Supplementary Materials

to the manuscript of Sergey P. Gavrish, Yaroslaw D. Lampeka, Philip Lightfoot and Hans Pritzkow “The crystal and molecular structures of the related nickel(II) complexes of open-chain and macrocyclic oxamide-based ligands and the peculiarities of water aggregates in their crystal lattices”

Table S1

The parameters of hydrogen bonds for the nickel(II) complexes of oxamide-derived ligands with standard uncertainties (s.u.) in parentheses

D-H…A	H…A/Å	∠DHA/°	D…A/Å
		$NiL^1 \cdot 4H_2O$	
N(1)-H(11)…O(1)[a]	2.03(2)	173(2)	2.928(4)
N(4)-H(41)…O(2)[a]	2.11(2)	171(2)	2.983(4)
N(4)-H(42)…O(2)[b]	2.23(2)	161(2)	3.064(4)
O(3)-H(31)…O(2)[c]	2.09(3)	177(2)	2.732(4)
O(3)-H(32)…O(5)	1.98(4)	180(2)	2.659(4)
O(4)-H(41)…O(1)	1.96(3)	174(2)	2.744(4)
O(4)-H(42)…O(6)[d]	1.82(4)	174(2)	2.651(4)
O(5)-H(51)…O(3)[e]	2.02(4)	172(2)	2.765(4)
O(5)-H(52)…O(4)	1.98(3)	170(2)	2.749(4)
O(6)-H(61)…O(4)	2.02(4)	178(2)	2.759(4)
O(6)-H(62)…O(3)[d]	2.01(3)	170(2)	2.740(4)
		$NiL^2 \cdot 3H_2O$	
O(3)-H(19)…O(4)	2.16(3)	155(3)	2.835(5)
O(4)-H(20)…O(5)[f]	1.89(3)	169(3)	2.815(4)
O(4)-H(21)…O(3)[g]	2.21(3)	157(3)	2.786(5)
O(3)-H(18)…O(1)	2.10(3)	164(3)	2.773(4)
O(5)-H(22)…O(2)	2.03(3)	171(3)	2.855(3)
O(5)-H(23)… O(2)[h]	2.04(3)	159(3)	2.794(3)

Symmetry codes: [a] [x, y-1, z]; [b] [x+1/2, -y+3/2, z]; [c] [-x+2, -y+2, z+1/2]; [d] [x-1/2, -y+5/2, z]; [e] [x-1/2, -y+3/2, z]; [f] [-x+1, -y+1, -z+1]; [g] [-x+1, -y+2, -z+1]; [h] [-x, -y+1, -z+1].

Table S2

The ^{1}H NMR chemical shifts δ (ppm), coupling constants J (Hz) and H-C-C-H dihedral angles φ (°)[a] for the macrocyclic complex NiL^{2}

H	δ	H-H	J	φ
e	2.695	**e-g**	12.7	156.4
f	2.803	**e-h**	6.5	36.3
g	2.776	**f-g**	5.1	36.4
h	3.158	**f-h**	0.6	83.7
		e-f	-11.3	
		g-h	-13.7	
c	3.642	**c-d**	-12.4	
d	3.663			

[a] Parameters taken from structural data.