

**Table S1. Crystallographic data, experimental parameters, and refinement of the magnesium comenate structure (according to X-ray diffraction data)**

Parameter	Value
Gross formula	C <sub>12</sub> H <sub>22</sub> MgO <sub>18</sub>
<i>M</i> , g/mol	478.60
Temperature, K	293(2)
Crystallographic system	triclinic
Space group	P-1
<i>a</i> , Å	6.7265(2)
<i>b</i> , Å	7.0802(2)
<i>c</i> , Å	10.7367(4)
$\alpha$ , deg.	103.337(3)
$\beta$ , deg.	96.095(2)
$\gamma$ , deg.	103.071(2)
<i>V</i> , Å <sup>3</sup>	477.84(3)
<i>Z</i>	1
$\rho$ (calc.), g/cm <sup>3</sup>	1.663
$\mu$ , mm <sup>-1</sup>	1.711
<i>F</i> (000)	250.0
Crystal size, mm	0.417 × 0.324 × 0.307
Radiation	Cu K $\alpha$ ( $\lambda$ = 1.54184)
Data collection range 2 $\Theta$ , deg	8.584-152.2
Ranges <i>h</i> , <i>k</i> , <i>l</i>	-8 ≤ <i>h</i> ≤ 8, -8 ≤ <i>k</i> ≤ 8, -12 ≤ <i>l</i> ≤ 13
Number of measured reflections	9635
Number of independent reflections ( <i>R</i> <sub>int</sub> , <i>R</i> <sub><math>\sigma</math></sub> )	1990 (0.0180, 0.0104)
Data/Restrictions/Parameters	1990/0/179
GOOF by <i>F</i> <sup>2</sup>	1.107
<i>R</i> - factor ( <i>I</i> > 2 $\sigma$ ( <i>I</i> ))	<i>R</i> <sub>1</sub> = 0.0248, w <i>R</i> <sub>2</sub> = 0.0655
<i>R</i> - factor (all data)	<i>R</i> <sub>1</sub> = 0.0251, w <i>R</i> <sub>2</sub> = 0.0657
$\Delta Q_{\max}/\Delta Q_{\min}$ , e Å <sup>-3</sup>	0.38/-0.21

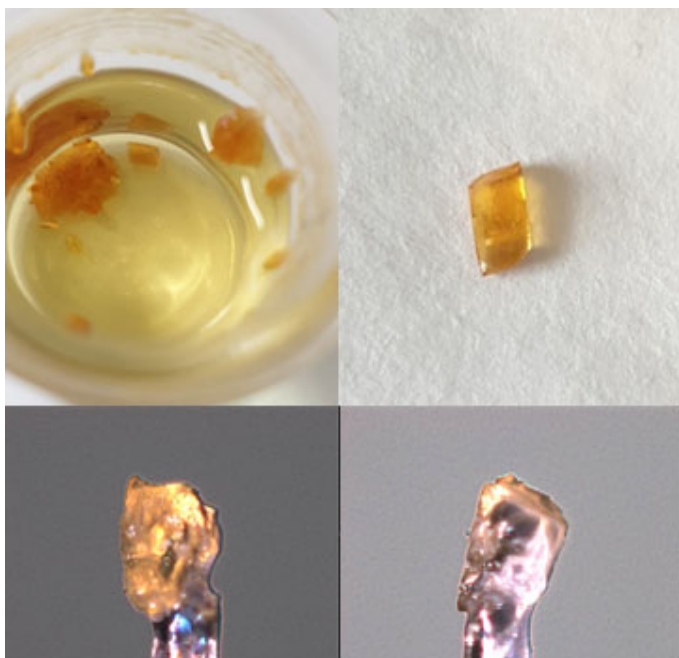
**Table S2. Main bond lengths for [Mg(HCom)<sub>2</sub>(H<sub>2</sub>O)<sub>6</sub>].2H<sub>2</sub>O**

Bond	<i>d</i> , Å	Bond	<i>d</i> , Å
Mg(1)–O(2 <sup>1</sup> )	2.0684(8)	O(8)–C(5)	1.3481(13)
Mg(1)–O(2)	2.0684(7)	O(7)–C(4)	1.2498(13)
Mg(1)–O(1 <sup>1</sup> )	2.0841(8)	O(4)–C(1)	1.2508(13)
Mg(1)–O(1)	2.0841(8)	C(5)–C(4)	1.4512(14)
Mg(1)–O(3)	2.0400(8)	C(5)–C(6)	1.3519(15)
Mg(1)–O(3 <sup>1</sup> )	2.0400(8)	C(4)–C(3)	1.4403(14)
O(6)–C(2)	1.3467(12)	C(2)–C(1)	1.5230(14)
O(6)–C(6)	1.3583(13)	C(2)–C(3)	1.3510(15)
O(5)–C(1)	1.2463(13)		

Note: <sup>1</sup>-X,1-Y,2-Z**Table S3. Main values of bond angles for [Mg(HCom)<sub>2</sub>(H<sub>2</sub>O)<sub>6</sub>].2H<sub>2</sub>O**

Angle	ω, degree	Angle	ω, degree
O(2)Mg(1)O(2 <sup>1</sup> )	180.0	C(2)O(6)C(6)	118.94(8)
O(2 <sup>1</sup> )Mg(1)O(1 <sup>1</sup> )	90.83(3)	O(8)C(5)C(4)	120.80(9)
O(2)Mg(1)O(1)	90.83(3)	O(8)C(5)C(6)	119.27(9)
O(2 <sup>1</sup> )Mg(1)O(1)	89.17(3)	C(6)C(5)C(4)	119.90(10)
O(2)Mg(1)O(1 <sup>1</sup> )	89.17(3)	O(7)C(4)C(5)	121.06(9)
O(1 <sup>1</sup> )Mg(1)O(1)	180.00(3)	O(7)C(4)C(3)	124.32(9)
O(3 <sup>1</sup> )Mg(1)O(2 <sup>1</sup> )	86.85(3)	C(3)C(4)C(5)	114.60(9)
O(3)Mg(1)O(2)	86.85(3)	O(6)C(2)C(1)	112.80(9)
O(3 <sup>1</sup> )Mg(1)O(2)	93.15(3)	O(6)C(2)C(3)	122.42(9)
O(3)Mg(1)O(2 <sup>1</sup> )	93.15(3)	C(3)C(2)C(1)	124.77(9)
O(3 <sup>1</sup> )Mg(1)O(1 <sup>1</sup> )	90.32(3)	C(5)C(6)O(6)	122.96(9)
O(3)Mg(1)O(1)	90.32(3)	O(5)C(1)O(4)	127.81(10)
O(3)Mg(1)O(1 <sup>1</sup> )	89.68(3)	O(5)C(1)C(2)	115.19(9)
O(3 <sup>1</sup> )Mg(1)O(1)	89.68(3)	O(4)C(1)C(2)	116.99(9)
O(3 <sup>1</sup> )Mg(1)O(3)	180.0	C(2)C(3)C(4)	121.06(10)

Note: <sup>1</sup>-X,1-Y,2-Z



**Figure S1.** Several single crystals were obtained, the size of which is suitable for X-ray diffraction studies.