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Perfect alignment of ribosomal protein S3 in creating an evolutionary tree
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Early attempts to use genomic analysis to define a tree of life used sequence alignment of ribosomal RNA. Subsequent analysis focused on proteins thought to be common to all species, revealed significant divergences from the rRNA based trees and the discrepancies have been attributed to horizontal gene transfer. Because the S2 bacterial ribosomal proteins are unlikely to have been affected by horizontal gene transfer, we examined the S3 ribosomal protein in search of a reliable method to use sequence alignment and divergence to trace species evolution. The amino acid length of bacterial ribosomal protein S3 has changed little throughout evolution. The search vector MGX XX(20)X(0,20)[DSTJX](3)[KKX](18)XX(0,15)X(3)[PA]XX(0,10)GSTA][KRX(6)GX(1)X(2)NQSC][X(3)XX(12)XX(7)XX(3)][LIV][XX(7)XX][LMT][GXX(2)GS][L][LIV][X(0,100) retrieves and aligns over 1800 S3 ribosomal proteins from SwissPro/TEMBL. Fully conserved positions in the fingerprint and those where occupancy is limited to two amino acids is dominated by Gly, Ala, Arg, and Pro residues (GARP) and the sites in which GARP is 100% conserved act as markers for perfect sequence alignment. Because the output contains more highly conserved residues than the input, the critical importance of conserved glycines is further established. Accuracy of alignment is tested by separating Gram-positive (G+) from Gram-negative (G-) bacteria. Certain amino acid positions within the fingerprint are capable of achieving such a separation, providing insight into the evolutionary history of the ribosomal protein S3. Accurate alignment also reveals homology between the sequences of the S3 ribosomal proteins of cyanobacteria and chloroplasts. The accuracy of a perfect sequence alignment can also be assessed by tracing its divergence through phylum, class, order, family, genus, species and strain. The percent of residues in the S3 protein that are fully conserved rises from 5% in all bacterial phylum to 98% in Escherichia coli and the number of conserved residues of GARP increases from 5 to 74. The amino acid sequence and three dimensional structure of the S3 proteins of all species and strains of a single genus of bacteria have undergone no significant change over billions of years of DNA replication. Mapping the most highly conserved GARP residues onto the three-dimensional structure of S3 reveals the role of S3 in ribosomal function. Support in part by: Mr Roy Hill Foundation and the generous help of a number of High School students from the Buffalo NY area.

Keywords: crystal chemistry, crystal design, coordination polymer

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Underlying nets in three-periodic coordination polymers
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We discuss a recently developed approach to formalize the analysis of extended architectures by successive simplifications of a crystal structure perceived as a periodic net. The approach has been implemented into the program package TOPOS that allows one to simplify and classify coordination polymers of any complexity in an automated mode [1]. Using TOPOS, we retrieved 6620 3-periodic coordination polymers from the Cambridge Structural Database and represented them in a standard way as underlying nets. The topological classification of both 975 interpenetrating and 5645 single 3-periodic underlying nets have been performed and compared.

The topological properties of coordination polymers can be formalized with the concept of underlying net. The nodes and edges of the underlying net correspond to structural groups and links between them. To obtain an underlying net for valence-bonded coordination polymers we use two types of their representation. The standard representation considers metal atoms and organic ligands as structure units, ignoring extra-framework ions and molecules. In the cluster representation the structural units include polyatomic coordination groups. We define topological type, the basic taxon to be used in the systematic of coordination polymers, as a set of crystal structures with the same underlying net.

In general, the distributions of interpenetrating 3D motifs on topological types and main interpenetration parameters are similar to the data of 2004 [2]. In particular, the most abundant topologies (dia, pe, srs, ths) remain the same. The typical interpenetrating motifs are 3-, 4-, or 6-coordinated.

For single nets the leaders are basically the same as for interpenetrating nets; 6 nets (dia, pe, srs, cds, pts, nbo) are among the ten most frequent nets in both samples. The top list of single nets contains a wider range of coordinations: 3-, 4-, 5-, 6-, 8-, or 3,6-coordinated.

The data on the abundance of underlying nets provide wide opportunities to find relations between the chemical composition of a coordination polymers and the topological properties of the corresponding underlying net. The most symmetrical (regular) nets for most widespread coordination figures (triangle, square, tetrahedron, octahedron, cube) are srs, nbo, dia, peu and bu, respectively, and these nets are the most abundant.

We have arranged the ways of the influence of coordination features on proteins thought to be common to all species, revealed significant change over billions of years of DNA replication. Mapping the most highly conserved GARP residues onto the three-dimensional structure of S3 in the ribosome provides insight into the reason for their conservation and the role of S3 in ribosomal function. Support in part by: Mr Roy Carver, Stafford Graduate Fellowship, Caerus Forum Fund, The East Hill Foundation and the generous help of a number of High School students from the Buffalo NY area.

Keywords: crystal chemistry, crystal design, coordination polymer

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Structural relationships in some monoclinic layered compounds
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The lamellar structure of thortveitite Sc3Si2O7 (S.G. C12/m1), was reported by Zachariasen [1]. This structure offers the possibility of have structural modifications changing the sandwich and silicon by other cations as (iron/indium) and germanium respectively, keeping the layered character of the crystalline arrangement. Atomic substitution in the thortveitite Fe3Ge2O7 (S.G. C12/m1) reduces its symmetry to thortveitite-like YFe2GeO5 (S.G. P12/m1) [2]. The aim
of this work was to determine 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/m1) when iron is partially substituted by yttrium in the layered thortveitite FeInGeO₆. The symmetry reduction promoted by the incorporation of yttrium in the formula YₓInₓFeGeO₆ (x = 0, 0.25, 0.50, 0.75, 0.90 and 1.0), is explained by mean of the crystallographic group-subgroup relationships.

Keywords: symmetry relations, klasengleiche subgroups, thortveitite

MS09.P03

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 fragments, such as the identification of close contacts and complex interfaces, we are looking at using atom pairs for which can be computed in O(N_x + N_y), where x and y are the number of atoms in fragments A and B, respectively. We are using atom pairs for which display significant excess density in an interface, or on a molecular surface, which should tend to bridge an interface. Use of only the atoms in A and B within a reasonable distance of (LRSA(A) ∪ LRSA(B)), (−LRSA(A ∪ B)) would help to pre-prune the search tree for these calculations.

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Keywords: complex interface, molecular_surface, contact

MS09.P04

Odd n-fatty acids CₙH₂O₂ and their alloys on the X-ray powder diffraction data

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Saturated fatty acids CₙH₂O₂ 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 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 CₙH₂O₂–C₁₀H₂O₂ and CₙH₂O₂–C₈H₂O₂ as well as quaternary one C₉H₂O₂–C₇H₂O₂– C₈H₂O₂ 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 bkl, 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: C₁₃H₂O₂–C₁₀H₂O₂ (studied compositions, mol. % C₁₀H₂O₂: 10, 33, 50, 67, and 70) and C₁₀H₂O₂–C₈H₂O₂ (studied compositions, mol. % C₈H₂O₂: 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 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.) C₁₀H₂O₂: C₉H₂O₂ = 1:1 represents peaks of only the original components. In our opinion, the limitation of the isomorphic miscibility should be caused by the dimeric nature of fatty acid molecules.

Apart from this, structural (thermal) deformations and polymorphic transitions of stearinic acid C₁₆H₃₃O₂, were studied in view of the variety its polymorphic modifications; high temperature X-ray powder diffraction method was used.