

The structure of $\text{Li}_4\text{NbO}_4\text{F}$ a joint neutron x-ray refinement.

M. Elcombe¹, L. Noren²

¹ *Bragg Institute, ANSTO, Lucas Heights, NSW, Australia*

² *Research School of Chemistry, Australian National University, Canberra, ACT, Australia*

A recent report (1) in the literature suggests that the electrically neutral compound $\text{Li}_4\text{NbO}_4\text{F}$ is cubic, with the NaCl structure and with statistical distribution of the anions and cations on their respective sites. It is difficult to imagine Nb^{5+} substituting for Li^{1+} without some form of structural relaxation. High-resolution neutron and x-ray patterns have been collected and the former shows FCC symmetry with only one atom per unit cell and the latter shows approximately primitive cubic symmetry with half the cell size. This anomaly can be explained in terms of the specific neutron and x-ray scattering factors of the constituent elements and a unique structure has been determined. Energy minimisation techniques have been used to simulate the displacements of the atoms from their highly symmetric sites in order to explain both the observed thermal parameters and the under/over bonding of the Nb and Li ions.

(1) *Advanced Inorganic Fluorides: Synthesis, Characterisation and Applications*, T Nakajima, B Zemva and A Tressaud (editors) Elsevier Science (2000) section 5.3.4 pp151-2.