Electronic Supplementary Material for CrystEngComm

Supporting Information

Observation of helical water chains reversibly inlayed in magnesium imidazole-4,5-dicarboxylate

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Materials and general methods

All the solvents and reagents for synthesis were commercially available and used as received. FT-IR spectra were recorded on a Bruker IFS 66v/S apparatus. The dry sample powder is mixed with KBr and treated directly in the purpose-made IR cell. Elemental analyses were performed on a Perkin-Elmer 2400 Series II analyzer. PXRD study was executed on a Rigaku X-ray diffractometer at 40 kV, 100 mA for Cu Kα radiation (λ = 1.5406 Å). Emission spectrum was taken on a Perkin Elmer LS50B luminescence spectrophotometer.

Table S1 Crystal data and structure refinement summary

[Mg(imdc)(H$_2$O)$_2$](H$_2$O)$_{1.5}$ (**1**)	
Chemical formula	$C_5H_9N_2O_{7.5}Mg$
Fw	241.45
Space group	*C*2/c
a / Å	13.936(3)
b / Å	11.642(2)
c / Å	12.090(2)
β / °	108.27(3)
V / Å^3	1862.4(6)
D_c / g cm^{-3}	1.722
Z	8
μ(Mo-Kα) / mm^{-1}	0.220
F(000)	1000
Data / restraints / parameters	1676/0/141
Goodness-of-fit on F^2	1.064
R^a/wR^b	0.0291/0.0861

[a] $R = \sum(||F_o|-|F_c||)/\sum|F_o|$. [b] $wR = [\sum(|F_o|^2 - |F_c|^2)^2/\sum(F_o^2)]^{1/2}$

Table S2 Selected bond parameters (Å, °) for complex **1**

Mg(1)-O(2)	2.0139(12)	Mg(1)-O(3)	2.0188(12)
Mg(1)-O(2W)	2.0713(15)	Mg(1)-O(4)#1	2.1137(12)
Mg(1)-O(1W)	2.1492(14)	Mg(1)-N(2)#1	2.1500(13)
O(2)-Mg(1)-O(3)	95.16(5)	O(2)-Mg(1)-O(2W)	94.88(6)
O(3)-Mg(1)-O(2W)	90.37(5)	O(2)-Mg(1)-O(4)#1	93.14(5)
O(3)-Mg(1)-O(4)#1	170.23(5)	O(2W)-Mg(1)-O(4)#1	94.06(5)
O(2)-Mg(1)-O(1W)	84.11(5)	O(3)-Mg(1)-O(1W)	89.64(5)
O(2W)-Mg(1)-O(1W)	178.98(6)	O(4)#1-Mg(1)-O(1W)	86.10(5)
O(2)-Mg(1)-N(2)#1	166.95(5)	O(3)-Mg(1)-N(2)#1	95.15(5)
O(2W)-Mg(1)-N(2)#1	93.04(6)	O(4)#1-Mg(1)-N(2)#1	75.94(5)
O(1W)-Mg(1)-N(2)#1	87.98(5)		

Symmetry codes: #1: $-x + 0.5, y + 0.5, -z + 0.5$; #2: $-x + 0.5, y - 0.5, -z + 0.5$.

Table S3 Hydrogen-bonding geometry (Å, °) for **1**

D–*H*···*A*	*H*···*A*	*D*···*A*	*D*–*H*···*A*
N1-H1A···O1#1	1.917	2.788	163
O1W-H1WA···O1#2	1.976	2.788	171
O1W-H1WB···O3W	2.017	2.833	174
O2W-H2WA···O3W#3	2.052	2.861	173
O2W-H2WB···O1#4	2.173	2.966	160
O2W-H2WB···O2#4	2.351	3.046	142
O3W-H3WA···O4#5	2.181	2.900	146
O3W-H3WA···O3#5	2.646	3.289	136
O3W-H3WB···O4W#6	2.034	2.822	158
O4W-H4WA···O1W#2	2.137	2.876	150

Symmetry codes: #1: -*x* + 1, -*y* + 1, -*z*; #2: -*x* + 1, *y*, -*z* + 0.5; #3: -*x* + 0.5, *y* - 0.5, -*z* + 0.5; #4: -*x* + 0.5, -*y* + 1.5, -*z*; #5: -*x* + 0.5, -*y* + 1.5, -*z*; #6: -*x* + 1, -*y* + 2, -*z* + 1.