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Journal of Applied Crystallography
ISSN 0021-8898
Editor: Gernot Kostorz
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# computer program abstracts

Journal of
Applied
Crystallography

ISSN 0021-8898

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This category provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing ones. Submissions should follow the standard format given in *J. Appl. Cryst.* (1985). **18**, 189–190, also available from **Crystallography Journals Online** at http://journals.iucr.org/j/services/authorservices.html.

# VRML general position diagrams of the magnetic subperiodic groups

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Received 18 November 2003 Accepted 16 December 2003

**Keywords:** subperiodic groups; frieze groups; rod groups; layer groups; general position diagrams; VRML; three-dimensional visualization

## 1. The crystallographic problem

The standard representation of the general position diagrams of the non-magnetic subperiodic groups, *i.e.* frieze, rod and layer groups, are two-dimensional (*International Tables for Crystallography*, 2002, and references therein). For rod and layer groups these are two-dimensional projections of three-dimensional diagrams. With this program, we have developed three-dimensional general position diagrams of all magnetic subperiodic groups, which includes all non-magnetic 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 diagrams for the non-magnetic layer groups (Tshudy & Litvin, 1998), the three-dimensional diagrams were developed using a commercial product (*AutoCAD2002* by Autodesk), with a second commercial product (*Vrmlout* for *AutoCAD* by Xanadu s.r.o.) 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.par-allelgraphics.com/products/cortona/), or a VRML stand-alone viewer, such as *VRMLview* (http://www.sim.no/products/VRMLview/). The NIST Web site http://cic.nist.gov/vrml/vbdetect.html lists many plugins, applets and programs to view VRML files on Windows, Linux and Mac operating systems.

The diagrams are stored on a 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 162 files containing 953 magnetic subperiodic group diagrams use 119 Mbyte of storage space.

#### 5. Documentation

Two pdf files, based on the work of Litvin (1999), are included: *Magnetic Subperiodic Group Numbering* lists the numbering used for the magnetic subperiodic groups and *Guide to Magnetic Subperiodic Groups* gives a general introduction to magnetic subperiodic groups.

# 6. Availability

Zipped VRML diagram files (21.7 Mbyte) and documentation (0.26 Mbyte) can be downloaded from http://www.bk.psu.edu/faculty/litvin/Download.html. Alternatively, the diagram and documentation files, on CD, can be obtained gratis by e-mailing the correspondence author.

This work was supported by the National Science Foundation through grant No. DMR-0074550.

#### References

International Tables for Crystallography (2002). Vol. E, Subperiodic Groups, edited by V. Kopsky & D. B. Litvin. Dordrecht: Kluwer Academic Publishers.

Litvin, D. B. (1999). Acta Cryst. A55, 963–964.Tshudy, D. K. & Litvin, D. B. (1998). J. Appl. Cryst. 31, 973.