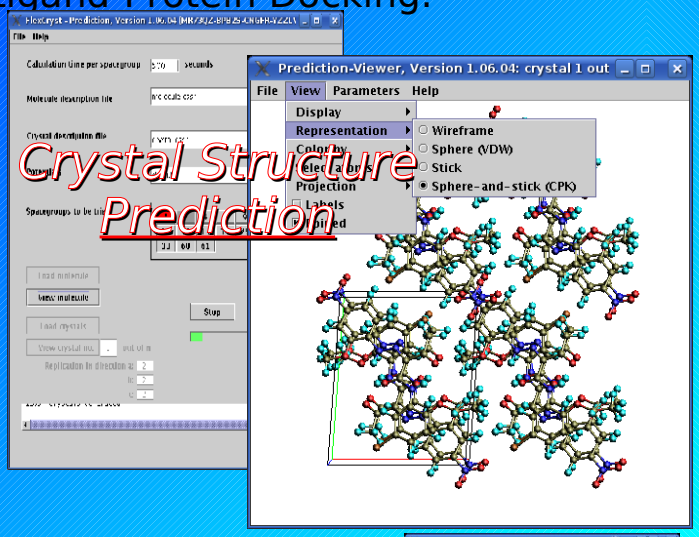
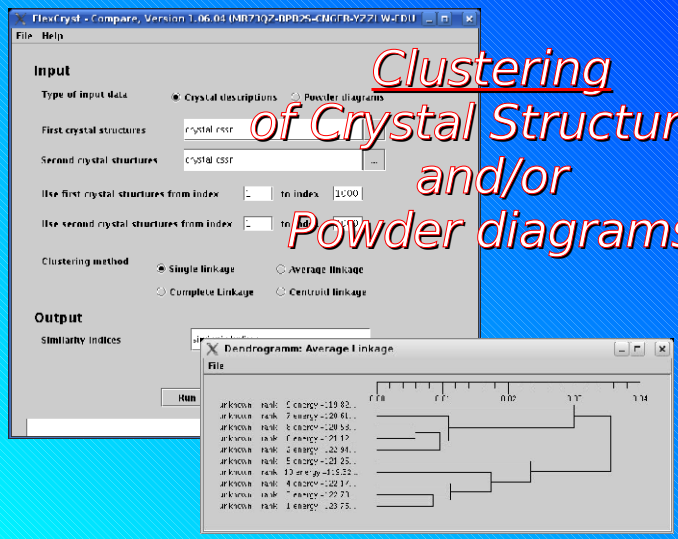
FlexCryst

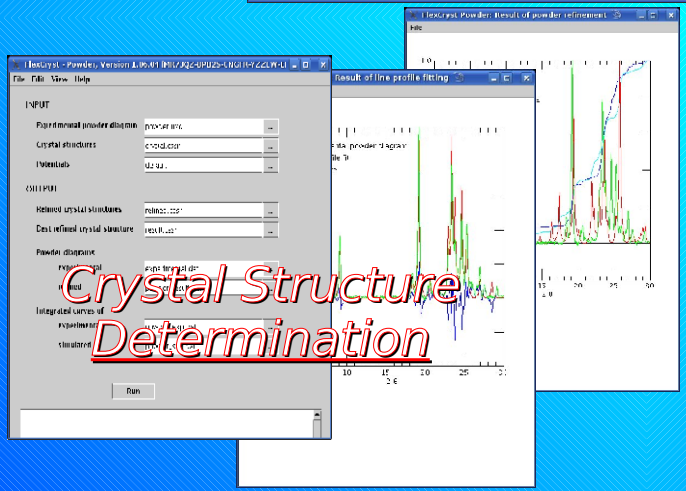
FlexCryst is a collection of programs for research in fields of crystallography, pharmacy, and chemistry. The programs are integrated in a common environment. Each of these programs can be handled, sold, and licensed independently on the other modules. Presently the suit of programs contains the modules: Crystal Structure Prediction, Crystal Structure Determination, Prediction of Sublimation Energy, Comparison and Clustering of Powder Diagrams and/or Crystal Structures, and Ligand-Protein Docking.



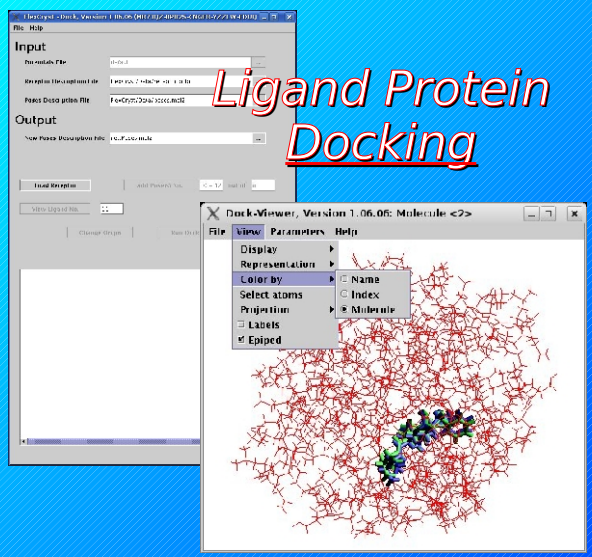
Crystal Structure Prediction



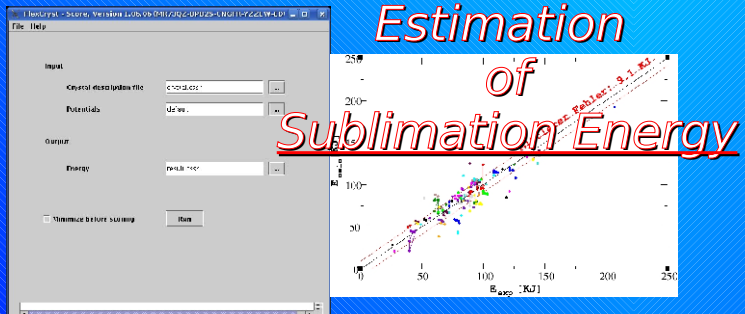
Clustering of Crystal Structures and/or Powder diagrams



Crystal Structure Determination



Ligand Protein Docking



Estimation of Sublimation Energy

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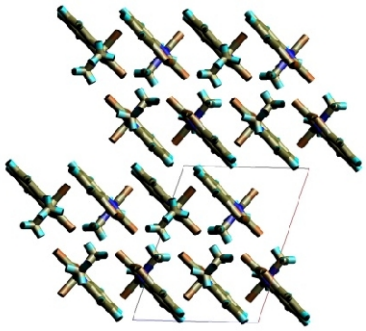
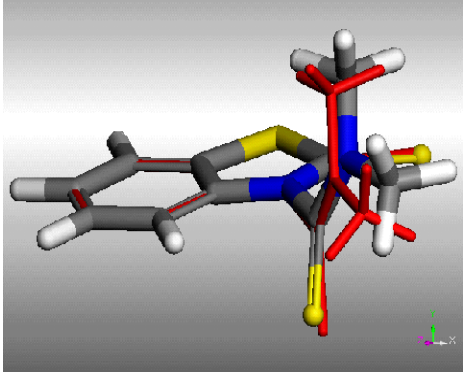
Online Presentations:

FlexCryst: A tool for molecular simulations in biochemistry and crystallography
(21 April 2008, Pula, Italy)
A new similarity index for determination and comparison of crystal structures
(3 March 2008, Erlangen, Germany)
Crystal modeling in der organischen und metallorganischen Chemie, Habilitation, June 2006
Crystal Structures of trans- and cis-octenes, Acta Cryst (2005). A61, C290-C291

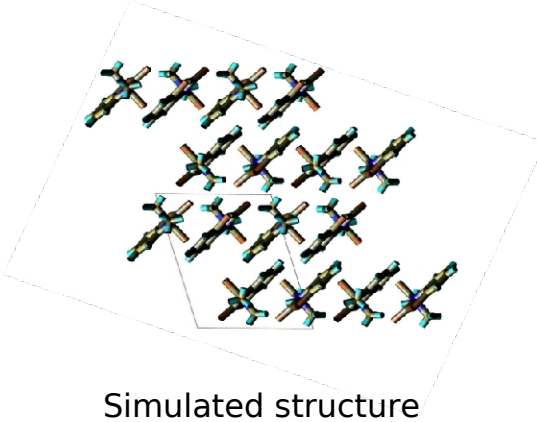
www.FlexCryst.com



experimental structure



Molecular conformation



Simulated structure (rank 2)

Crystal Structure Prediction

This module gives the possibility to perform calculations for rigid organic and organometallic compounds in the most common space groups. As input information it needs the molecular geometry. The module gives possibility to calculate also flexible molecules with known or previously derived conformation. The conformation has to be highly accurate and all atoms must have ordinary environment. The experimental crystal structure can be commonly found among the first hundred predicted crystal structures.

Applications:

- *Investigations on possible polymorphism. One unique substance (drug, pigment) can occur in several crystal structures (polymorphs). These different polymorphs have different properties and can be patented separately.*
- *Crystal structure determination. Together with additional information, e.g. powder diagrams, the experimental structure can be selected between the predicted structures.*
- *Thermodynamical properties of possible crystal structures. All predicted crystal structures have similar energy, which allow to predict the sublimation energy of a given molecule.*

Publications

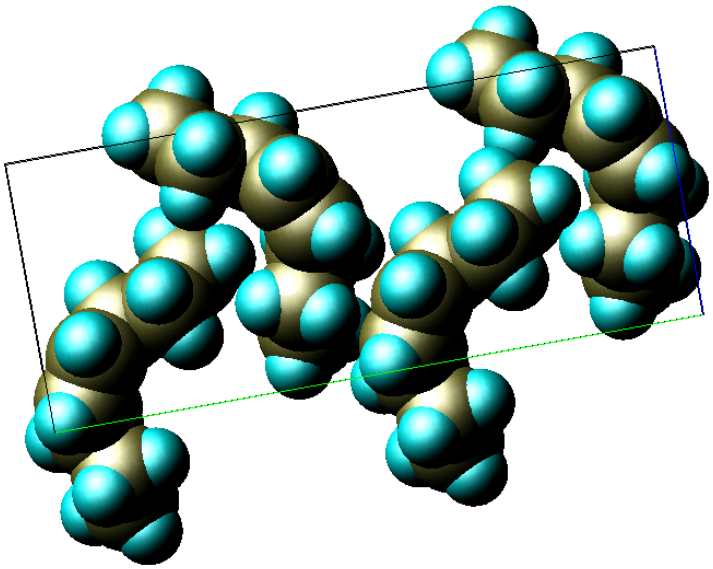
D.W.M. Hofmann and J. Apostolakis
Crystal structure prediction by data mining
J.Mol.Struc.(Theochem), 647, 17-39 (2003).

J. Apostolakis, D.W.M. Hofmann, and T. Lengauer
Derivation of a scoring function for crystal structure prediction
Acta Cryst A, A57, 442-450 (2001)

D.W.M. Hofmann, and T. Lengauer
Prediction of Crystal Structures for Organic Molecules
J.Mol.Struc.(Theochem) 474, 13-23 (1999).

D.W.M. Hofmann, and T. Lengauer
Crystal Structure Prediction based on Statistical Potentials
J.Mol.Mod. 4, 132-144 (1998).

home



Crystal Structure Determination

This module allows crystal structure determination from indexed and un-indexed powder diagrams. It is implemented with a new similarity index for automated comparison of powder diagrams which is valid for refinement in cases of large deviations in the cell constants and overlapping picks. The refinement according to this index closes the gap between crystal structure prediction and automated crystal structure determination. As input information it needs the molecular geometry and the powder diagram.

Publications:

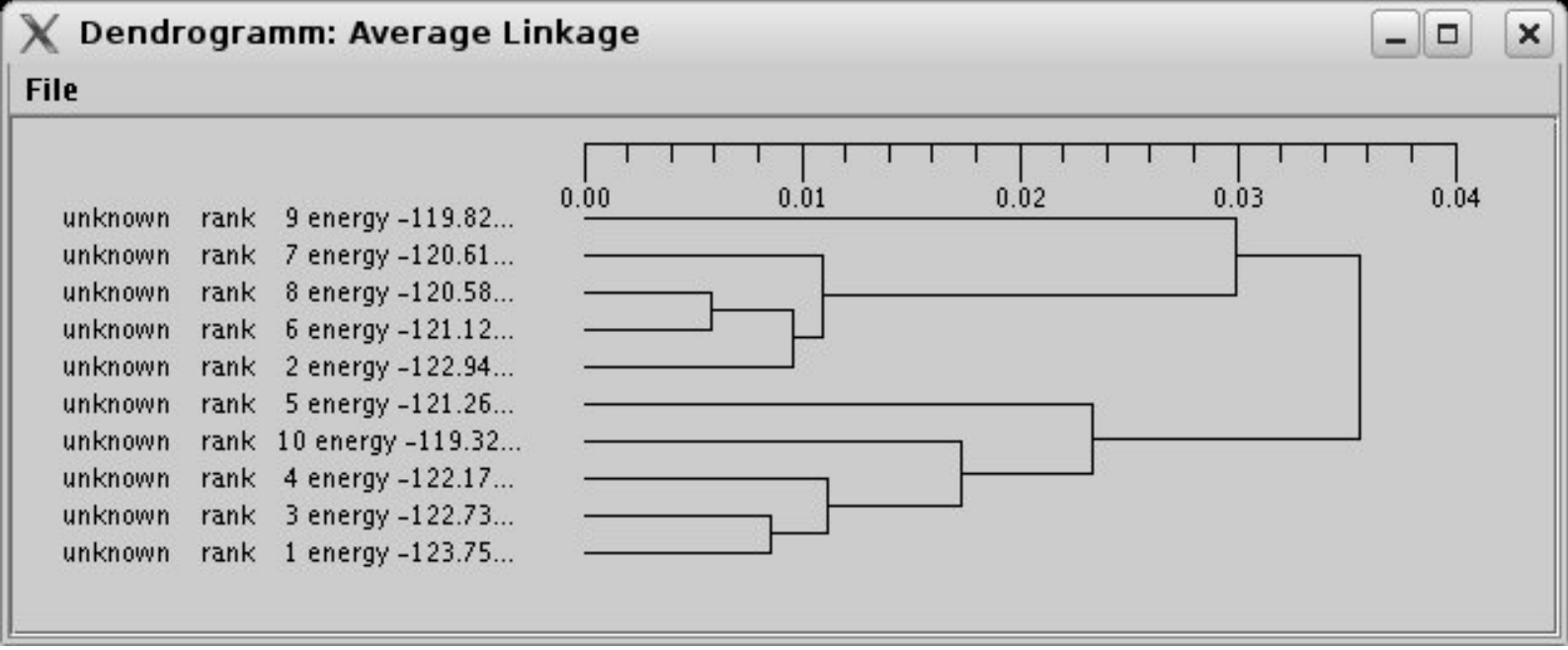
D.W.M. Hofmann and L.N. Kuleshova
A New similarity index for crystal structure determination from X-ray powder diagrams.
Journal of Applied Crystallography (2005) 38, 861-866.

D.W.M. Hofmann and L.N. Kuleshova.
A Method for Automated Determination of the Crystal Structures from X-ray Powder Diffr
Crystallography Reports. (2006). 51. 452-460.

M.U. Schmidt, D.W.M.Hofmann, C. Buchsbaum, and H.J.Metz
Crystal Structures of Pigment Red 170 and Derivatives, as Determined by X-ray Powder I
Angewandte Chemie Int. Ed. (2006) 45, 1313-1317.

C. Schauerte, C. Buchsbaum, L. Fink, D. W. M. Hofmann, M.U. Schmidt, J. Knipping, and R. Boese,
Crystal Structures of trans- and cis-octenes
Acta Cryst (2005). A61, C290-C291

home



Clustering of Crystal Structures and/or Powder diagrams

This module allows the comparison and clustering of crystal structures and powder diagrams. The results are visualized in dendrograms. The module offers for the clustering the most common linkages, simple, average, centroid, and complex linkage.

Applications:

- *Search and elimination of manifold structures or powder diagrams in data bases, this refers to experimental data bases as well as to virtual data bases generated by programs.*
- *Search and recognition of a new crystal structures or powder diagrams within existing data bases*
- *Clustering of powder diagrams and crystal structures for aims of polymorph's screening. The program recognizes the similarity of polymorphs even if they belong to different space groups and/or have different parameters of cell.*

Publications:

D.W.M. Hofmann and L.N.Kuleshova.
A Method for Automated Determination of the Crystal Structures from X-ray Powder Diffractio
Crystallography Reports. (2006). 51. 452-460.

D.W.M.Hofmann and L.N.Kuleshova
A New similarity index for crystal structure determination from X-ray powder diagrams.
Journal of Applied Crystallography (2005) 38, 861-866.

D.W.M. Hofmann, L.N. Kuleshova, F. Hofmann
Application of a new similarity index for the crystal structure determination and cluster analysis of po
(DGK, 3 March 2008, Erlangen, Germany)

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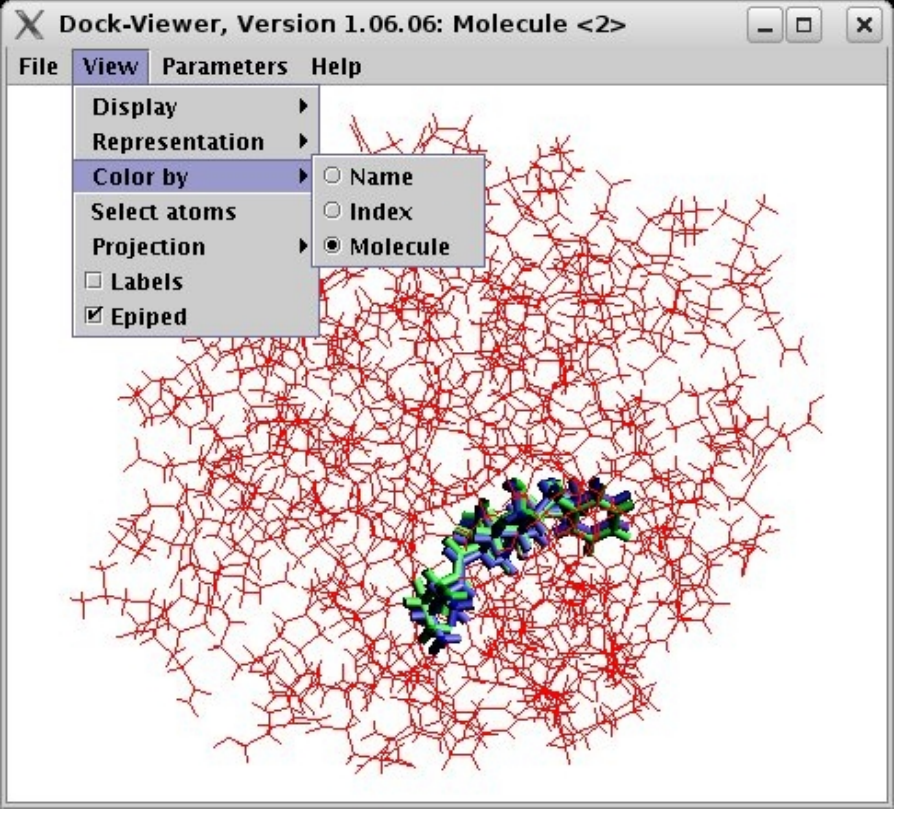


Ligand-Protein Docking

This module fits for investigations of drugs and pigments. These substances are very often rigid (e.g. Clopidogrel, progesterone, caffeine, and nicotine). Flexible drugs loose during docking degrees of freedom, which comes along with a decrease of the entropy. In result the binding affinity of flexible molecules is lower than for rigid molecules. However, flexible molecules show much more often a biological activity and are more practical to find leading structures for drug design. Due to the flexibility they can easier conform themselves to a given pocket of a protein.

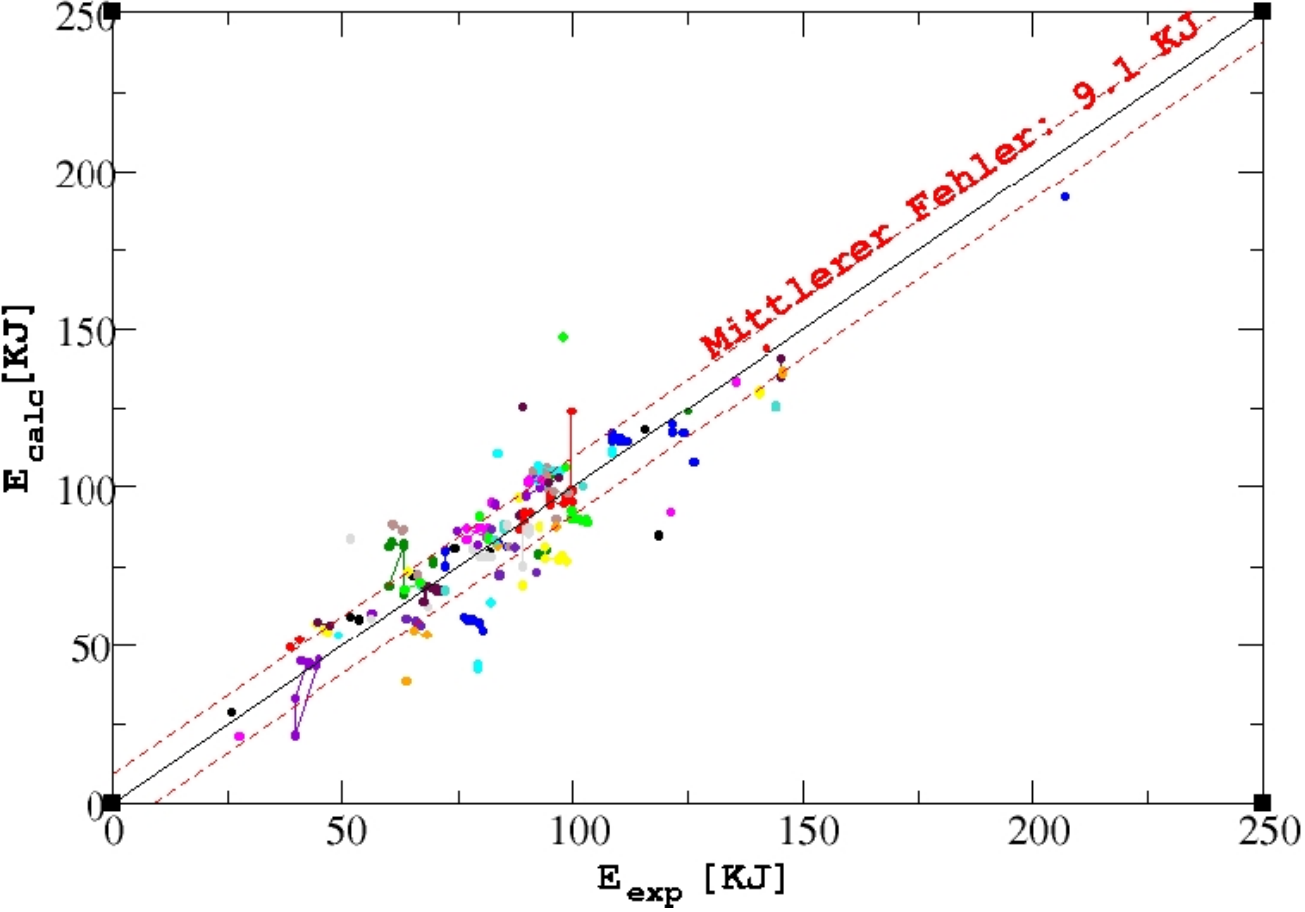
Applications:

- *(Re-)ranking of poses of Ligand-Protein complexes, which might be generated with some other programs*
- *Thermodynamical investigations of complexes, e.g. solubility*

Publications:

J. Apostolakis, D.W.M. Hofmann, and T. Lengauer
Using simple learning machines to derive a new potential for molecular modeling
Rational Approaches to drug design, H.-D. Höltje und W.Sippl, Prous Science, Barcelona, 2001, 125-134.

home



Estimation of Sublimation Energy

This module calculates the sublimation energy for a given crystal structure. The structure can contain several different molecules in the asymmetric cell. The sublimation energy can be estimated with an accuracy of 9.1 KJ/mole, which is correlated to the experimental accuracy. In the database some structures (shown in same color) occur manifolded with slightly different coordinates. The resulting energy difference determines the mean error.

Applications:

A wide variety of solid substances occurs in crystalline or microcrystalline state (e.g. drugs or pigments). One of the most important properties is the sublimation energy. Further properties (solubility, for example) can be derived from this energy.

Publications:

D. W. M. Hofmann, L. N. Kuleshova and M.Yu Antipin
Supramolecular Synthons and Crystal structure prediction of Organic Compounds
Crystal Growth & Design (2004) 4, 1395-1402.

Л.Н. Кулешова, Д.В.М. Хоффманн, М.Ю. Антипин
Систематические исследования общих закономерностей строения и предсказание кристаллической структуры органических соединений
Кристаллография (2005) 50, 199-208

D.W.M. Hofmann
Crystal Modeling in der organischen und metallorganischen Chemie
Habilitation, Frankfurt a. Main, 2004

home