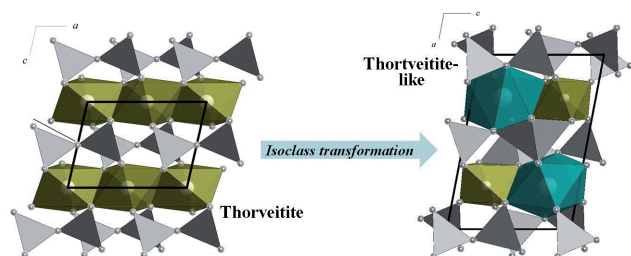


of this work was to determinate the structural relations between the space groups of the basic structure of layered thortveitite (S.G.  $C12/m1$ ) and its derivative structure named thortveitite-like (S.G.  $P12_1/m1$ ) when iron is partially substituted by yttrium in the layered thortveitite  $FeInGe_2O_7$ . The symmetry reduction promoted by the incorporation of yttrium in the formula  $Y_xIn_{1-x}FeGe_2O_7$  ( $x = 0, 0.25, 0.50, 0.75, 0.90$  and  $1.0$ ), is explained by mean of the crystallographic group-subgroup relationships.



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**Keywords:** symmetry relations, klassengleiche subgroups, thortveitite

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**Using Lee-Richards Surfaces to calculate close contacts and complex interfaces**

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The calculation of geometric interactions among macromolecular fragments, such as the identification of close contacts and complex interface regions, normally involves atom-by-atom comparisons of coordinates. In a brute-force calculation distance search involving molecular fragment  $A$  with  $N_A$  atoms and fragment  $B$  with  $N_B$ ,  $O(N_A N_B)$  distances need to be computed. A calculation using Levinthal cubing, Voronoi diagrams, NearTrees or other partitioning schemes can reduce this time to

$$O(\min(N_A \log(N_A) + N_B \log(N_A), N_B \log(N_B) + N_A \log(N_B))) \\ = O((N_A + N_B)(\log(\min(N_A, N_B))))$$

which is excellent for fragments of very different sizes but problematic for fragments of similar sizes. It is difficult to reduce the time further with any atom-by-atom based scheme. An alternative is to base the analysis of an interface on the electron density or a pseudo-density, which should display significant excess density in an interface, or on a molecular surface, which should tend to bridge an interface. Use of the Pseudo-Gaussian Approximation to Lee-Richards Surfaces (PGALRS) algorithm [2] to compute Lee-Richards surfaces [3] combined with use of a NearTree [1] to partition space allows generation of a molecular surface in linear time and identification of atoms forming a surface ( $L RSA()$ ) in linear time. The atoms in the interface are then

$$(L RSA(A) \cup L RSA(B)) \cap (\neg L RSA(A \cup B))$$

which can be computed in  $O(N_A + N_B)$  time. This calculation is sufficient for identification of close contracts and an efficient first approximation for interface identification. We are looking at using atom pairs for

more accurate interface identification. Use of only the atoms in  $A$  and  $B$  within a reasonable distance of  $(L RSA(A) \cup L RSA(B)) \cap (\neg L RSA(A \cup B))$  would help to pre-prune the search tree for these calculations.

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**Keywords:** complex\_interface, molecular\_surface, contact

### MS09.P04

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**Odd n-fatty acids  $C_nH_{2n}O_2$  and their alloys on the X-ray powder diffraction data**

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Saturated fatty acids  $C_nH_{2n}O_2$  play important role in the life of plants and animals. Some even ones (even number  $n$ ) were specified in the literature including our works. We refined X-ray characteristics of six even acids ( $n = 12, 14, 16, 18, 20,$  and  $22$ ) [1]; determined thermal deformations and polymorphic transformations of three acids ( $n = 12, 14$  and  $16$ ); synthesized double alloys  $C_{12}H_{24}O_2-C_{14}H_{28}O_2$  and  $C_{14}H_{28}O_2-C_{16}H_{32}O_2$  as well as quaternary one  $C_{12}H_{24}O_2-C_{14}H_{28}O_2-C_{16}H_{32}O_2$  in relative binary and ternary systems; and revealed rather limited isomorphism in these mixtures [1, 2].

Oppositely, odd fatty acids (odd  $n$ ) have a weak state of knowledge because of their less spread in the nature [3]. For example, information about odd acids missed in the ICDD bank [4]. In this work we present results of X-ray powder diffraction study of odd fatty acids.

X-ray characteristics (crystal system, polymorph modification, indices  $hkl$ , elementary cell parameters, space group, etc.) of four odd fatty acids with  $n = 13, 15, 17,$  and  $19$  (homological purity 98–99 %) were obtained for the first time. In particular it was found that odd acids could crystallize at room temperature in monoclinic polymorphs of single and double layers.

Limits of solid solutions were established for two binary systems of odd components:  $C_{13}H_{26}O_2-C_{15}H_{30}O_2$  (studied compositions, mol. %  $C_{15}H_{30}O_2$ : 10, 33, 50, 67, and 90) and  $C_{15}H_{30}O_2-C_{17}H_{34}O_2$  (studied compositions, mol. %  $C_{17}H_{34}O_2$ : 10, 25, 33, 50, 67, 75, and 90). Our experiments showed rather limited isomorphism too, like in binary systems of even components [1, 2]. Thus, rather limited isomorphism specifies n-fatty acids even in systems of one parity. This differs principally n-fatty acids from n-paraffins, which molecules mix together in wide ranges forming solid solutions easily [5].

The diffractograms of the majority of melted binary mixtures of odd n-fatty acids displayed peaks of binary acid compound. Remarkable, the binary compounds are the new acids. They are presented by dimers combined of two molecules of different lengths. Herewith, we identified on these diffractograms also peaks of solid solutions, which compositions are nearly close to those of the excess components.

In binary systems of mixed parity, binary compounds of fatty acids do not apparently form after melting. For example, the diffractogram of the melted mixture (mol.)  $C_{18}H_{36}O_2 : C_{19}H_{38}O_2 = 1:1$  represents peaks of only the original components. In our opinion, the limitation of the isomorphous miscibility should be caused by the dimeric nature of fatty acid molecules.

Apart from this, structural (thermal) deformations and polymorphic transitions of stearic acid  $C_{18}H_{36}O_2$  were studied in view of the variety its polymorphic modifications; high temperature X-ray powder diffraction method was used.