

Comprehensive study of the synthetic Tychite $\text{Na}_6\text{Mg}_2(\text{CO}_3)_4\text{SO}_4$: synthesis, structure and conductive properties

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Supplementary information

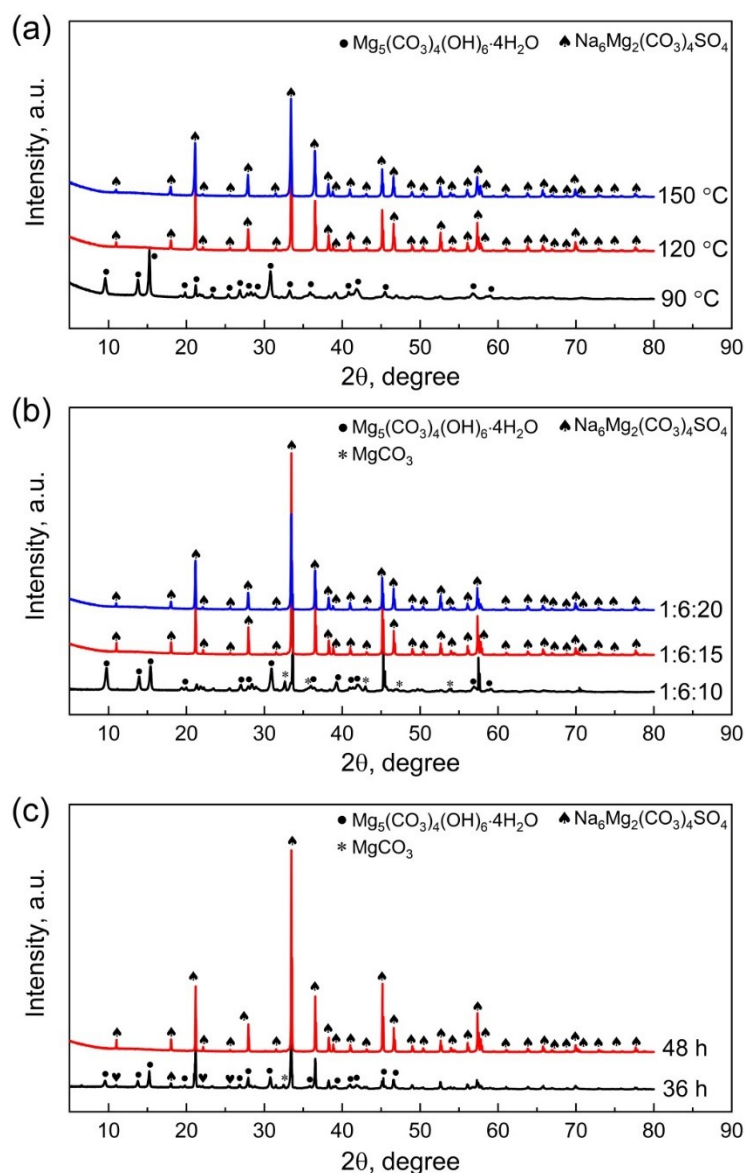


Fig. S1 XRD patterns of $\text{Na}_6\text{Mg}_2(\text{CO}_3)_4\text{SO}_4$ obtained at different synthesis temperatures (a), molar ratio of reagents (b) and synthesis time (c).

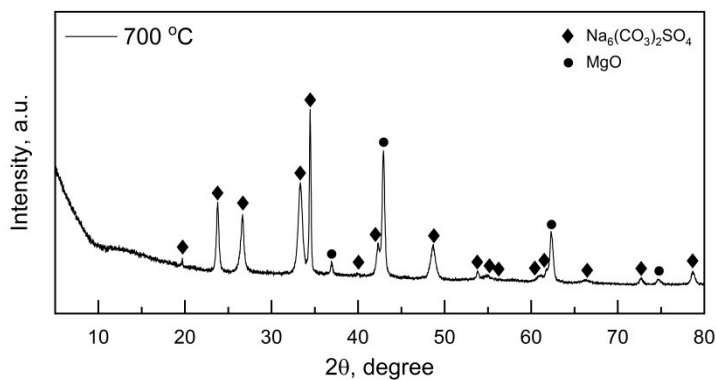


Fig. S2 XRD pattern of the decomposed $\text{Na}_6\text{Mg}_2(\text{CO}_3)_4\text{SO}_4$

Table S1. Rietveld refined lattice parameters of the $\text{Na}_6\text{Mg}_2(\text{CO}_3)_4\text{SO}_4$

Formula	$\text{Na}_6\text{Mg}_2(\text{CO}_3)_4\text{SO}_4$
Space Group	$Fd\text{-}3$
a , Å	13.9073(3)
V , Å ³	2689.9(2)
GOF	1.33
R_p , %	4.36
R_{wp} , %	5.61

Table S2. Atomic coordinates for $\text{Na}_6\text{Mg}_2(\text{CO}_3)_4\text{SO}_4$.

Atom	Wyckoff	x/a	y/b	z/c	Occupancy
S	8a	0.1250	0.1250	0.1250	1.0
Mg	16d	0.0000	0.5000	0.0000	1.0
C	32e	0.0321(1)	0.7179(1)	0.0321(1)	1.0
Na	48f	0.3434(1)	0.1250	0.1250	1.0
O1	96g	0.2664(1)	0.2259(1)	0.3529(1)	1.0
O2	32e	0.0626(2)	0.0626(2)	0.0626(2)	1.0

Table S3. Selected bond lengths for $\text{Na}_6\text{Mg}_2(\text{CO}_3)_4\text{SO}_4$

Bonds	Distances, Å
Na-O1	2.4199(5)
Na-O1	2.4015(7)
Na-O2	2.4932(5)
Mg-O1	2.0851(5)
C-O1	1.2763(5)
S-O2	1.5019(1)

Table S4. Raman and FTIR bands for $\text{Na}_6\text{Mg}_2(\text{CO}_3)_4\text{SO}_4$.

Peak positions		Vibration modes
Raman	FTIR	
144, 249, 301	-	Lattice vibrations
464	-	ν_2 SO_4 symmetric bend
630	630	ν_4 SO_4 asymmetric bend
719	719	ν_4 CO_3 in-plane bending
-	883	ν_2 CO_3 out-of-plane bending
967	-	ν_1 SO_4 stretching mode
1101, 1109	1109	ν_1 CO_3 stretching mode
1135	-	ν_3 SO_4 asymmetric stretching
-	1462	ν_3 CO_3 asymmetric stretching
-	3438	ν_1 H_2O stretching mode