Subject: Re: Faulty SDF import
Posted by thomas on Fri, 23 Oct 2020 08:13:40 GMT
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Dear All,

there has been a bug in OpenChemLib regarding open valences of charge atoms in certain situations, which seems to have caused the issue. DataWarrior stores structures in a canonical representation. Therefore, it needs to resolve delocalized bonds into alternating single/double bonds when displaying. Because of the valence bug the charged nitrogen was not seen as having the needed open valence. The bug was fixed Sep. 30 in OpenChemLib, but took till yesterday to materialize in a DataWarrior build.

Thank you all for reporting.

Thomas