

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  $\text{KNi}_x\text{Mn}_{1-x}[\text{Cr}(\text{CN})_6]$ . We apply the same 35% HF functional and basis sets as were used in our recent study of the  $\text{KM}^{\text{II}}[\text{Cr}^{\text{III}}(\text{CN})_6]$  ( $\text{M} = \text{V}, \text{Mn}, \text{Ni}$ ) [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  $\text{M}^{\text{III}}(\text{CN})_6$  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  $\text{M}^{\text{III}}(\text{CN})_6$  vacancies necessitate the use of idealised models containing charge-balancing cations. Efforts to synthesise high quality  $\text{CsM}^{\text{II}}[\text{Cr}^{\text{III}}(\text{CN})_6]$  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<sup>a</sup>, Pavel Afonine<sup>b</sup>, Dušan Turk<sup>a</sup>, <sup>a</sup>*Jozef Stefan Institute, Department of Biochemistry, Molecular and Structural Biology, Ljubljana, Slovenia.* <sup>b</sup>*Lawrence Berkeley National Laboratory, Berkeley, USA.* E-mail: jure.praznikar@ijs.si

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The concept of Kick 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 of *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 phospholipaseA2 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*

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Langasite family is one of the most attractive single crystals in promising piezoelectric materials. These crystals with general formula  $\text{A}_3\text{B}_1\text{C}_3\text{D}_2\text{O}_{14}$  have  $\text{La}_3\text{Ga}_5\text{SiO}_{14}$  ( $\text{La}_3\text{GaGa}_3(\text{Ga}_{0.5}\text{Si}_{0.5})_2\text{O}_{14}$ ) 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  $\text{A}_3\text{B}_1\text{C}_3\text{D}_2\text{O}_{14}$  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