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OLEX: new software for visualization and analysis of extended crystal structures

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We have developed new software (*OLEX*) for the visualization and analysis of extended crystal structures. This software has a Windows-compatible mouse-driven graphical interface which gives full control over all structural elements. *OLEX* provides the user with tools to construct topological networks, visualize interpenetrating or overlapping fragments, and analyse networks constructed fully or partially by exploiting short interactions. It is also easy to generate conventional ellipsoid, ball-and-stick or packing plots.

1. Introduction

In recent years, the number of extended and complex polymeric structures reported has grown dramatically as a result of intense interest in the unique properties of these compounds (*e.g.* Eddaoudi *et al.*, 2001; Tabares *et al.*, 2001; Jin *et al.*, 2002; Barnett & Champness, 2003; Blake *et al.*, 1999). The analysis and structural classification of such compounds is a very important part of their characterization, allowing them to be described and compared with related compounds in the same or different class. However, this analysis is demanding and requires specially designed tools and powerful three-dimensional graphics. Most structure visualization software currently available is designed and optimized for discrete (*i.e.* molecular) species, and the analysis and interpretation of extended structures using such software is, therefore, problematic. Common complications arising during the analysis of extended frameworks involve topologically irrelevant structural elements such as hydrogen atoms, counteranions and guest molecules: an interactive interface based on structural component selection and a clear data hierarchy is, therefore, a key prerequisite for efficient and reliable analysis.

The topological analysis of extended frameworks plays an important role in structure analysis, description and classification. Such an analysis normally consists of three steps: selection of topological nodes, construction of the topological network and evaluation of the topological term. Automation of the last two steps is very beneficial, since when the construction of the topological network and evaluation of the topological term are performed manually, there is a high likelihood of error (Power & Tracy, 1998; Carlucci *et al.*, 2002).

2. Program description

The software can import structural data *via* a number of crystallographic file formats (*SHELXL* model files, CIF, MDL MOL, PBD), generate the extended structure if required, and produce a picture. Extended structures can be exported as MOL files and pictures as bitmaps or JPEG files.

The *OLEX* graphical system is built on OpenGL (Silicon Graphics). The Windows implementation of OpenGL allows the use of up to eight uniform or directional light sources, different material properties and lighting models (which define ambient scene light intensity and how reflection angles are calculated). The *OLEX* background designer allows pictures to be superimposed on semi-transparent backgrounds and predefined or user-defined gradients.

As *OLEX* has been designed for use with extended structures, the mouse-driven interface is an essential part of the program. The interface is flexible, giving the user a choice of how to carry out a particular operation. For example, almost all operations on structural elements can be performed using either screen selections or a list-based method. Standard operations such as the measurement of interatomic distances, valence angles or dihedral angles are also supported, as is viewing along crystallographic directions. Additional facilities include atom labelling, adjustable atom and bond radii and the determination of the current view direction. Tools specifically related to the analysis of topology and short interactions are described in §2.2 below.

2.1. Data organization

As the logic and interface of the program are highly dependent on its internal data representation, knowledge of the data hierarchy is important for understanding the functionality of the software. The largest block of data within *OLEX* is that describing the structure, the components of which are intramolecular bonds, fragments with no covalent connections between them, and the network, which is represented by network nodes and inter-node connections. Fragments consist of atoms connected by covalent bonds. Information relating to atoms, covalent bonds and intermolecular interactions is designated by fragment, and fragments, atoms and bonds are related so that the properties of any fragment can be accessed by selecting any of its atoms or bonds, while selecting a bond gives access to the properties of the atoms linked through it.

2.2. Special features

As mentioned above, we have designed the software specifically to be used to visualize and analyse extended structures and, therefore, it possesses some unique functions. Networks having large pores commonly exhibit interpenetration, and visualizing them is difficult unless the fragments can be made clearly distinguishable. The solution adopted in *OLEX* is to display all elements of a particular fragment in a single colour. The same technique can be used to visualize layered structures or large overlapping discrete entities, such as overlapping C_{60} molecules (O'Neil *et al.*, 2002) or bulky fragments (Blake *et al.*, 2001).

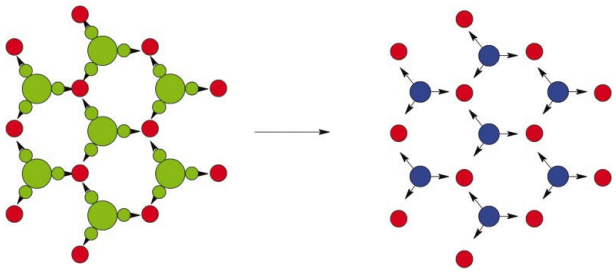

Figure 1
Illustration of the transformation of a covalent network to the multinodal topological equivalent. Metal centres are shown as red circles and ligands as blue circles or green figures.

Analysing structures where the framework is constructed of short interactions can also be laborious because standard software does not allow such a network to be considered as a single entity. *OLEX* solves this problem by allowing the user to transform a list of short interactions into covalent bonds within the analysis procedure and perform further framework analysis in the normal way [*e.g.* see Blake *et al.* (2001) for an example of a hydrogen-bonded framework].

The most advanced function of *OLEX* is the construction of topological networks and the evaluation of topological (*Schläfli*) symbols (Wells, 1977). The topological networks represent structural connectivity and are usually based on physical nodes. In the case of networks constructed from bidentate ligands and metal centres, the latter have the role of topological nodes and these networks can readily be transformed to topological ones by replacing the ligands with network bonds. Another kind of network is constructed from metal centres and multidentate ligands. The connectivity of such networks can be correctly shown using two types of nodes, one based on the metal centres and the other representing ligand connectivity (See Fig. 1). Thus, while it is common for metal centres to fulfil the role of topological nodes, it is sometimes also necessary to consider the ligands as nodes.

2.3. User interface

The *OLEX* interface is mouse-driven and Windows compliant, and consists of a main window, toolboxes and dialogs. The main window has a menu, a toolbar with buttons and a status bar used to show bond lengths and angles. The toolboxes include rotation controls, viewing controls and a fragment navigator.

3. Software environment

OLEX runs under Windows 98/Me and NT4/2000/XP. The user interface and main program are written in Borland C++.

4. Documentation

The software is supplied with an HTML-format manual containing installation notes, system requirements and a description of the interface.

5. Availability

The software is available from the principal author upon e-mail request.

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