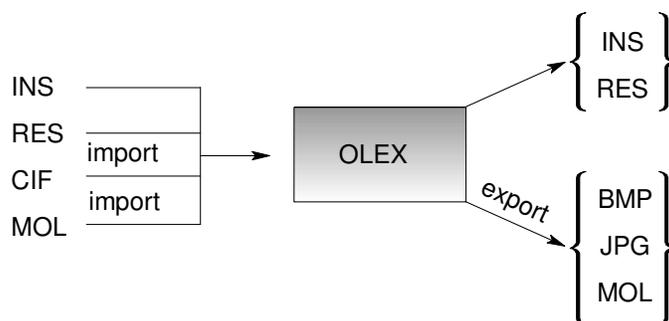


DEVELOPMENT OF A NEW SOFTWARE FOR X-RAY  
STRUCTURE ANALYSIS AND VISUALISATION

Oleg V. Dolomanov,\* Neil. R Champness and Martin Schröder.

School of Chemistry, University of Nottingham, University Park, Nottingham, NG7  
2RD, UK.

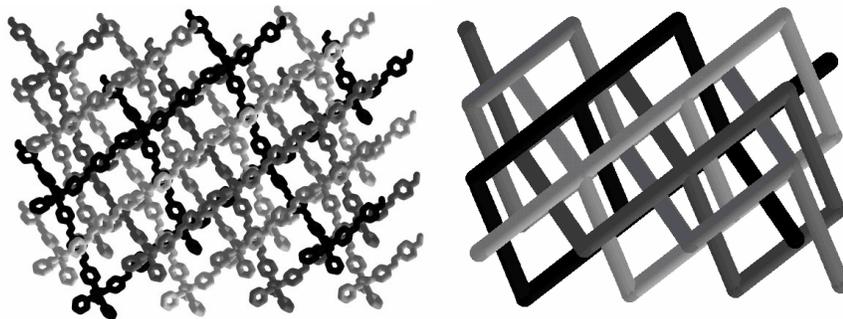
A new program which allows visualisation and topological analysis of X-ray structures has been developed. The program has both a user-friendly interface and allows easy data access supporting the file formats shown in scheme 1.



Scheme 1. Input and output files. SHELX Ins and Res-files are fully supported.

A mouse driven Windows compliant program interface is allowing access to individual atoms or bonds or even to extended arrays. Pictures generated in this program can be exported as high resolution image files and imported into other programs, including Word and almost any graphics programs.

One of the main features of the program is the topology analysis which allows identification and highlighting of individual molecules, frameworks or fragments. This includes interpretation of H-bonds or other short interactions. Illustrated below is an example of the visualisation of an interpenetrating 4,4 grid.



Scheme 2. Structural and topological illustration of interpenetrating 4,4 grid.