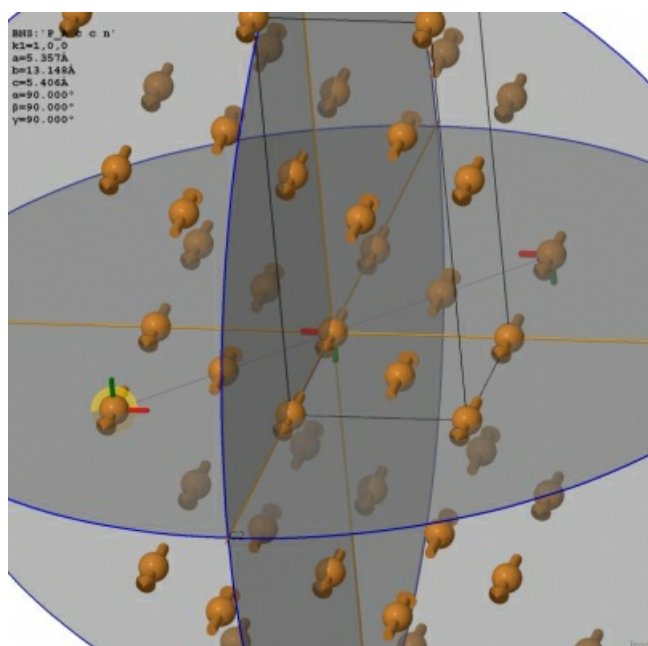


CIF1 to CIF2: lessons learned in the development of jmol

Robert Mark Hanson¹

¹Department Of Chemistry, St. Olaf College, Northfield, United States
E-mail: hansonr@stolaf.edu

The many evolving variations of the Crystallographic Information Format pose substantial challenges for developers of tools such as Jmol that read and write a wide variety of file formats. Jmol, for instance, has been developed to handle parsing of standard "CIF1" format as well as macromolecular (mmCIF), magnetic (magCIF), and modulated structure (msCIF) formats, including their combinations, such data files for incommensurately modulated magnetic structures. In addition, Jmol must read similar information from non-CIF formats – PDB, and MMTF for macromolecular data; Jana2006 for incommensurately modulated structures. For maintenance purposes as well as the preservation of developer sanity, a layered approach was taken for the design of these readers in Jmol. Thus, the basic CIF1 reader is "subclassed" to become a CIF2 or mmCIF reader and fitted with relevant parsers for CIF1, CIF2, and specialized [3+n] modulation-related data. The result is a complex but manageable set of modules that work seamlessly to provide a unified crystallographic package. This presentation will focus on challenges in working with CIF1 and CIF2 formats, the development of a JSON version of these formats for testing purposes, and limitations in Jmol in relation to their implementations.



Keywords: [Jmol](#), [visualization](#), [incommensurate](#)