Subject: Faulty SDF import
Posted by richards99 on Mon, 19 Oct 2020 09:30:37 GMT
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Hi,
There are still issues with regards the import of SDF files and its interpretation of the bonding.
This time it is not down to specified aromatic bonds but simply kekulised bonds.

Take for instance this SMILES string of a protonated heterocycle.
CNC1=C2C=C3OCCOC3=CC2=[NH+]C=C1

When this is saved as an SDF file using Marvin for instance, and then imported into DataWarrior the bonding is completely wrong.
I have attached the SDF of this smiles string above.

The output it provides is attached

File Attachments

1) Screenshot 2020-10-19 at 10.28.58.png, downloaded 573 times
2) untitled_molecule_file.sdf, downloaded 336 times