Contents

Chapter 1

Rasmol extensions to ROD

An extension to ROD has been written to display the structure being fitted in the molecular graphics package rasmol[1]. Rasmol allows visualisation of the structure in 3d.

1.1 Quick Start

Rasmol version 2.6 or greater for UNIX is required.

To get started, do the following:

1. Start rasmol in the same directory as rod.

2. Run the following commands in rasmol.

   ROD> *extensions walker activate return*

   ROD> *extensions walker rasmol display*

1.2 Description of extension (ext.wal)

Rasmol version 2.6 or later for UNIX is required. I'm told that it doesn't work on windows.

1.3 ext.wal

1.3.1 ext.wal.set

ext.wal.set.rasmol

host The machine rasmol is run on. *port* The port rasmol is listening on - 21069 by default. *filename* The filename of the temporary xyz structure file.

ext.wal.set.xyz

xrepeats The number of unit cells in x direction. *yrepeats* The number of unit cells in y direction.

1.3.2 ext.wal.rasmol

display - send structure to rasmol *command* - send a command directly to rasmol

1.4 Details of implementation

Rod saves the structure to a temporary xyz file (defined by the ext.wal.set.rasmol.filename), and then communicates with rasmol using BSD style sockets. Usually, rasmol would be run on the same machine as ROD, and *host* would therefore be set to localhost. It is possible however for rod and rasmol to run on different machines. At present it is necessary rod and rasmol share a filesystem to store the structure file.

The ext.wal.rasmol.command option makes it possible to send a rasmol command from within rod. For example it would be possible to change atom colour from within rod.

1.5 Further work

It is only possible for one rasmol process to listen on the standard port. If someone else gets there first, then you will have to work out how to get rasmol to listen on a different port so rod can talk to it.

Ideally it would not be necessary to save the structure to a temporary file, but just pass the structure down the socket connection. This would make running rod on one machine, and rasmol on another much simpler. It is currently not possible to do this with rasmol.

Bibliography

[1] Roger Sayle and E. James Milner-White. Rasmol: Biomolecular graphics for all. *Trends in Biochemical Sciences (TIBS)*, 20(9):374, September 1995.