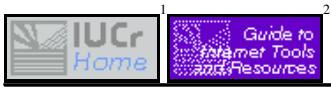

VRML – Virtual Reality Modeling Language

VRML is to 3D graphics what HTML is to text: it is a common format that can be displayed on any computer using a standard WWW browser (for instance Netscape 3.0[3] or Explorer 3.0[4] equipped with a viewer like Live3D[5], the SGI Cosmo Player[6] or the Microsoft VRML Add–In[7]...).

It allows the user to click on links to other objects (hypertext mark–up). As a trivial example, the following file displays two spheres in 3D, with the address of another VRML object (bcc.wrl[8]) anchored to the first sphere.

```
#VRML V1.0 ascii
WWWAnchor{name "http://www.ill.fr/dif/vrml/bcc.wrl" Sphere{}}
Translation {translation 1 1 1 } Sphere {}
```

Complex 3D crystal structures can be described in VRML, including space filling, ball–and–stick, co–ordination polyhedra *etc*.. They can be explored from the inside with full interactivity. The translation of three dimensional crystallographic objects into VRML is facilitated by way of converters able to change a conventional set of coordinates into a standard .wrl file. There is no need to speak VRML like a specialist.

VRML Authoring for Crystallographers: The tool market is growing with either downloadable converters such as pdb2vrml[9], xtal–3d[10], CRYSTAL[11], MOLDA[12] and STRUVIR[13] or online builders (send your data and receive the corresponding .wrl file in return) such as Builder 1.2[14] for membranes, PDB to VRML[15], the Crystal Packing Visualization by VRML[16] system, the Chemical VRML Generation Service[17] and xtal–3d[18] which is able to access to the Inorganic Crystal Structure Database.[19]

Example VRML Files: A non–exhaustive list includes Chemical Examples[20], 3D Scenarios of Biomolecules[21], Silicates[22] (aluminosilicates and zeolites announced), the ILL's Gallery[23], an Introduction to Crystal Structures[24], the JICST Crystal Structure Database[25], 6–connected 3D nets[26], the IUMSC Database[27], Biological Macromolecules[28], ... Some of them were built using the above converters.

General Documentation: It is recommended to read the FAQ[29], to visit the VRML repository[30]

1 http://www.iucr.ac.uk/iucr–top/welcome.html
2 int.index.html
3 http://home.netscape.com/comprod/mirror/client_download.html
4 http://www.microsoft.com/ie/ie.htm
5 http://home.netscape.com/eng/live3d/
6 http://vrml.sgi.com/cosmoplayer/download.html
7 http://www.microsoft.com/ie/ie3/vrml.htm
8 http://www.ill.fr/dif/vrml/bcc.wrl
9 http://ws05.pc.chemie.th–darmstadt.de/vrml/pdb2vrml.html
10 http://www.ill.fr/dif/3D_crystals.html
11 http://tutor.oc.chemie.th–darmstadt.de/Poly/VRML/crystal.html
12 http://cssj.chem.sci.hiroshima–u.ac.jp/molda/molda.htm
13 http://fluo.univ–lemans.fr:8001/vrml/struvir.html
14 http://bellatrix.pcl.ox.ac.uk/people/alan/WebSpace/builder/form.html
15 http://ws05.pc.chemie.th–darmstadt.de/vrml/urlvis.html
16 http://laue.biochem.ubc.ca:8080/cgi–bin/ssis/banff/xpack.html
17 http://schiele.organik.uni–erlangen.de/services/vrml.html
18 http://www.ill.fr/dif/xtal–3d.html
19 http://www.ill.fr/dif/icsd/welcome.html
20 http://www.ch.ic.ac.uk/VRML/
21 http://ws05.pc.chemie.th–darmstadt.de/vrml/
22 http://tutor.oc.chemie.th–darmstadt.de/Poly/VRML/silicat_e.html
23 http://193.49.43.3/dif/3D_crystals.html
24 http://mama.minmet.uq.oz.au/~darcy/vrml/index.html
25 http://fact.jicst.go.jp/cr–vrml.html
26 http://fluo.univ–lemans.fr:8001/vrml/6c3d/6c3dnets.html
27 http://www.iumsc.indiana.edu/database/iumsclookup.html
28 http://www.imb–jena.de/VRML.html
29 http://vag.vrml.org/VRML_FAQ.html
30 http://www.sdsc.edu/vrml/

and its list of Browsers,[31] to subscribe to the VRML Forum,[32] to respect the VRML versions 1.0[33] and 2.0[34] specifications, to consider the SGI site[35] and the Yahoo[36] selection, to read and post messages to the comp.lang.vrml[37] Newsgroup.

Conclusion: As a general tool for 3D visualization in crystallography VRML was unexpected. The real usefulness of current or future possibilities like 3D mark–up, multi–user connections, links to sound or other media is an open question. Not everything that uses VRML will necessarily be an Internet application. Producers of drawing programs for crystallography should consider at least offering a .wrl output file option to their users. Availability of free PC converters should boost VRML applications in crystallography. Finally, without the possibility to save high quality 2D projections of a selected 3D view and to print them, crystallographers at large might not adopt the baby. At the moment quality depends on your maximum screen resolution.

What is New since IUCr XVII?

- The conference *VRML as a tool for exploring complex structures*[38] given at the IUCr XVII Congress (Seattle, USA, August 8–17, 1996) is online (abstract, full text, transparencies and VRML example files).
- The demo of the latest version of Crystallographica[39] including a VRML export function is available.
- Plot your 3D–diffraction scans at ILL by Surf3d.[40]
- Download the free MSI WebLab[41] Viewer and test its VRML export function.

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[31] http://www.sdsc.edu/vrml/browsers.html
[32] http://vrml.wired.com/
[33] http://vrml.wired.com/vrml.tech/vrml10–3.html
[34] http://vag.vrml.org/VRML2.0/FINAL/
[35] http://webspace.sgi.com/Repository/indexch.html
[36] http://www.yahoo.com/Computers_and_Internet/Internet/World_Wide_Web/Virtual_Reality_Modeling_Language_VRML_/
[37] news:comp.lang.vrml
[38] http://pcb4122.univ–lemans.fr/vrml/seattle/seattle.html
[39] http://www.demon.co.uk/oxcryo/cgraph.html
[40] http://www.ill.fr/dif/surf/welcome.html
[41] http://www.msi.com/weblab/index.html
[42] int.index.html
[43] mailto:hewat@ill.fr
[44] mailto:armel@fluo.univ–lemans.fr
[45] http://fluo.univ–lemans.fr:8001/vrml/intvrml.html