

Graphics Programs that will read SHELX or CIF files

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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/

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

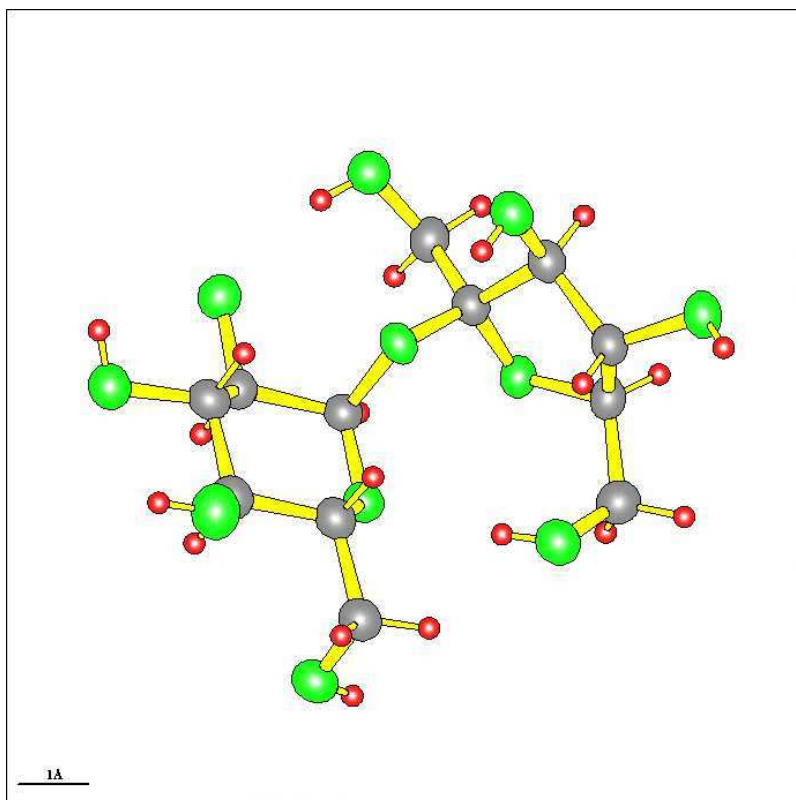
Rasmol

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

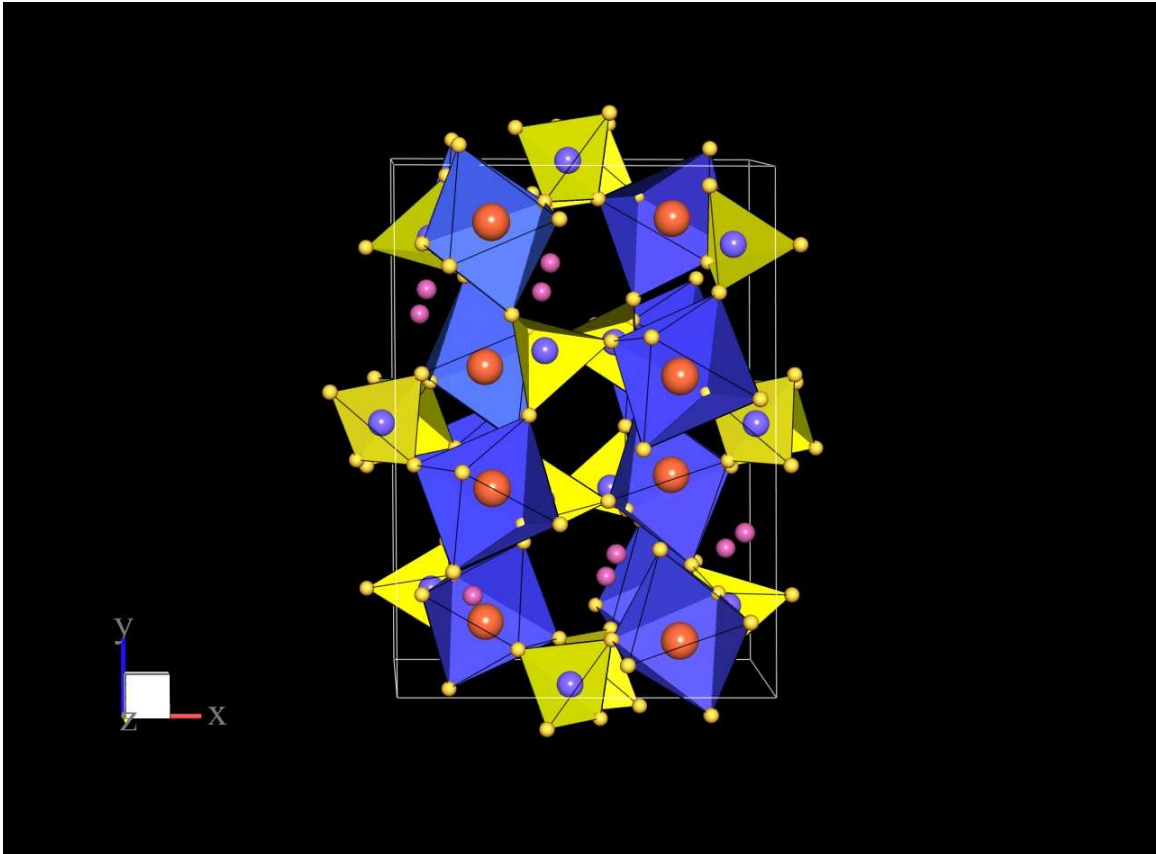
<http://www.umass.edu/microbio/rasmol/>

Examples

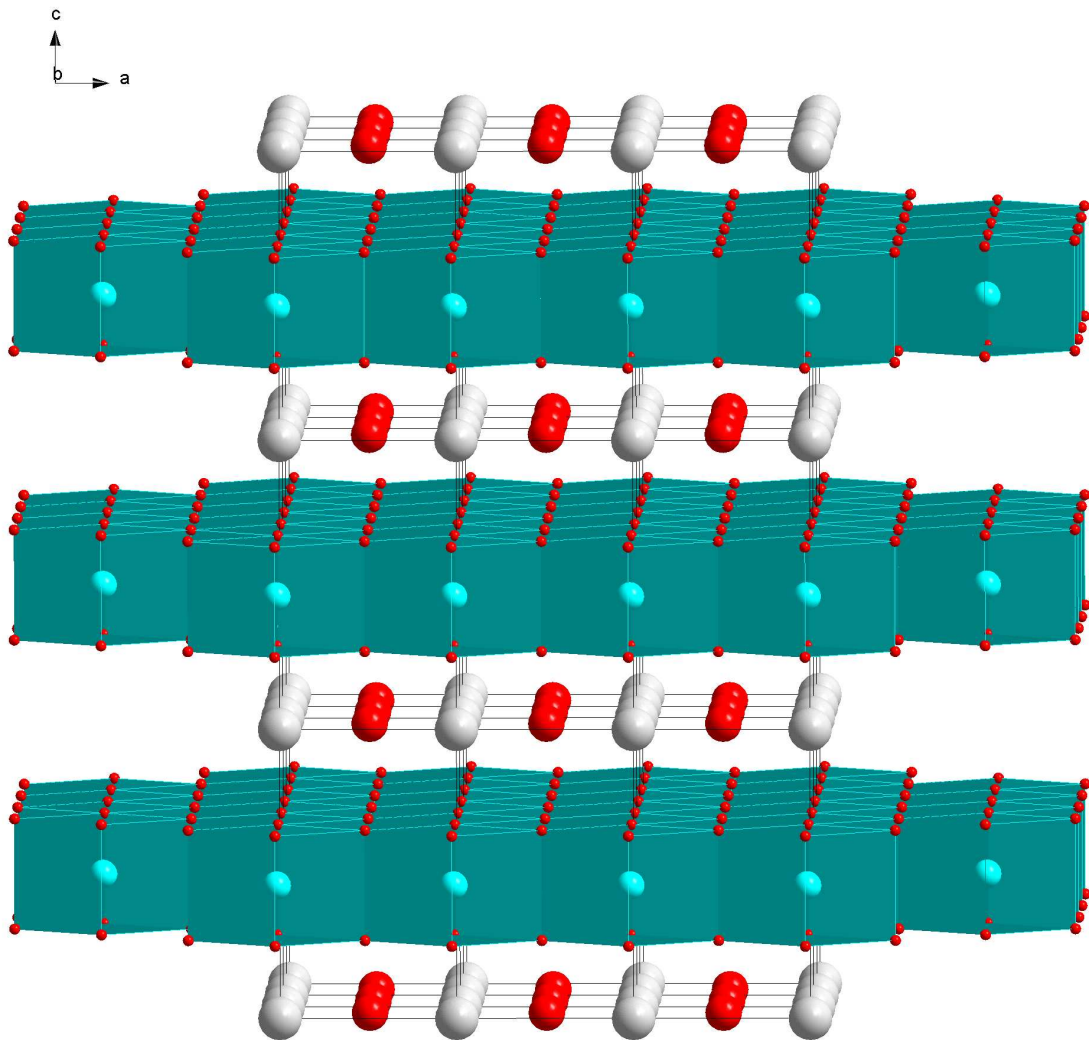
Gretep

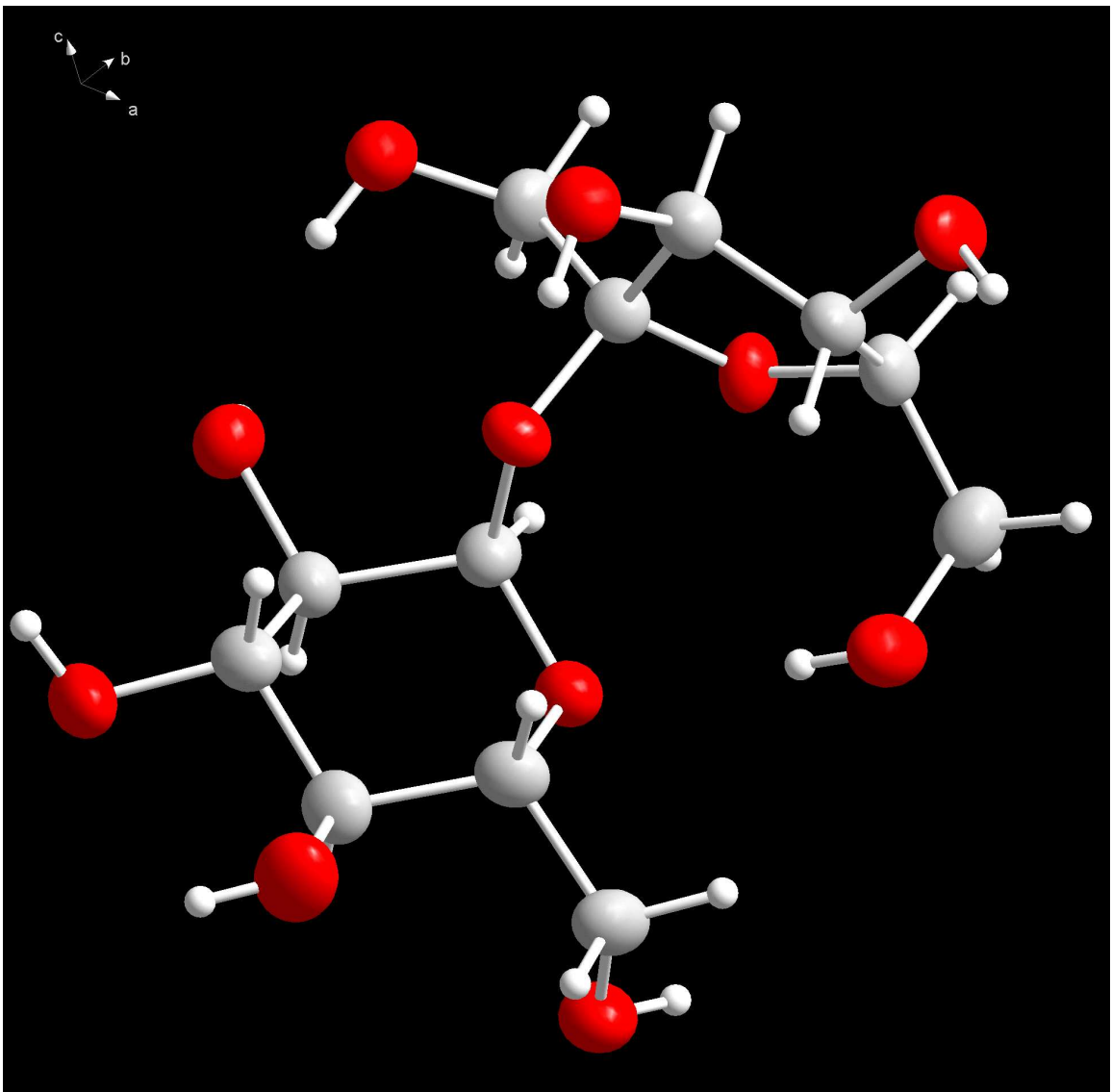


Balls and Sticks example

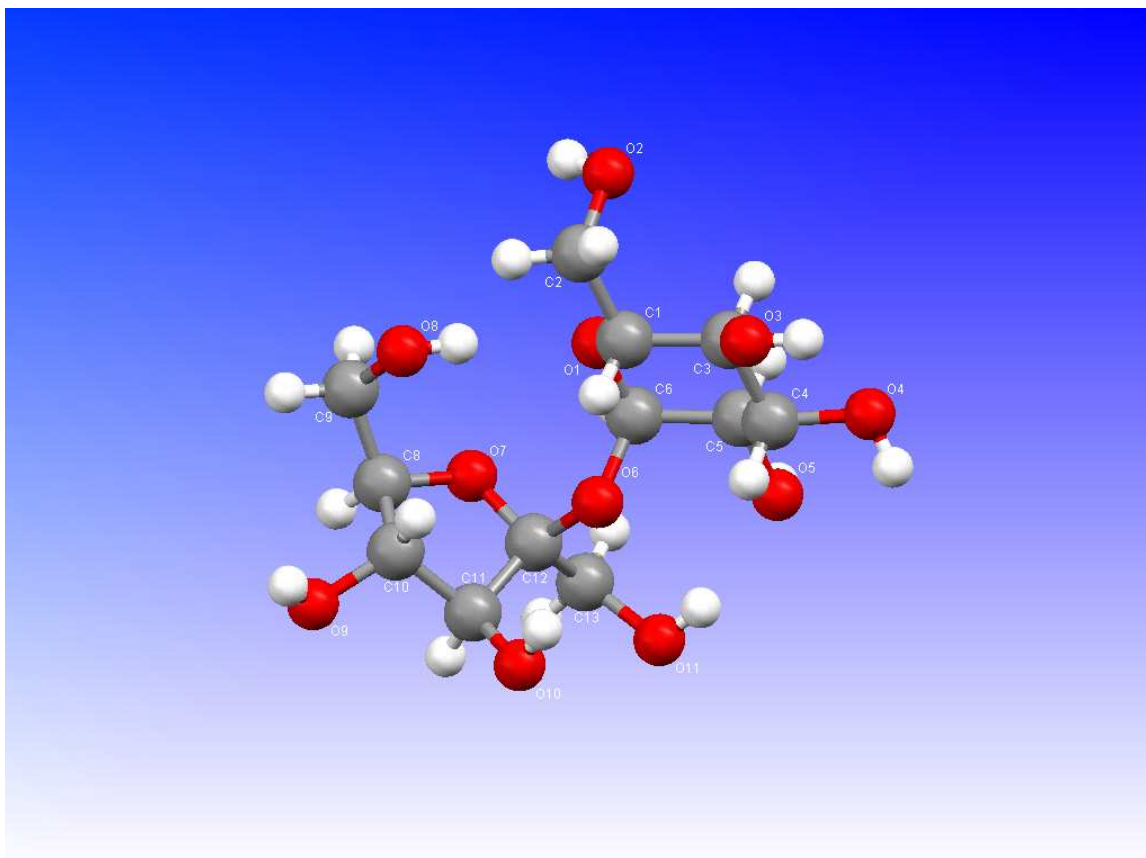


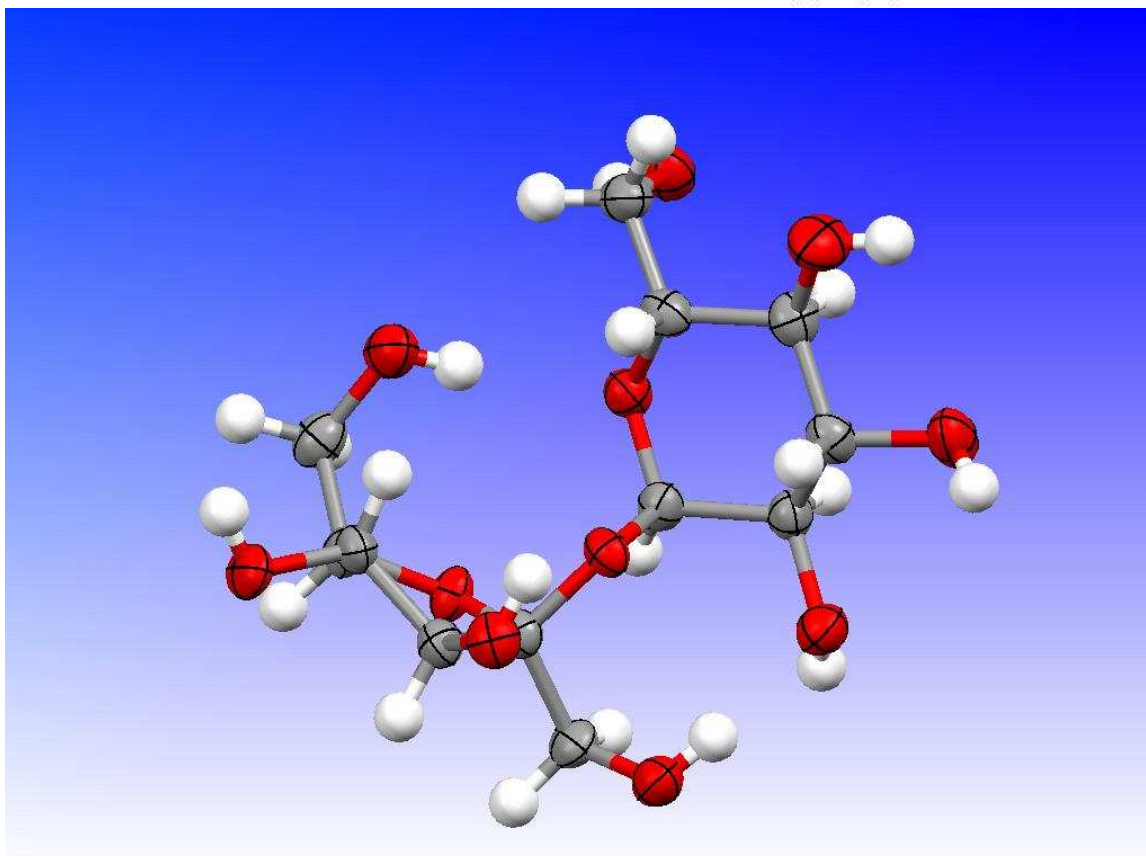
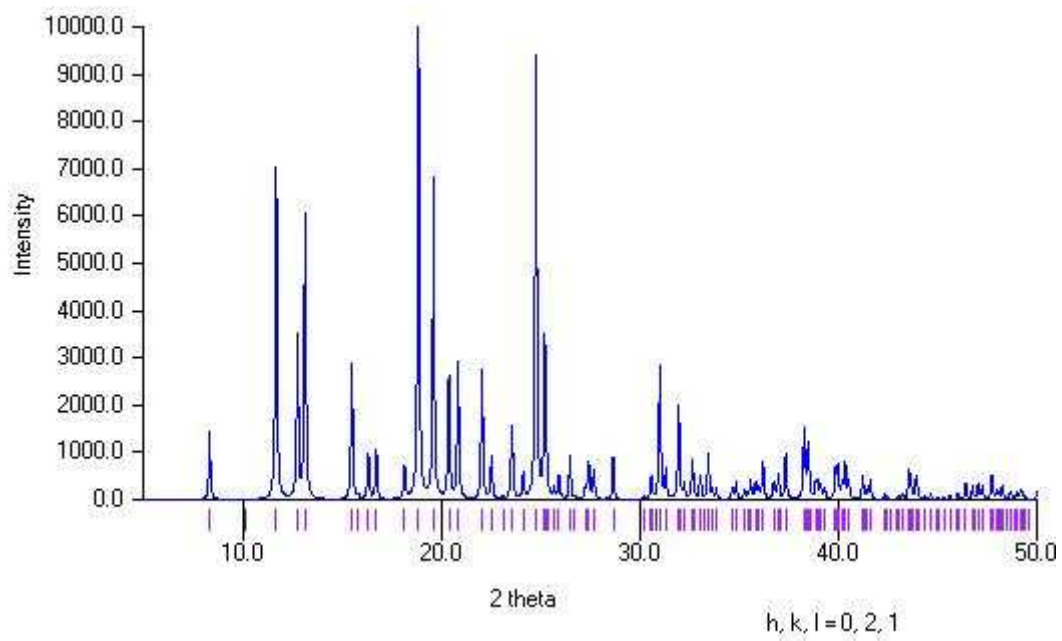
Diamond 2.0

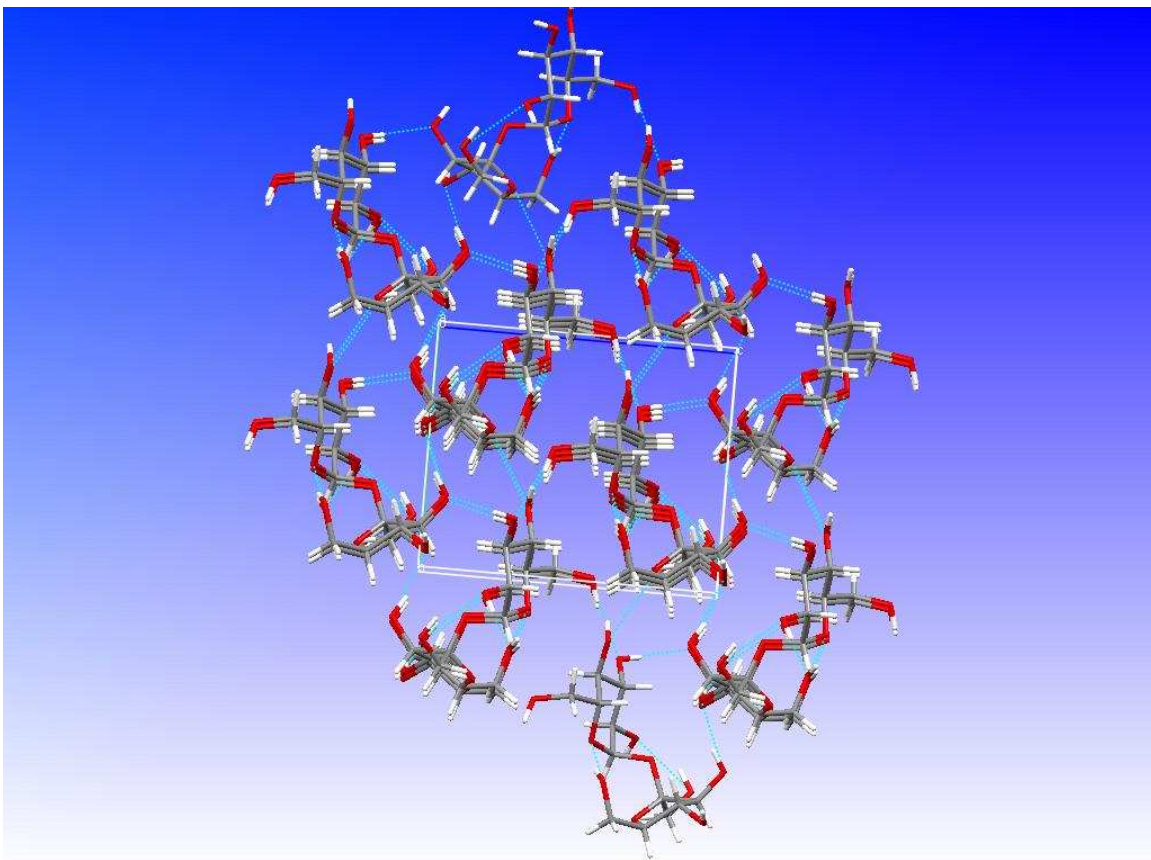




Mercury







RASMOL

