

Research and teaching tools: A SHELX/POV-Ray interface (X-Seed) and simulation of a diffractometer (SMART1k)

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X-Seed is a crystallographic software tool with two primary objectives: (1) to serve as a graphical user interface to the SHELX software package and (2) to produce publication/presentation quality molecular graphics using POV-Ray. X-Seed was first released in 2009 to meet needs that were not completely filled by other crystallographic packages. Between 2009 and 2016 several updates were implemented through versions 1 to 3 of X-Seed but these early versions only supported SHELX-97. Owing to the growth in popularity of alternative programs such as Olex², shelXle and others, the author resisted updating X-Seed to support the latest versions of the SHELX suite (he expected X-Seed to “die a natural death”). However, over the 2016/2017 period he finally yielded to continued pressure from long-time X-Seed users to make the changes, which resulted in the recent release of version 4.

The Ewald sphere concept is difficult to teach effectively, but it is central to understanding diffraction geometry. SMART1k was developed as a visual aid for students of crystallography. The program simulates the operation of a diffractometer equipped with platform geometry. The most illustrative feature of the program is its ability to superimpose the reciprocal lattice and the Ewald sphere onto the simulated diffractometer.

X-Seed and SMART1k are freeware programs that run under Windows operating systems implemented on either an IBM-compatible or an Apple computer.