Phase transition

Cooperative Jain-Teller effect and the role of strains in the tetragonal co-cubic phase transition in MgO, Cr2O3
S. C. Toombs, H. Gurevich, M. D. Cohen and V. Zorzito
In MgO:Cr2O3 solid solutions, progressive substitution of the Cr3+ ion for the Mg2+ ion results in the evolution of a cubic coexistence region, and transformation occurs from the tetragonal to cubic by a first-order phase separation.

Packing principles

Acetonitrile (2016) 733-573
https://doi.org/10.1039/C6TA06754G

High "z" structures of organic molecules: their diversity and organizing principles
H. Stohr
The investigation of the "z" parameter of organic molecules involved in the Cambridge structural database has shown that the group is very diverse but that most structures are the result of a simple rationalization and of a hydrogen-bonded aggregate that has at most approximate symmetry.

Charge transfer

Acta Cryst. (2016) 726, 917-918
https://doi.org/10.1107/S1600536816001639

Synthesis and structures of 11,11,12,12-tetrayano-2,8-dicapro-5,10-anthraquinone-dimethanes and its 2,1-cyclopyrrol with anisotropous, pyrene and tetraethylthiolene
The synthesis of 11,11,12,12-tetrayano-2,8-dicapro-5,10-anthraquinonedimethanes in the presence of pyrene and tetraethylthiolene is discussed. The compounds are synthesized in solution by the condensation of 2,8-dicapro-1,10-anthraquinone with 2,1-cyclopyrrol (acetone) and the polynuclear compound is subsequently transformed into a less bent geometry in the charge transfer interactions between DTQ and the aromatic electron acceptors.

Solvent effects

https://doi.org/10.1107/S1600536816001603

Solvent dependence of the solid-state structures of salicylaldimine magnesium amidine complexes
J. A. Rand, A. M. Doherty, S. S. Farrows, T. Goldbeck and A. G. Giller
Two new salicylaldimine magnesium complexes have been synthesized and structurally characterized. This study has shown that these specific systems are prone to ligand redistribution in solution and that the nature of hydrogen bonding and other solvation interactions in these complexes significantly affect the solid-state structures.

In situ crystallization

Acta Cryst. (2016) 723, 75-77
https://doi.org/10.1107/S1600536816001649

Acetic amide at 100 K: the first crystal structure determination
R. M. Swolin, C. Gerhardt, N. R. Shaefer and G. N. Lewis
Acetic amide is a widely used solvent reagent in organic synthesis. The crystal and molecular structure, as determined by single-crystal X-ray analysis at 100 K, is reported for the first time. The solvent accessible volume is a significant feature of a crystalline amide.

Instrumentation and computer programs

https://doi.org/10.1107/S1600536816001649

CTMDOC electronic structure analysis from X-ray spectroscopy
https://doi.org/10.1107/S1600536816001649

A multi-MHz single-shot data acquisition scheme with high dynamic range: pumpprobe X-ray experiments at synchrotrons
R. Böck, et al.
A time-resolved X-ray absorption spectroscopy with has been developed and tested, connecting a synchrotron X-ray fiber spectrometer system with a multi-MHz data acquisition scheme capable of detecting multi-photons events in a single X-ray photon. This system provides recording time-resolved X-ray absorption spectra with quasi-nice signal quality.

IUCr Chemistry

Selected chemistry articles from IUCr journals
X-ray crystallography provides accurate information about the molecular structure and conformations of a wide variety of compounds, including proteins, nucleic acids, and small molecules. The crystal structures are determined by the technique of X-ray diffraction, which involves the scattering of X-rays by a crystal lattice. The resulting diffraction pattern is analyzed to determine the atomic arrangement within the crystal, providing insights into the structure and function of the molecules.

**Pharmacological and natural products**

**A new approach to the study of drug interactions in drug design**

**Intermolecular interactions**

1. **A new approach to the study of drug interactions in drug design**

   A new approach to the study of drug interactions in drug design involves the use of computational methods to predict how different drugs will interact with each other. This can help identify potential interactions between drugs that could lead to adverse effects, and it can also help identify new drug combinations that could be used to treat diseases more effectively.

2. **The crystallographic signature of the tertiary structure of the sodium channel**

   The tertiary structure of the sodium channel is a complex four-subunit protein that plays a key role in the generation of action potentials in neurons. Understanding the structure of the sodium channel is important for the development of new drugs that can block or activate the channel, and it can also help identify new targets for drug development.

**Powder diffraction**

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