B1 16:00 – 16:15

CORRELATION ANALYSIS – HELPFUL TOOL FOR DESIGNING CRYSTALLINE MATERIALS

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Statistical analysis of structural parameters retrieved from *Inorganic Structural Data Base*[1] can be easily used as a base for designing new crystalline materials having particular properties. The type and degree of correlation is site and constitution dependent. Therefore, except the total samples for different structures, some selected subsets of data have been analyzed with only one variable ion occupying given site. Structural parameters are not equally sensitive to changes imposed by the change of the crystal constitution.

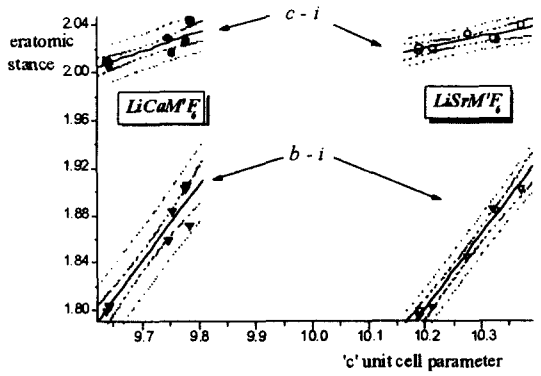

Fig.1. Linear relations between interatomic distances and the 'c' unit cell parameter for the $LiCaM'F_6$ and $LiSrM'F_6$ subsets (with exception of a-i distance which does not correlate).

An effective ion radius have been proposed in order to establish unknown concentration of doping ions only on the basis of known unit cell parameter or one of the interatomic distances. The authors have been investigated garnet, colquiriite-like and perovskite-fluoride structures.

[1] G. Bergerhoff, R. Hundt, R. Sievers, I.D. Brown, J. Chem. Inf. Comput. Sci., 23, (1983),66; G. Bergerhoff, R. Sievers, Nachr. Dokum., 40, (1989), 27

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