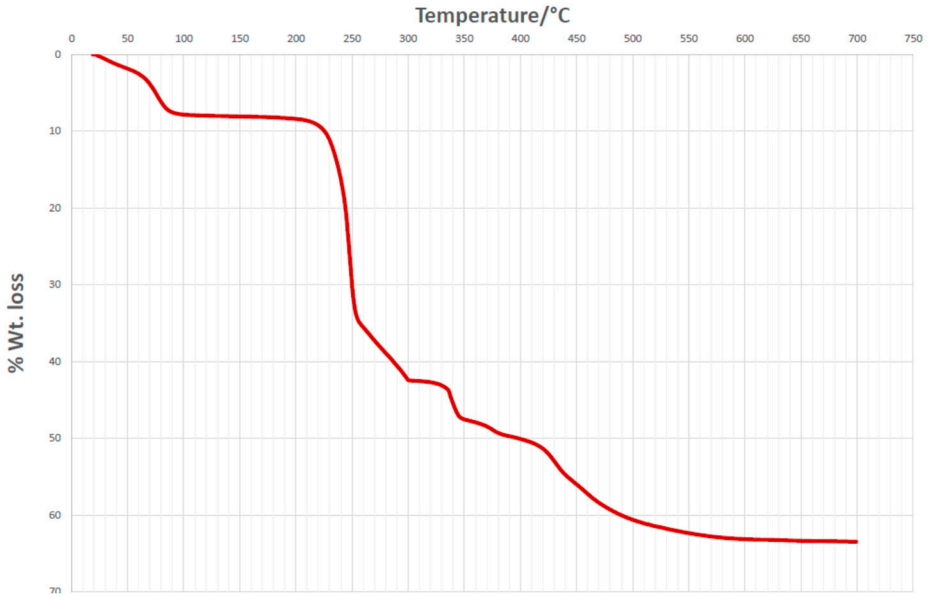

Figure S6. TGA of compound **4.**

3) Additional information for the crystal structures of compounds **1**-**4**

Table S1. Selected bond angles (°) for the coordination center in compounds **1** and **2**[†].

Compound	**1**	**2**	
		Angles	
O(1)–Cu(1)–O(6)$^{\#1}$	95.89(13)	O(1)–Cu(1)–O(6)$^{\#3}$	95.87(11)
O(1)–Cu(1)–O(2)$^{\#1}$	96.83(11)	O(1)–Cu(1)–O(2)$^{\#3}$	97.98(9)
O(1)–Cu(1)–O(3)$^{\#1}$	92.36(13)	O(1)–Cu(1)–O(3)$^{\#3}$	92.38(11)
O(1)–Cu(1)–N(1)$^{\#1}$	173.20(13)	O(1)–Cu(1)–N(1)$^{\#3}$	173.74(11)
O(6)$^{\#1}$–Cu(1)–O(2)$^{\#1}$	92.80(12)	O(6)$^{\#3}$–Cu(1)–O(2)$^{\#3}$	92.23(10)
O(6)$^{\#1}$–Cu(1)–O(3)$^{\#1}$	156.58(13)	O(6)$^{\#3}$–Cu(1)–O(3)$^{\#3}$	156.91(11)
O(6)$^{\#1}$–Cu(1)–N(1)$^{\#1}$	89.18(13)	O(6)$^{\#3}$–Cu(1)–N(1)$^{\#3}$	89.20(11)
O(3)$^{\#1}$–Cu(1)–O(2)$^{\#1}$	107.96(13)	O(3)$^{\#3}$–Cu(1)–O(2)$^{\#3}$	107.95(11)
O(3)$^{\#1}$–Cu(1)–N(1)$^{\#1}$	84.67(13)	O(3)$^{\#3}$–Cu(1)–N(1)$^{\#3}$	84.29(11)
N(1)$^{\#1}$–Cu(1)–O(2)$^{\#1}$	78.35(11)	N(1)$^{\#3}$–Cu(1)–O(2)$^{\#3}$	78.11(10)
O(7)–Cu(2)–O(8)$^{\#2}$	92.76(12)	O(7)–Cu(2)–O(8)$^{\#4}$	93.74(10)
O(7)–Cu(2)–O(9)$^{\#2}$	95.83(14)	O(7)–Cu(2)–O(12)$^{\#4}$	96.88(12)
O(7)–Cu(2)–O(12)$^{\#2}$	96.16(14)	O(7)–Cu(2)–O(9)$^{\#4}$	95.76(12)
O(7)–Cu(2)–N(2)$^{\#2}$	169.76(13)	O(7)–Cu(2)–N(2)$^{\#4}$	170.51(12)
O(9)$^{\#2}$–Cu(2)–O(8)$^{\#2}$	114.86(13)	O(12)$^{\#4}$–Cu(2)–O(8)$^{\#4}$	90.96(11)
O(9)$^{\#2}$–Cu(2)–N(2)$^{\#2}$	83.74(13)	O(12)$^{\#4}$–Cu(2)–O(9)$^{\#4}$	148.97(12)
O(12)$^{\#2}$–Cu(2)–O(8)$^{\#2}$	92.00(13)	O(12)$^{\#4}$–Cu(2)–N(2)$^{\#4}$	88.68(11)
O(12)$^{\#2}$–Cu(2)–O(9)$^{\#2}$	149.90(14)	O(9)$^{\#4}$–Cu(2)–O(8)$^{\#4}$	116.35(12)
O(12)$^{\#2}$–Cu(2)–N(2)$^{\#2}$	89.11(13)	O(9)$^{\#4}$–Cu(2)–N(2)$^{\#4}$	83.14(11)
N(2)$^{\#2}$–Cu(2)–O(8)$^{\#2}$	78.24(12)	N(2)$^{\#4}$–Cu(2)–O(8)$^{\#4}$	78.44(10)
O(2W)–Cu(3)–O(5)	86.95(13)	O(2W)–Cu(3)–O(5)	87.11(11)
O(2W)–Cu(3)–O(1W)	92.83(12)	O(2W)–Cu(3)–O(4W)	92.89(11)
O(2W)–Cu(3)–O(4W)	92.51(13)	O(2W)–Cu(3)–O(3W)	93.46(11)
O(5)–Cu(3)–O(1W)	97.07(12)	O(5)–Cu(3)–O(4W)	168.95(11)
O(5)–Cu(3)–O(4W)	168.75(13)	O(5)–Cu(3)–O(3W)	97.81(10)
O(4W)–Cu(3)–O(1W)	94.18(13)	O(4W)–Cu(3)–O(3W)	93.22(11)
O(3W)–Cu(3)–O(2W)	168.65(14)	O(1W)–Cu(3)–O(2W)	168.28(12)
O(3W)–Cu(3)–O(5)	90.35(16)	O(1W)–Cu(3)–O(5)	89.23(12)
O(3W)–Cu(3)–O(1W)	98.44(14)	O(1W)–Cu(3)–O(4W)	88.57(13)
O(3W)–Cu(3)–O(4W)	87.99(16)	O(1W)–Cu(3)–O(3W)	98.07(12)

[†]Symmetry codes: $^{\#1}$ -x+1/2, y+1/2, -z+3/2; $^{\#2}$ -x+1/2, y-1/2, -z+5/2; $^{\#3}$ -x+3/2, y+1/2, -z+3/2; $^{\#4}$ -x+1/2, y-1/2, -z+3/2;

Table S2. Selected bond angles (°) for the coordination center in compounds **3** and **4**[†].

Compound	**3**	**4**	
		Angles	
O(1)#5–Cu(1)–O(3)	89.55(17)	O(5)–Cu(1)–O(3)	176.52(13)
O(1)#5–Cu(1)–N(1)	172.90(18)	O(5)–Cu(1)–O(1)	87.90(10)
O(5)–Cu(1)–O(1)$^{\#5}$	91.24(17)	O(5)–Cu(1)–O(1)$^{\#9}$	92.93(10)
O(5)–Cu(1)–O(3)	177.70(17)	O(5)–Cu(1)–N(1)	92.70(10)
O(5)–Cu(1)–N(1)	92.74(17)	O(3)–Cu(1)–O(1)$^{\#9}$	88.28(10)
O(3)–Cu(1)–N(1)	86.70(17)	O(3)–Cu(1)–O(1)	88.63(10)
O(1)–Na(1)–O(3)$^{\#6}$	173.31(14)	O(3)–Cu(1)–N(1)	86.48(9)
O(5)–Na(1)–O(1)	73.95(14)	O(1)#9–Cu(1)–O(1)	106.8(7)
O(5)–Na(1)–O(3)$^{\#6}$	102.58(14)	O(1)#9–Cu(1)–N(1)	171.37(11)
O(5)–Na(1)–O(3)$^{\#7}$	138.01(17)	N(1)–Cu(1)–O(1)	79.93(10)
O(5)–Na(1)–O(4)$^{\#6}$	130.71(17)	O(5)–Na(1)–O(3)$^{\#10}$	103.80(9)
O(5)–Na(1)–O(2)$^{\#5}$	82.79(14)	O(5)–Na(1)–O(3)$^{\#11}$	136.66(11)
O(3)$^{\#7}$–Na(1)–O(1)	64.19(13)	O(5)–Na(1)–O(2)$^{\#9}$	81.98(8)
O(3)$^{\#7}$–Na(1)–O(3)$^{\#6}$	119.40(15)	O(5)–Na(1)–O(6)$^{\#12}$	83.27(9)
O(3)$^{\#7}$–Na(1)–O(2)$^{\#5}$	78.57(14)	O(5)–Na(1)–O(4)$^{\#10}$	126.45(10)
O(6)$^{\#8}$–Na(1)–O(1)	83.24(15)	O(5)–Na(1)–O(1)	72.82(9)

O(6)$^{\#8}$–Na(1)–O(5)	78.93(15)	O(3)$^{\#11}$–Na(1)–O(3)$^{\#10}$	119.24(10)
O(6)$^{\#8}$–Na(1)–O(3)$^{\#6}$	90.50(15)	O(3)$^{\#11}$–Na(1)–O(2)$^{\#9}$	75.42(8)
O(6)$^{\#8}$–Na(1)–O(3)$^{\#7}$	98.70(16)	O(3)$^{\#11}$–Na(1)–O(4)$^{\#10}$	83.65(9)
O(6)$^{\#8}$–Na(1)–O(4)$^{\#6}$	129.36(17)	O(3)$^{\#11}$–Na(1)–O(1)	64.35(8)
O(6)$^{\#8}$–Na(1)–O(2)$^{\#5}$	148.87(16)	O(2)$^{\#9}$–Na(1)–O(3)$^{\#10}$	115.64(8)
O(4)$^{\#6}$–Na(1)–O(1)	138.12(16)	O(6)$^{\#12}$–Na(1)–O(3)$^{\#11}$	98.65(10)
O(4)$^{\#6}$–Na(1)–O(3)$^{\#6}$	48.40(13)	O(6)$^{\#12}$–Na(1)–O(3)$^{\#10}$	92.85(8)
O(4)$^{\#6}$–Na(1)–O(3)$^{\#}$7	83.15(15)	O(6)$^{\#12}$–Na(1)–O(2)$^{\#9}$	150.31(9)
O(4)$^{\#6}$–Na(1)–O(2)$^{\#5}$	81.46(14)	O(6)$^{\#12}$–Na(1)–O(4)$^{\#10}$	132.20(10)
O(2)$^{\#5}$–Na(1)–O(1)	67.52(13)	O(6)$^{\#12}$–Na(1)–O(1)	84.70(8)
O(2)$^{\#5}$–Na(1)–O(3)$^{\#6}$	118.12(14)	O(4)$^{\#10}$–Na(1)–O(3)$^{\#10}$	48.06(8)
		O(4)$^{\#10}$–Na(1)–O(2)$^{\#9}$	76.75(9)
		O(4)$^{\#10}$–Na(1)–O(1)	135.63(10)
		O(1)–Na(1)–O(3)$^{\#10}$	176.01(9)
		O(1)–Na(1)–O(2)$^{\#9}$	66.37(8)

†Symmetry codes: $^{\#5}$ -x+1, y+1/2, -z+1/2; $^{\#6}$ x+1/2, y, -z+1/2; $^{\#7}$ -x+1, y-1/2, -z+1/2; $^{\#8}$ -x+3/2, y-1/2, z; $^{\#9}$ -x+1/2,-y+1/2,z-1/2; $^{\#10}$ -x+1/2,y+1/2,z; $^{\#11}$ -x+1/2,-y+1/2,z+1/2; $^{\#12}$ x,-y+1,z+1/2

Table S3. Hydrogen bonds for **1** [Å and °]*.

D-H...A	*d*(D-H)	*d*(H...A)	*d*(D...A)	<(DHA)
O(2W)-H(2WA)...O(3)$^{\#1}$	0.85	1.84	2.674(4)	167.9
O(2W)-H(2WB)...O(8)$^{\#5}$	0.85	1.90	2.687(5)	153.4
O(3W)-H(3WA)...O(12)$^{\#6}$	0.85	1.90	2.754(5)	177.2
O(3W)-H(3WB)...O(7)$^{\#5}$	0.85	2.06	2.853(5)	153.4
O(4W)-H(4WA)...O(11)$^{\#6}$	0.86	1.87	2.707(5)	164.1
O(4W)-H(4WB)...O(4)#1	0.86	1.95	2.764(5)	157.2
O(1W)-H(1WA)...O(5W)	0.86	1.86	2.697(6)	163.0
O(1W)-H(1WB)...O(6W)	0.86	1.98	2.800(8)	158.5

*Symmetry transformations used to generate equivalent atoms: $^{\#1}$ −x + 1/2, y + 1/2, −z + 3/2; $^{\#5}$ −x + 1, −y + 2, −z + 2; $^{\#6}$ x + 1/2, −y + 3/2, z − 1/2.

Table S4. Hydrogen bonds for **2** [Å and °]*

D-H...A	*d*(D-H)	*d*(H...A)	*d*(D...A)	<(DHA)
O(2W)-H(2WA)...O(10)$^{\#5}$	0.87	1.83	2.669(4)	159.5
O(2W)-H(2WB)...O(3)$^{\#1}$	0.87	1.81	2.669(3)	167.8
O(4W)-H(4WA)...O(4)$^{\#1}$	0.87	1.92	2.750(4)	160.4
O(4W)-H(4WB)...O(11)$^{\#6}$	0.87	1.87	2.724(4)	166.0
O(3W)-H(3WA)...O(12)$^{\#6}$	0.85	1.95	2.766(4)	160.8
O(3W)-H(3WB)...O(9)$^{\#5}$	0.85	2.03	2.856(4)	162.6

O(1W)-H(1WA)...O(13)	0.85	1.88	2.711(6)	164.2
O(1W)-H(1WB)...O(5W)	0.85	1.86	2.700(5)	169.2
C(4)-H(4B)...O(13)[#1]	0.97	2.65	3.442(8)	138.7
O(13)-H(13)...O(11)[#3]	0.82	2.28	3.019(7)	149.4

*Symmetry transformations used to generate equivalent atoms: [#1] −x + 3/2, y + 1/2, −z + 3/2; [#5] −x + 1, −y + 1, −z + 1; [#6] x + 1/2, −y + 1/2, z − 1/2