Subject: Re: Converting COD2020 to SDF
Posted by nbehrnd on Thu, 28 Jan 2021 21:56:31 GMT
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Possibly codcif2sdf is part of the tools used for at least two reasons: Using only Openbabel (including release 3.1.0) would not retain the bibliographic information in the .sdf written which show up in DW's display.

An other reason is sometimes both crystallographic motif as well as symmetry of the unit cell are needed to complete the molecule's appearance as one would draw it in a notebook. By choice of the unit cell this may look like the molecule were broken. And it is the reconstruction of intramolecular atom connectivity where OpenBabel may more frequently encounter problems, than codcif2sdf. As an illustration, I attach both COD's .cif about a simple triazine, as well as the rewritten form as .sdf, once by OpenBabel, once by codcif2sdf.

Once the individual entries are rewritten for the organic chemist's eye, they may be stacked into a .sdf of multiple models and read as-such by DataWarrior. Possibly Thomas or/and the maintainer's of COD developed some template scripts to automate the whole process including formatting, and checks for plausibility and consistency. Given the scope and coverage of COD and TCOD often complementary to the ones e.g., by CCDC and ICSD, additional mirrors most likely are welcomed enthusiastically.

Norwid

TCOD, the sibling of COD mentioned: https://www.crystallography.net/tcod/

File Attachments

1) 7050214.cif, downloaded 423 times
2) triazene_obabel.sdf, downloaded 424 times
3) triazene_cod.sdf, downloaded 423 times