BIOVIA MATERIALS STUDIO SYNTHIA

DATASHEET

BIOVIA Materials Studio Synthia calculates polymer properties using advanced Quantitative Structure-Property Relationships (QSPRs). It allows researchers to rapidly screen candidate polymers for a wide range of properties, and allows the property prediction of copolymer blends.

WHAT DOES BIOVIA MATERIALS STUDIO SYNTHIA DO?

BIOVIA Materials Studio Synthia uses pre-defined correlations to evaluate a wide range of polymer properties. Using these empirical correlation methods, large numbers of polymers, or copolymers of varying composition, can be rapidly screened for desired properties. QSPR methods are fast, provide large numbers of properties, and are the easiest modeling tool to use.

Understanding quantitative structure-property relationships helps chemists to prioritize candidate polymers for synthesis and testing. Previous QSPR approaches have relied on statistical interpolation from observed structure-property relationships using functional group contribution methods. These approaches restricted property prediction to those polymers comprised of a specific set of known chemical groups.

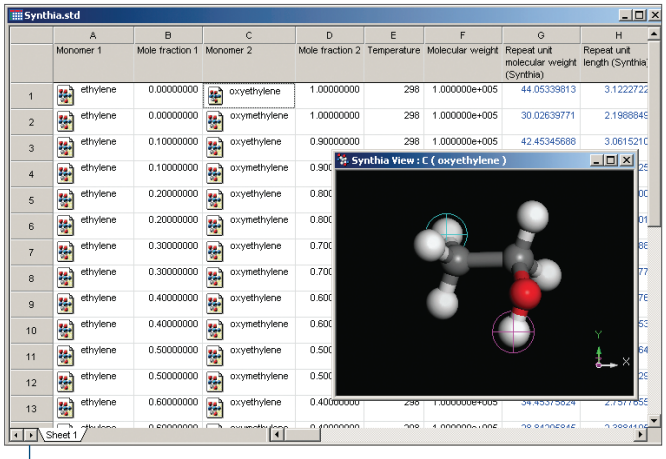

Figure 1: A plot of the mole fraction dependence of solubility parameter for a random copolymer consisting of two different monomer units. These complex properties can be obtained quickly and easily using the BIOVIA Materials Studio Synthia module.

BIOVIA Materials Studio Synthia is a significant advance in QSPR. BIOVIA Materials Studio Synthia uses topological information - specifically, connectivity indices derived from graph theory - and so is essentially based upon individual atoms and bonds. With no database of functional group contributions required, properties can be predicted for polymers comprised of the nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, and bromine.

BIOVIA Materials Studio Synthia is based on work conducted by Dr. Jozef Bicerano of The Dow Chemical Company, where the methodology has been extensively tested in practical work.

THE BIOVIA MATERIALS STUDIO ADVANTAGE

MS Modeling, BIOVIA Material Studio's modeling and simulation suite, runs as a Windows® client on your PC, and provides a comprehensive BIOVIA Materials Studio Synthia 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. The introduction of BIOVIA Materials Studio Synthia into this toolkit makes it easy to take advantage of the existing functionality of BIOVIA Materials Studio, such as the study table document. The comprehensive spreadsheet-like environment is used for accessing, comparing and analyzing results, and allows the storage of all predictions, making it easy to track work.

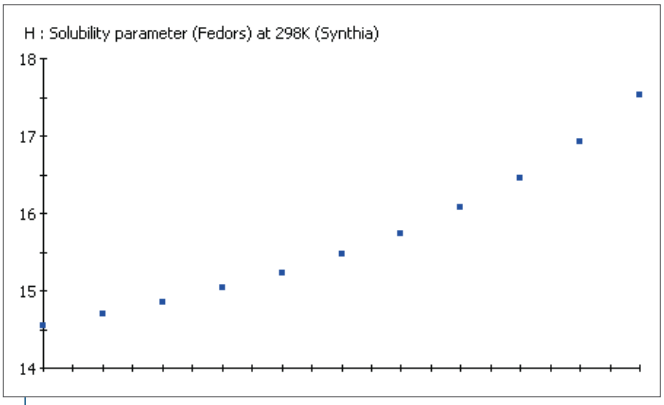

Figure 2: BIOVIA Materials Studio Synthia results are stored in a study table allowing you to store, plot, or sort results using the study table tools. Monomers can be edited in the study table and their properties updated giving you a fast method of screening new repeat units.

Polymer property data can be plotted using the integral charting tools or pasted into other Windows productivity tools, allowing for easy communication of results.

The 3D representation of each polymer repeat unit structure can be found by clicking on the monomer cell. The large numbers of polymer repeat units stored in libraries in MS Modeling means you may not even have to sketch your polymer of interest; however if the required repeat unit is not in the standard library, BIOVIA Materials Studio's advanced sketching tools make it a matter of following a few simple steps to sketch novel units and add them to your library.

BIOVIA Materials Studio Synthia can be used to predict properties for a single repeat unit, a series of homopolymers, or complex random copolymers. All this functionality is accessed from a single, simple, graphical user-interface.

FEATURES

- Rapidly estimate polymer properties by using empirical methods
- Predict a wide range of thermodynamic, mechanical, and transport properties for bulk amorphous homopolymers and random copolymers
- Make predictions for polymers so novel that the properties of interest are not documented
- Use study tables and charts to examine results for both homopolymer and copolymer calculations
- Use the study table, with the structural descriptors and a QSAR license, to generate custom correlations,
- Calculate the following types of properties:
- Structural properties
- Thermophysical properties
- Electrical, optical, and magnetic properties
- Mechanical properties
- Chain stiffness and entanglement properties
- Transport properties.

To learn more about BIOVIA Materials Studio, go to **accelrys.com/materials-studio**

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