

# Supporting information

## A new hydrate of magnesium carbonate: $\text{MgCO}_3 \cdot 6\text{H}_2\text{O}$

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### Experimental conditions and characterization

**Table S1** Conditions of the attempts for crystallization of hydrated magnesium carbonates.

Attempt	molalitiy( $\text{Mg}^{2+}$ ) in mol/kg( $\text{H}_2\text{O}$ )	$\text{CO}_2$ -pressure, duration of $\text{CO}_2$ discharge in hours	Temperature in K	Duration and conditions of storage	Product phases according to XRPD
V6	0,248	1 bar, 18 h	278.15	12 d, not stirred	$\text{MgCO}_3 \cdot 3\text{H}_2\text{O}$
V7	0,124	1 bar, 23 h	273.15	6 d, stirred	$\text{MgCO}_3 \cdot 3\text{H}_2\text{O}$
V8	0,124	1 bar, 22 h	273.15	2 d, stirred	$\text{MgCO}_3 \cdot 3\text{H}_2\text{O}$
V9	0,356	1 bar, 24 h	273.15	3 d, stirred	unknown phase <sup>a)</sup>
V10	0,388	1 bar, 24 h	273.15	1 d, stirred	unknown phase <sup>a)</sup>
V11	0,385	1 bar, 22 h	273.15	16 d, not stirred	$\text{MgCO}_3 \cdot 3\text{H}_2\text{O}$ + unknown phase <sup>b)</sup>

a) very fine crystals – too small for single crystal diffraction, b) crystals for suitable for single crystal diffraction.

**Table S2** Comparison of band positions in Raman spectra of different magnesium carbonate hydrates.

$\text{MgCO}_3 \cdot 3\text{H}_2\text{O}$ (Coleyshaw <i>et al.</i> , 2003)	$\text{MgCO}_3 \cdot 5\text{H}_2\text{O}$ (Coleyshaw <i>et al.</i> , 2003)	$\text{MgCO}_3 \cdot 6\text{H}_2\text{O}$ , present work	Assignment (Coleyshaw <i>et al.</i> , 2003)
2431, 2350	2628, 3264	3200	$\nu(\text{OH})$
	1705		$\delta(\text{HOH})$
1516, 1423	1514, 1424	1414	$\nu^{\text{as}}(\text{CO})$
1095	1098	1089	$\nu^{\text{s}}(\text{CO})$
713, 781	698, 774	710	$\delta^{\text{as}}(\text{CO})$
223	225	349, 299, 238, 190, 171, 151, 116	lattice vibrations

v valence vibration,  $\delta$  deformation vibration, s symmetric, as asymmetric