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Quasiperiodic Structures Constructed by Projection in Two Stages

Shelomo I. Ben-Abraham[a], Alexander Quandt[b], [a]*Department of Physics, Ben-Gurion University, Beer-Sheba, Israel.* [b]*Institut für Physik, Ernst-Moritz-Arndt Universität, Greifswald, Germany.* E-mail: benabr@bgumail.bgu.ac.il

Pentagonal, octagonal; decagonal and dodecagonal structures have been observed in several alloy systems. These structures are quasiperiodic in a plane and periodic in its perpendicular direction. Crystals aperiodic in one direction have been known for decades. It is interesting to study intermediate structures in which the periodic and quasiperiodi directions are intrinsically connected. That may be done by projecting a a periodic structure in $D(>3)$ dimensions into three-dimensional space so that a second projection be quasiperiodic in a plane. We have achieved this earlier in the octagonal case [1] and partly in the dodecagonal case [2]. Here we present an improved dodecagonal version, as well as a new look at the pentagonal, or rather decagonal case. In the dodecagonal case we cut and project first the four-dimensional root lattice D_4 into $\mathbf{R}^3$ and then into a suitable irrational $\mathbf{R}^2$. In the pentagonal/decagonal case we start with the five-dimensional simple cubic lattice $\mathbf{Z}^5$.

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Keywords: quasicrystallography, partly quasiperiodic structures, two-stage projection

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Hydrogen Bonding in new Hybrid Compounds

Nourredine Benali-Cherif, *Institut des Sciences Exactes, Technologie et Informatique, Centre Universitaire de Khenchela*. *40000-Khenchela, Algérie*. E-mail: benalicherif@hotmail.com

Studies of organic-inorganic hybrid materials, including amino acids and various inorganic acids **[1,2,3],** have received a great deal of attention in recent years, because of their electrical, magnetic and optical properties **[4]**. Hydrogen bonds in hybrid compounds are of interest because of their widespread biological occurrence. The potential importance of hydrogen bonding in the structure and function of biomolecules is well established [5], in particular, N-H…O hydrogen bonds are predominant in determining the formation of secondary structure elements in proteins, and base-pairing in nucleic acids and their biomolecular interactions.

The present structure analysis of new hybrid compounds, was undertaken as part of our systematic investigation of organic-inorganic hybrid materials, including organic cations and various inorganic acids, to study the nature of hydrogen bonding in the crystalline forms of these compounds **[6,7,8,9]**.
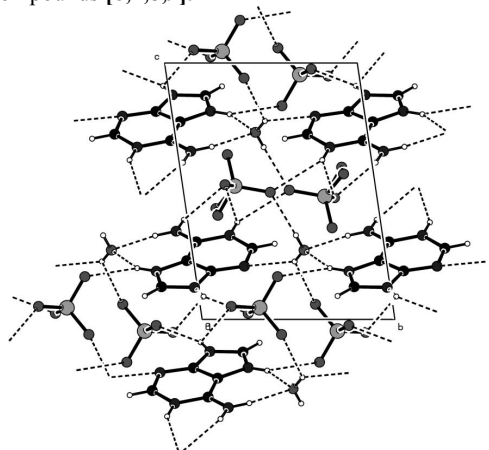
Figure. *View of diprotonated adeninium diperchlorate hydrate at 120 K **[10]**, showing the immediate hydrogen-bonded surroundings of anions and cation.*

The crystal structure of these compounds is built up from intricate cation-anion, anion-anion and/or cation-cation hydrogen bonds, resulting in two-dimensional and/or three-dimensional comparable networks.

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Keywords: hydrogen bonding, hybrid compounds, network

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Non-redundant Graph Representation of Polyhedral Networks

Hans-Joachim Klein, *Inst. of Computer Science and Applied Mathematics, Univ. of Kiel, Germany*. E-mail: hjk@is.informatik.uni-kiel.de

Infinite homogeneous networks in crystal structures with a single kind of coordination polyhedron and a single kind of connection between polyhedra can be represented by so-called quotient graphs or direction-labeled graphs [1],[2]. These finite graphs may be obtained from periodic nets by graph folding based upon translational symmetries. Taking all given symmetries into account this folding can be generalized such that so-called symmetry-labeled graphs are obtained [3]. We show how to further reduce this representation form by checking whether edges exist which may be generated by applying symmetry operations to other edges. A similar proceeding can be applied to polyhedra graphs [4]. In these graphs nodes represent geometrical or topological views of polyhedra. Edges represent connections between polyhedra with vertices involved in the connections as labels. A suitable representation of faces in topological views allows to reflect the main characteristics of a given polyhedral network when polyhedra are assumed to be rigid bodies.

In both cases, the minimal graph forms are well-suited for enumeration processes since they allow to avoid the generation of isomorphic graphs in an early stage. A further application is the improvement of indexes supporting the efficient search for isomorphic substructures in large collections of crystal structures.

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P.23.04.3

Ring Topology and Strain in pure Silica Zeolites

Jose Luis Jorda, German Sastre, Avelino Corma, *Instituto de Tecnologia Quimica CSIC-UPV. Avda. Los Naranjos s/n, 46022 Valencia (Spain)*. E-mail: gsastre@itq.upv.es

Framework stability in zeolites has been the subject of many studies and whether the source of structural instability is or not related with the number of rings and its distribution remains unclear. Only rough estimations of strain associated to 4-, 5- and 6-MR (membered rings) have been given. Also it is argued that 3-MR are utterly unstable although no calculations have been reported.

This study analyses rings in pure silica zeolites and strains associated to rings through the values of OSiO angles. A software code has been updated which calculates: (i) OSiO (and SiOSi) angles against ring size, (ii) strain associated to OSiO angles of each topologically unique Si atom, (iii) individual rings in each structure and ring-strain according to the classical quadratic term in OSiO.

In MEI topology, Si1 is the most strained atom, against the classical explanation that Si4, to which the 3-MR are associated, should be the most unstable. Nevertheless, it is true that amongst the