

Supporting Information

Synthesis and crystallographic characterisation of $\text{Mg}(\text{H}_2\text{dhtp})(\text{H}_2\text{O})_5 \cdot \text{H}_2\text{O}$

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Table S.1. Selected bond lengths [\AA] and angles [$^\circ$] for $\text{Mg}(\text{H}_2\text{dhtp})(\text{H}_2\text{O})_5 \cdot \text{H}_2\text{O}$

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 $\text{Mg}(\text{H}_2\text{dhtp})(\text{H}_2\text{O})_5 \cdot \text{H}_2\text{O}$ [\AA and $^\circ$]

D-H \cdots A	d(D-H)	d(H \cdots A)	d(D \cdots A)	$\angle(\text{DHA})$
O(3)-H(3) \cdots O(2)	0.84	1.79	2.5334(14)	147.2
O(6)-H(6) \cdots O(5)	0.84	1.75	2.4926(14)	147.0
O(2W)-H(2A) \cdots 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:** $-x+1, -y+1, -z+1$

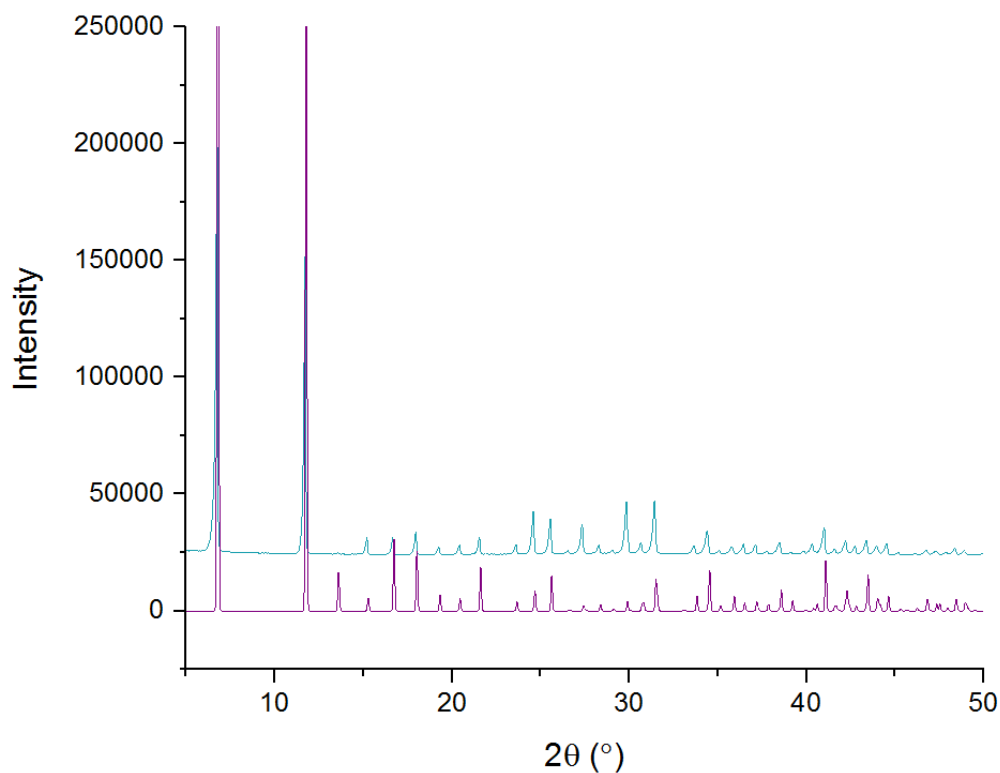


Fig. S.1. Powder XRD patterns for CPO-27-Mg. Teal – as-synthesised; Purple – simulated spectrum at a factor of 100

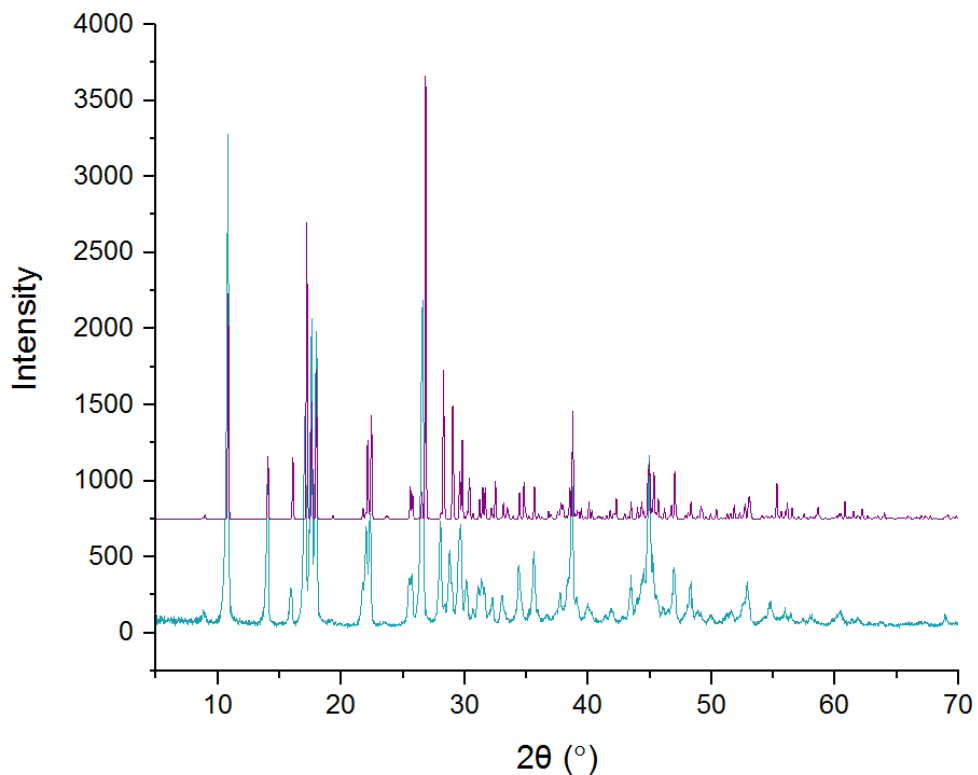


Fig. S.2. Powder XRD spectra for monomeric species, $\text{Mg}(\text{H}_2\text{dhtp})(\text{H}_2\text{O})_5 \cdot \text{H}_2\text{O}$. Teal – as-synthesised; Purple – simulated from single crystal data at a factor of 100

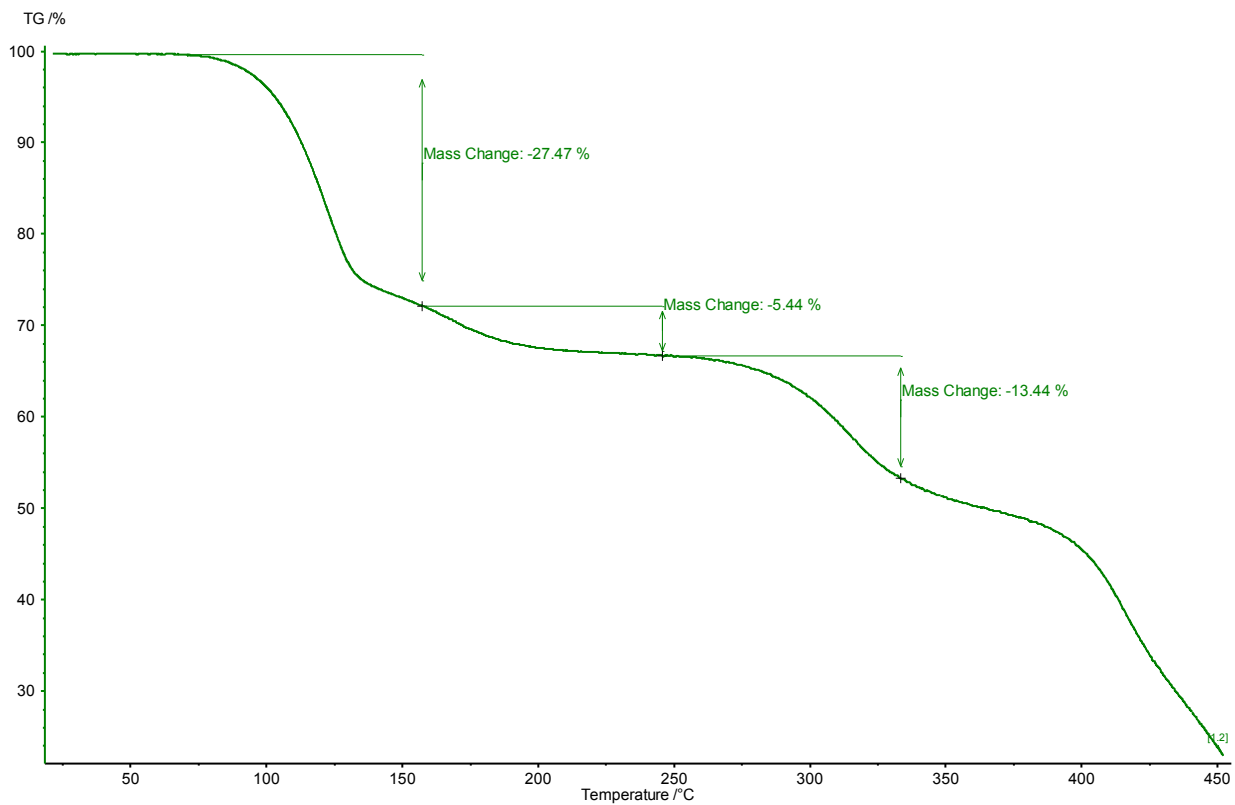


Fig. S.3. Thermogravimetric analysis (TGA) showing three mass changes of 27.47, 5.44 and 13.44% corresponding to the loss of $5\text{H}_2\text{O}$, H_2O and CO_2 respectively

Eq. (S.1). Thermogravimetric analysis calculations

$$328.52 \text{ gmol}^{-1} \times 0.2747\% = 90.24 \text{ gmol}^{-1} \quad 5\text{H}_2\text{O}$$

$$328.52 \text{ gmol}^{-1} \times 0.0544\% = 17.87 \text{ gmol}^{-1} \quad \text{H}_2\text{O}$$

$$328.52 \text{ gmol}^{-1} \times 0.1344\% = 44.15 \text{ gmol}^{-1} \quad \text{CO}_2$$

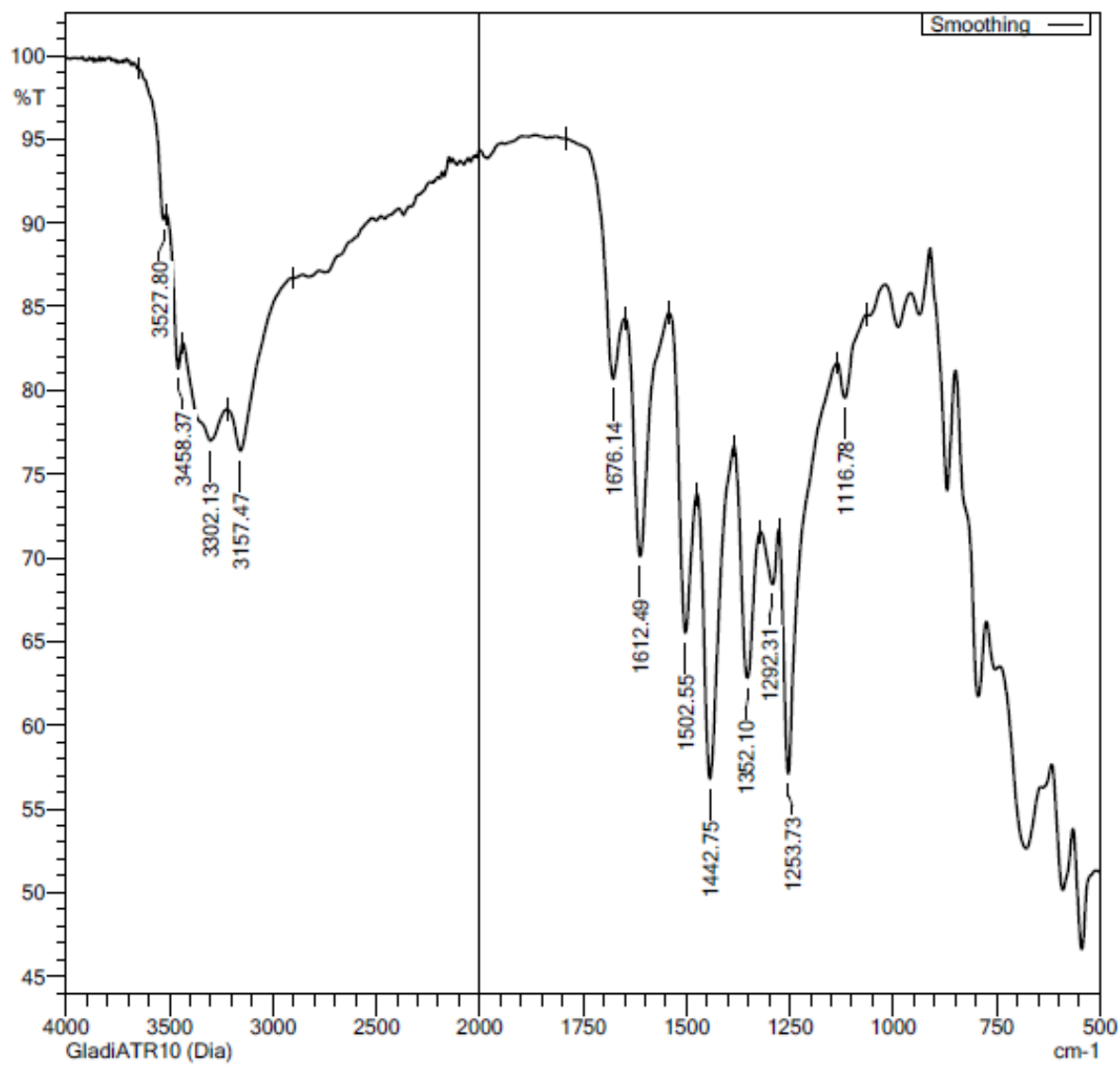


Fig. S.4. Infra-red spectrum of $\text{Mg}(\text{H}_2\text{dhtp})(\text{H}_2\text{O})_5 \cdot \text{H}_2\text{O}$