langasite structure could be achived by optimal values of the radius ($r_i$, Å) and electronegativity ($\chi_i$) of atoms: $r_A$ = 1.02 ÷ 1.42 Å, $\chi_A$ = 0.85 ÷ 2.1 (the A site), $r_B$ = 0.53 ÷ 0.75 Å, $\chi_B$ = 1.5 ÷ 2.1 (the B site), $r_C$ = 0.37 ÷ 0.60 Å, $\chi_C$ = 1.5 ÷ 1.8 (the C site), and $r_D$ = 0.25 ÷ 0.50Å, $\chi_D$ = 1.5 ÷ 1.8 (the D site). It was found that the cell parameters must belong to the *a*=~7.95÷8.67Å and *c*=~4.80÷5.44Å intervals. Moreover, the intervals of all interatomic distances (A-O, B-O, C-O, D-O, O-O) and the atoms coordinates (A, B, C, D, O) were distinguished, which were ascribed to distinctive characteristics of langasite structure.

The relationship between the lattice parameters (*a, c*), the ionic radius of the A atom, the composition of the D site, and some interatomic distances (for example, O-O), on the one hand, and piezoelectric constants ($d_{ij}$), the electromechanical coupling factors ($k_{ij}$), the relative dielectric coefficients ($\varepsilon_i$), the elastic stiffness coefficients ($c_{ij}$), and elastic compliances ($s_{ij}$), on the other hand, has been corroborated or found.

Our study is intended for the establishment of distinctive indications of langasite structure for an application of information technology. This allows to process a large quantity of information for the prediction new compositions and property characteristics.

**MS14 P10**

**The mean-square Friedel intensity difference in *P*1 with a centrosymmetric substructure**

U. Shmueli[a], H. D. Flack,[b] [a]*School of Chemistry, Tel Aviv University, Israel.,* [b]*Laboratoire de Cristallographie, University of Geneva, Switzerland.* E-mail: ushmueli@post.tau.ac.il

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For non-centrosymmetric structures in space group *P*1 containing a centrosymmetric substructure, analytical expressions have been obtained for various functions of the diffraction intensity of Friedel opposites. These functions are the average intensity of Friedel opposites, the mean difference in intensity of Friedel opposites and the mean-square difference in intensity of Friedel opposites. A Bijvoet intensity ratio is defined for the evaluation of resonant scattering effects in non-centrosymmetric and pseudo-centrosymmetric structures. Analysis of these expressions confirms that both resonant and non-resonant atoms are necessary to produce differences in intensity between Friedel opposites and also shows that in some circumstances atoms may lie on a centrosymmetric substructure without diminishing the Bijvoet intensity ratio. The effects of the real component of resonant scattering, of the variation of the scattering factors with $\sin\theta/\lambda$, of isotropic atomic displacement parameters, of a crystal twinned by inversion, of atoms in special positions and of weak reflections are considered. Software is available for the evaluation of the Bijvoet intensity ratio[1].

[1] Flack, H. D.Shmueli, U., *Acta Cryst.*, 2007, A63, *In press*.