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Supporting Information

for the

Cadmium(II) Coordination Polymers Based on Substituted Malonic Acid: Synthesis, Characterization and Photoluminescent Properties

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Table S1. Summary of the Crystal Data and Refinement Details for complexes **1-4**

	1·0.5H$_2$O	**2**	**3**	**4**
Formula	$C_{24}H_{37}Cd_6O_{30.5}$	$C_5H_8CdO_5$	$C_7H_{12}CdO_5$	$C_{10}H_{10}CdO_5$
M	1487.82	260.51	286.56	322.58
Crystal system	trigonal	monoclinic	orthorhombic	orthorhombic
Space group	R-3	*P21/c*	*Pbca*	*Pbca*
a, Å	17.908(2)	10.520(2)	9.2530(19)	9.39660(10)
b, Å	17.908(2)	9.2650(19)	7.8740(16)	7.88530(10)
c, Å	10.9400(9)	7.8960(16)	25.531(5)	29.8510(4)
α deg	90	90	90	90
β, deg	90	104.74(3)	90	90
γ, deg	120.00	90	90	90
V, Å^3	3038.3(6)	744.3(3)	1860.1(7)	2211.81(5)
Z	3	4	8	8
ρ_{calc} (Mg m^{-3})	2.418	2.325	2.046	1.937
F(000)	2064	504	1120	1264
μ (Mo-K$_\alpha$) (mm^{-1})	3.199	3.162	2.541	1.976
Number parameters/restrains	95/6	108/2	120/0	153/2
Goodness-of-fit (*S*)	1.338	1.103	1.088	1.393
R1, $I > 2\sigma(I)$ (all)	0.0360 (0.0382)	0.0444 (0.0447)	0.0401 (0.0409)	0.0363 (0.0426)
wR2, $I > 2\sigma(I)$ (all)	0.0729 (0.0735)	0.1239 (0.1243)	0.1091 (0.1100)	0.0616 (0.0633)
Max/min electron density (e Å^{-3})	0.696 / -1.053	1.366 / -2.761	1.057 / -2.241	0.995 / -0.837
Measured reflections (R_{int})	1714 (0.060)	3686 (0.0444)	14442 (0.0693)	21771 (0.0243)
Independent reflections [$I > 2\sigma(I)$]	1711 (1662)	1553 (1526)	1902 (1816)	3090 (2715)

Table S2. Selected bond lengths [A˚] and angles [deg] for **1**.

Cd(1)-O(2)	2.272(3)	Cd(1)-O(4)	2.276(3)
Cd(1)-O(1a)	2.399(3)	Cd(1)-O(4b)	2.637(3)
Cd(1)-O(2a)	2.465(3)	Cd(1)-O(1W)	2.287(3)
Cd(1)-O(3b)	2.277(3)		
O(2)-Cd(1)-O(4)	84.67(10)	O(1a)-Cd(1)-O(1W)	86.76(13)
O(2)-Cd(1)-O(1W)	86.60(11)	O(1a)-Cd(1)-O(2a)	53.19(10)
O(2)-Cd(1)-O(1a)	78.68(11)	O(1a)-Cd(1)-O(3b)	139.93(11)
O(2)-Cd(1)-O(2a)	131.86(10)	O(1a)-Cd(1)-O(4b)	167.24(10)
O(2)-Cd(1)-O(3b)	141.37(11)	O(2a)-Cd(1)-O(1W)	89.43(11)
O(2)-Cd(1)-O(4b)	89.29(10)	O(2a)-Cd(1)-O(3b)	86.74(10)
O(4)-Cd(1)-O(1W)	171.12(10)	O(2a)-Cd(1)-O(4b)	138.55(9)
O(4)-Cd(1)-O(1a)	89.95(12)	O(3b)-Cd(1)-O(1W)	93.32(12)
O(4)-Cd(1)-O(2a)	131.86(10)	O(3b)-Cd(1)-O(4b)	52.12(10)
O(4)-Cd(1)-O(3b)	94.51(12)	O(4b)-Cd(1)-O(1W)	88.29(12)
O(4)-Cd(1)-O(4b)	93.19(15)		

Symmetry codes: (a) = -*y*+1/3, *x*-*y*+2/3, *z*-1/3, (b) = *x*-*y*+2/3, *x*+1/3, -*z*+1/3.

Table S3. Selected bond lengths [A˚] and angles [deg] for **2**

Cd(1)-O(1a)	2.218(4)	Cd(1)-O(4)	2.401(3)
Cd(1)-O(2)	2.264(4)	Cd(1)-O(4b)	2.279(3)
Cd(1)-O(3c)	2.389(4)	Cd(1)-O(1W)	2.279(3)
O(1a)-Cd(1)-O(2)	81.76(13)	O(2)-Cd(1)-O(4b)	149.76(13)
O(1a)-Cd(1)-O(4)	156.96(12)	O(4)-Cd(1)-O(1W)	78.26(12)
O(1a)-Cd(1)-O(1W)	118.65(14)	O(4)-Cd(1)-O(3c)	80.54(12)
O(1a)-Cd(1)-O(3c)	84.82(14)	O(4)-Cd(1)-O(4b)	73.62(12)
O(1a)-Cd(1)-O(4b)	121.86(13)	O(1W)-Cd(1)-O(3c)	156.17(12)
O(2)-Cd(1)-O(4)	78.64(11)	O(1W)-Cd(1)-O(4b)	81.74(12)
O(2)-Cd(1)-O(1W)	104.32(15)	O(3c)-Cd(1)-O(4b)	78.64(11)
O(2)-Cd(1)-O(3c)	81.86(16)		

Symmetry codes: (a) = *x*, -*y*+1/2, *z*-1/2; (b) = a(**2**) = -*x*+2, -y+1, -*z*+1; (c) = -*x*+2, *y*-1/2, -*z*+3/2

a(**2**) = nomenclature of symmetry used for clarity in the manuscript

Table S3. Selected bond lengths [A˚] and angles [deg] for **3** and **4**.

	3	**4**
Cd(1)-O(2)	2.406(2)	2.411(2)
Cd(1)-O(4)	2.267(3)	2.263(2)
Cd(1)-O(1f)	2.410(2)	2.461(3)
Cd(1)-O(2e)	2.279(2)	2.261(2)
Cd(1)-O(3d)	2.218(3)	2.246(2)
Cd(1)-O(1W)	2.279(3)	2.318(3)
O(2)-Cd(1)-O(4)	78.71(8)	78.11(8)
O(2)-Cd(1)-O(1f)	79.56(8)	83.35(8)
O(2)-Cd(1)-O(2e)	155.95(9)	75.44(9)
O(2)-Cd(1)-O(3d)	155.95(9)	155.87(8)
O(2)-Cd(1)-O(1W)	78.39(8)	76.43(9)
O(4)-Cd(1)-O(1f)	82.04(9)	78.35(9)
O(4)-Cd(1)-O(2e)	149.01(8)	148.82(9)
O(4)-Cd(1)-O(3d)	81.46(9)	79.35(9)
O(4)-Cd(1)-O(1W)	104.89(9)	104.38(10)
O(1W)-Cd(1)-O(1f)	155.01(8)	158.41(9)
O(1W)-Cd(1)-O(2e)	81.29(8)	85.20(10)
O(1W)-Cd(1)-O(3d)	120.18(9)	117.80(10)
O(1f)-Cd(1)-O(2e)	81.07(8)	82.45(8)
O(1f)-Cd(1)-O(3d)	84.35(9)	83.79(9)
O(2e)-Cd(1)-O(3d)	122.26(9)	122.80(9)

Symmetry codes: (d) = -*x*+3/2, *y*-1/2, *z*; (e) = a(**3**) = a(**4**) = -*x*+1, -y, -*z*+1; (f) = *x*+1/2, -*y*+1/2, -*z*+1

a(**3**) = a(**4**) = nomenclature of symmetry used for clarity in the manuscript

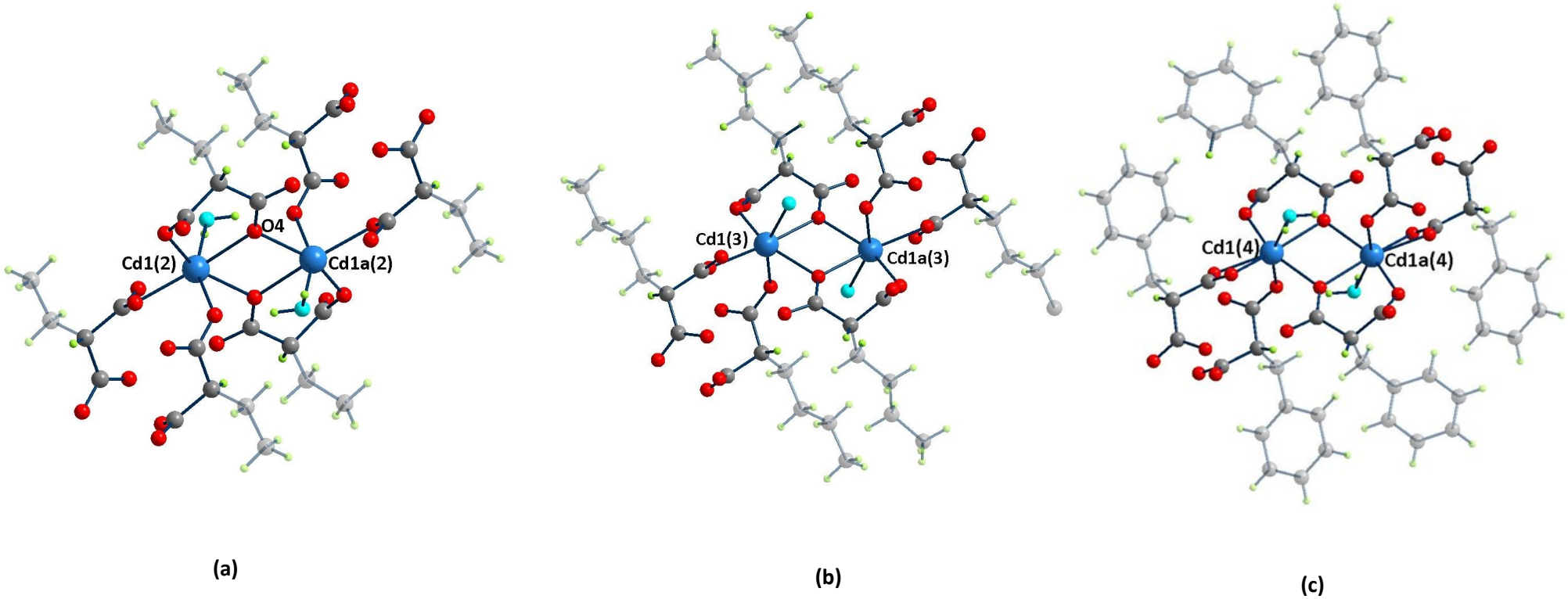


Fig. S1. Detail of the dinuclear units present in complexes **2** (a), **3** (b) and **4** (c)

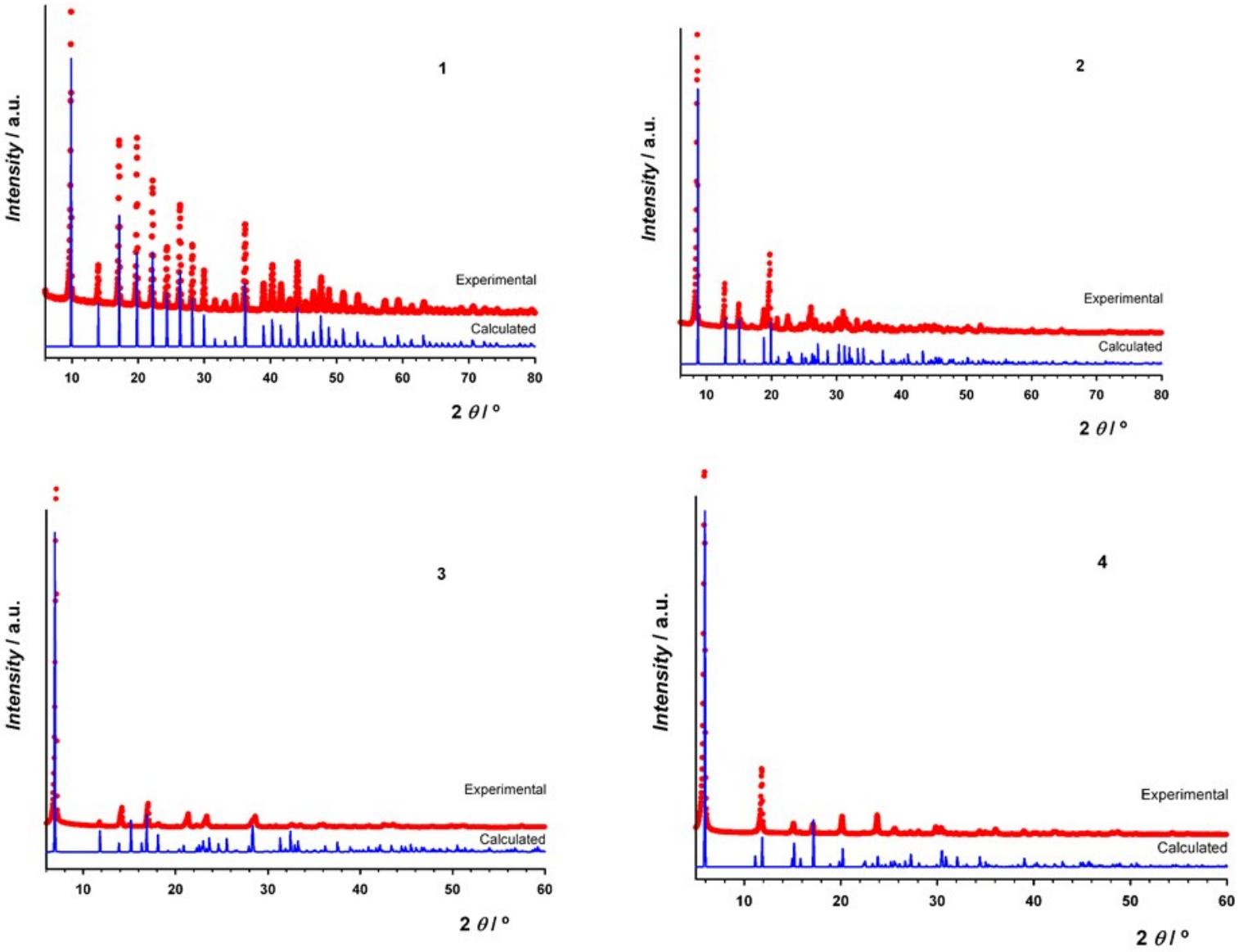


Fig. S2. X-ray diffraction patterns for complexes **1-4**.

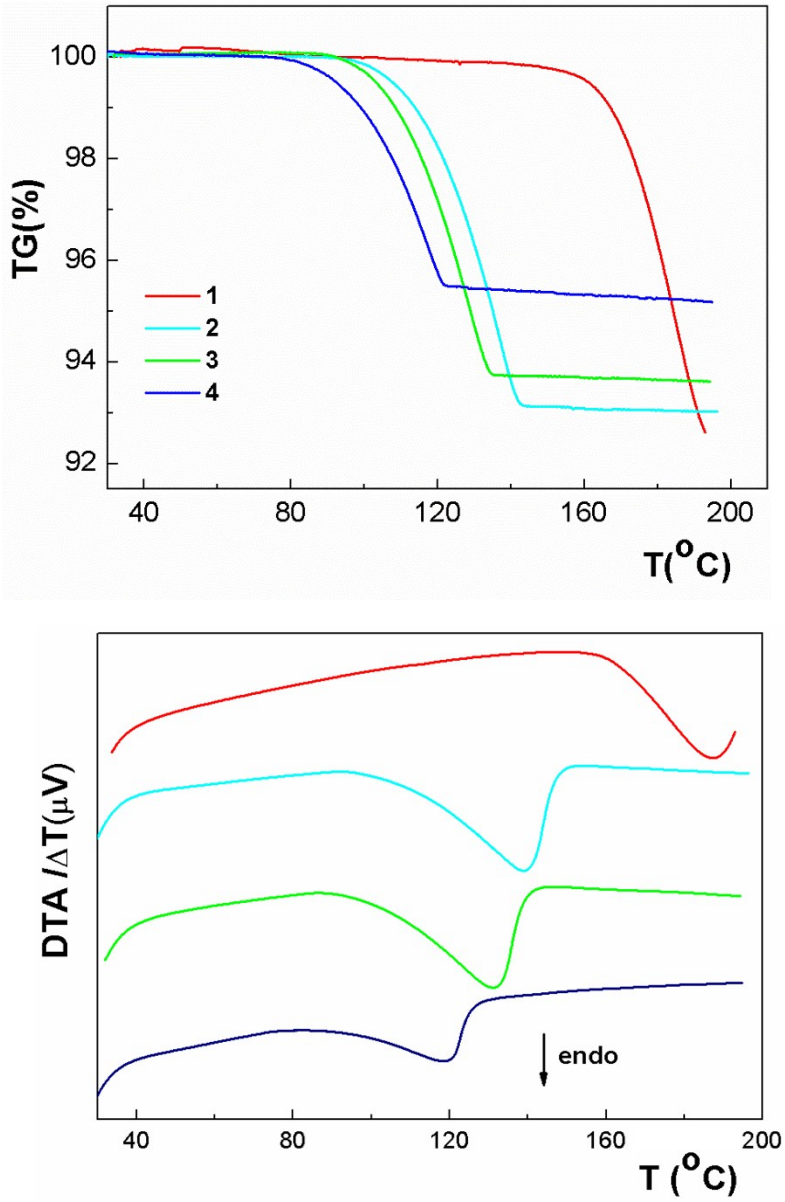
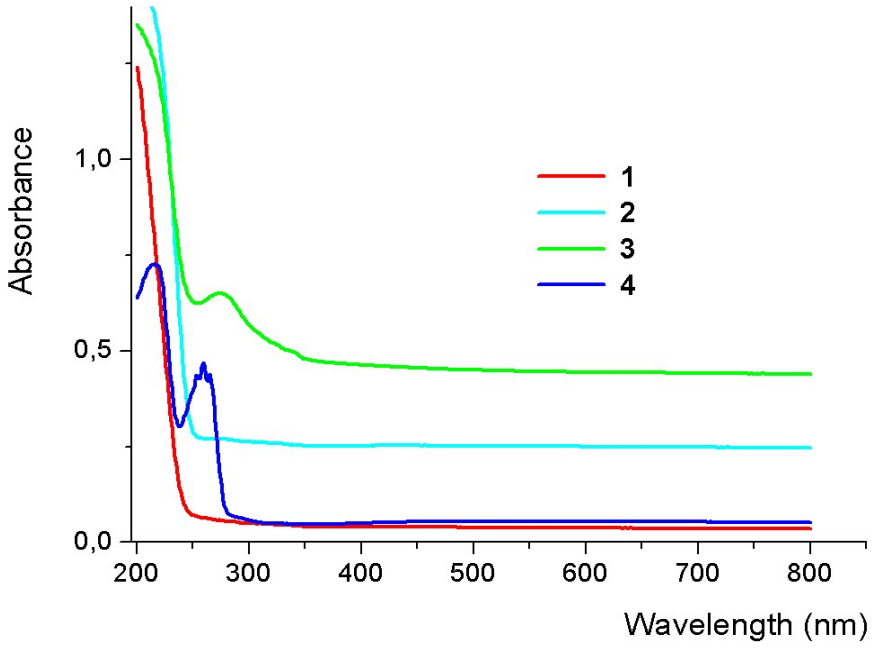
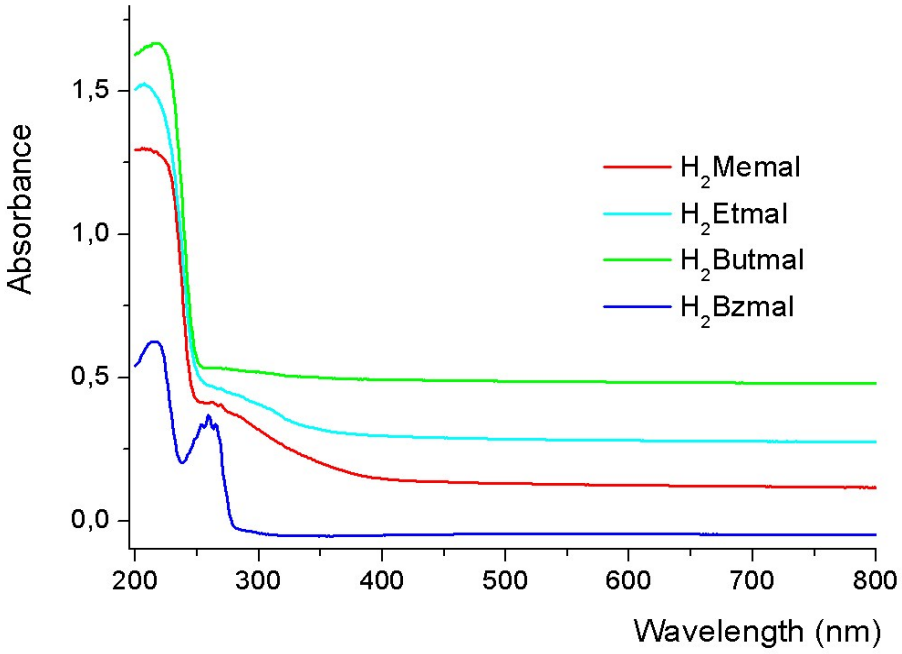


Fig. S3. TG/DTA curves of the complexes **1** (red), **2** (cyan), **3** (green) and **4** (blue). TG = mass loss (percent); DTA = ΔT/(μV) (↓ endo process).



(a)



(b)

Fig. S4. (a) UV-Vis absorption spectra of the complexes **1** (red), **2** (cyan), **3** (green) and **4** (blue).; (b) UV-Vis absorption spectra of the Methyl-(H_2Memal), ethyl- (H_2Etmal), butyl-(H_2Butmal) and benzyl malonic (H_2Bzmal) acids. Some of the spectra are vertically shifted for clarity.

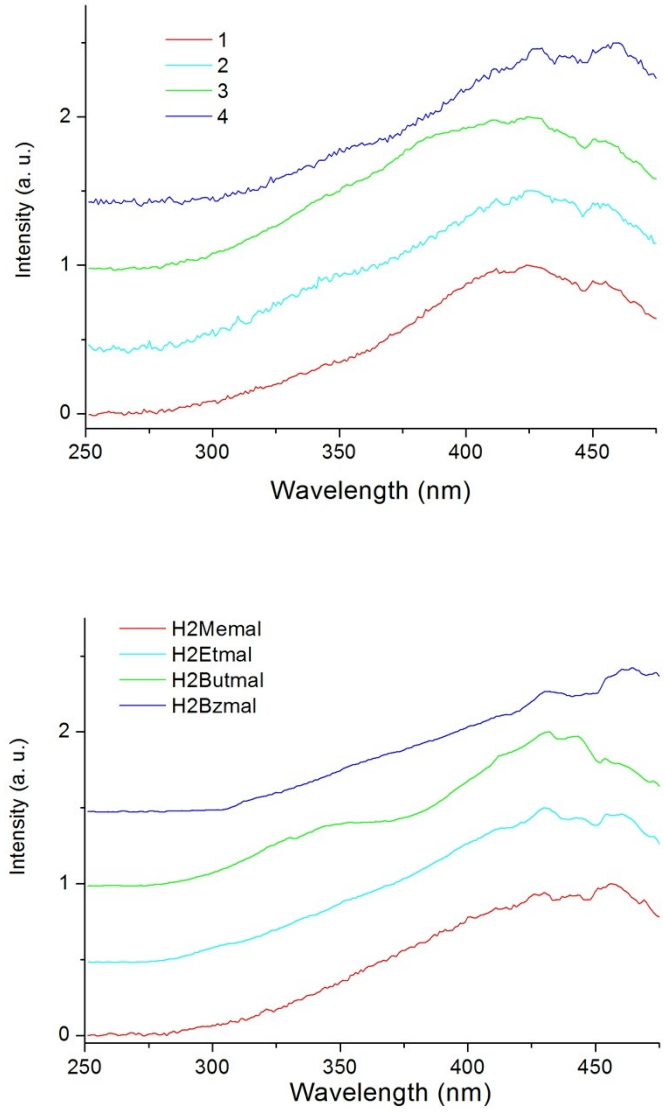


Figure S5. (a) UV-Vis excitation spectra of the complexes 1 (red), 2 (cyan), 3 (green) and 4 (blue) under detection at 500 nm; (b) UV-Vis excitation spectra of the Methyl-(H_2Memal), ethyl- (H_2Etmal), butyl- (H_2Butmal) and benzyl malonic (H_2Bzmal) acids under detection at 500 nm.