

Supplementary Materials

The anion impact on dimensionality of cadmium(II) complexes with nicotinamide

Željka Soldin ^{1,*}, Boris-Marko Kukovec ^{2,*}, Milica Kovačić ³, Marijana Đaković ¹ and Zora Popović ¹

¹ Division of General and Inorganic Chemistry, Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, HR-10000 Zagreb, Croatia; zeljka.chem@pmf.hr (Ž.S.); mdjakovic@chem.pmf.hr (M.Đ.); zpopovic@chem.pmf.hr (Z.P.)

² Department of Physical Chemistry, Faculty of Chemistry and Technology, University of Split, Ruđera Boškovića 35, HR-21000 Split, Croatia; bmkukovec@ktf-split.hr (B.-M.K.)

³ Institute for Medical Research and Occupational Health, Ksaverska cesta 2, HR-10000 Zagreb, Croatia; mkovacic@imi.hr (M.K.)

* Correspondence: zeljka.chem@pmf.hr (Ž.S.); bmkukovec@ktf-split.hr (B.-M.K.)

1. Crystal structures

Table S1. Selected bond lengths (Å) and angles (°) for [Cd(CH₃COO)₂(nia)₂]₂ (**1**), [[Cd(nia)₄](ClO₄)₂]_n (**2**) and [Cd(H₂O)₃(nia)₃](ClO₄)₂·nia (**3**).

1		2		3	
Bond lengths					
Cd1–N1	2.348(3)	Cd1–N1	2.349(2)	Cd1–N1	2.336(3)
Cd1–N3	2.312(3)	Cd1–N3	2.338(2)	Cd1–N3	2.321(3)
Cd1–O3	2.465(3)	Cd1–O1	2.329(2)	Cd1–N5	2.316(3)
Cd1–O4	2.360(4)			Cd1–O5	2.323(3)
Cd1–O5	2.277(4)			Cd1–O6	2.395(4)
Cd1–O6	2.365(4)			Cd1–O7	2.301(3)
Bond angles					
O5–Cd1–N3	89.8(1)	O1–Cd1–N3 ⁱⁱ	90.50(7)	O7–Cd1–N5	87.8(1)
O5–Cd1–N1	90.2(1)	O1–Cd1–N3	89.50(7)	O7–Cd1–N3	91.7(1)
N3–Cd1–N1	179.0(1)	O1–Cd1–N1	95.30(6)	N5–Cd1–N3	93.4(1)
O5–Cd1–O4	100.3(3)	N3–Cd1–N1	98.64(7)	O7–Cd1–O5	177.9(1)
N3–Cd1–O4	95.0(1)	O1–Cd1–N1 ⁱⁱ	84.70(6)	N5–Cd1–O5	92.5(1)
N1–Cd1–O4	86.0(1)	N3–Cd1–N1 ⁱⁱ	81.36(7)	N3–Cd1–O5	90.3(1)
O5–Cd1–O6	123.9(3)			O7–Cd1–N1	91.3(1)
N3–Cd1–O6	90.3(1)			N5–Cd1–N1	171.9(1)
N1–Cd1–O6	88.9(1)			N3–Cd1–N1	94.6(1)
O4–Cd1–O6	135.5(1)			O5–Cd1–N1	88.2(1)
O5–Cd1–O3	154.0(3)			O7–Cd1–O6	87.8(2)
N3–Cd1–O3	90.1(1)			N5–Cd1–O6	84.6(1)
N1–Cd1–O3	90.4(1)			N3–Cd1–O6	177.9(1)
O4–Cd1–O3	53.8(1)			O5–Cd1–O6	90.2(2)
O6–Cd1–O3	82.1(1)			N1–Cd1–O6	87.4(1)

Symmetry code (ii) $-x+1, -y, -z$.

Table S2. The hydrogen bond geometry for [Cd(CH₃COO)₂(nia)₂]₂ (**1**), {[Cd(nia)₄](ClO₄)₂]_n (**2**) and [Cd(H₂O)₃(nia)₃](ClO₄)₂·nia (**3**).

D–H...A	<i>d</i> (D–H)/Å	<i>d</i> (H...A)/Å	<i>d</i> (D...A)/ Å	∠(D–H...A)/°	Symmetry code on A
1					
N2–H12N...O2	0.87	1.99	2.856(5)	170	<i>x</i> , <i>y</i> +1, <i>z</i>
N4–H14N...O1	0.88	2.50	3.020(5)	119	<i>x</i> , <i>y</i> –1, <i>z</i>
N2–H22N...O4	0.86	2.45	2.879(7)	111	– <i>x</i> –1, 1/2+ <i>y</i> , 1/2– <i>z</i>
N4–H24N...O3	0.87	2.30	3.151(7)	169	– <i>x</i> , –1/2+ <i>y</i> , 1/2– <i>z</i>
C3–H3...O4	0.93	2.59	3.450(5)	154	– <i>x</i> –1, 1/2+ <i>y</i> , 1/2– <i>z</i>
C9–H9...O3	0.93	2.33	3.219(7)	160	– <i>x</i> , –1/2+ <i>y</i> , 1/2– <i>z</i>
C10–H10...O1	0.93	2.37	3.148(9)	142	– <i>x</i> , –1/2+ <i>y</i> , 1/2– <i>z</i>
2					
N2–H12N...O6	0.85(4)	2.18(3)	2.980(4)	158(3)	<i>x</i> , <i>y</i> , <i>z</i>
N4–H14N...O3	0.88(4)	2.13(3)	3.010(4)	177(3)	<i>x</i> , –1/2– <i>y</i> , –1/2+ <i>z</i>
N2–H22N...O2	0.91(3)	2.16(3)	3.004(3)	153(3)	– <i>x</i> +1, 1/2+ <i>y</i> , 1/2– <i>z</i>
N4–H24N...O2	0.97(4)	2.00(4)	2.920(4)	159(4)	– <i>x</i> , – <i>y</i> –1, – <i>z</i>
C3–H3...O4	0.93	2.46	3.321(4)	154	– <i>x</i> , 1/2+ <i>y</i> , 1/2– <i>z</i>
C5–H5...O3	0.93	2.41	3.272(3)	155	– <i>x</i> +1, 1/2+ <i>y</i> , 1/2– <i>z</i>
3					
N2–H12N...O4	0.86(1)	2.12(1)	2.970(4)	172(4)	– <i>x</i> , – <i>y</i> +1, – <i>z</i> +2
N2–H22N...O9	0.86(1)	2.27(1)	3.112(4)	169(4)	– <i>x</i> +1/2, <i>y</i> –1/2, – <i>z</i> +3/2
N4–H24N...O3	0.86(1)	2.06(1)	2.913(4)	173(4)	<i>x</i> +3/2, – <i>y</i> +3/2, <i>z</i> +1/2
N6–H16N...O1	0.86(1)	2.03(2)	2.849(4)	159(4)	<i>x</i> –1/2, – <i>y</i> +3/2, <i>z</i> –1/2
N6–H26N...O2	0.86(1)	2.06(1)	2.921(4)	173(4)	<i>x</i> –3/2, – <i>y</i> +3/2, <i>z</i> –1/2
N8–H18N...O1	0.86(1)	2.07(1)	2.932(4)	177(5)	– <i>x</i> , – <i>y</i> +1, – <i>z</i> +2
N8–H28N...O10	0.86(1)	2.19(2)	3.011(5)	160(4)	– <i>x</i> –1/2, <i>y</i> –1/2, – <i>z</i> +3/2
O5–H15O...O3	0.83(1)	1.98(2)	2.777(4)	162(4)	<i>x</i> +1, <i>y</i> , <i>z</i>
O5–H25O...O13	0.82(1)	2.08(1)	2.898(5)	172(4)	<i>x</i> , <i>y</i> , <i>z</i>
O6–H16O...O12	0.82(1)	2.36(1)	3.171(7)	177(6)	– <i>x</i> +1, – <i>y</i> +1, – <i>z</i> +1
O7–H17O...O8	0.81(1)	2.11(2)	2.893(4)	163(4)	<i>x</i> , <i>y</i> , <i>z</i>
O7–H27O...N7	0.82(1)	1.89(1)	2.692(4)	167(4)	<i>x</i> , <i>y</i> , <i>z</i>
C11–H11...O8	0.93	2.44	3.361(5)	172	<i>x</i> , <i>y</i> , <i>z</i>
C16–H16...O4	0.93	2.56	3.229(4)	129	<i>x</i> +1/2, – <i>y</i> +3/2, <i>z</i> –1/2
C17–H17...O10	0.93	2.41	3.275(5)	154	<i>x</i> +1, <i>y</i> , <i>z</i>
C22–H22...O15	0.93	2.52	3.286(6)	139	– <i>x</i> +1, – <i>y</i> +1, – <i>z</i> +1

2. IR spectra

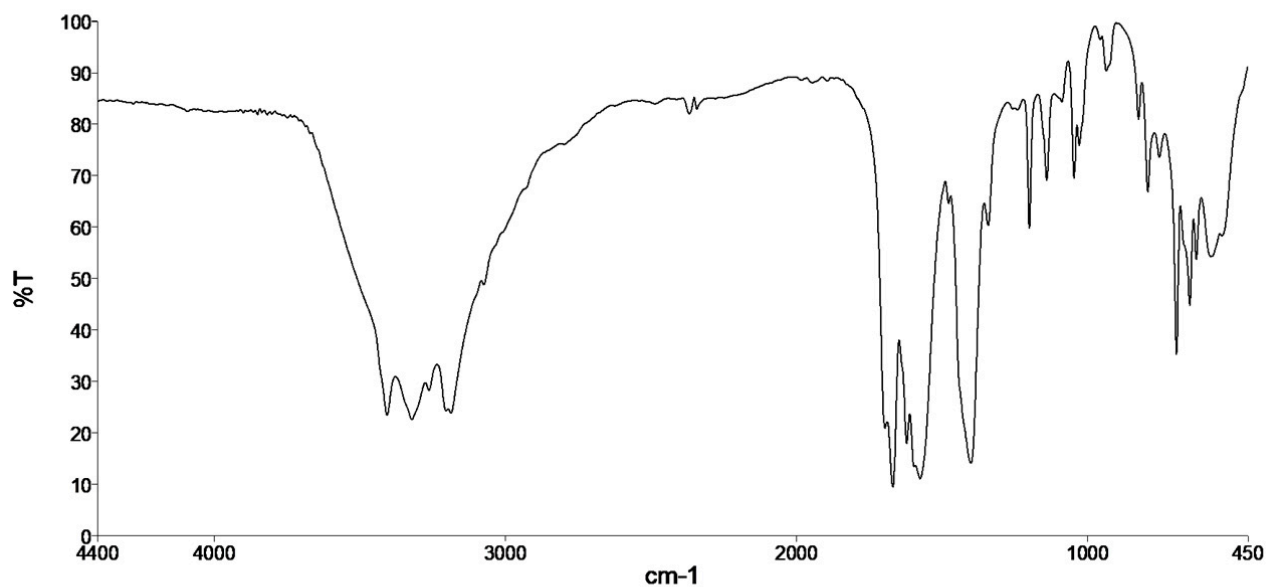


Figure S1. IR spectrum of $[\text{Cd}(\text{CH}_3\text{COO})_2(\text{nia})_2]$ (1).

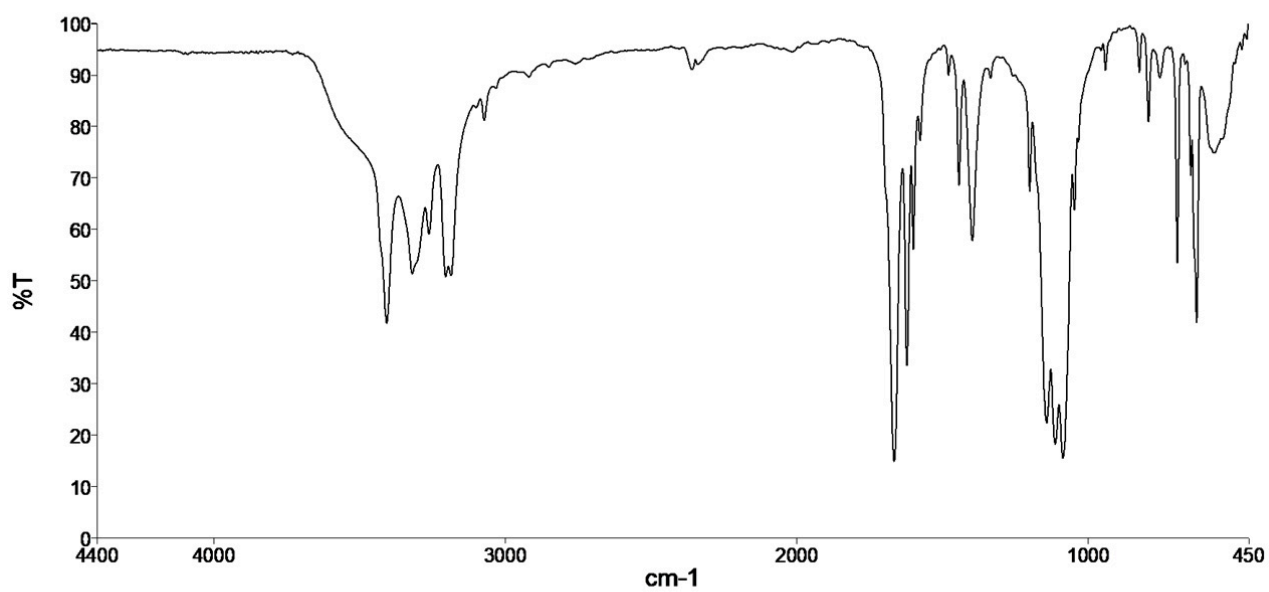


Figure S2. IR spectrum of $[\text{Cd}(\text{nia})_4](\text{ClO}_4)_2$ (2).

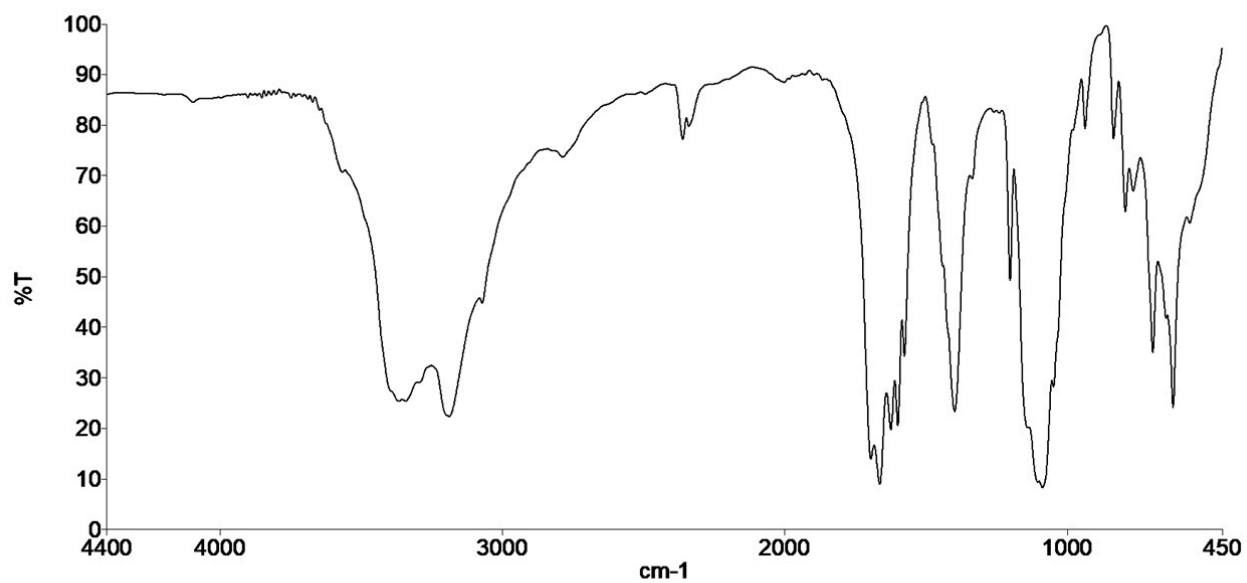


Figure S3. IR spectrum of $[\text{Cd}(\text{H}_2\text{O})_3(\text{nia})_3](\text{ClO}_4)_2 \cdot \text{nia}$ (**3**).

3. TGA/DTA curves

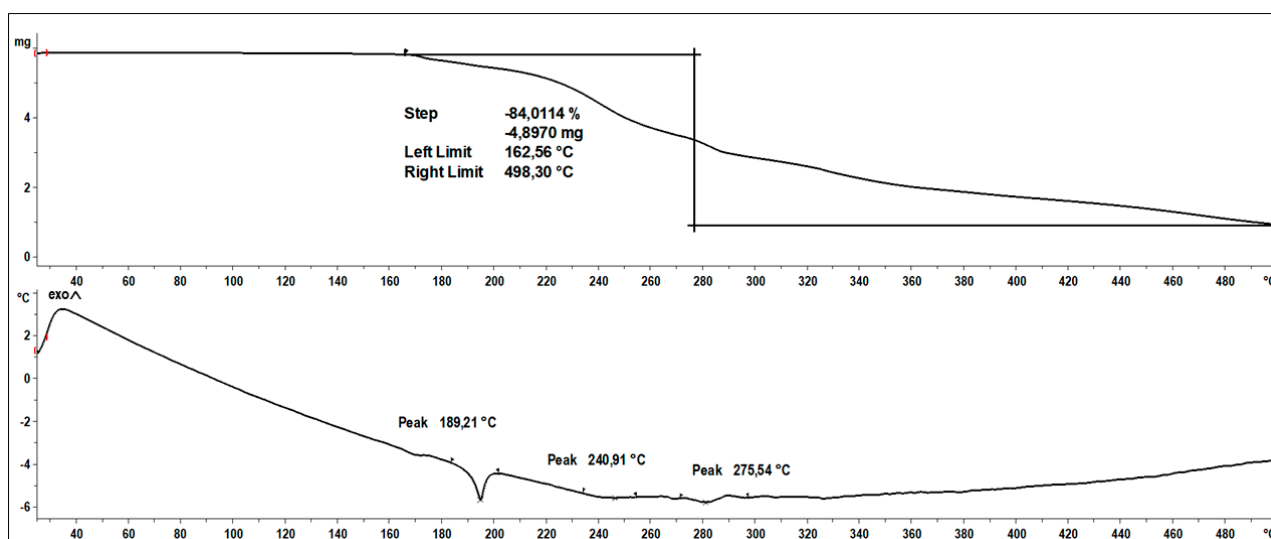


Figure S4. TGA/DTA curves of $[\text{Cd}(\text{CH}_3\text{COO})_2(\text{nia})_2]_2$ (1).

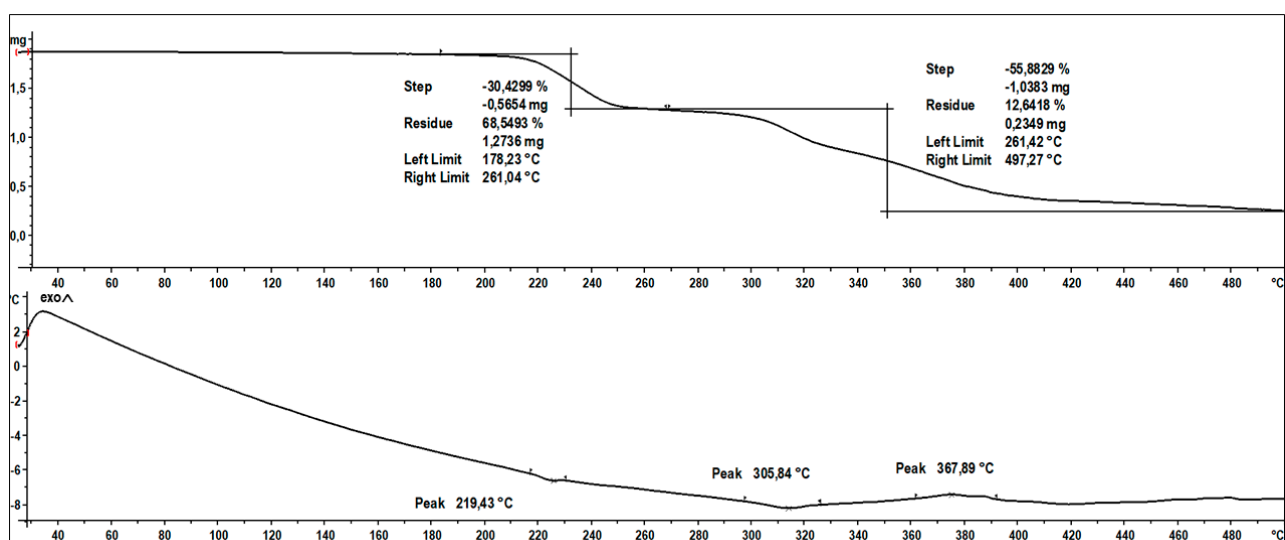


Figure S5. TGA/DTA curves of $\{[\text{Cd}(\text{nia})_4](\text{ClO}_4)_2\}_n$ (2).

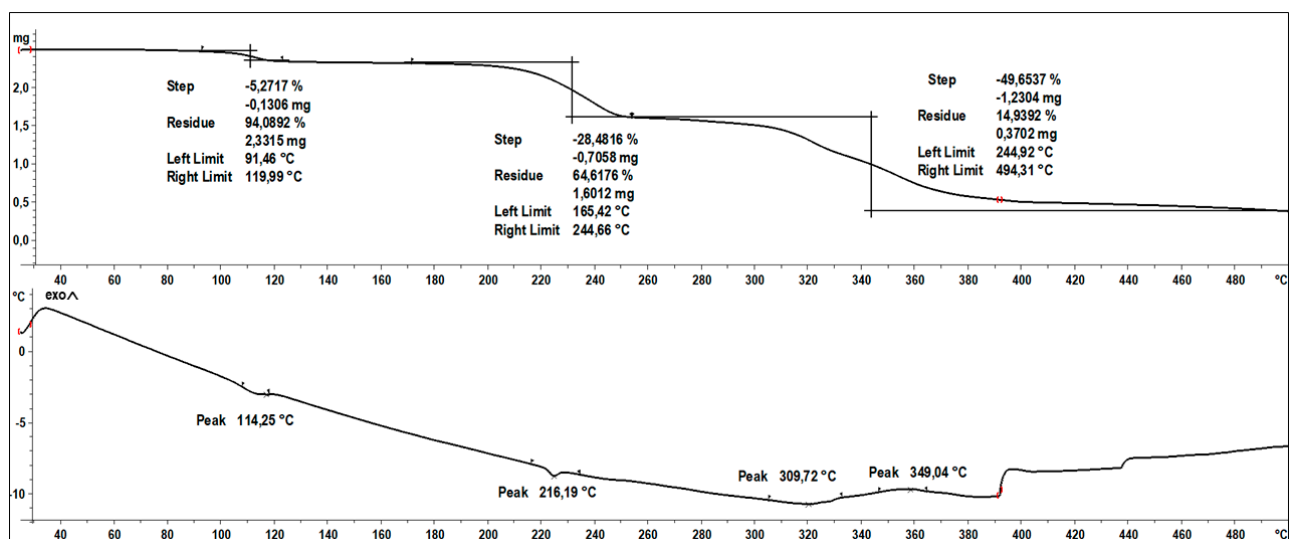


Figure S6. TGA/DTA curves of $[\text{Cd}(\text{H}_2\text{O})_3(\text{nia})_3](\text{ClO}_4)_2 \cdot \text{nia}$ (**3**).