Mononuclear discrete complexes and coordination polymers based on metal(II) chelidonate complexes with aromatic N,N-chelating ligands

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Supplementary material

Table S1. Selected bond lengths (Å) and angles (º) for the coordination polymers **1** and **2**.

1		**2**	
Cu–O4	1.908(3)	Zn1–O6	1.987(5)
Cu–O6^{i}	1.940(3)	Zn1–O14	2.011(5)
Cu–O6^{ii}	2.564(3)	Zn1–O1w	2.089(5)
Cu–N1	1.983(3)	Zn1–N3	2.100(6)
Cu–N2	1.992(3)	Zn1–N4	2.122(7)
		Zn2–O16	2.007(5)
		Zn2–O4^{i}	2.023(5)
		Zn2–N2	2.093(6)
		Zn2–O2w	2.093(5)
		Zn2–N1	2.118(6)
O4–Cu–O6^{i}	97.46(12)	O6–Zn1–O14	97.3(2)
O4–Cu–N1	91.91(13)	O6–Zn1–O1w	99.7(2)
O6^{i}–Cu–N1	169.60(12)	O14–Zn1–O1w	86.4(2)
O4–Cu–N2	166.75(14)	O6–Zn1–N3	126.8(2)
O6^{i}–Cu–N2	90.44(13)	O14–Zn1–N3	135.0(2)
N1–Cu–N2	81.23(14)	O1w–Zn1–N3	94.0(2)
O4–Cu–O6^{ii}	96.02(12)	O6–Zn1–N4	95.5(3)
O6^{i}–Cu–O6^{ii}	85.56(11)	O14–Zn1–N4	92.4(3)
N1–Cu–O6^{ii}	88.99(12)	O1w–Zn1–N4	164.8(2)
N2–Cu–O6^{ii}	95.19(12)	N3–Zn1–N4	76.2(2)
		O16–Zn2–O4^{i}	100.7(3)
i = x, 3/2-y, z-1/2		O16–Zn2–N2	132.0(2)
ii = 1-x, ½+y, 1.5-z		O4^{i}–Zn2–N2	126.4(2)
		O16–Zn2–O2w	87.5(2)
		O4^{i}–Zn2–O2w	97.9(2)
		N2–Zn2–O2w	94.2(2)
		O16–Zn2–N1	92.8(2)
		O4^{i}–Zn2–N1	93.5(2)
		N2–Zn2–N1	77.0(3)
		O2w–Zn2–N1	168.4(2)
		i = x-1, y ,z-1	

Table S2. Selected interatomic bond lengths (Å) and angles (º) for the mononuclear complexes **3**–**6**

Compound	**3**	**4**	**5**	**6**
M–O1w	2.004(3)	2.033(2)	2.090(5)	2.095(4)
M–O2w	1.992(3)	2.077(2)	2.096(6)	2.094(4)
M–O11	2.032(2)	2.045(2)	2.028(5)	
M–N1	2.177(3)	2.194(3)	2.059(6)	2.152(4)
M–N2	2.092(3)	2.154(2)	2.096(6)	2.189(4)
M–O3w		2.229(2)	2.055(6)	
M–N11				2.201(4)
M–N12				2.130(4)
O2w–M–O1w	117.60(13)	88.28(10)	90.5(2)	93.64(15)
O11–M–O2w	93.73(11)	87.49(9)	85.1(2)	
O1w–M–O11	96.96(11)	97.31(10)	94.8(2)	
O2w–M–N2	121.22(13)	95.64(10)	93.3(2)	168.74(15)
O1w–M–N2	120.34(12)	94.48(10)	94.5(2)	92.12(14)
O11–M–N2	88.59(10)	167.89(9)	170.5(2)	
O2w–M–N1	90.39(12)	91.35(10)	94.6(2)	92.64(15)
O1w–M–N1	92.79(11)	171.12(10)	172.8(2)	96.09(14)
N1–M–O11	166.17(10)	91.53(9)	90.7(2)	
N2–M–N1	78.00(10)	76.73(10)	80.1(2)	77.12(15)
O1w–M–O3w		91.34(11)	88.4(2)	
O11–M–O3w		88.56(9)	90.9(2)	
O2w–M–O3w		175.95(9)	175.8(2)	
N2–M–O3w		88.41(9)	90.8(2)	
N1–M–O3w		89.64(11)	86.9(2)	
O2w–M–N12				94.21(16)
O1w–M–N12				91.62(15)
N12–M–N1				169.33(16)
N12–M–N2				95.29(16)
O2w–M–N11				88.48(15)
O1w–M–N11				168.40(15)
N12–M–N11				76.84(17)
N1–M–N11				95.20(16)
N2–M–N11				87.81(16)

Table S3. Main hydrogen bond distances (Å) and angles (º) for compounds **1**–**5**

Compound	D–H···A	d(D–H)	d(H···A)	d(D···A)	∠(DHA)
1[a]	C14–H14…O3^{i}	0.93	2.30	3.211(6)	167
	C15–H15…O5^{ii}	0.93	2.56	3.473(5)	166
	C19–H19…O3^{iii}	0.93	2.46	3.287(6)	148
2[b]	O1w…O3^{iii}			2.723(8)	
	O1w…O5^{iv}			2.731(9)	
	O2w…O13^{v}			2.760(8)	
	O2w…O3w^{i}			2.962(13)	
	O4w…O4^{iii}			2.920(2)	
	O4w…O16^{ii}			2.995(2)	
	C24–H24…O15^{i}	0.93	2.43	3.335(13)	165
	C27–H27…O15^{i}	0.93	2.49	3.421(13)	176
	C29–H29…O7^{vii}	0.93	2.49	3.263(14)	141
	C39–H39…O5^{vi}	0.93	2.48	3.282(13)	144
	C38–H38…O13^{viii}	0.93	2.56	3.390(12)	149
	C37–H37…O17^{vii}	0.93	2.53	3.453(13)	171
	C34–H34…O17^{vii}	0.93	2.49	3.411(14)	169
4[c]	O4w…O13^{i}			2.903(5)	
	O4w…O3^{ii}			2.945(6)	
	O2w–H2wA…O12^{iii}	0.75(8)	2.09(8)	2.831(3)	172
	O2w–H2wB…O14^{iii}	0.73(8)	1.98(8)	2.706(3)	174
	O1w–H1wA…O3^{iv}	0.72(8)	2.00(8)	2.724(3)	175
	O1w–H1wB…O13^{v}	1.02(8)	1.65(8)	2.659(3)	168
	C4–H4…O13^{vi}	0.93	2.39	3.267(4)	156
5[d]	O3w…O6w			2.617(8)	
	O3w…O5w			2.828(8)	
	O5w…O3^{i}			2.832(9)	
	O5w…O3^{ii}			2.872(9)	
	O6w…O12^{iii}			2.755(8)	
	O6w…O52^{iii}			2.763(8)	
	O6w…O1^{iii}			2.967(7)	
	O2w…O51^{v}			2.711(8)	
	O2w…O52^{vi}			2.842(7)	
	C17-H17…O3^{iv}	0.93	2.45	3.333(10)	154

[a] i = -1+x, 5/2-y, -1/2+z; ii = -x, 2-y, 1-z; iii = -1+x, y, -1+z .

[b] i = 1-x, 1-y, -z; ii = 1-x, -y, -z; iii = 2-x, -y, 1-z; iv = x-1, y, z; v = 2-x, -y, -z; vi = 2-x, 1-y, 1-z; vii = 2-x, 1-y, -z; viii = x, 1+y, z.

[c] i = 2-x, 1-y, 1-z; ii = -1+x, 1+y, -1+z; iii = -1+x, y, z; iv = 1-x, 1-y, 2-z; v = -1+x,1+y,z; vi = 3-x, -y, 2-z.

[d] i = x, -y+1/2, z+1/2; ii = x, y, z+1; iii = -x+1, -y, -z+1; iv = x-1, 1/2 -y, ½+z; v = x-1, y, z; vi = 1-z, -y, -z.

Table S4. Main hydrogen bond distances (Å) and angles (º) for compound **6**

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠(DHA)
Tetrameric association of crystallization water molecules				
O4w…O6w			2.74(2)	
O3w…O5w^{iii}			2.69(1)	
O3w…O4w^{iv}			2.76(1)	
O3w…O6w^{iv}			2.86(2)	
Linkage of the cationic complex with the water tetramer				
O2w…O4w^{i}			2.651(6)	
C1–H1…O6w^{i}	0.93	2.62	3.28(2)	128
Linkage of chelidonate ion with the water tetramer				
O3w…O33			2.990(9)	
O4w…O36			2.693(7)	
O6w…O35			2.97(2)	
O5w…O34^{v}			2.738(8)	
O6w…O35^{iv}			2.92(2)	
C34–34…O6w^{iv}	0.93	2.34	3.22(2)	156
Linkage of the cationic complex with chelidonate ion				
O1w…O36^{i}			2.699(5)	
O1w…O32^{i}			2.720(5)	
O1w…O31^{i}			2.901(5)	
O2w…O32^{ii}			2.643(5)	
C2–H2…O35^{vi}	0.93	2.42	3.349(7)	174
C8–H8…O35^{vii}	0.93	2.61	3.401(7)	143

[a] i = x+1/2, -y+3/2, z+1/2; ii = 1-x, 2-y, 1-z; iii = 1+x, y, z; iv = 1-x, 1-y, -z; v = -x+1/2, y-1/2, -z+1/2; vi = 3/2-x, ½+y, ½-z; vii = 1+x, y, 1+z.