

Structural and compositional tuning of layered subnitrides; new complex nitride halides

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Supplementary information (ESI)

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Table ES1. Anisotropic temperature factors for $\text{Ca}_{2-x}\text{Sr}_x\text{NX}$ from PND.

Formula	100 x U_{anis}	U_{11}	U_{33}	U_{12}
Ca_{1.46}Sr_{0.54}NCl (1)	Ca / Sr	0.883 (19)	1.056 (32)	0.442 (9)
	N	0.947 (18)	1.199 (33)	0.474 (9)
	Cl	1.564 (21)	1.442 (31)	0.782 (11)
Ca_{0.94}Sr_{1.06}NCl (2)	Ca / Sr	0.905 (27)	1.089 (47)	0.453 (13)
	N	1.137 (28)	1.321 (51)	0.568 (14)
	Cl	1.540 (32)	1.842 (48)	0.770 (16)
Ca_{0.40}Sr_{1.60}NCl (3)	Ca / Sr	0.779 (17)	1.005 (32)	0.390 (9)
	N	0.938 (19)	1.289 (36)	0.469 (9)
	Cl	1.523 (22)	1.272 (34)	0.762 (11)
Ca_{1.52}Sr_{0.48}NBr (4)	Ca / Sr	0.783 (15)	1.139 (26)	0.391 (8)
	N	0.964 (14)	1.327 (27)	0.482 (7)
	Br	1.362 (19)	1.369 (33)	0.681 (9)
Ca_{0.95}Sr_{1.05}NBr (5)	Ca / Sr	0.724 (23)	1.165 (41)	0.362 (11)
	N	1.151 (24)	1.328 (45)	0.576 (12)
	Br	1.615 (32)	1.362 (56)	0.807 (16)
Ca_{0.18}Sr_{1.82}Br (6)	Ca / Sr	0.981 (17)	1.003 (28)	0.490 (8)
	N	1.025 (17)	1.215 (33)	0.513 (8)
	Br	1.382 (23)	1.478 (42)	0.691 (12)

$$U_{11} = U_{22}, U_{13} = U_{23}$$