

**THE STRUCTURE OF TWINNED  $\text{Ag}_4\text{Mn}_3\text{O}_8$ , A NOVEL OCTAHEDRAL FRAMEWORK WITH A TOPOLOGY RELATED TO THE ARCHETYPE CUBIC {10,3} NET**

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Preparative exploration of the system Ag-Mn-O under an elevated oxygen pressure yielded so far unknown  $\text{Ag}_4\text{Mn}_3\text{O}_8$ . All reflections in the diffraction pattern can be indexed assuming a large cubic cell with  $a_{\text{cubic}} = 26.7 \text{ \AA}$ . Integration on the basis of the large cubic cell leads to only approximately 10% of observed reflections. Furthermore conspicuous absences of reflections are observed (see figure) which are not in agreement with any of the known extinction rules of the space groups. All this indicates the presence of complex systematic twinning.

Indeed the observed distribution of reflections can be explained assuming a trigonal cell with  $a_{\text{trigonal}} = 12.5919(1)$  and  $c_{\text{trigonal}} = 15.4978(1) \text{ \AA}$  (space group  $P3_121$ ) in combination with one of the fourfold axis of the cubic system as twinning element. The structure resulting from the twin refinement with the program Jana 2000 (Petricek & Dusek, Institute of Physics, Praha) is characterized by the occurrence of  $\text{MnO}_6$ -octahedra. These are connected via common edges and form a complex framework in the cavities of which the  $\text{Ag}^+$  ions are incorporated. The framework can be topologically related to the archetype cubic {10,3} net. While the silver partial structure which is spatially separated from the anionic structure has only trigonal symmetry, the  $\text{MnO}_6$  framework shows a high pseudosymmetry of  $P4_332$  which is most probably the underlying reason for the observed twinning.

Figure: hk0 and hk1 layer (with respect to  $a_{\text{cubic}} = 26.7 \text{ \AA}$ ) calculated from Imaging plate data.

**Keywords:** TWINNING,  $\text{AG}_4\text{MN}_3\text{O}_8$ , CUBIC NET

**SEARCH FOR STRUCTURE-FORMING COMPONENTS IN MOLECULAR CRYSTALS OF BINARY COMPOUNDS: A TOPOLOGICAL APPROACH**

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Molecular crystal structures of 81 polymorphs of binary compounds are investigated with the method of coordination sequences and with the uniformity criterion for atomic sublattices, implemented in the program package for multipurpose crystal-chemical analysis TOPOS. It is shown that using these tools one can estimate semi-quantitatively the relative force of intermolecular interactions and to find so-called structure-forming lattice, i.e. the atomic sublattice, where the most stable long-wavelength phonons are likely to spread. When a crystal consists of molecules with distinguished central atoms, the polarizability of surrounding atoms is found to dictate mainly the composition of the structure-forming lattice. If the polarizability is small, crystal structure is formed by molecules as a whole, otherwise surrounding atoms form the structure basis themselves, and it is their lattice that often is one of the close packings. It is shown that if the central atom of a molecule has stereoactive lone pair the central atom can form the structure-forming lattice together with surrounding atoms. The binary compounds were taken as the investigation objects to verify the conclusions of the method using standard crystal structure data and clear qualitative chemical concepts. The results obtained make wider the application field of the procedure of topological analysis of crystal sublattices, and allow one to use this procedure to investigate more complicated molecular compounds, where the intuitive qualitative conclusions are not so obvious.

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**Keywords:** STRUCTURE-FORMING PACKING TOPOLOGICAL ANALYSIS UNIFORMITY

**ENERGY FUNCTIONALS OF A PHYSICAL SYSTEM INDUCED BY A DIFFEOMORPHISMS GROUP**

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Additional terms induced by the symmetry of a physical system in the energy functional have been derived for the finite symmetry groups. It turns out, that, in the case when the symmetry group is a diffeomorphisms group, different topological invariants can be introduced to this energy functional. It has been found, that the equations of motion for an energy functional with a given topological invariant lead to the series of functionals depending on physical fields but not in the form of polynomials. Moreover, these functionals are parametrized by the solutions of these equations of motion formulated for the connection, which defines this topological invariant. The functionals under consideration have been expanded into power series in the physical fields. The polynomials obtained as a result of this expansion create the whole family of the Ginzburg-Landau functionals.

**Keywords:** SYMMETRY, TOPOLOGICAL INVARIANTS, ENERGY FUNCTIONAL

**CRYSTALLOGRAPHIC DATA IN THE PAULING FILE**

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The PAULING FILE is a long-term project aimed at creating tools for scientists working with inorganic materials. A comprehensive, phase-oriented database will group four kinds of data under the same computer frame: constitution data, structural data, diffraction data, and a broad range of physical properties. The first part of the project is limited to binary phases [1].

The structural part of the binary database contains 28'300 entries, with or without atom coordinates. For the first category, two presentations are proposed, one identical to the published data, and one directly comparable for all isotopic compounds. The latter is derived in a three-step procedure: 1) checking and correction of symmetry, 2) standardization following the method proposed by Parthe and Gelato, 3) comparison with the standardized data of the type-defining database entry.

All crystallographic data have been checked with an extensive package of software modules. Each structure type has been analyzed for interatomic distances and atomic environments, and a search based on atomic environment types (coordination polyhedra) is possible.

A 'phase' has been assigned to each database entry, based on information concerning structure, colloquial name, stability conditions, etc. These links make it possible to retrieve constitution, structure, diffraction, and property data reported for the same compound.

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References

[1] PAULING FILE, Binaries Edition for PC, MPDS, 2002. Distributor Crystal Impact, Bonn.

**Keywords:** PAULING FILE DATABASE INORGANIC COMPOUNDS