Visualisation of Chemistry Data with the Open Source software, Jmol and JSpecView

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The most notable Open Source tools for display of molecular graphics and spectra are Jmol and JSpecView. Both have been in existence from before 2000, but it is perhaps only since 2006, when active development of MDL Chime ceased, that their usage bases significantly expanded. (Jmol, for instance, recently passed its 500,000th download mark.)

2012 represents another milestone in the history of these tools with the decision to merge code and to develop direct interoperability. As an important step in this progress, we have designed and implemented new JCAMP-DX extensions that allow a single file to be read by both programs, indicating multiple structures, spectra, and peak assignments relating to NMR, IR/Raman, and mass spectrometry. Examples of these files and their use with web pages and the stand-alone Jmol application will be demonstrated, including exercises in the interpretation of IR, NMR, and MS data as well as symmetry and group theory

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