has also been used to tune the interaction strength and pole orientation in the bulk magnetisation of a series of recently synthesised PBA's [2]. We have commenced a theoretical study of the effects of change in pressure and composition parameter, x, upon the trimetallic PBA KNi_xMn_{1-x} [Cr (CN)$_6$]. We apply the same 35% HF functional and basis sets as were used in our recent study of the KM^{II} [Cr^{III} (CN)$_6$] (M =V, Mn, Ni) [3] system. Our initial optimisations of structures at different Mn/Ni ratios indicate an adherence to Vegard's Law, which postulates a linear relationship between the lattice constant of substitutional alloys and their composition. We note that similar behaviour has also been observed in mixed oxide lattices [4].

Experimentally, PBAs often prove difficult to crystallise, are generally highly insoluble, contain large numbers of water molecules and M^{III} (CN)$_6$ vacancies and possess low crystal symmetries. While the first two issues clearly offer no impediment to theoretical approaches, the presence of the disordered water molecules and M^{III} (CN)$_6$ vacancies necessitate the use of idealised models containing charge-balancing cations. Efforts to synthesise high quality CsM^{II} [Cr^{III} (CN)$_6$] crystals with minimal water content are currently under way, with the aim of permitting a direct comparison between experimental and theoretical properties both at equilibrium and under pressure. Experimental findings of early results from the synthesis will be presented.

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MS14 P08

Validation of "Kick maps". Jure Pražnikar[a], Pavel Afonine[b,] Dušan Turk[a], [a]*Jozef Stefan Institute, Department of Biochemistry, Molecular and Structural Biology, Ljubljana, Slovenija.* [b]*Lawrence Berkeley National Laboratory, Berkeley, USA.* E-mail: jure.praznikar@ijs.si

Keywords: model building, electron density, maximum likelihood

The concept of Kkick map has been in use for a while as a part of MAIN [1] distributions. However, apart from occasional comparisons, kick maps have not been systematically analyzed and compared against *2Fobs-Fcalc* least square and maximum likelihood maps calculated with unit or likelihood-weighted weights. The kick map is an average of a series *2Fobs-Fcalc* maps, where each *Fcalc* set was calculated from kicked atomic positions generated with a different random number seed. Kick of an atomic position is a random displacement along X, Y, and Z coordinate.
Validation involved convergence of a map as results of different number of repeats, kick size and resolution. The

resulting maps were compared with maximum likelihood weighted maps, LSQ weighted maps among themselves and against the *Fcalc* map of the final model. The tests were carried out with the initial structures of the phospholipaseA2 [4] and stefin B tetramer [5]. Tests with phospholipasesA2 shows that maximum likelihood and kick maps are better than traditional least square map. Linear correlation for both maps was 0.69 when compared with *Fcalc* map of final model. Local differences reveal that both maps have their virtues and "weak" points. Tests with stefin B tetramer show that the kick map gave better correlation than traditional least square and maximum likelihood map (stefin B initial structure required partial model rebuilding due to conformational change). The linear correlation coefficient of kick map against "true" map was 6% higher than that of the maximum likelihood map.

The kick map is comparable to maximum likelihood map and is occasionally closer to the "true" map. Therefore it can be successfully applied as an alternative approach on map calculations based on molecular models especially during the early stages of model building and refinement, when model bias plays a crucial role.

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MS14 P09

Crystallochemical design of langasite family compounds and information technology Tyunina E, Kuz'micheva G. *Lomonosov State Academy of Fine Chemical Technology, Moscow, Russia*
E-mail: tyunina_elena@mail.ru

Keywords: langasite, crystallochemical design, information technology

Langasite family is one of the most attractive single crystals in promising piezoelectric materials. These crystals with general formula $A_3B_1C_3D_2O_{14}$ have $La_3Ga_5SiO_{14}$ ($La_3GaGa_3(Ga_{0.5}$ $Si_{0.5})_2O_{14}$) structure and belong to the sp.gr. P321. There are four kinds of cation sites in the structure. A and B atoms are located on a dodecahedral (CN=8) sites and an octahedral (CN=6) ones, respectively. C and D atoms occupy tetrahedral (CN=4) and trigonal-pyramidal (CN=3+1) sites. There are three crystallographic positions for oxygen atoms. The most interesting part of material design is how to improve piezoelectricity by the substitution of other metal one.
In this work, we demonstrate relationship between composition, structural peculiarities and some properties of langasite family compounds and suggest an information technology for prediction new compositions with required properties set.
Well-known 216 compounds of $A_3B_1C_3D_2O_{14}$ general composition were divided into four groups. Compounds of the I-st (26.3 %) and the II-nd (27.6 %) groups have langasite structure confirmed and unverified by the structural analysis, respectively. Compounds of the III-rd group (23.5 %) have not langasite structure. Samples of the IV-th group (22.6 %) contain both langasite phase and impurities. According to crystallochemical analysis, the

langasite structure could be achived by optimal values of the radius (r_i, Å) and electronegativity (χ_i) of atoms: r_A = 1.02 ÷ 1.42 Å, χ_A = 0.85 ÷ 2.1 (the A site), r_B = 0.53 ÷ 0.75 Å, χ_B = 1.5 ÷ 2.1 (the B site), r_C = 0.37 ÷ 0.60 Å, χ_C = 1.5 ÷ 1.8 (the C site), and r_D = 0.25 ÷ 0.50Å, χ_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 (ε_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

Keywords: resonant scattering, absolute structure, intensity statistics

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].

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