

# Graphics Programs that will read SHELX or CIF files

J. Reibenspies,  
N. Bhuvanesh

ver 1.0.0

Free software.

Gretep : Reads SHELX files and CIF files and outputs thermal ellipsoid plots.

<http://www.bio.net/bionet/mm/xtal-log/2000-September/004413.html>

Note : You can generate a sphere of enclosure that includes all molecules or atoms within a stated radius of a central point.

Balls and Sticks. Reads SHELX files and outputs POLYHEDRAL plots

<http://www.softbug.com/toycrate/bs/index.html>

Mercury : CCDC suite :

[http://www.ccdc.cam.ac.uk/products/csd\\_system/mercury/](http://www.ccdc.cam.ac.uk/products/csd_system/mercury/)

Features, Ellipsoids, Simulated powder patterns, unit cells, gradient backgrounds, labels

Rasmol

Disadvantage : will not read shelx files or output thermal ellipsoid plots.

<http://www.umass.edu/microbio/rasmol/>

ORTEP-3

<http://www.chem.gla.ac.uk/~louis/software/ortep3/>

Note : Need to register with Louis J. Farrugia

<http://www.chem.gla.ac.uk/~louis/software/licenseform.html>

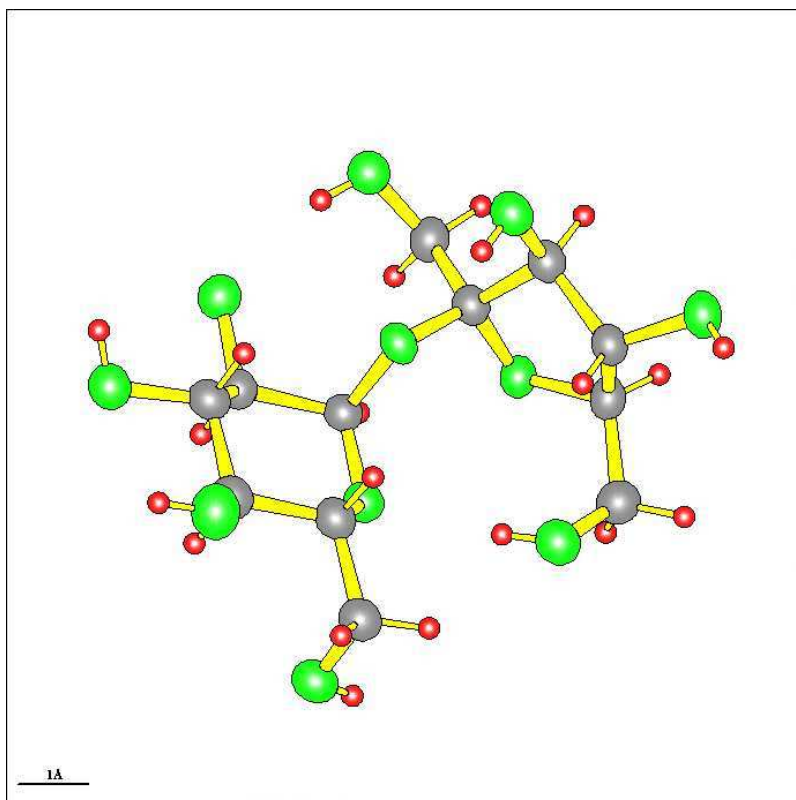
### **Commercial Software**

Diamond

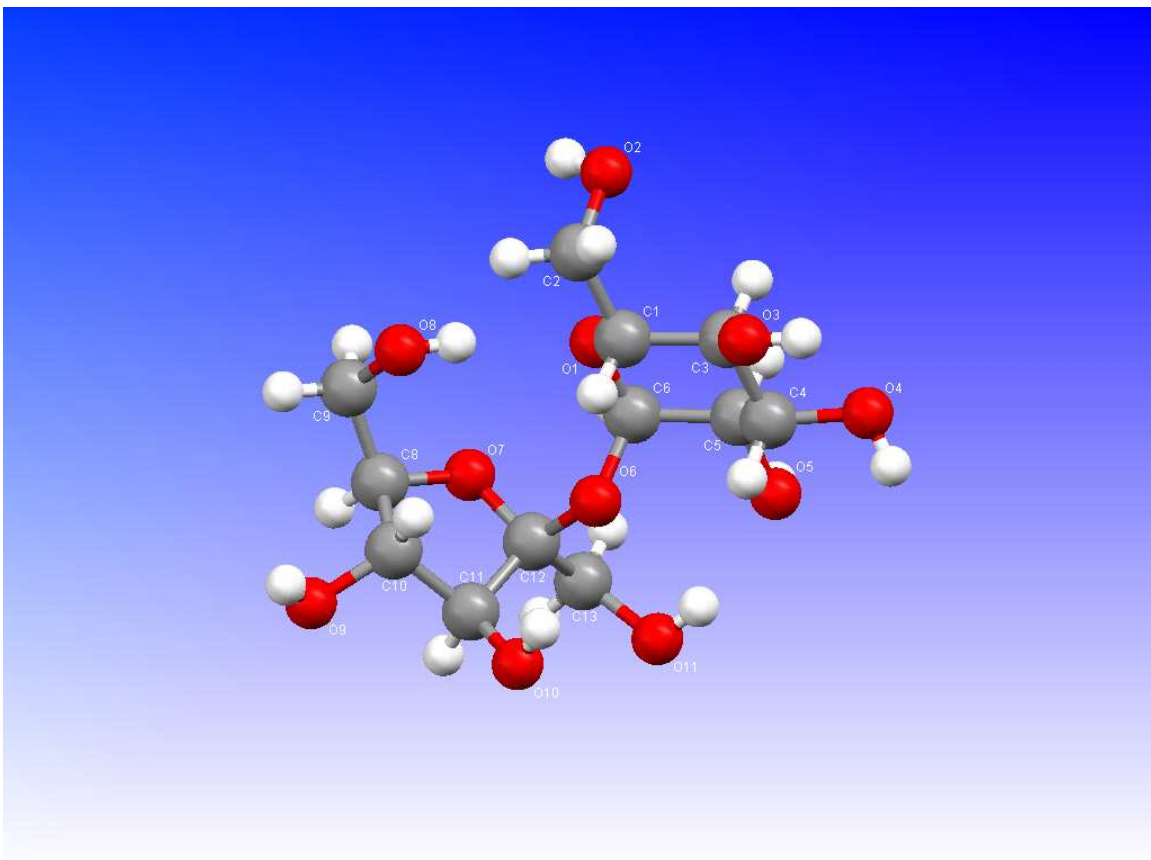
<http://www.crystalimpact.com/diamond/>

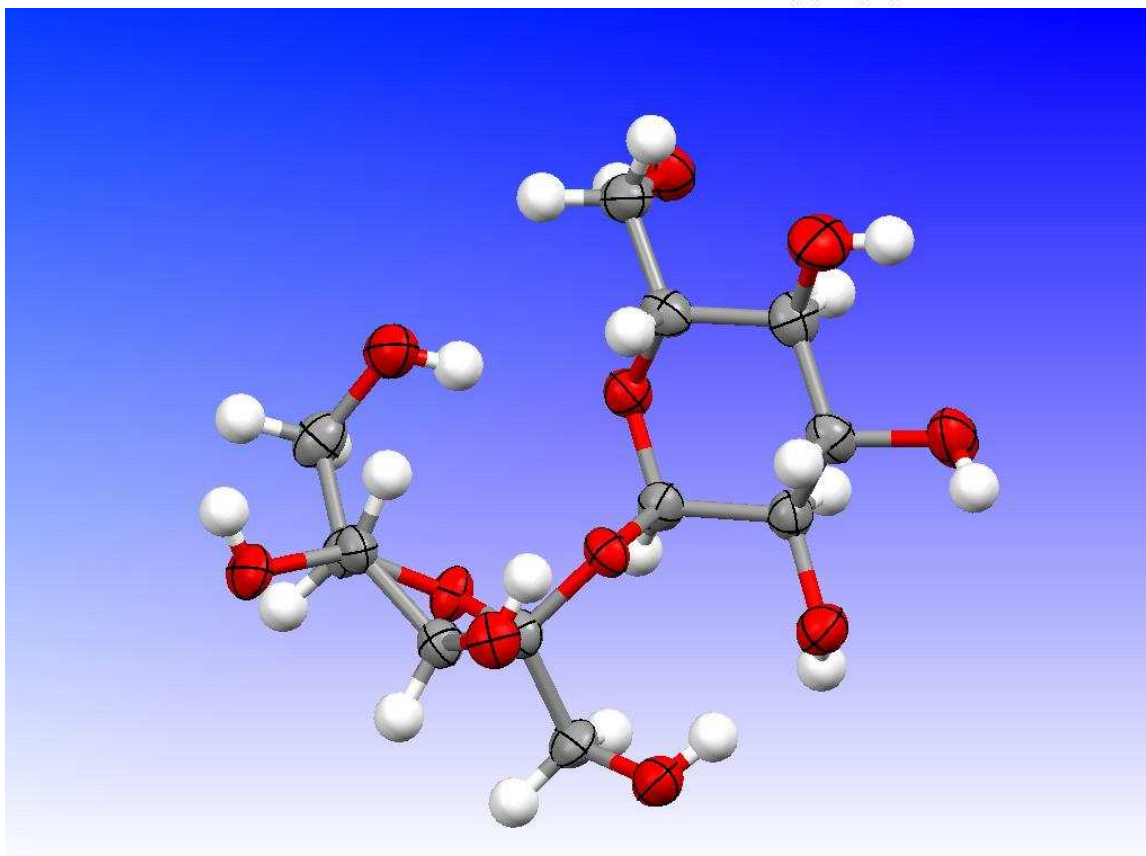
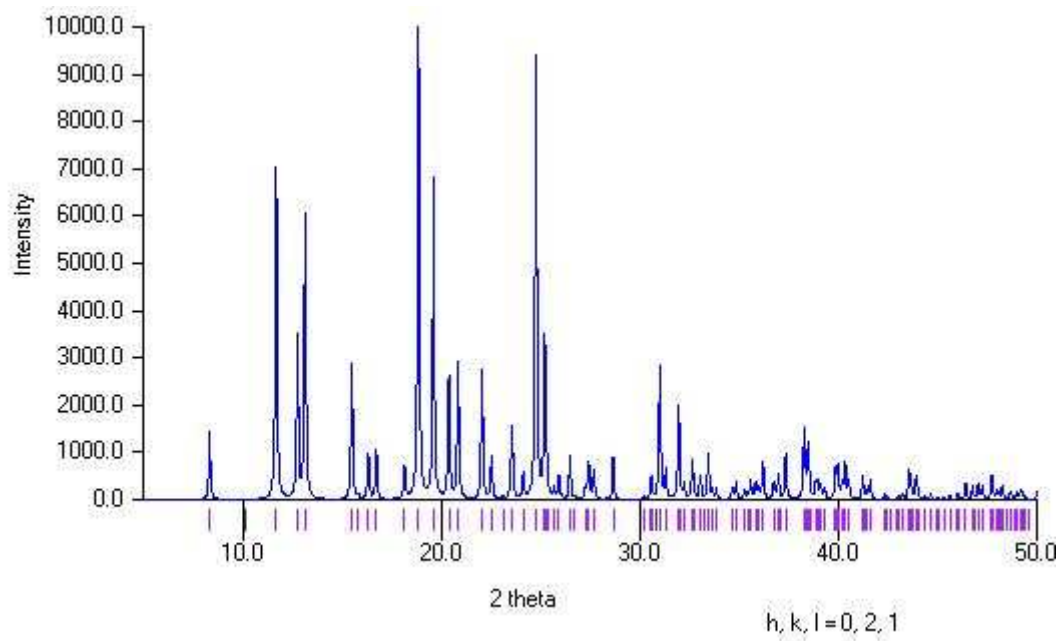
Examples

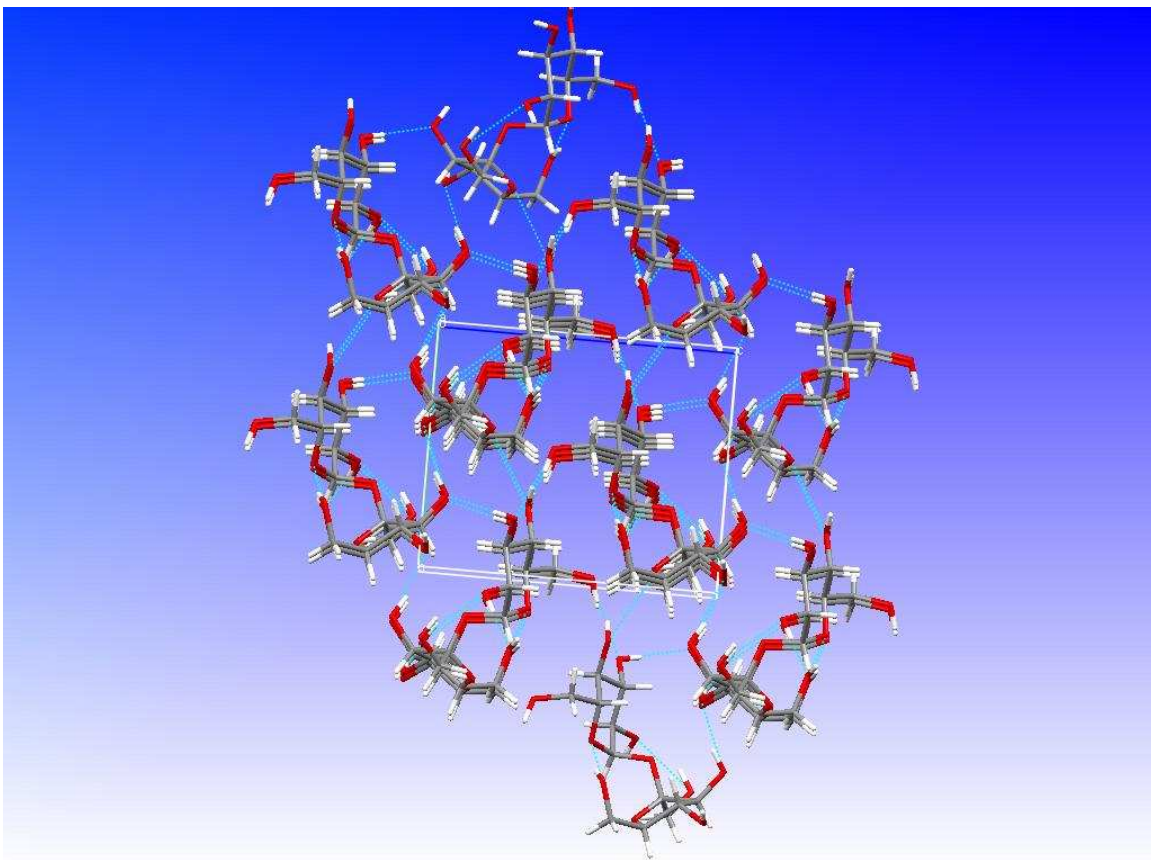
Gretep



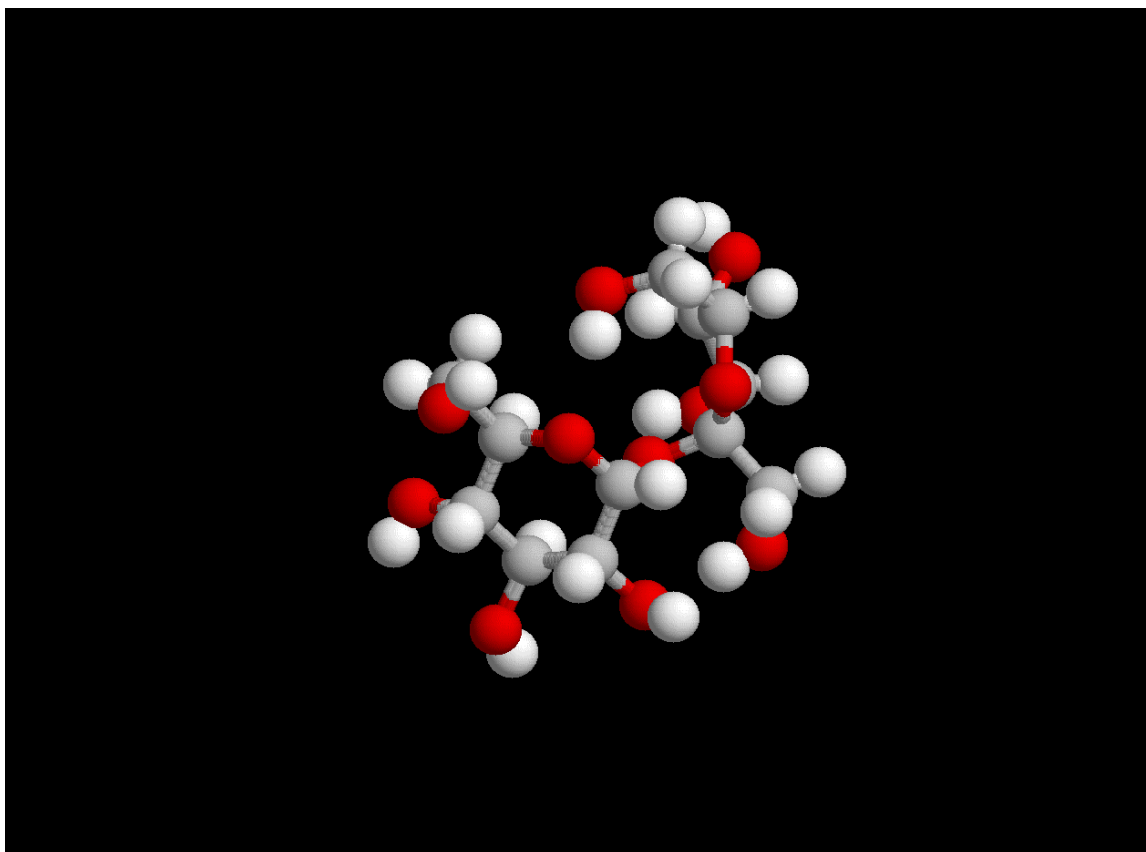
**Mercury**



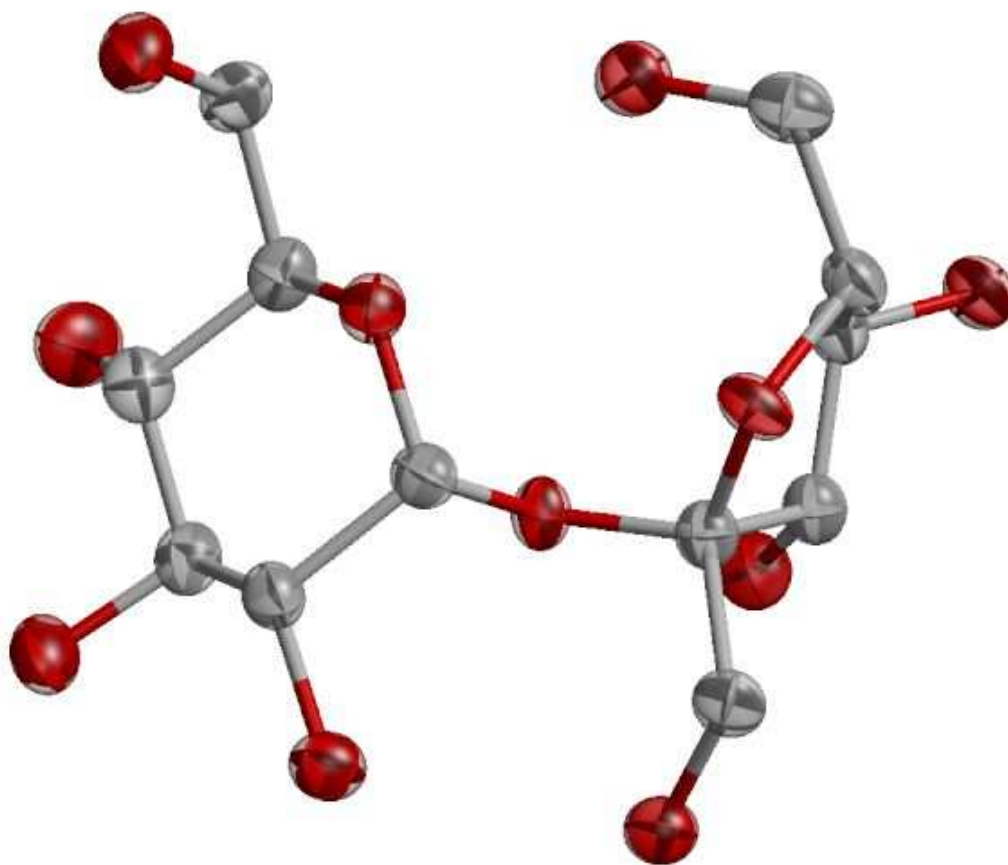




## RASMOL

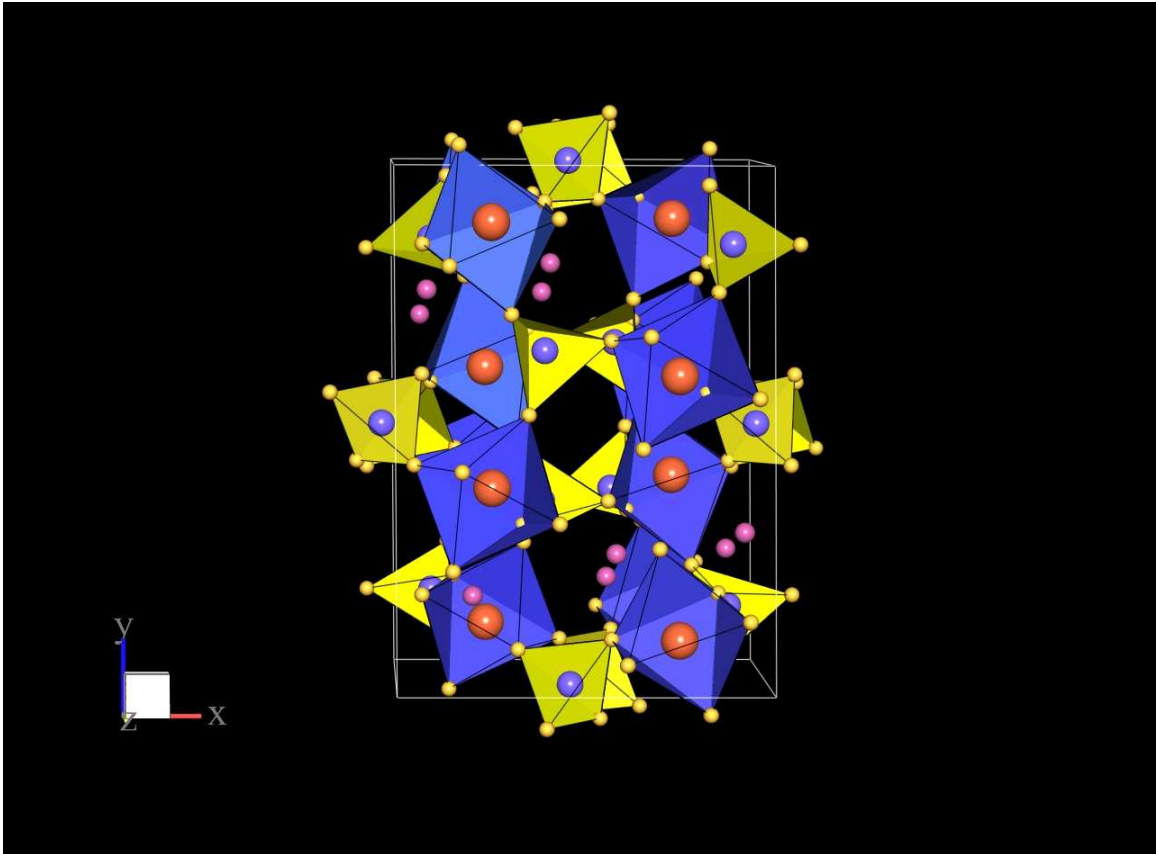


Ortep-3





## Balls and Sticks example



## Diamond 2.0

