Supplementary Material (ESI) for Chemical Communications

Supplementary material to accompany 'Zeotype nitride-chlorides with a predicted topology'

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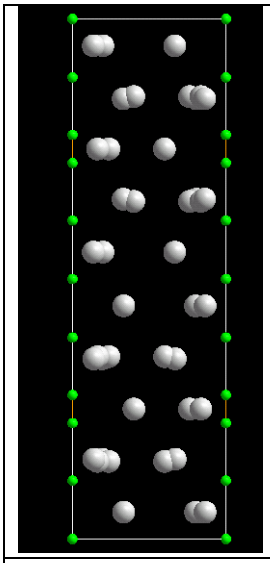
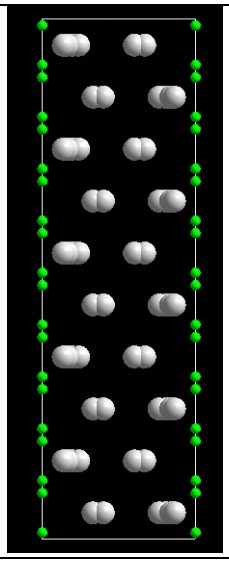
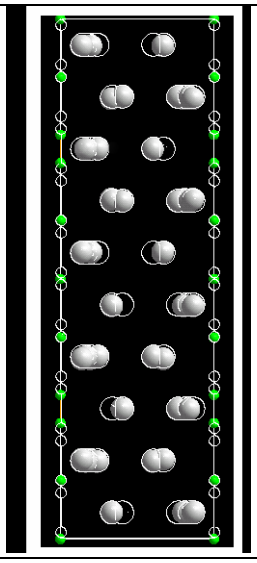
Comparison of chloride positions in 1 and 2

		
Barium / Chloride positions in 2 (chloride in green)	**Barium / Chloride positions in 1 (five unit cells of compound 1 along c are drawn)**	**Overlay of positions. Solid circles refer to atoms in 2.**

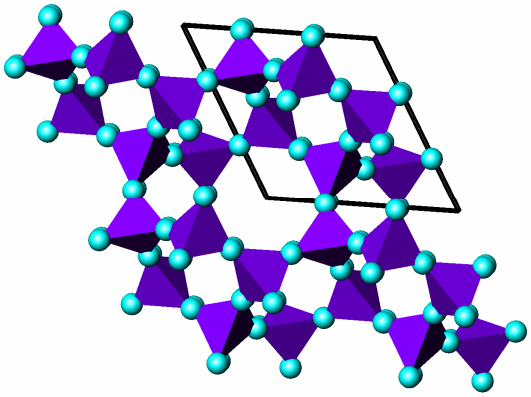
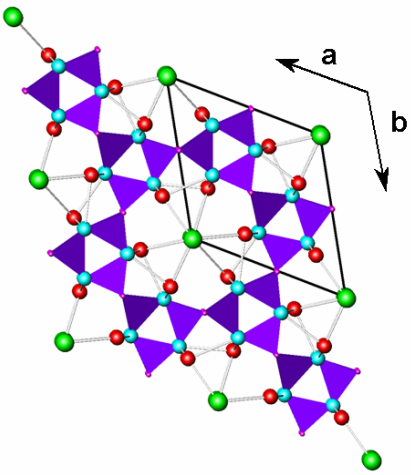
	
Theoretical SiO_2 framework (Foster *et al.*)	**Experimentally determined framework**

Table 1. Crystal data and structure refinement for $Ba_3Ta_3N_6Cl$.

Identification code	**1**	
Empirical formula	Ba6 Cl2 N12 Ta6	
Formula weight	2148.76	
Temperature	150(2) K	
Wavelength	0.78480 Å	
Crystal system	Hexagonal	
Space group	P-62c	
Unit cell dimensions	a = 10.1455(7) Å	α= 90°.
	b = 10.1455(7) Å	β= 90°.
	c = 5.9770(8) Å	γ = 120°.
Volume	532.80(9) $Å^3$	
Z	1	
Density (calculated)	6.697 Mg/m^3	
Absorption coefficient	41.797 mm^{-1}	
F(000)	892	
Crystal size	0.025 × 0.015 × 0.015 mm^3	
Theta range for data collection	4.44 to 32.82°.	
Index ranges	-1<=h<=13, -12<=k<=6, -7<=l<=8	
Reflections collected	1322	
Independent reflections	487 [R(int) = 0.0619]	
Completeness to theta = 31.00°	99.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	487 / 0 / 21	
Goodness-of-fit on F^2	1.084	
Final R indices [I>2sigma(I)]	R1 = 0.0443, wR2 = 0.1091	
R indices (all data)	R1 = 0.0455, wR2 = 0.1105	
Absolute structure parameter	0.01(5)	
Largest diff. peak and hole	4.130 and -3.091 $e.Å^{-3}$	

Table 2. Crystal data and structure refinement for $Ba_{15}Ta_{15}N_{33}Cl_4$.

Identification code	**2**	
Empirical formula	Ba30 Cl8 N67.333 Ta30	
Formula weight	10770.97	
Temperature	150(2) K	
Wavelength	0.78480 Å	
Crystal system	Hexagonal	
Space group	P -6 2 c	
Unit cell dimensions	a = 10.1545(3) Å	α= 90°.
	b = 10.1545(3) Å	β= 90°.
	c = 29.9170(18) Å	γ = 120°.
Volume	2671.6(2) $Å^3$	
Z	1	
Density (calculated)	6.695 Mg/m^3	
Absorption coefficient	41.632 mm^{-1}	
F(000)	4475	
Crystal size	0.030 × 0.015 × 0.015 mm^3	
Theta range for data collection	3.95 to 33.14°.	
Index ranges	-13<=h<=9, -13<=k<=13, -41<=l<=39	
Reflections collected	16811	
Independent reflections	2480 [R(int) = 0.1003]	
Completeness to theta = 31.00°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6809 and 0.3681	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2480 / 0 / 81	
Goodness-of-fit on F^2	0.948	
Final R indices [I>2sigma(I)]	R1 = 0.0474, wR2 = 0.1233	
R indices (all data)	R1 = 0.0701, wR2 = 0.1456	
Absolute structure parameter	-0.08(3)	
Largest diff. peak and hole	5.478 and -2.949 $e.Å^{-3}$	

Table 3. Crystal data and structure refinement for $Ba_3Si_3N_5OCl$.

Identification code	**3**	
Empirical formula	Ba6 Cl2 N10 O2 Si6	
Formula weight	1235.58	
Temperature	150(2) K	
Wavelength	0.78480 Å	
Crystal system	Hexagonal	
Space group	P -6 2 c	
Unit cell dimensions	a = 9.5604(13) Å	α= 90°.
	b = 9.5604(13) Å	β= 90°.
	c = 5.5520(15) Å	γ = 120°.
Volume	439.47(15) $Å^3$	
Z	1	
Density (calculated)	4.669 Mg/m^3	
Absorption coefficient	13.966 mm^{-1}	
F(000)	540	
Crystal size	0.04 × 0.01 × 0.01 mm^3	
Theta range for data collection	4.71 to 32.70°.	
Index ranges	-12<=h<=5, -10<=k<=12, -7<=l<=6	
Reflections collected	1267	
Independent reflections	403 [R(int) = 0.0499]	
Completeness to theta = 31.00°	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1 and 0.728	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	403 / 0 / 28	
Goodness-of-fit on F^2	1.258	
Final R indices [I>2sigma(I)]	R1 = 0.0504, wR2 = 0.1074	
R indices (all data)	R1 = 0.0593, wR2 = 0.1119	
Absolute structure parameter	0.25(14)	
Largest diff. peak and hole	1.494 and -1.493 $e.Å^{-3}$	