m28.p11

The Constructions of Algebraic Geometry and Symmetry Laws of Gas Hydrate Structure

A.L. Talis, O.A. Belyaev, I.A. Ronova, A.A. Reu[a], G.F. Tereschenko

A.N.Nesmeyanov Institute for Organoelement Compound,Moscow, Russia, [a]Russian Institute for Mineral Synthesis (VNIISIMS), Alexandrov,Vladimir Region, Russia

Keywords: gas hydrates, algebraic geometry, topological methods

Despite the substantial (and growing) number of publications on gas hydrates, our understanding of symmetry aspects of their structure, formation mechanisms, and phase transitions is still incomplete. The adequate mapping of the symmetry of tetrahedrally coordinated water framework of gas hydrates requires a change in the Euclidean basis of the structural crystallography to a more general basis of projective/algebraic geometry. This is due, in particular, to the fact that the point symmetry group of the dodecahedron - the principal polyhedral cavity of the gas hydrate - is noncrystallographic. The main result of our work is the determination graphs of the polyhedral cavities of gas hydrates as the Euclidian implementations of the incidence graphs of specific subconfigurations of the finite projective plane PG(2,q), q=2,3,4. The number of specific subconfigurations of PG(2,q), q=2,3,4 is relatively small, and, therefore (like the simple forms in classical crystallography), all polyhedral cavities of gas hydrates can be enumerated. As an example, the graphs of 20-vertex polyhedral cavities are defined as subgraphs of the corresponding graphs of the Desargues configurations. It is shown that the polyhedral cavity of gas hydrate by means of reshuffling of the minimum number of bonds can be transformed into a diamond-like cluster corresponging to the ”conjugate” subconfiguration of the same configuration. Thus, a set of conjugate subconfigurations defines a chain of hypothetical phase transitions in gas hydrates. Spatial unions of the polyhedral cavities of gas hydrates are also determined by constructions of algebraic geometry, in particular, by a fibration for the substructures of 8D lattice E_8 [1]. Various model of crystalline and non-crystalline [2] gas hydrates will correspond to the various fibrations associated with this main fibration. The point group of the lattice E_8 is of $2^{14}3^55^27$=696729600th order and contains the symmetry group of the polytope
(a 4D analogue of the dodecahedron) whose unit cell is the dodecahedron
. The principal result of our work is the construction of models of mutual transformations of gas hydrate rods and other tetrahedrally coordinated structures. The main advantage of the developed approach is the possibility of finding a minimal number of hydrogen bonds that one needs to reshuffle (or break) in order to realize all symmetrically allowable transformations in gas hydrates.
The work has been partially funded by RFBR (project # 05-03-32539) and RAS (program #7).

[1] Talis A.L. Structural Characteristics of Gas Hydrates within the Framework of Generalized Crystallography// Cryst. Reports, V. 48, N° 3, 2003, P. 347-350.
[2] Schmitz J., Peters J., Trebin. H.-R.Z. An icosahedral quasicrystalline for amorphous semiconductors. Phys, Rev B, 1996, v.100, p.57-62.

m28.p12

Crystal engineering with tricyclic quinazoline derivatives

Kambarali K. Turgunov, Akmal Tojiboev, Bahodir Tashkhodjaev

S. Yunusov Institute of Chemistry of Plant Substances, Tashkent, Uzbekistan. E-mail: kk_turgunov@rambler.ru

Keywords: crystal engineering, hydrogen bonding, supramolecular assemblies

Crystal engineering is a flourishing field of research in modern chemistry, practiced by scientists with interest in the modeling, design, synthesis and applications of crystalline solids with predefined and desired aggregation of molecules and ions. Tricyclic quinazoline derivatives are potentially valuable synthons in crystal engineering: their electron donating nitrogen atom holds out the promise of different complexes with a range of electron acceptors.
Researches relating to crystal structures of trimethilene-, tetramethylene- and pentamethylene-3,4-dihydroqunazoline hydrochloride dihydrates showed that there are formed identically five-membered hydrogen bonded chains in presence of chlorine ion and water molecules[1-2]. Resent investigations of crystal structures of selected tricyclic quinazolines with some ”guest” molecules showed the formation an isostructural supramolecular assemblies also. Since varying the quinazoline molecule does not result in a change to the basic state structure, we conclude that this arrangements is energetically favourable. Such observations are significant in crystal engineering terms since they offer the possibility of designing new materials through control of hydrogen bonding.

[1] CCDC refcodes: FIFQUG, ZIZYAI.
[2] K.K.Turgunov, B.Tashkhodzhaev, L.V.Molchanov, Kh.M.Shakhidoyatov. *Chemistry of Natural Compounds,* 2003, Vol. 39, Issue 4, pp.379-382.