SUPPLEMENTARY INFORMATION for

Novel Cd(II) Coordination Polymers afforded with EDTA or trans-1,2-CDTA chelators and Imidazole, Adenine or 9-(2-Hydroxyethyl)adenine Coligands

Jeannette Carolina Belmont-Sánchez,[1] María Eugenia García-Rubiño,[2] Antonio Frontera,[3] Antonio Matilla-Hernández,[1] Alfonso Castiñeiras,[4] Juan Niclós-Gutiérrez*[1]

[1] University of Granada, Department of Inorganic Chemistry, Faculty of Pharmacy, 18071 Granada, Spain.

[2] Universidad de Granada, Departmento de Fisicoquímica, Facultad de Farmacia, 18071 Granada, Spain.

[3] Departament de Química, Universitat de les Illes Balears, Crta. de Valldemossa km 7.5, 07122 Palma de Mallorca (Baleares), SPAIN; toni.frontera@uib.es

[4] University of Santiago de Compostela, Department of Inorganic Chemistry, Faculty of Pharmacy, 15782 Santiago de Compostela, Spain.

- Correspondence: jniclos@ugr.es; (J.N.-G.)

INDEX OF CONTEXT

Table S1. Crystal Data and Structure Refinement for Compounds **1**-**3**.

Table S2. Selected Coordination Bond Lengths [Å] and Angles [°] for Compounds **1**-**3**.

Table S3. Hydrogen bonding data for Compounds **1**-**3**.

Table S4. Inter-molecular π,π-Stacking Interaction Parameters [Å, °] for Compounds **2** -**3**.

Table S5. Summary of the Results and Assignations in the Thermogravimetric Analysis of the Compound $[Cd(H_2EDTA)(H_2O)]\cdot 2H_2O$.

Table S6. Summary of the Results and Assignations in the Thermogravimetric Analysis of Compound $\{[Cd(\mu_3\text{-EDTA})(Him)\cdot Cd(Him)(H_2O)_2]\cdot H_2O\}_n$ (**1**).

Table S7. Summary of the Results and Assignations in the Thermogravimetric Analysis of Compound $[Cd(\mu_4\text{-CDTA})(Hade)\cdot Cd(Hade)_2]_n$ (**2**).

Table S8. Summary of the Results and Assignations in the Thermogravimetric Analysis of Compound $\{[Cd(\mu_3\text{-EDTA})(H_2O)\cdot Cd(H9heade)(H_2O)]\cdot 2H_2O\}_n$ (**3**).

Table S9. Coordination Number of Cd(II) chelated by distinct anions of H_4EDTA acid.

Table S1. Crystal Data and Structure Refinement for Compounds {[Cd(μ3-EDTA)(Him)·Cd(Him)(H2O)2]·H2O}n (**1**), {[Cd(μ4-CDTA)(Hade)·Cd(Hade)2]}n (**2**) and {[Cd(μ3-EDTA)(H2O)·Cd(H9heade)(H2O)]·2H2O}n (**3**).

Compound	**1**	**2**	**3**
Empirical formula	$C_{16}H_{26}Cd_2N_6O_{11}$	$C_{29}H_{33}Cd_2N_{17}O_8$	$C_{17}H_{33}Cd_2N_7O_{15}$
Formula weight	703.23	972.52	800.30
Temperature / K	100(2)	100(2)	298(2)
Wavelength / Å	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/n$	$P2_1/n$
Unit cell dimensions			
a / Å	9.7935(9)	16.903(2)	8.1917(8)
b / Å	16.2316(15)	8.5967(13)	12.6335(14)
c / Å	14.9467(12)	23.899(3)	28.474(3)
α / º	90	90	90
β / º	92.474(5)	104.414(4)	96.097(2)
γ / º	90	90	90
Volume / Å^{-3}	2373.8(4)	3363.4(8)	2030.1(5)
Z	4	4	4
Calc. density / Mg/m^3	1.968	1.921	1.814
Absorp. coefc. / mm^{-1}	1.860	1.345	1.529
F(000)	1392	1944	1600
Crystal size	0.26×0.20×0.12	0.21×0.07×0.05	0.12×0.10×0.08
θ range / º	2.081–30.561	2.488–28.440	2.161–27.531
Limiting indices / h,k,l	–14/13, –23/23, –21/21	-22/21, 0/11, 0/31	–9/10, –16/16, –37/32
Refl. collect / unique [R_{int}]	54392/7244 [0.0798]	10710/10710 [0.0463]	32562/6751 [0.1056)
Completeness θ / º	25.242/100.0	25.242/99.5	25.242/100.0
Absorp. correct.	Multi-scan	Multi-scan	Multi-scan
Max. /min. transm.	1.000/0.868	1.000/0.853	1.000/0.869
Data / parameters	7244/316	10710/510	6751/363
Goodness-of-fit on F^2	1.030	1.100	1.006
Final R indices	R_1 = 0.0358, wR_2 = 0.0620	R_1 = 0.0470, wR_2 = 0.1307	R_1 = 0.0457, wR_2 = 0.0763
R indices (all data)	R_1 = 0.0514, wR_2 = 0.0676	R_1 = 0.0542, wR_2 = 0.1363	R_1 = 0.0938, wR_2 = 0.0875
Largest dif. peak/hole / eÅ^{-3}	0.875/–1.036	2.001/–0.654	0.929/–0.596

Table S2. Selected Coordination Bond Lengths [Å] and Angles [°] for Compounds {[Cd(μ3-EDTA)(Him)·Cd(Him)(H_2O)2]·H_2O}n (**1**), {[Cd(μ4-CDTA)(Hade)·Cd(Hade)2]}n (**2**) and {[Cd(μ3-EDTA)(H_2O)·Cd(H9heade)(H_2O)]·2H_2O}n (**3**).

Compound 1		**Compound 2**		**Compound 3**	
Distances					
Cd1-N1	2.224(2)	Cd1-O11 [a]	2.253(5)	Cd1-O2	2.232(4)
Cd1-O13[a]	2.3365(19)	Cd1-O11	2.253(5)	Cd1-O24	2.341(3)
Cd1-O21	2.3893(19)	Cd1-O41[b]	2.308(4)	Cd1-O28	2.418(3)
Cd1-N10	2.395(2)	Cd1-O41 [c]	2.308(4)	Cd1-O35	2.344(3)
Cd1-N20	2.406(2)	Cd1-N13	2.366(5)	Cd1-O39	2.332(3)
Cd1-O11	2.4366(19)	Cd1-N13 [a]	2.366(5)	Cd1-N21	2.425(3)
Cd1-O23	2.5556(19)	Cd2-O12	2.277(5)	Cd1-N32	2.383(3)
Cd2-O14	2.1942(19)	Cd2-O31	2.305(5)	Cd2-O1	2.305(3)
Cd2-N3	2.205(2)	Cd2-N23	2.332(5)	Cd2-O25	2.229(3)
Cd2-O12	2.2133(18)	Cd2-O22	2.344(5)	Cd2-O28 [a]	2.411(3)
Cd2-O1	2.2952(19)	Cd2-O42	2.364(5)	Cd2-O29 [a]	2.445(3)
Cd2-O2	2.3413(19)	Cd2-N1	2.457(5)	Cd2-O36 [b]	2.268(3)
Cd1-Cd2	5.1953(5)	Cd2-N2	2.469(5)	Cd2-N7	2.267(4)
		Cd3-O32[c]	2.250(4)		
		Cd3-O32[d]	2.250(4)		
		Cd3-O21 [e]	2.270(4)		
		Cd3-O21	2.270(4)		
		Cd3-N33	2.380(5)		
		Cd3-N33 [e]	2.380(5)		
Angles					
N1-Cd1-O13 [a]	104.61(8)	O11 [a] -Cd1-O11	180.0	O2-Cd1-O24	96.23(14)
N1-Cd1-O21	94.31(8)	O11 [a] -Cd1-O41 [b]	98.30(17)	O2-Cd1-O28	79.73(12)
O13 [a] -Cd1-O21	160.46(7)	O11-Cd1-O41 [b]	81.70(17)	O2-Cd1-O35	97.30(14)
N1-Cd1-N10	149.97(8)	O11 [a] -Cd1-O41 [c]	81.70(17)	O2-Cd1-O39	78.46(13)
O13 [a] -Cd1-N10	71.74(7)	O11-Cd1-O41 [c]	98.30(17)	O2-Cd1-N21	141.22(13)
O21-Cd1-N10	94.26(7)	O41 [b] -Cd1-O41 [c]	180.0	O2-Cd1-N32	143.26(14)
N1-Cd1-N20	134.32(8)	O11 [a] -Cd1-N13	89.13(18)	O24-Cd1-O28	100.87(11)
O13 [a] -Cd1-N20	93.46(7)	O11-Cd1-N13	90.87(18)	O24-Cd1-O35	166.08(11)
O21-Cd1-N20	69.33(7)	O41 [b] -Cd1-N13	78.43(17)	O24-Cd1-N21	71.28(11)
N10-Cd1-N20	75.46(7)	O41 [c] -Cd1-N13	101.57(17)	O24-Cd1-N32	99.47(12)
N1-Cd1-O11	84.14(7)	O11 [a] -Cd1-N13 [a]	90.87(18)	O28-Cd1-N21	67.54(11)
O13 [a] -Cd1-O11	109.02(7)	O11-Cd1-N13 [a]	89.13(18)	O35-Cd1-O28	78.38(10)
O21-Cd1-O11	77.31(6)	O41 [b] -Cd1-N13 [a]	101.57(17)	O35-Cd1-N21	95.93(12)
N10-Cd1-O11	69.82(7)	O41 [c] -Cd1-N13 [a]	78.43(17)	O35-Cd1-N32	71.26(11)
N20-Cd1-O11	129.12(7)	N13-Cd1-N13 [a]	180.0	O39-Cd1-O24	83.29(11)
N1-Cd1-O23	78.15(7)	O12-Cd2-O31	163.0(2)	O39-Cd1-O28	158.12(10)
O13 [a] -Cd1-O23	75.48(6)	O12-Cd2-N23	104.1(2)	O39-Cd1-O35	102.65(12)
O21-Cd1-O23	104.28(6)	O31-Cd2-N23	92.09(19)	O39-Cd1-N21	133.22(11)
N10-Cd1-O23	127.03(7)	O12-Cd2-O22	106.0(2)	O39-Cd1-N32	70.72(12)
N20-Cd1-O23	66.21(7)	O31-Cd2-O22	82.18(19)	N32-Cd1-O28	128.69(11)
O11-Cd1-O23	162.28(6)	N23-Cd2-O22	78.09(18)	N32-Cd1-N21	75.50(12)
O14-Cd2-N3	114.96(8)	O12-Cd2-O42	83.8(2)	O1-Cd2-O28 [a]	80.24(10)
O14-Cd2-O12	99.51(7)	O31-Cd2-O42	93.6(2)	O1-Cd2-O29 [a]	82.04(11)
N3-Cd2-O12	145.24(8)	N23-Cd2-O42	81.65(19)	O25-Cd2-O1	98.95(12)
O14-Cd2-O1	86.47(7)	O22-Cd2-O42	159.10(19)	O25-Cd2-O28 [a]	78.84(10)

N3-Cd2-O1	92.61(8)	O12-Cd2-N1	70.07(18)	O25-Cd2-O29 [a]	131.97(11)
O12-Cd2-O1	84.78(7)	O31-Cd2-N1	100.22(18)	O25-Cd2-O36 [b]	92.10(12)
O14-Cd2-O2	105.37(7)	N23-Cd2-N1	142.31(17)	O25-Cd2-N7	117.49(12)
N3-Cd2-O2	92.02(8)	O22-Cd2-N1	68.66(17)	O28 [a] -Cd2-O29 [a]	53.80(10)
O12-Cd2-O2	82.69(7)	O42-Cd2-N1	132.18(17)	O36 [b] -Cd2-O1	166.94(12)
O1-Cd2-O2	164.00(7)	O12-Cd2-N2	91.95(18)	O36 [b] -Cd2-O28 [a]	108.90(10)
		O31-Cd2-N2	71.57(16)	O36 [b] -Cd2-O29 [a]	95.75(12)
		N23-Cd2-N2	144.46(16)	N7-Cd2-O1	84.88(12)
		O22-Cd2-N2	128.04(17)	N7-Cd2-O28 [a]	159.59(11)
		O42-Cd2-N2	68.60(18)	N7-Cd2-O29 [a]	110.45(12)
		N1-Cd2-N2	72.92(16)	N7-Cd2-O36 [b]	83.86(12)
		O32 [c] -Cd3-O32 [d]	180.0		
		O32 [c] -Cd3-O21 [e]	86.88(18)		
		O32 [d] -Cd3-O21 [e]	93.12(18)		
		O32 [c] -Cd3-O21	93.12(18)		
		O32 [d] -Cd3-O21	86.88(18)		
		O21 [e] -Cd3-O21	180.0		
		O32 [c] -Cd3-N33	101.24(18)		
		O32 [d] -Cd3-N33	78.76(18)		
		O21 [e] -Cd3-N33	91.91(18)		
		O21-Cd3-N33	88.09(18)		
		O32 [c] -Cd3-N33 [e]	78.76(18)		
		O32 [d] -Cd3-N33 [e]	101.24(18)		
		O21 [e] -Cd3-N33 [e]	88.09(18)		
		O21-Cd3-N33 [e]	91.91(18)		
		N33-Cd3-N33 [e]	180.0		

Symmetry codes

a: x+1,y,z	a: -x+2,-y+2,-z	a: -x+1/2,y+1/2,-z+3/2
	b: -x+2,-y+1,-z	b: -x+3/2,y+1/2,-z+3/2
	c: x,y+1,z	
	d: -x+1,-y+1,-z	
	e: -x+1,-y+2,-z	

Table S3. Hydrogen Bonding data for Compounds {[Cd(μ_3-EDTA)(Him)·Cd(Him)(H_2O)$_2$]·H_2O}$_n$ (**1**), {[Cd(μ_4-CDTA)(Hade)·Cd(Hade)$_2$]}$_n$ (**2**) and {[Cd(μ_3-EDTA)(H_2O)·Cd(H9heade)(H_2O)]·2H_2O}$_n$ (**3**). Superscript Letters Refer to the Symmetry Codes.

Compound	D–H···A	D···A (Å)	∠DHA (°)	Symmetry code
1	O1–H1W1···O24^c	2.694(3)	170.5	x-1,-y+1/2,z-1/2
	O1–H1W2···O22^d	2.636(3)	176.5	x,-y+1/2,z-1/2
	O2–H2W1···O21	2.759(3)	174.3	
	O2–H2W2···O24^b	2.777(3)	169.0	x-1,y,z
	O3–H3W1···O12	2.739(3)	171.5	
	O3–H3W2···O22^e	2.701(3)	165.3	-x+1,y+1/2,-z+1/2
	N2–H2A···O24^f	2.768(3)	173.9	-x+2,-y,-z
	N4–H4A···O3^d	2.717(3)	175.7	x,-y+1/2,z-1/2
2	N16–H16A···N37^g	3.014(8)	178.4	-x+3/2,y-1/2,-z+1/2
	N16–H16B···N31^h	3.080(8)	161.3	-x+3/2,y+1/2,-z+1/2
	N19–H19A···O11^a	2.969(7)	132.0	-x+2,-y+2,-z
	N26–H26A···N27^h	2.949(8)	171.5	-x+3/2,y+1/2,-z+1/2
	N29–H29A···O42	2.713(8)	137.2	
	N36–H36A···N17^g	3.028(8)	165.7	-x+3/2,y-1/2,-z+1/2
	N36–H36B···N11^h	3.086(8)	165.1	-x+3/2,y+1/2,-z+1/2
	N39–H39A···O31^c	2.810(7)	155.2	x,y+1,z
3	N6–H6B···O29^a	3.067(5)	153.6	-x+1/2,y+1/2,-z+3/2
	O1–H1A···O40^e	2.649(5)	165.7	x-1,y,z
	O1–H1B···O35^a	2.773(4)	174.5	-x+1/2,y+1/2,-z+3/2
	O2–H2A···O25^c	2.685(5)	162.4	-x+1/2,y-1/2,-z+3/2
	O2–H2B···O12	2.745(5)	144.9	
	O12–H12···O3	2.666(5)	171.	
	O3–H3A···N1^f	2.805(5)	162.5	-x,-y+1,-z+1
	O3–H3B···O40^e	2.749(5)	150.1	x-1,y,z
	O4–H4A···O36^b	2.938(7)	143.2	-x+3/2,y+1/2,-z+3/2
	O4–H4B···N3^g	2.961(6)	169.9	-x+1,-y+1,-z+1

Table S4. Inter-molecular π,π-Stacking Interaction Parameters [Å, °] for. Compounds {[Cd(μ_4-CDTA)(Hade)·Cd(Hade)$_2$]}$_n$ (**2**) and {[Cd(μ_3-EDTA)(H_2O)·Cd(H9heade)(H_2O)]·2H_2O}$_n$ (**3**).*

Comp.	Ring	π···π	Cg-Cg	α	IPD	SA	Symmetry code
2	Cg2 = N27/C25/C24/N29/C28 Cg4 = N11/C12/N13/C14/C15/C16	Cg2–Cg4^b	3.449(4)	1.174	3.295(3)	1.017	x,-1+y,z
	Cg3 = N37/C35/C34/N39/C38 Cg5 = N21/C22/N23/C24/C25/C26	Cg3- Cg5^c	3.514(4)	3.604	3.426(3)	0.782	x,1+y,z
3	Cg4 = N1/C2/N3/C4/C5/C6	Cg4-Cg4^f	3.668(3)	0.00	3.267(2)	1.667	-x, 1-y, 1-z

*CgI/CgJ = centroids of the corresponding stacked rings. Cg-Cg = inter-centroid distance, α = dihedral angle between mean ring planes, IPD = mean interplanar distance and SA = mean slippage angle (angle subtended by the inter-centroids vector to the plane normal). For other details see Janiak, C. J. *Chem. Soc. Dalton Trans.* **2000**, 3885–3898.

Table S.5 . Summary of the Results and Assignations in the Thermogravimetric Analysis of the Compound [Cd(H_2EDTA)(H_2O)]·2H_2O.

			Weight (%)		
Step or R	Temp. (°C)	Time (min)	Exp.	Cal.	Evolved gasses or residue (R)
1	35-165	0-13	8.166	7.090	2 H_2O*
2	165-275	13-27	1.081	3.945	1 H_2O*
3	275-400	27-40	11.393		H_2O, CO_2,
4	400-480	40-47	14.270		H_2O, CO_2, CO, CH_4, $H_2C{=}CH_2$ (t), N_2O, NO, NO_2
5	480-660	47-60	31.807		H_2O, CO_2, CO, CH_4, N_2O, NO, NO_2
R	660	70	33.242	28.118	CdO
R	950	93	33.291	28.118	CdO

*** Calculated values for only the loss of water or aqua ligand. t = trace amounts.**

[≠]For the molecular and crystal structure of this compound see ACAQOK in CSD Database or Polyakova, I. N.; Poznyak, A. L.; Sergienko, V. S.; Stopolyanskaya, L. V. Crystal Structures of Acid Ethylenediaminotetraacetates [Cd(H_2Edta) (H_2O)] ·2H_2O and [Mn(H_2O)$_4$][Mn(HEdta]·4H_2O, *Crystallogr. Rep.* **2001**, *46*, 40-45.

Table S.6. Summary of the Results and Assignations in the Thermogravimetric Analysis of Compound {[Cd(μ_3-EDTA)(Him)·Cd(Him)(H_2O)$_2$]·H_2O}$_n$ (**1**).

			Weight (%)		
Step or R	Temp. (°C)	Time (min)	Exp.	Cal.	Evolved gasses or residue ®
1	r.t-185	2-17	7.757	7.090	3 H_2O*, CO_2 (t)
2	185-300	17-28	1.057	3.945	H_2O*, CO_2 (t)
3	300-370	28-35	15.760		H_2O, CO_2
4	370-440	35-43	25.395		H_2O, CO_2, CO, CH_4, $H_2C{=}CH_2$ (t), N_2O, NO
5	440-560	43-57	12.555		H_2O, CO_2, CO(t), CH_4, NH_3, N_2O, NO, NO_2
R	560	57	37.452	36.520	2 CdO
R	950	94	37.222	36.520	2 CdO

*** Calculated only for the loss of water and aqua ligand. t = trace amounts.**

Table S.7. Summary of the Results and Assignations in the Thermogravimetric Analysis of Compound $[Cd(\mu_4\text{-CDTA})(Hade)\cdot Cd(Hade)_2]_n$ (**2**).

			Weight (%)		
Step or R	Temp. (°C)	Time (min)	Exp.	Cal.	Evolved gasses or residue ®
1	25-185	2-17	7.757	7.090	4 H_2O*, CO_2 (t)**
2	185-300	17-28	1.057	3.945	H_2O*, CO_2 (t)**
3	300-370	28-35	15.760		H_2O, CO_2
4	370-440	35-43	25.395		H_2O, CO_2, CO, CH_4, $H_2C{=}CH_2$ (t)**, N_2O, NO
5	440-560	43-57	12.555		H_2O, CO_2, CO(t)**, CH_4, NH_3, N_2O, NO, NO_2
R	560	57	37.452	24.586	2 CdO
R	950	94	37.222	34.926	$CdO\cdot Cd(NO_3)_2$

- CAUTION! Calculated for the water loss from an empirical formula $\{[Cd(\mu_4\text{-CDTA})(Hade)\cdot Cd(Hade)_2]\cdot \mathbf{4}H_2O\}_n$. All other calculated values also refer to this formula. ** t = trace amounts.

Table S.8. Summary of the Results and Assignations in the Thermogravimetric Analysis of Compound $\{[Cd(\mu_3\text{-EDTA})(H_2O)\cdot Cd(H9heade)(H_2O)]\cdot 2H_2O\}_n$ (**3**).*

			Weight (%)		
Step or R	Temp. (°C)	Time (min)	Exp.	Cal.	Evolved gasses or residue ®
1	r.t-90	0-7	2.306*	13.516*	6 H_2O*, CO_2 (t)**
2	90-130	7-11	1.403*		
3	130-220	11-21	5.496*		
4	220-325	21-32	4.311		
5	325-405	32-38	9.531		H_2O, CO_2, CO
6	405-475	38-46	14.180	-	H_2O, CO_2, CO, CH_4, $H_2C{=}CH_2$ (t)
7	475-570	46-54	25.085	-	H_2O, CO_2, CO, CH_4, NH_3, N_2O, NO, NO_2
8	570-636	54-64	3.493	-	H_2O, CO_2, CO, CH_4, NH_3, N_2O, NO, NO_2
R	635	64	34.205	32.090	2 CdO
R	950	93	34.016	32.090	2 CdO

- CAUTION! Calculated for the water loss to an empirical formula $\{[Cd(\mu_3\text{-EDTA})(H_2O)\cdot Cd(H9heade)\ (H_2O)]\cdot \mathbf{4}H_2O\}_n$. All other calculated values also refer to this formula. ** t = trace amounts.

Table S.9. Coordination Number of Cd(II) chelated by different anions of H_4EDTA acid.

Chelating anion	Denticity as chelators	Seventh donor	ACRONIM in CSD	CN Cd-EDTA chelate	CN Cd non-chelated
H_2EDTA^{2-}	hexadentate	O-aqua	ACAQOK	7	-
	hexadentate	O-aqua	1992206*	7	-
	pentadentate	S-donor	LOFKAT	6**	-
	tetradentate	N-donor	IFELIP	6***	
$HEDTA^{3-}$	hexadentate	O-aqua	BOLMAQ01	7	6
	hexadentate	O-aqua	TUGNEQ	7	6
$EDTA^{4-}$	hexadentate	O-aqua	BENVUN	7	-
		O-aqua	BENWAU	7	-
		O-carboxylate	BINBOP10	7	6
		O-aqua	CDEDTA11	7	6
		O-carboxylate	FAFJON	7	7
		O-aqua	SOXXIN	7	6
		O-aqua	SOXXOT	7	6

*Deposition Number from: Belmont-Sánchez, C. B.; Ruiz-González, N.; Frontera, A.; Matilla-Hernández, A.; Castiñeiras, A.; Juan Niclós-Gutiérrez, J. Anion-cation recognition pattern, thermal stability and DFT-calculations in the crystal structure of H_2dap[Cd(HEDTA)(H_2O)] salt (H_2dap = H_2(N3,N7)-2,6-diaminopurinium(1+) ion), *Crystals*, 10 (2020) 304.

** Reached with an S(exocyclic-thio donor)-triazole coligand.

*** Reached with two N(heterocyclic donor)-guanazole coligands.