Supporting Information

Synthesis and crystallographic characterisation of $Mg(H_2dhtp)(H_2O)_5 \cdot H_2O$

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Table S.1. Selected bond lengths [Å] and angles [°] for $Mg(H_2dhtp)(H_2O)_5 \cdot H_2O$

Mg(1)-O(1)	2.0231(11)	O(2W)-Mg(1)-O(5W)	91.90(4)
Mg(1)-O(2W)	2.0402(11)	O(4W)-Mg(1)-O(5W)	89.57(4)
Mg(1)-O(4W)	2.0416(11)	O(1)-Mg(1)-O(3W)	95.69(4)
Mg(1)-O(5W)	2.0490(11)	O(2W)-Mg(1)-O(3W)	92.15(4)
Mg(1)-O(3W)	2.0903(10)	O(4W)-Mg(1)-O(3W)	90.49(4)
Mg(1)-O(1W)	2.1134(10)	O(5W)-Mg(1)-O(3W)	85.78(4)
		O(1)-Mg(1)-O(1W)	90.78(4)
O(1)-Mg(1)-O(2W)	88.73(4)	O(2W)-Mg(1)-O(1W)	91.01(4)
O(1)-Mg(1)-O(4W)	89.74(4)	O(4W)-Mg(1)-O(1W)	86.50(4)
O(2W)-Mg(1)-O(4W)	177.07(5)	O(5W)-Mg(1)-O(1W)	87.72(4)
O(1)-Mg(1)-O(5W)	178.38(5)	O(3W)-Mg(1)-O(1W)	172.86(4)

Table S.2. Hydrogen bonds for $Mg(H_2dhtp)(H_2O)_5 \cdot H_2O$ [Å and °]

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(3)-H(3)···O(2)	0.84	1.79	2.5334(14)	147.2
O(6)-H(6)···O(5)	0.84	1.75	2.4926(14)	147.0
O(2W)-H(2A)···O(6W)	0.892(9)	1.900(10)	2.7825(14)	170.0(15)
$O(6W)-H(6A)\cdots O(1W)^{I}$	0.898(9)	2.168(10)	3.0020(14)	154.1(14)
$O(5W)-H(5A)\cdots O(5)^{II}$	0.897(9)	1.819(9)	2.7154(14)	177.0(16)
$O(3W)-H(3W)\cdots O(4)^{II}$	0.911(9)	1.731(10)	2.6275(13)	167.4(15)
$O(2W)-H(2W)\cdots O(6)^{III}$	0.881(9)	1.958(10)	2.8236(14)	167.3(15)
$O(3W)-H(3A)\cdots O(2)^{IV}$	0.897(9)	1.924(11)	2.7617(14)	154.7(15)
$O(4W)-H(4A)\cdots O(3W)^{V}$	0.886(9)	1.849(9)	2.7334(13)	176.4(16)
$O(4W)-H(4W)\cdots O(2)^{V}$	0.887(9)	1.885(11)	2.7361(13)	160.2(15)
$O(5W)-H(5W)\cdots O(3)^{VI}$	0.891(9)	1.856(10)	2.7416(14)	172.7(16)
$O(6W)-H(6W)\cdots O(4)^{VII}$	0.892(9)	1.853(10)	2.7397(15)	172.1(17)

Symmetry transformations used to generate equivalent atoms:

I: x, y-1, z **II:** x+1/2, -y+3/2, z-1/2 **III:** -x+1/2, y-1/2, -z+1/2

IV: -x+3/2, y-1/2, -z+1/2 **V:** -x+3/2, y+1/2, -z+1/2

VI: x-1/2, -y+3/2, z-1/2 **VII:** -x+1, -y+1, -z+1

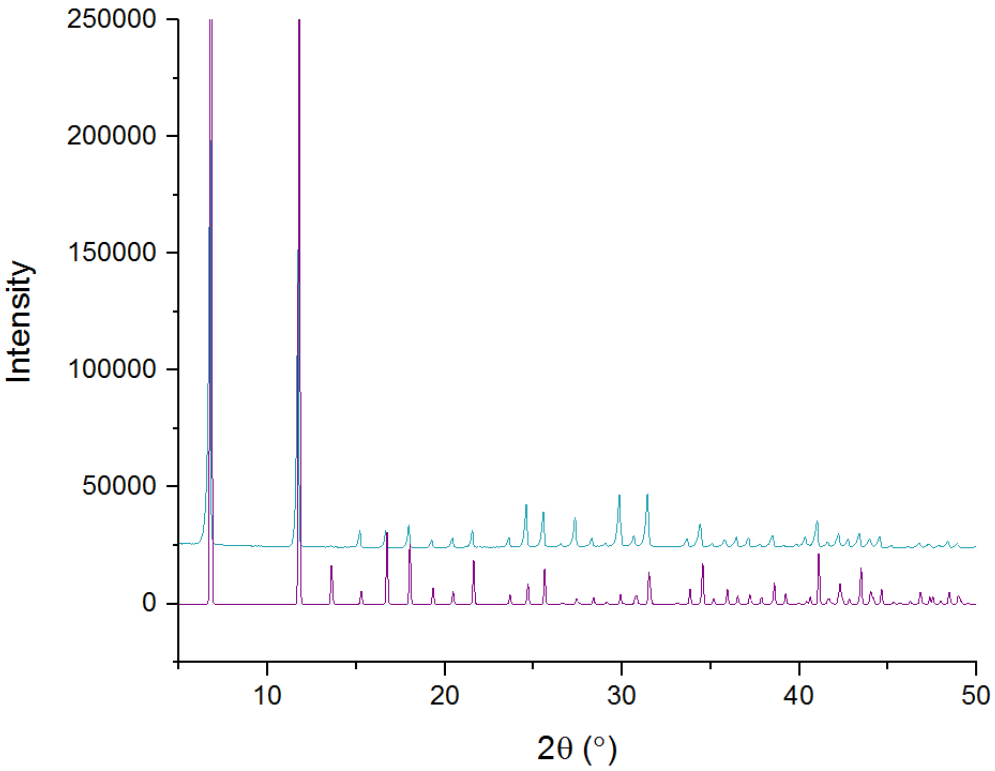

Fig. S.1. Powder XRD patterns for CPO-27-Mg. Teal – as-synthesised; Purple – simulated spectrum at a factor of 100

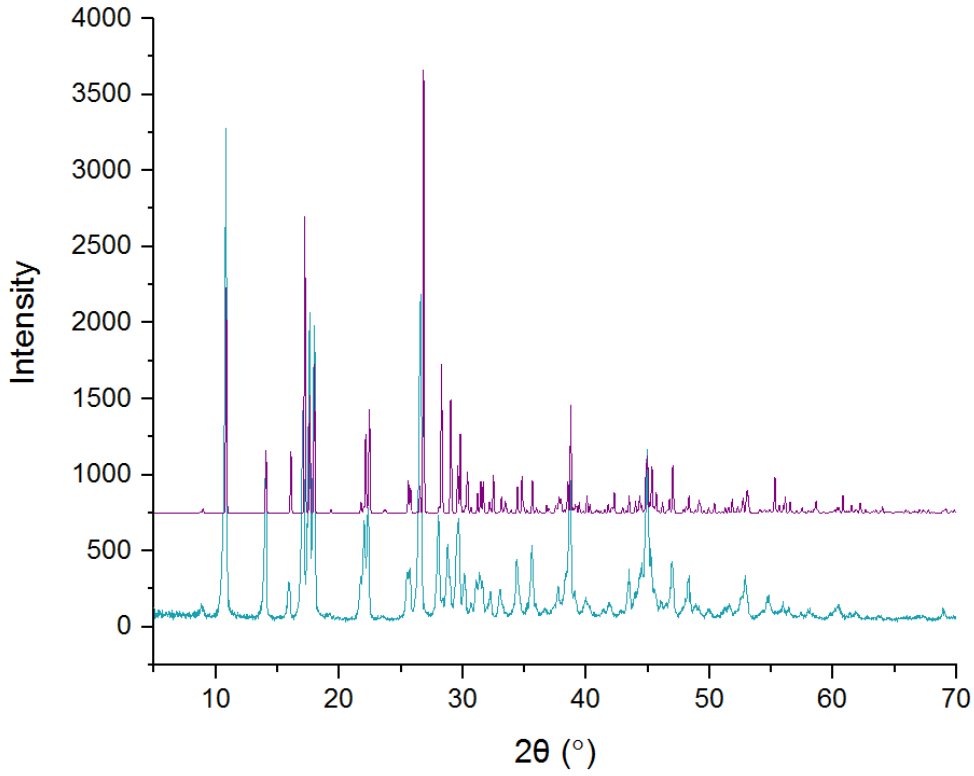

Fig. S.2. Powder XRD spectra for monomeric species, $Mg(H_2dhtp)(H_2O)_5 \bullet H_2O$. Teal – as-synthesised; Purple – simulated from single crystal data at a factor of 100

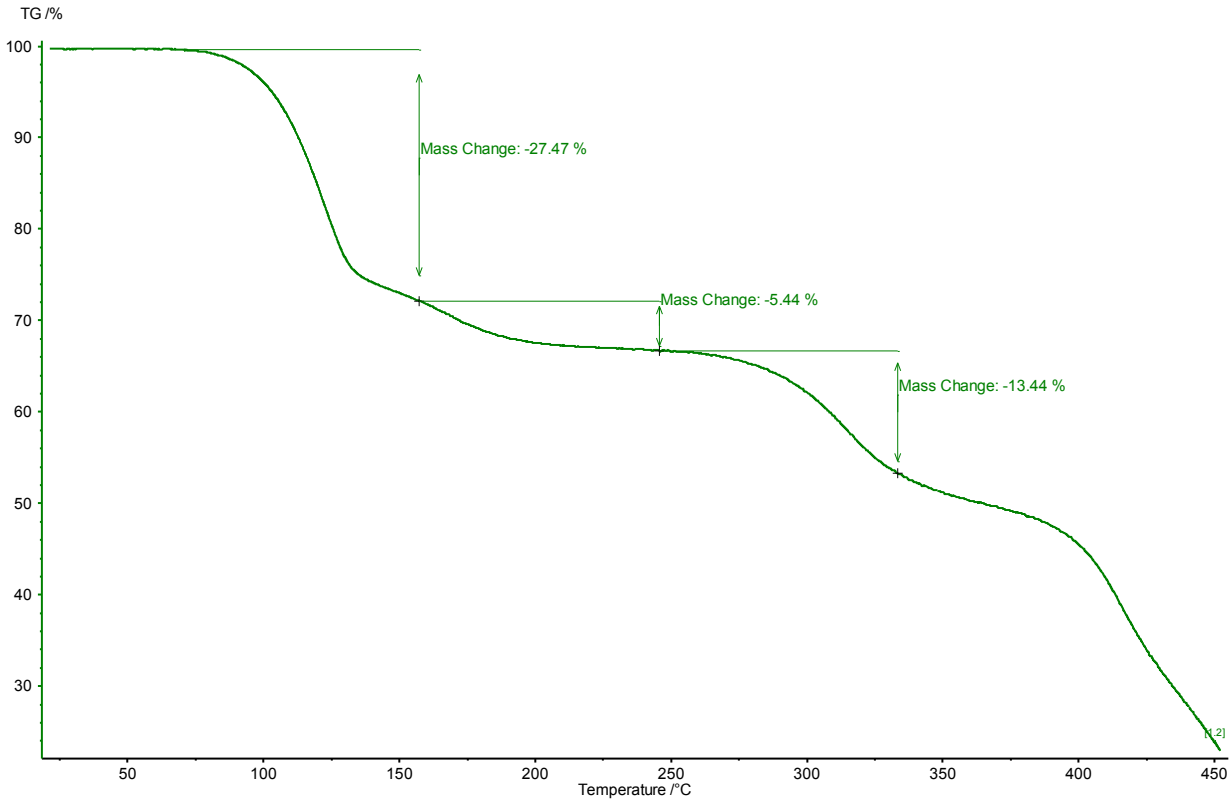

Fig. S.3. Thermogravimetric analysis (TGA) showing three mass changes of 27.47, 5.44 and 13.44% corresponding to the loss of $5H_2O$, H_2O and CO_2 respectively

Eq. (S.1). Thermogravimetric analysis calculations

$328.52\ gmol^{-1} \times 0.2747\% = 90.24\ gmol^{-1}$ $5H_2O$

$328.52\ gmol^{-1} \times 0.0544\% = 17.87\ gmol^{-1}$ H_2O

$328.52\ gmol^{-1} \times 0.1344\% = 44.15\ gmol^{-1}$ CO_2

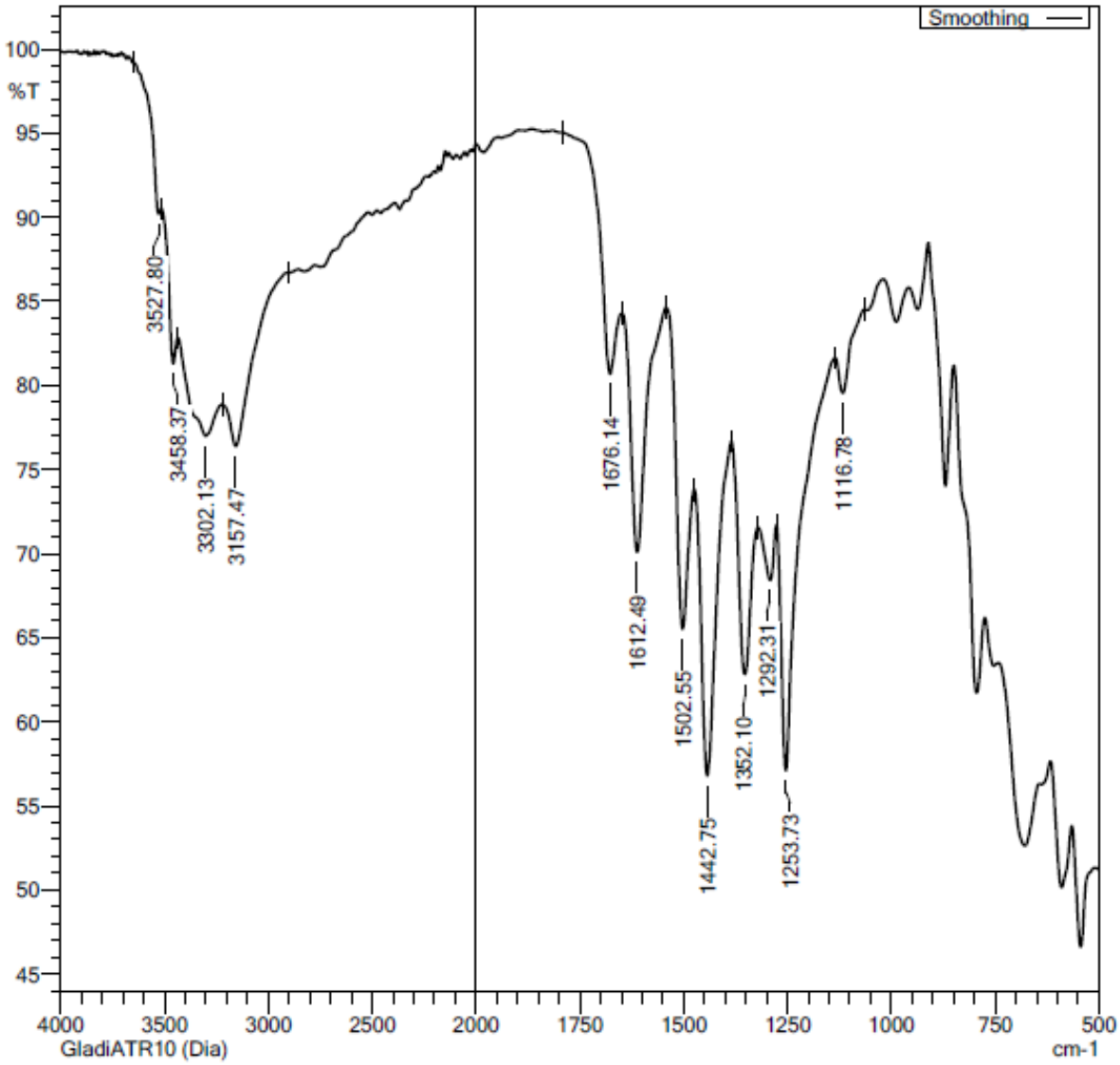

Fig. S.4. Infra-red spectrum of $Mg(H_2dhtp)(H_2O)_5 \cdot H_2O$