accelrys®

Materials Studio

Analyze hydrogen bond topographies in molecular crystals

Classify predicted polymorphs regarding their connectivity information

Score predicted polymorphs using related structures from the CSD

Motif

Motif expands Accelrys' toolset for crystal engineering efforts. It is a tool designed to analyze connectivity information in molecular crystals, providing a qualitative and quantitative analysis method of hydrogen bond topologies. Combined with the predictive capabilities of Polymorph, Motif helps categorizing proposed packing arrangements and introduces a similarity measure to related structures available in the Cambridge Structural Database (CSD), allowing for a statistical scoring of proposed structures.

Polymorphism affects a wide array of materials properties, including solubility, bioavailability, mechanical stability, and manufacturability. For researchers dealing with solidification processes, selecting an optimal form introduces both challenges and opportunities. Motif supports these scientific efforts by generating knowledge about hydrogen bond topologies. This knowledge can help categorizing the tremendously complex design space, spanned not only by often numerous polymorphs, but also by salts, solvents, and co-crystals.

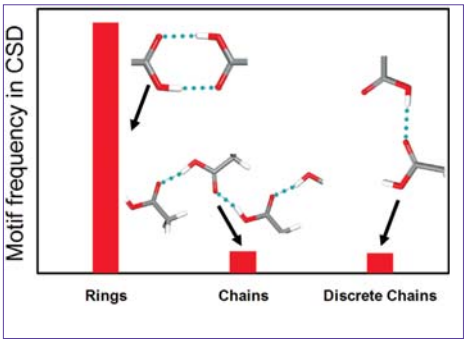
What does Motif do?

Motif interfaces with the Cambridge Structural Database (CSD) [1] exploiting Cambridge Crystallographic Data Centre's (CCDC) Mercury functionality [2]. Motif answers the important question: Do molecules with comparable architecture crystallize in similar bonding configurations as the proposed new structure?

Motif supports two primary workflows: To extract connectivity information of molecular crystals and to compare this connectivity information to experimentally know structures.

The first workflow uses previously defined contact points – typically hydrogen bond acceptors/donors or ionic contacts – to search for bonding motifs: Rings, infinite and finite chains, discrete motifs, and intermolecular contacts.

The second workflow queries the Cambridge Structural Database (CSD) for similar or related structures and their bonding motifs. Motif uses a similarity measure – based on Tanimoto coefficients – to gauge whether the bonding motifs of comparable CSD structures match those of the analyzed structure. As a result a similarity score is assigned to the analyzed structure. This allows for a statistical comparison of a proposed new polymorph and previously known structures with similar molecular architecture.



Hydrogen bond motifs of carboxyl groups together with their statistical occurence

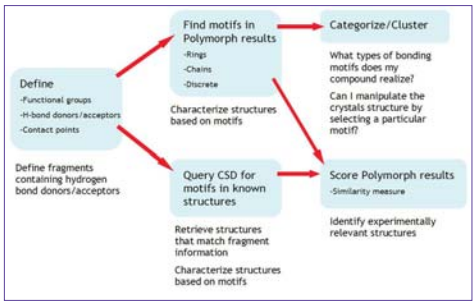
How does Motif benefit you?

Motif is a tool designed to support crystal engineering efforts. Motif adds an additional level of analysis and ranking capability when used together with Polymorph, Accelrys' predictive crystal packing tool. Statistical ranking/scoring of packing results from Polymorph can add an additional layer of confidence to the results. In addition, classification of motifs gives valuable knowledge that can be used in the context of crystal engineering efforts, e.g. selective crystallization strategies [3].

Features

Motif searches are driven by an interactive setup step in which chemical knowledge of functional groups involved in hydrogen bonding, donor and acceptor sites, and classes of potential bonding motifs, is translated into a database query that can be sent to the CSD. Motif simplifies this setup by:

- Interactive definition of functional groups using the Materials Studio "Set" concept
- Creation of contact points via manual selection or automatic processing using fully configurable lists of donor/acceptor atoms
- Support for ionic contact points for salt selection studies



Motif workflows

Motif allows for:

- Simple selection of motifs for query building
- Scoring function based on Taminoto coefficients
- Scoring against CSD entries or against input list, i.e. Polymorph output
- Reuse of previous CSD search results
- Client-server architecture for CSD access across your organization

The Materials Studio advantage

Motif is available through Material Studio's modeling and simulation suite that runs as a Windows® client on your PC, and provides a comprehensive range of software tools. Flexible client/server computing harnesses the power of a range of server technologies, to access leading methods in computational chemistry and materials science, delivering results direct to your desktop.

Results generated by Motif can be analyzed using Materials Studio's spreadsheet-like study table environment. The study table allows for a condensed representation of the results, associating crystal structures with motif formulas, number of motifs found, scoring information, as well as collecting related structures retrieved from the CSD. The resulting structural information can be further enriched as Materials Studio gives integrated access to related modeling and simulation functionality including morphology prediction, lattice energy evaluations based on molecular and quantum mechanics, advanced visualization, prediction of powder X-ray pattern, and statistical analysis.

System Requirements:

For Materials Studio system requirements see www.accelrys.com/products/materials-studio/system-requirements.html

References

[1] F. H. Allen, *Acta Cryst.*, 2002, B**58**, 380-388.
[2] C. F. Macrae, P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor, M. Towler and J. van de Streek, J. *Appl. Cryst.*, 2006, **39**, 453-457.
[3] Cross,W., Blagden, N., Davey, R., Pritchard, R., Neumann, M., Roberts, R., and Rowe, R., J. *Crystal Growth & Design*, 2003, **3**(2), 151-158.

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