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Product review

X-Seed — A Software Tool for Supramolecular Crystallography

Leonard J. Barbour*

Department of Chemistry, University of Missouri-Columbia, Columbia MO, 65211, USA

Abstract—X-Seed is a software tool for X-ray crystallographers and runs under any of the 32-bit Microsoft Windows operating systems including 95, 98, Millennium Edition, 2000 and XP. Many of its features are tailored to meet the needs of scientists interested in solid-state supramolecular chemistry. The two primary functions of the software are (i) to serve as a graphical interface to the SHELX-97 program suite, and (ii) to produce high-quality molecular graphics images. In addition to these features, many other useful functions are also implemented in order to facilitate the process of crystal structure solution, refinement, analysis and presentation.

Owing to the high level of precision and accuracy to which intra- and intermolecular parameters can be measured using X-ray crystallography, this powerful technique has contributed greatly to the growth of the rapidly expanding field of Supramolecular Chemistry.[1] Generally, the metric parameters of supramolecular building blocks are well known and we are no longer interested exclusively in their molecular structures, but also in their extended structures. Since the three-dimensional assembly of molecules is controlled by relatively feeble interactions, multicomponent systems often display crystallographic disorder and, consequently, produce weak diffraction patterns. Furthermore, when presenting such structures to the scientific community, it is usually desirable to draw attention to very specific features of the intermolecular arrangement and conventional packing diagrams are often inadequate for this purpose. Clearly the elucidation and subsequent presentation of supramolecular crystal structures can be a daunting and protracted undertaking, and it is therefore of great value to employ software that is sympathetic to these tasks.

This contribution describes the program X-Seed,[2] which is specifically designed to address the requirements of supramolecular chemists whilst still being of use for routine crystallography. X-Seed provides a graphical user interface (GUI) to several non-interactive utilities that are generally regarded as being among the foremost programs of their kind, but that do not possess user-friendly interfaces. The program was designed to take advantage of the flexibility offered by these utilities without sacrificing their power. This is an important consideration since the determination of crystal structures, once the realm only of specialists, has in recent years become widely practiced by scientists not specifically trained as crystallographers. Indeed, the advent of modern instruments for the rapid measurement of diffraction data has contributed vastly to the recent surge in crystal structure reports.

The widely used and trusted crystallographic software suite SHELX-97[3] provides a feature-rich set of tools for structure solution, refinement and analysis. The programs SHELXS-97 and SHELXL-97 operate non-interactively, utilizing ASCII text files both for the input of instructions and data, and for the output of computed results. These programs have evolved over a period of several decades, during which time they have seen widespread use, and are universally recognized for their power and reliability. Whilst providing data and instructions by means of text files allows a high degree of flexibility, the coding of such files is usually a frustrating and time-consuming task. Fortunately, this mode of operation is readily adaptable to the implementation of a GUI whereby data and instructions can be conveniently manipulated by means of a mouse and dialog boxes. Such a GUI program can then generate the text instruction files accordingly and even launch the appropriate application at the click of a button. Since the utility application does not pause for input, the GUI would simply wait for it to terminate, and then scan the output text file to extract and display the computed results in a meaningful and useful fashion. Such a GUI

*Corresponding author. E-mail: barbourl@missouri.edu

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needs to be designed carefully to 'wrap around' the utility programs in order to provide the user with an optimal balance of simplicity and power. Although several GUI programs have been developed in recent years to interface with the SHELXL-97 suite of programs, it is not within the scope of the present contribution to provide a comprehensive review of the subject.

POV-Ray[4] is a free ray-tracing program that can be obtained from its dedicated web site http://www.povray.org. This program utilizes a unique and intricate set of commands to render an image representing a scene. A scene consists of any number of definable objects and light sources. X-Seed had been designed to generate POV-Ray scene files in order to produce high-quality

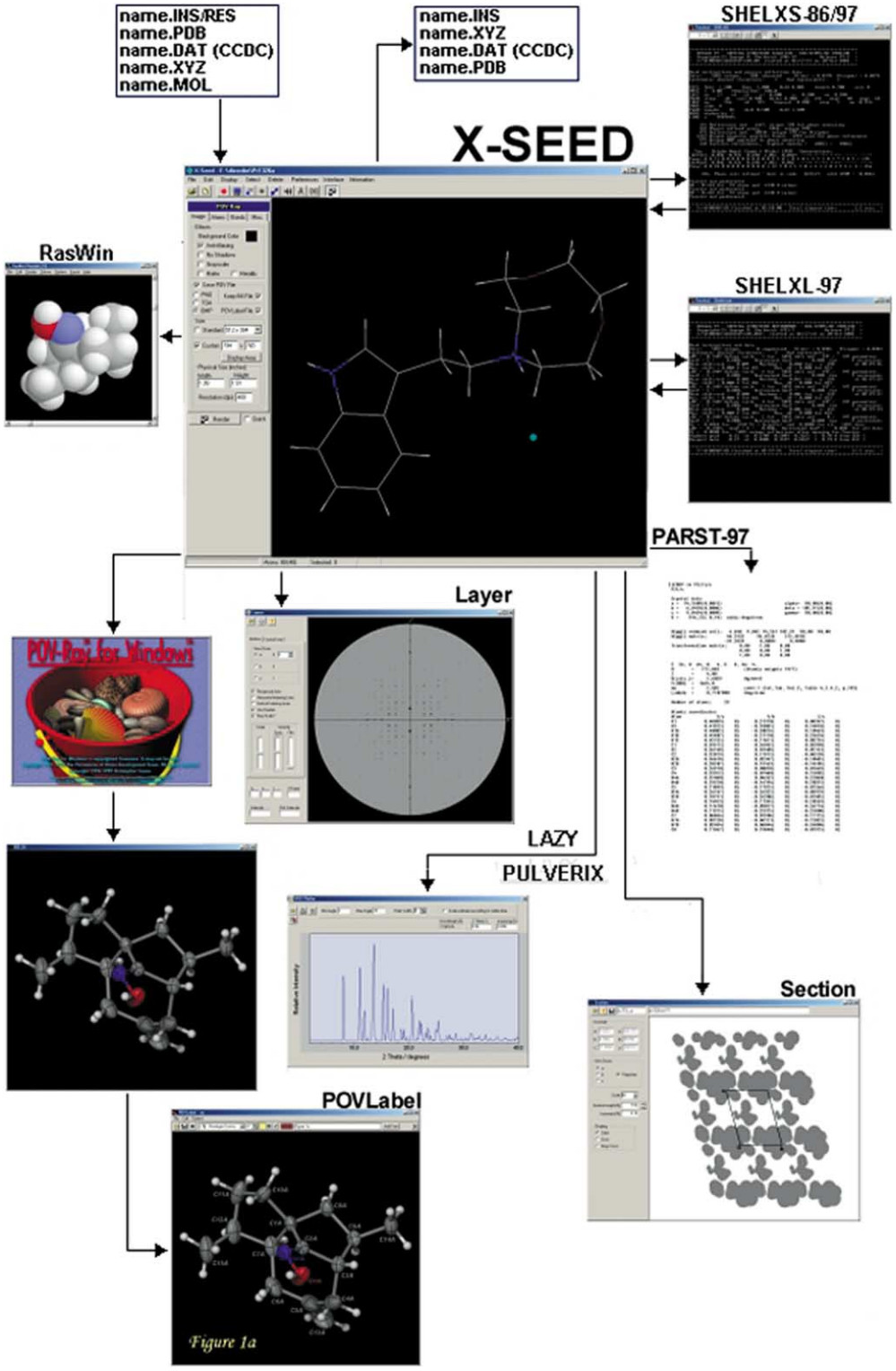

Figure 1. Schematic overview of the X-Seed software system.

molecular graphics images. The desired attributes of objects such as atoms and bonds can easily be set within X-Seed, which can then invoke POV-Ray on request. In recent years the use of ray-traced images has become commonplace in journal articles as well as poster and oral presentations. Examples of ray-traced images produced by X-Seed/POV-Ray can be found on the X-Seed web site (http://x-seed.net), in journal articles by the author[5] and other X-Seed users,[6] as well as the cover of this journal.

A brief outline describing typical implementation of X-Seed is given in Fig. 1. While it would not be feasible to provide a comprehensive list of features in this contribution, the following deserve note:

1. complete SHELX support — even complicated and disordered structures can be modeled without use of a text editor;
2. interactive creation of packing diagrams;
3. convenient measurement of interatomic contacts, as well as bond and torsion angles;
4. when creating ray-traced images, atoms and bonds can be assigned attributes individually or collectively (attributes include colors, radii, thermal ellipsoid surfaces, bond fragmentation and variants of all of these);
5. hydrogen bonds can be located and used as criteria for expanding a packing diagram;
6. centroids of any collection of atoms can be generated and used for measurement and display (e.g., to display a contact between a metal ion and an aromatic ring);
7. ray-traced images can include semi-transparent van der Waals volumes.

It should also be noted that X-Seed interfaces with other crystallographic utilities such as Lazy-Pulverix,[7] PARST,[8] Layer,[9] Section[10] and Rasmol,[11] and can import structures retrieved from the Cambridge Crystallographic Database. Further information regarding X-Seed can be obtained from its web site, and from the author.

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