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VRML general position diagrams of magnetic space groups

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Three-dimensional general position diagrams of the superfamilies of all non-cubic magnetic space groups have been developed. The diagrams can be rotated and zoomed to aid in the visualization of the general position diagrams and include both the general positions of the atoms and the general orientations of the associated magnetic moments.

1. The crystallographic problem

The standard representation of the general position diagrams of the non-magnetic space groups is two dimensional (*International Tables for Crystallography*, 2002), *i.e.* two-dimensional projections of three-dimensional diagrams. We have developed the 1502 three-dimensional general position diagrams of the superfamilies of all non-cubic magnetic space groups, which includes all non-magnetic non-cubic cases. Each diagram can be rotated and zoomed to aid in the visualization of the general position diagram and includes both the general positions of the atoms and the general orientations of the associated magnetic moments.

2. Method of solution

Similar to the development of the VRML (virtual reality modeling language) general position diagrams for subperiodic groups (Cordisco & Litvin, 2004), the three-dimensional diagrams were developed using a commercial product (*AutoCAD2002* by Autodesk, http://www.autodesk.com). A second commercial product (*Vrmlout for AutoCAD* by XANADU s.r.o., http://www.xanadu.cz) was used to convert the diagrams to VRML format. The general positions are represented by spheres and the associated magnetic moments by arrows.

3. Software environment

Needed to view the diagrams are a Web browser, such as *Netscape*, with a VRML plug-in, *e.g. Cortona VRML Client* (http://www.parallelgraphics.com/products/cortona/), or a VRML stand-alone viewer, such as *VRMLview* (http://www.sim.no/products/SIM_VRMLview/index_html). The NIST Website http://cic.nist.gov/vrml/vbdetect.html lists many plug-ins, applets and stand-alone programs to view VRML files on Windows, Linux and Mac operating systems.

The diagrams are stored on hard disk or CD and loaded individually into the Web browser or VRML viewer.

4. Hardware environment

The diagrams can be viewed on any platform that supports viewing of VRML files. Stored on a hard-disk drive or CD, the 1502 files, each containing one general position diagram, use 740 Mbyte of storage space.

5. Documentation

The numbering and symbols of the magnetic groups, references to these groups, and an explicit list of the coset representatives which define each group are given by Litvin (2001) and the deposited supplementary monograph *Magnetic Space Group Types*. Both the paper and the monograph are available at http://journals.iucr.org/ or from the author at http://www.bk.psu.edu/faculty/litvin/Download. html.

6. Availability

The 1502 general position diagrams on CD can be obtained gratis by e-mailing the correspondence author. The diagrams may also be downloaded from http://www.bk.psu.edu/faculty/litvin/Download. html.

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