

P.08.15.3

Acta Cryst. (2005). A61, C352

The Ternary Fluoride Lithium at Low Temperature

Malika Hamadène^a, A. Guehria^a, S. Dahaoui^b, C. Lecomte^b,
^aLaboratoire de Cristallographie et de Thermodynamique, Faculté de Chimie, USTHB, BP 32 El-Alia, BEZ, Alger, Algérie. ^bLCM3B, Université de Nancy I, Vandoeuvres, 54506, France. E-mail: mal_hamadene@hotmail.com

The structure of Li_3InF_6 α , at room-temperature (Ta), may be described into two unit cells 1 and 2 with $P2_1/m$ symmetry [1]. All Li atoms are disordered since the octahedral Li atoms occupy fully sites with relatively high thermal parameters and the tetrahedral Li atoms are located on 2 partially occupied independent sites [2][3].

The structure of the low-temperature form is solved and refined at 100K in a superlattice. This latter leads to a cell identical with the cell 2 but with the a double c-axis. The mirror plane is replaced by a glide plane and the resulting space group is $P2_1/c$. The structure is closely related to that of the Ta form. The change is associated with shifts of all atoms (the largest shifts occurred for the Li atoms), change in Li coordination number (6, 5 and 4). Significant differences are observed in some Li-F bond lengths. The disorder of Li ions disappears at low temperature : the two original tetrahedral Li atoms occupy fully sites in the " superstructure" while the octahedral Li atoms show normal displacement parameters. It is noteworthy that the octahedral Li atoms at room-temperature are rather oscillating between two positions but not statistically disordered.

[1] Hamadène M., Ravez J., Grannec J., Laïdoudi-Guehria A., *Mat. Letters*, 1996, **27**, 33. [2] Hamadène M., Balegroune F., Laïdoudi-Guehria A., Grannec J., Ravez J, *J. Chem. Cryst.*, submitted. [3] Hamadène M., Balegroune F., Laïdoudi-Guehria A., Grannec J., Ravez J, *Communication ecm22*, Budapest, 25-28 August 2004.

Keywords: low temperature structure, superlattice, disorder