

## Electronic Supplementary Material

### Synthesis and crystal structure of three new cadmium tartrates with open frameworks

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**Figure S1.** Powder X-ray diffraction pattern of compound **I** pure.

**Figure S2.** Powder X-ray diffraction pattern of sample containing compound **II** as a predominant phase with lower contributions of compounds **I** and **III**.

**Figure S3.** Powder X-ray diffraction pattern of sample containing compound **III** as a predominant phase with a lower contribution of compound **IV**.

**Figure S4.** Powder X-ray diffraction pattern of compound **IV** pure.

**Table S1.** Selected bond lengths (Å) and angles (°) for compounds **I**, **II** and **III**.

**Table S2.** Selected hydrogen bond distances (Å) and angles (°) for compounds **I**, **II** and **III**.

**Figure S5.** Topological Analysis for Compound **I**.

**Figure S6.** Topological Analysis for Compound **IV**.

**Table S3.** Topologies of reported cadmium tartrates

**Table S1.** Selected bond lengths (Å) and angles (°) for compounds **I**<sup>a</sup>, **II**<sup>b</sup> and **III**<sup>c</sup>

<b>I</b>	Cd1—O6 <sup>i</sup>	2.276(3)	Cd2—O11 <sup>iii</sup>	2.302(3)
	Cd1—O7	2.298(3)	Cd2—O15	2.334(3)
	Cd1—O12 <sup>i</sup>	2.323(3)	Cd3—O8	2.203(3)
	Cd1—O1	2.371(3)	Cd3—O17	2.235(3)
	Cd1—O4 <sup>i</sup>	2.446(3)	Cd3—O16 <sup>i</sup>	2.357(3)
	Cd1—O9	2.476(3)	Cd3—O19	2.371(3)
	Cd1—O10 <sup>i</sup>	2.562(3)	Cd3—O1 <sup>iv</sup>	2.404(3)
	Cd1—O3	2.599(3)	Cd3—O2 <sup>iv</sup>	2.446(3)
	Cd2—O5	2.248(3)	Cd1...Cd2 <sup>viii</sup>	4.7722(4)
	Cd2—O14 <sup>ii</sup>	2.285(3)	Cd1...Cd3 <sup>v</sup>	4.4791(4)
	Cd2—O13	2.286(3)	O12 <sup>iii</sup> —Cd2—O15	178.43(9)
	O6 <sup>i</sup> —Cd1—O4 <sup>i</sup>	69.09(9)	O11 <sup>iii</sup> —Cd2—O12 <sup>iii</sup>	52.83(9)
	O7—Cd1—O9	69.07(8)	O8—Cd3—O17	111.14(11)
	O12 <sup>i</sup> —Cd1—O10 <sup>i</sup>	67.02(8)	O17—Cd3—O1 <sup>iv</sup>	82.75(10)
	O1—Cd1—O3	65.18(8)	O8—Cd3—O2 <sup>iv</sup>	111.54(10)
	O5—Cd2—O14 <sup>ii</sup>	92.07(10)	O1 <sup>iv</sup> —Cd3—O2 <sup>iv</sup>	53.89(9)
	O14 <sup>ii</sup> —Cd2—O13	105.0(1)	O16 <sup>i</sup> —Cd3—O19	172.31(12)
	O5—Cd2—O11 <sup>iii</sup>	90.20(11)	Cd1 <sup>vi</sup> —O12—Cd2 <sup>vii</sup>	146.31(12)
	O13—Cd2—O11 <sup>iii</sup>	91.31(10)	Cd1—O1—Cd3 <sup>v</sup>	139.41(11)
	O13—Cd2—O15	70.15(9)		
<b>II</b>	Cd1—O11	2.286(6)	Cd3—O2	2.203(6)
	Cd1—O10 <sup>i</sup>	2.296(6)	Cd3—O12 <sup>ii</sup>	2.208(6)
	Cd1—O10	2.365(6)	Cd3—O6 <sup>iii</sup>	2.245(6)
	Cd1—O1	2.379(6)	Cd3—O8 <sup>i</sup>	2.318(6)
	Cd1—O4	2.386(5)	Cd3—O7 <sup>i</sup>	2.489(5)
	Cd1—O3	2.395(6)	Cd3—O5 <sup>iii</sup>	2.604(6)
	Cd1—O13	2.410(6)	Cd3—C5 <sup>i</sup>	2.735(7)
	Cd2—O4	2.275(6)	Cd1...Cd2	3.5495(8)
	Cd2—O14	2.295(7)	Cd1...Cd1 <sup>i</sup>	3.6237(9)
	Cd2—O7	2.321(6)	Cd1...Cd2 <sup>i</sup>	3.5260(8)
	Cd2—O4 <sup>i</sup>	2.324(6)	Cd2...Cd2 <sup>i</sup>	3.5257(8)
	Cd2—O5	2.327(6)	Cd2...Cd3 <sup>iii</sup>	4.8372(9)
	Cd2—O10	2.371(5)	Cd2...Cd3 <sup>i</sup>	4.5594(9)
	Cd2—O9	2.572(6)	O4 <sup>i</sup> —Cd2—O10	81.16(19)
	O11—Cd1—O10	72.02(19)	O7—Cd2—O9	66.6(2)
	O10 <sup>i</sup> —Cd1—O10	77.6(2)	O10—Cd2—O9	66.51(19)
	O10 <sup>i</sup> —Cd1—O4	81.41(19)	O4 <sup>i</sup> —O4—O10	61.27(19)
	O10—Cd1—O4	79.83(18)	O4 <sup>i</sup> —O10—O4	57.67(18)
	O1—Cd1—O4	80.0(2)	O4 <sup>i</sup> —O4—O10 <sup>i</sup>	61.07(19)
	O1—Cd1—O3	69.2(2)	O5—O9—O14	43.67(16)
	O4—Cd1—O3	68.72(19)	O5—O14—O9	43.56(16)
	O4—O10—O10 <sup>i</sup>	61.47(18)	O9—O5—O14	92.77(23)
	O10 <sup>i</sup> —O4—O10	57.26(17)	O8 <sup>i</sup> —Cd3—O7 <sup>i</sup>	54.71(19)
	O10 <sup>i</sup> —O10—O4 <sup>i</sup>	61.27(18)	O6 <sup>iii</sup> —Cd3—O5 <sup>iii</sup>	53.4(2)
	O11—O3—O13	43.33(16)	O6 <sup>ix</sup> —O8—O7	70.30(24)
	O11—O13—O3	52.37(19)	O8 <sup>viii</sup> —O6—O7 <sup>viii</sup>	39.84(17)
	O3—O11—O13	84.30(24)	O6 <sup>ix</sup> —O7—O8	69.86(24)
	O4—Cd2—O4 <sup>i</sup>	79.61(19)	O5 <sup>iii</sup> —O2—O12 <sup>ii</sup>	63.84(20)

	O4—Cd2—O5	73.4(2)	O2 <sup>v</sup> —O12—O5 <sup>vi</sup>	61.97(19)
	O4—Cd2—O10	81.97(19)	O2 <sup>iv</sup> —O5—O12 <sup>vii</sup>	54.20(18)
	O7—Cd2—O10	84.4(2)		
<b>III</b>	Cd1—O11	2.212(3)	Cd2—O1	2.229(2)
	Cd1—O2 <sup>i</sup>	2.233(3)	Cd2—O13	2.233(3)
	Cd1—O5	2.241(3)	Cd2—O7	2.299(3)
	Cd1—O8 <sup>ii</sup>	2.249(3)	Cd2—O9	2.312(3)
	Cd1—O10	2.411(3)	Cd2—O3	2.360(3)
	Cd1—O4	2.442(3)	Cd1...Cd2	5.776(1)
	Cd2—O6 <sup>iii</sup>	2.179(2)	O6 <sup>iii</sup> —Cd2—O1	114.00(11)
	O11—Cd1—O2 <sup>i</sup>	90.58(11)	O6 <sup>iii</sup> —Cd2—O7	87.29(10)
	O2 <sup>i</sup> —Cd1—O5	102.23(12)	O1—Cd2—O9	89.4(1)
	O11—Cd1—O10	71.55(9)	O7—Cd2—O9	69.82(9)
	O5—Cd1—O10	92.43(10)	O1—Cd2—O3	71.59(10)
	O5—Cd1—O4	70.47(9)	O13—Cd2—O3	164.83(11)
	O8 <sup>ii</sup> —Cd1—O4	158.29(10)		

<sup>a</sup> Symmetry codes: (i)  $-1+x, y, z$ ; (ii)  $-0.5+x, 0.5-y, 1-z$ ; (iii)  $2-x, -0.5+y, 0.5-z$ ; (iv)  $0.5-x, 1-y, 0.5+z$ ; (v)  $0.5-x, 1-y, -0.5+z$ ; (vi)  $1+x, y, z$ ; (vii)  $2-x, 0.5+y, 0.5-z$ ; (viii)  $1-x, 0.5+y, 0.5-z$ .

<sup>b</sup> Symmetry codes: (i)  $-x, 1-y, z$ ; (ii)  $0.5-x, -0.5+y, 1-z$ ; (iii)  $0.5-x, -0.5+y, -z$ ; (iv)  $0.5-x, 0.5+y, -z$ ; (v)  $0.5-x, 0.5+y, 1-z$ ; (vi)  $x, y, 1+z$ ; (vii)  $x, y, -1+z$ ; (viii)  $0.5+x, 1.5-y, -z$ ; (ix)  $-0.5+x, 1.5-y, -z$ .

<sup>c</sup> Symmetry codes: (i)  $1-x, 0.5+y, 1-z$ ; (ii)  $-x, 0.5+y, -z$ ; (iii)  $-x, -0.5+y, 1-z$ .

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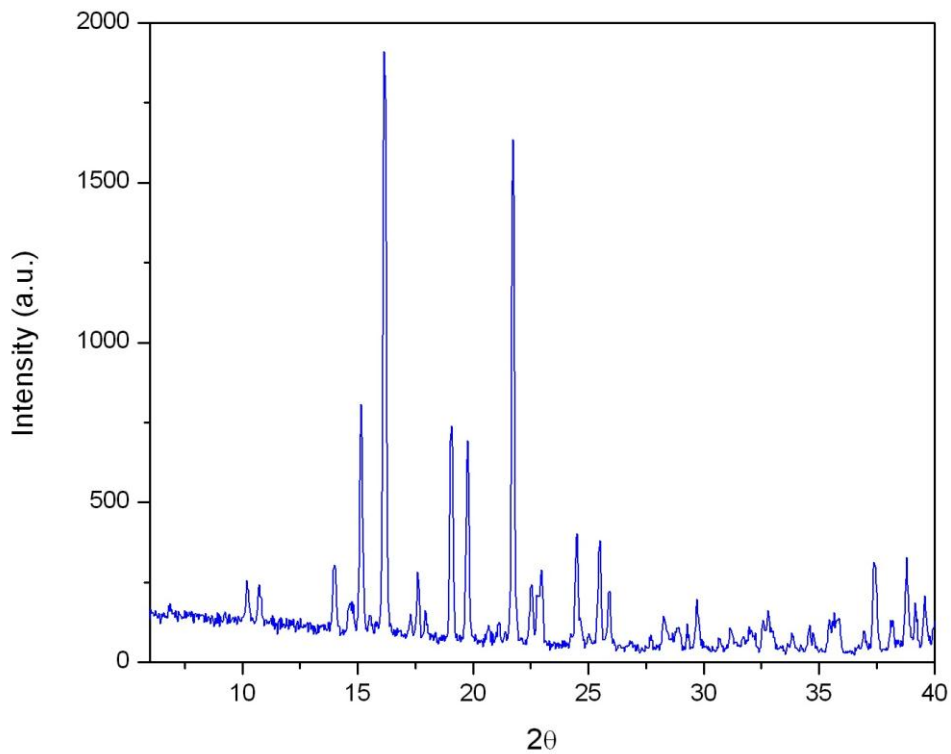
**Table S2.** Selected hydrogen bond distances (Å) and angles (°) for compounds **I**<sup>a</sup>, **II**<sup>b</sup> and **III**<sup>c</sup>

	<b>D-H...A</b>	<b>d(D-H)</b>	<b>d(H...A)</b>	<b>d(D...A)</b>	<b>&lt;DHA</b>
<b>I</b>	O4—H4...O9	0.847(10)	2.64(2)	3.435(4)	157.0(4)
	O10—H10A...O18	0.845(10)	1.918(18)	2.733(5)	162.0(5)
	O15—H15...O20	0.85(1)	1.828(15)	2.664(4)	167.0(5)
	O16—H16...O7 <sup>i</sup>	0.844(10)	2.15(4)	2.816(4)	136.0(4)
	O19—H19B...O18	0.851(10)	2.51(4)	3.184(5)	137.0(5)
	O20—H20A...O11 <sup>ii</sup>	0.8500	2.5000	3.258(5)	147.900
	O20—H20B...O16 <sup>iii</sup>	0.8500	2.3700	3.024(4)	133.600
<b>II</b>	O3—H3A...O16	0.8500(14)	1.789(14)	2.636(9)	174.0(11)
	O13—H13B...O15	0.8500(15)	2.05(5)	2.811(9)	149.0(9)
	O14—H14A...O19 <sup>i</sup>	0.8500(14)	1.931(11)	2.78(1)	178.0(12)
	O16—H16B...O15	0.8500(14)	1.98(4)	2.808(12)	163.0(13)
	O17—H17A...O2 <sup>ii</sup>	0.8500(14)	1.877(15)	2.701(9)	163.0(4)
	O17—H17B...O19 <sup>ii</sup>	0.8500(15)	2.41(6)	3.065(10)	134.0(7)
	O18—H18A...O9 <sup>iii</sup>	0.8500(14)	2.065(19)	2.906(9)	171.0(10)
	O18—H18B...O8 <sup>iv</sup>	0.8500(14)	2.01(5)	2.803(9)	154.0(10)
	O19—H19A...O12 <sup>iv</sup>	0.8500(14)	2.15(6)	2.920(9)	150.0(11)
	O19—H19B...O18	0.8500(14)	2.10(4)	2.897(10)	157.0(10)
	O20—H20A...O13	0.8500(14)	2.09(3)	2.904(7)	161.0(7)
	<b>III</b>	O3—H3A...O5 <sup>i</sup>	0.775(18)	2.49(3)	3.223(4)
O4—H4...O3		0.776(18)	2.47(3)	2.832(4)	110.3(19)
O9—H9...O15		0.773(18)	1.82(2)	2.584(4)	171.0(5)
O13—H13A...O12 <sup>ii</sup>		0.770(18)	1.88(3)	2.619(4)	161.0(7)
O14—H14A...O2		0.775(18)	2.53(5)	3.260(7)	157.0(9)
O14—H14B...O4		0.775(18)	2.41(6)	3.059(6)	142.0(9)
O15—H15B...O14		0.772(18)	2.18(4)	2.893(10)	153.0(8)
O16—H16A...O14		0.773(18)	2.34(9)	2.808(9)	120.0(9)
O16—H16B...O11		0.774(18)	2.00(3)	2.762(5)	166.0(10)

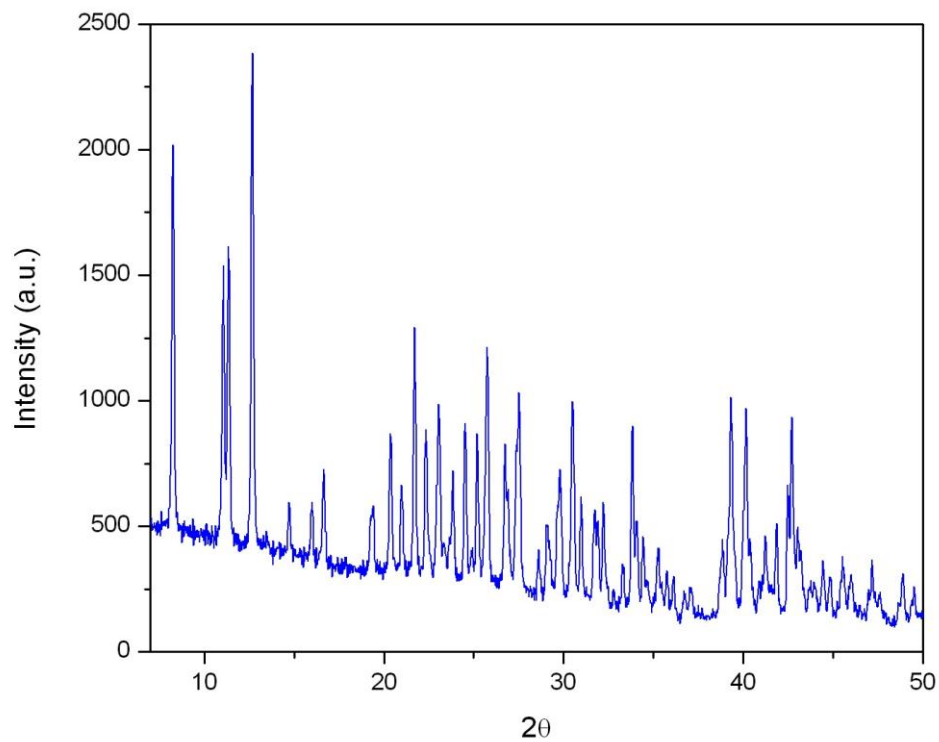
<sup>a</sup> Symmetry codes: (i) 1+x, y, z; (ii) 1-x, -0.5+y, 0.5-z; (iii) -1+x, y, z.

<sup>b</sup> Symmetry codes: (i) 0.5-x, 0.5+y, -z; (ii) x, y, 1+z; (iii) 1-x, 1-y, z; (iv) 0.5-x, -0.5+y, 1-z.

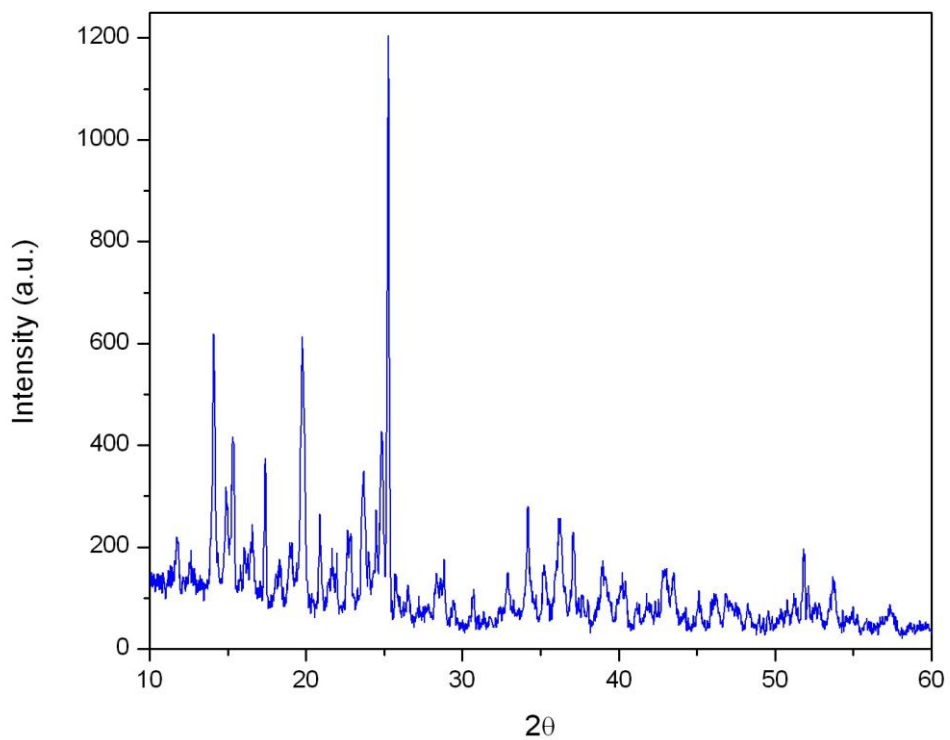
<sup>c</sup> Symmetry codes: (i) -x, -0.5+y, 1-z; (ii) 1-x, -0.5+y, -z.



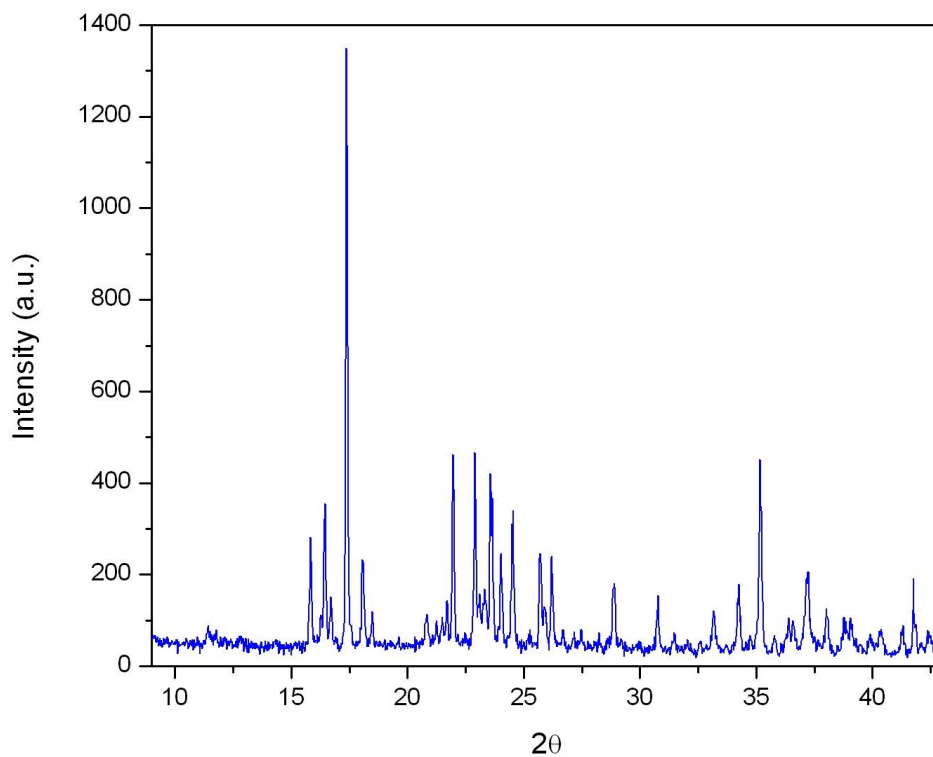
**Figure S1.** Powder X-ray diffraction pattern of compound **I** pure.



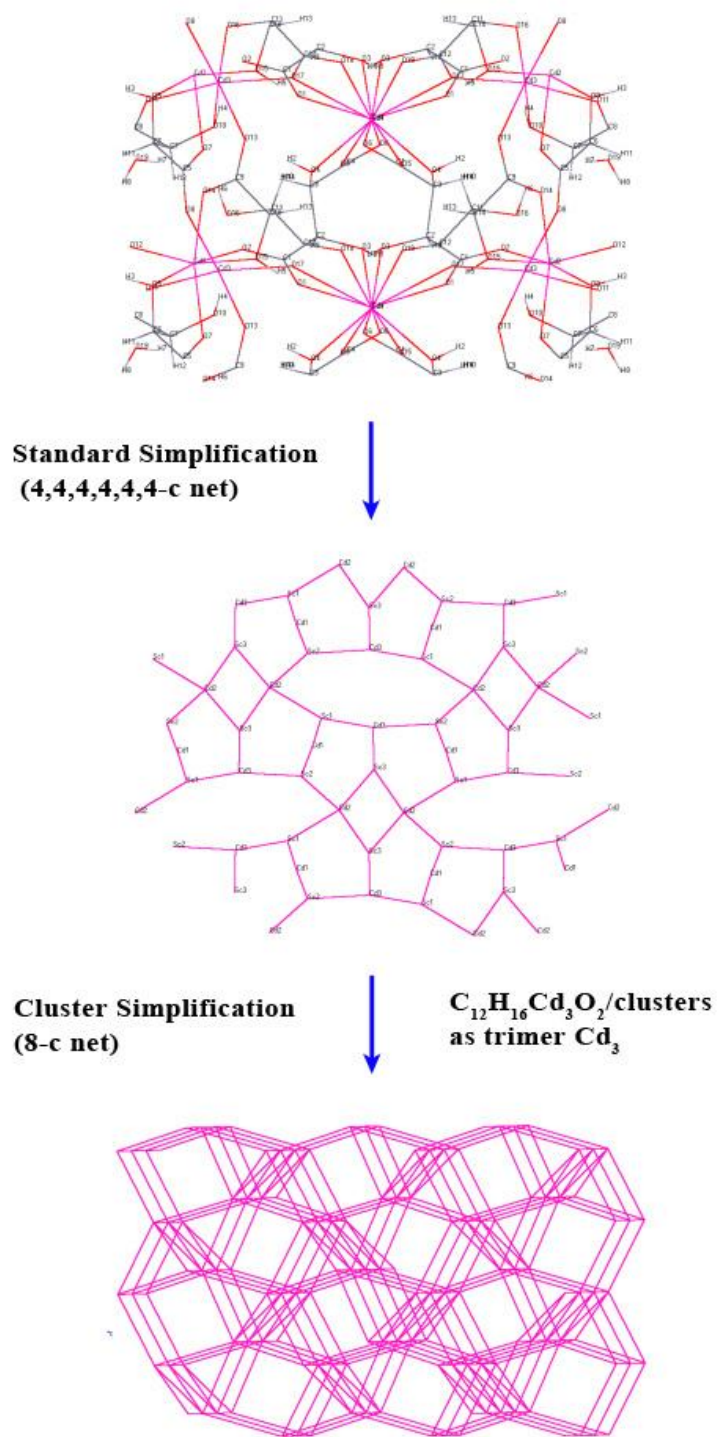
**Figure S2.** Powder X-ray diffraction pattern of sample containing compound **II** as a predominant phase with lower contributions of compounds **I** and **III**.



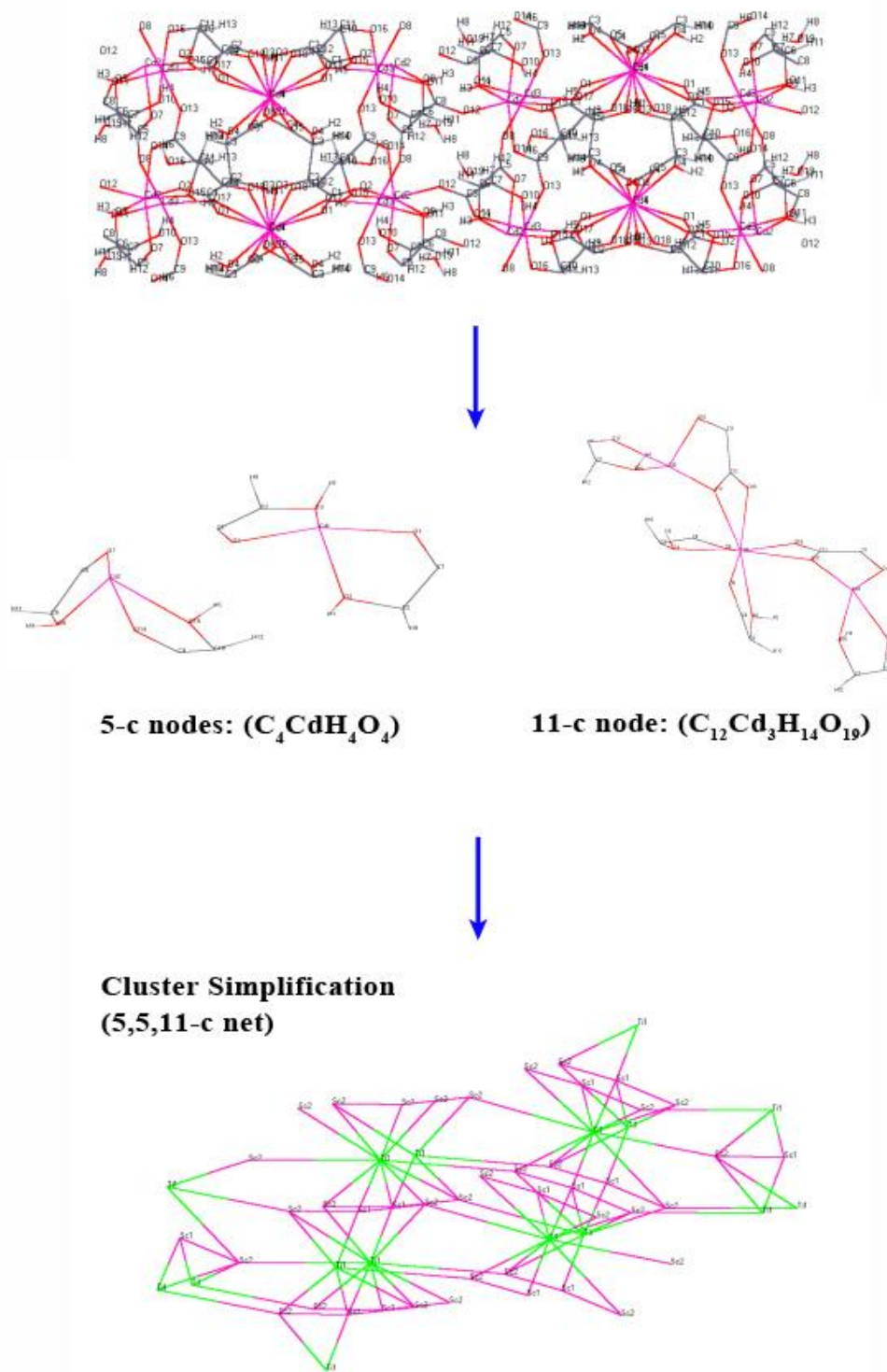
**Figure S3.** Powder X-ray diffraction pattern of sample containing compound **III** as a predominant phase with a lower contribution of compound **IV**.



**Figure S4.** Powder X-ray diffraction pattern of compound **IV** pure.



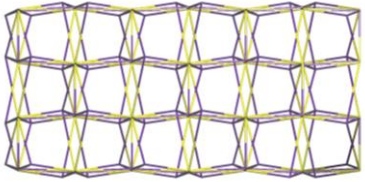
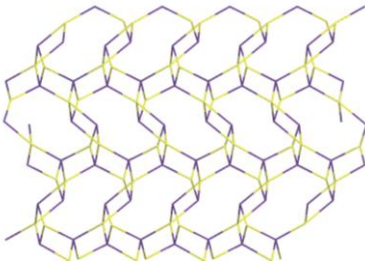
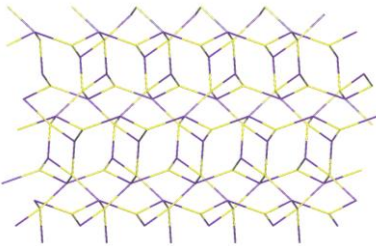
**Figure S5.** Topological Analysis for Compound I.



**Figure S6.** Topological Analysis for Compound IV.



**Table S3.** Topologies of reported cadmium tartrates

Chemical Formula <i>CSD Refcode</i> [Reference]	Topology Demonstration	Topological simplification	Node selection	Point Symbol (Schläfli Symbol)	Nodal Connectivity	Node Type
$[\text{Cd}(\text{C}_4\text{H}_4\text{O}_6)]_n$ <i>UPIXUN</i> [2a] $\{[\text{Cd}(\text{C}_4\text{H}_4\text{O}_6)] \cdot 0.167\text{H}_2\text{O}\}_n$ <i>XUBMEN</i> [2b]		Cluster Simplification	5-c nodes: $(\text{C}_4\text{CdH}_4\text{O}_4)$ 11-c nodes: $(\text{C}_{12}\text{Cd}_3 \text{H}_{14}\text{O}_{19})$	$\{3^2.4^6.5^2\}_2$ $\{3^4.4^{14}.5^{16}.6^{18}.7^2.8\}$ $\{3^4.4^3.5^2.6\}$	5,5,11-c	3-nodal
$\{[\text{Cd}_2(\mu\text{-C}_4\text{H}_4\text{O}_6)_2(\text{H}_2\text{O})] \cdot 3\text{H}_2\text{O}\}_\infty$ <i>HIXWIU01</i> [23] $\{[\text{Cd}_2(\text{C}_4\text{H}_4\text{O}_6)_2(\text{H}_2\text{O})] \cdot 3\text{H}_2\text{O}\}_n$ <i>HIXWIU</i> [24]		Standard simplification	3c-nodes: Tart(O1-O6) and Cd1 4c-nodes : Tart(O7-O12) and Cd2	$\{4.8^2\}\{4.8^4.10\}$	3,3,4,4-c	4-nodal
$[\text{Cd}_2(\text{C}_4\text{H}_4\text{O}_6)_2]_n$ <i>CCDC 791340</i> [25]		Standard simplification	4c-nodes: Tart, Cd1 and Cd2	$\{4.6^2.8^2.10\}$ $\{4.6^2.8^3\}\{4.6^3.8^2\}_2$	4,4,4-c	3-nodal