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Acta Cryst. (2011) A67, C268**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 52 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)[DST]X(3)[RK]X(18)XX(0,15)X(3)X[PA]XX^cX(0,10)[GSTA][KR]X(6)GX[LIVMT]X(2)[NQSCH]X(1,3)[LIVFCA]X(3)[LIV]XX(7)[LMT]X(2)GX(2)[GS]X(0,100) retrieves and aligns over 1800 S3 ribosomal proteins from SwissPro/TrEMBL. 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* 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 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.

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Acta Cryst. (2011) A67, C268**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 polynuclear coordination groups. We define *topological type*, the basic taxon to be used in the systematics 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**, **pcu**, **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**, **pcu**, **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**, **pcu** and **bcu**, respectively, and these nets are the most abundant.

We have arranged the ways of the influence of coordination features of metal centers and ligands on the overall topology of coordination polymers. We found that the number of possible overall topologies is essentially restricted by the geometrical-topological properties of coordination groups.

[1] V.A. Blatov, *IUCr CompComm Newsletter* **2006**, 7, 4-38; <http://www.topos.ssu.samara.ru>. [2] V.A. Blatov, L. Carlucci, G. Ciani, D.M. Proserpio, *CrystEngComm*, **2004**, 6, 377-395.

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Acta Cryst. (2011) A67, C268-C269**Structural relationships in some monoclinic layered compounds**

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The laminar structure of thortveitite Sc₂Si₂O₇ (S.G. C12/m1), was reported by Zachariassen [1]. This structure offers the possibility of have structural modifications changing the scandium and silicon by other cations as (iron/indium) and germanium respectively, keeping the layered character of the crystalline arrangement. Atomic substitution in the thortveitite FeInGe₂O₇ (S.G. C12/m1) reduces its symmetry to thortveitite-like YFeGe₂O₇ (S.G. P12₁/m1) [2]. The aim