

Electronic Supplementary Information (ESI) Ionic Liquid-Mediated Low-Temperature Formation of Hexagonal Titanium- Oxyhydroxyfluoride Particles

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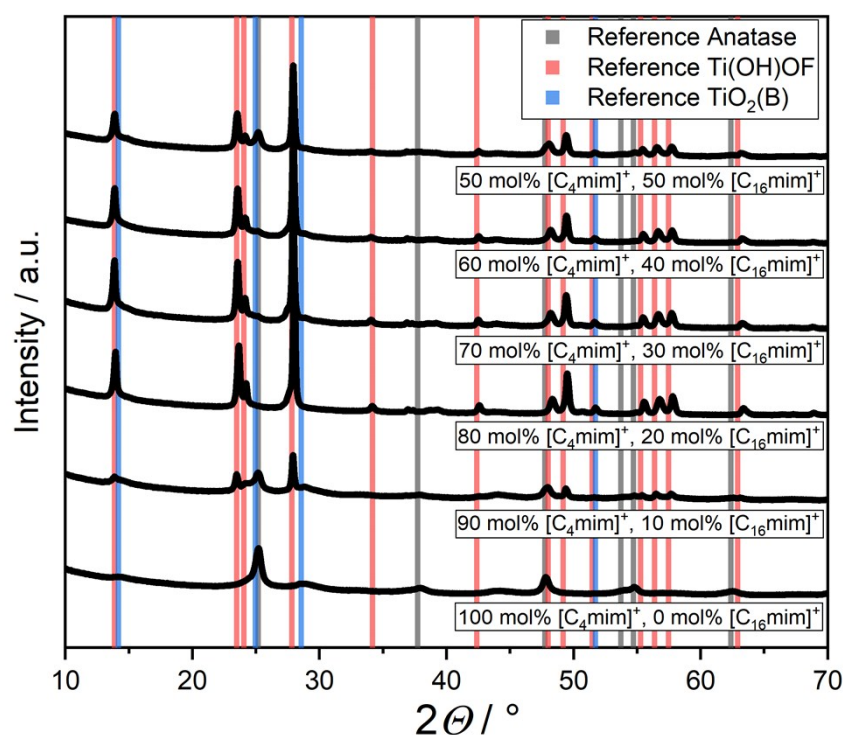


Figure S1 XRD patterns of the resulting products after the synthesis with different mixtures of ionic liquids.

Table S 1 Crystallographic data and refinement parameters.

	Ti(OH)OF · 0.66 H₂O	TiO₂(B)
Space group	<i>P6₃cm</i> (185)	<i>C2/m</i> (12)
Molecular weight (g/mol)	111.76	79.87
Z	6	8
Crystal system	Hexagonal	Monoclinic
Lattice parameters (Å)	<i>a</i> = 7.3866(5), <i>c</i> = 7.5697(5)	<i>a</i> = 12.670(4), <i>b</i> = 3.7711(11), <i>c</i> = 6.141(2), β = 106.36(4)
Cell volume (Å³)	357.68(4)	281.54(2)
Calculated density (g cm⁻³)	3.088	3.769
Data collection range	10° - 75°	
No. of parameters refined	85	
No. of bond lengths restrained	20	18
No. of bond angles restrained	0	0
Average apparent crystallite size (nm)	26.0(8)	8.9(1)
Phase composition (wt%)	72.7(2.0)	27.3(2.3)
R_B (%)	8.04	8.23
Conventional R_p, R_{wp}, R_e (%)	20.8, 21.2, 4.85	
GoF	4.3	

Table S 2 Selected interatomic distances for Ti(OH)OF · 0.66 H₂O.

	Bond length (Å)
Ti1-F1	
x1	1.860(9)
x1	1.929(9)
Ti1-O1	
x2	1.938(7)
x2	1.976(6)

Table S 3 Distortion of coordination polyhedral (δ) and valences ($\sum S_{ij}$) of the atoms in Ti(OH)OF · 0.66 H₂O.

Atom	δ (x10⁻⁴)	$\sum S_{ij}$
Ti1	4.042	4.12(3)
O1	174.081	1.64(1)
F1	3.375	1.39(2)

Table S 4 Structural parameters for Ti(OH)OF · 0.66 H₂O. The refined occupancies are expressed in terms of the ratio m/M: site multiplicity/multiplicity of a general position.

Atom	Wyckoff position	x	y	z	B(Å²)	Occupancy
Ti1	6c	0	0.5111(7)	0.8551(9)	0.20(2)	0.50000
O1	12d	0.1910(5)	0.4049(6)	0.883(1)	0.39(3)	1.00000
F1	6c	0	0.505(1)	1.1007(7)	1.82(4)	0.50000
O2	2a	0	0	0.8510(9)	0.39(3)	0.16667
O3	2a	0	0	1.1002(9)	0.39(3)	0.16667

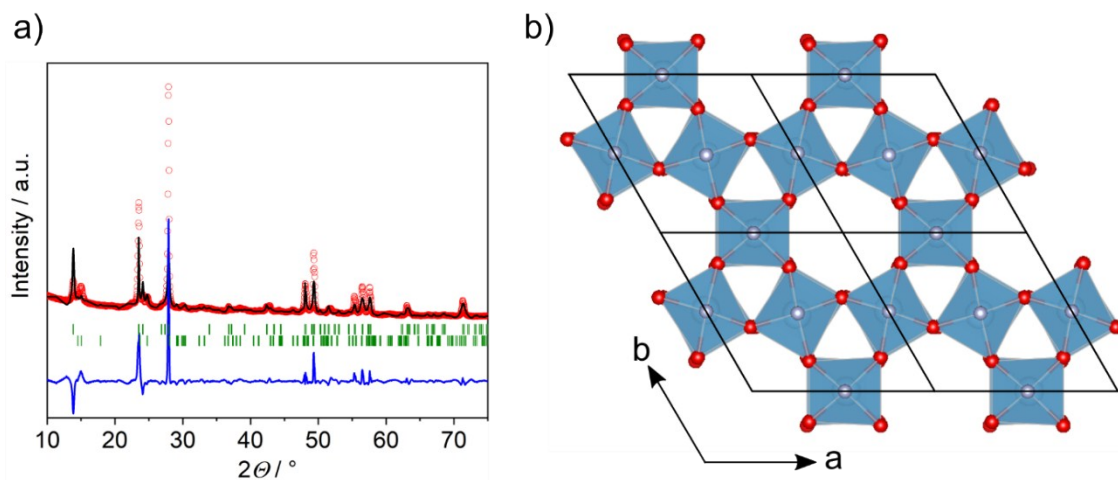


Figure S2 a) Rietveld refinement of structure b) without crystalline water inside of the channels.

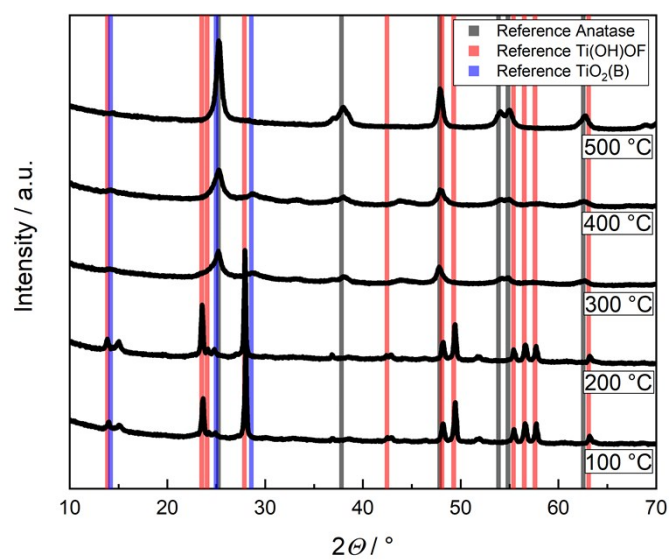


Figure S3 PXRD patterns of the product which was heated up to different temperatures.