Subject: C=C double bonds/search by extended stereochemistry
Posted by nbehrnd on Tue, 30 Nov 2021 16:11:02 GMT
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Hello Thomas,

my understanding of DataWarrior's manual is that the program internally stores the molecules in a format capable to discern and (if selecting .sdf v3000) export of double bonds including those without explicit assignment of (E)/(Z) configuration. As anticipated, the SMILES strings

C/C=C/C
C/C=C\C
CC=CC

yield three different representations of but-2-ene.

For a small test set (cf. double_bond.dwar and the screen photos in the .zip archive attached), I aimed to use the features of extended stereochemisty as a criterion to retain a sub set (Chemisty -> From Chemical Structure -> Add Substructure Count), including the unassigned double bond visualized as a crossed double bond. So far, the attempts failed.

As anticipated, the search pattern of (cis)-butene, retained both (cis)-butene and cyclohexene and withdrew the oxime. However -- contrasting to anticipation -- (trans)-butene and the unassigned butene equally were retained. Does the search for, e.g. crossed double bonds, require a particular instruction?

Version info: DataWarrior 5.5.0 for Linux in Debian 12/bookworm (branch testing), including the update as «development version» as fetched on Sunday, 2021-11-28.

Norwid

File Attachments

1) double_bonds.dwar, downloaded 657 times
2) double_bond_documentation.zip, downloaded 633 times