Subject: Re: Converting COD2020 to SDF
Posted by nbehrnd on Thu, 28 Jan 2021 14:36:13 GMT
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In case only a few structures are needed, and you are comfortable with the terminal / CLI you might consider the following:

Each COD dataset has its COD ID, a number which may be seen in DataWarrior and which may be used to
access the dataset e.g. on COD's text-based form
https://www.crystallography.net/cod/search.html.

The entry «cif» on COD's listed results directs you to the structure's model data set, which you may store on your computer. Among the cod-tools (https://wiki.crystallography.net/cod-tools/) which you may obtain as an archive, or as a bundle package (e.g., Linux Debian, or Ubuntu) is the tool codcif2sdf for the CLI / terminal, which offers the conversion of COD's .cif into the .sdf file. To run successfully, you need OpenBabel which equally is freely available.

The output may be redirected into a permanent record, e.g. calling

codcif2sdf 1505213.cif > example.sdf

Both a COD cif as well its conversion into the .sdf of a typical entry are attached below.

In the past, the conversion a COD .cif into a .sdf only with OpenBabel often was not as good as with codcif2sdf. Alternatively, use a visual program capable to read and write both file formats (e.g., Jmol, or CCDC's Mercury)

Norwid

File Attachments

1) 1505213.cif, downloaded 815 times
2) example.sdf, downloaded 812 times