Subject: 3D coordinates of hydrogen atom lost for structures containing positive charged nitrogen
Posted by zhentg on Mon, 23 Mar 2020 10:47:04 GMT
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Dear developers,

When I load SDF with 3D coordinates, I found if a structure contains positively charged nitrogen, then its hydrogen atom will disppear in DataWarrior. Furthermore, if the structure is exported to a new SDF file, the hydrogen atoms are still missing.

Could you help to check this?

Attached is the original SDF, a DataWarrior file created from the SDF, and a snapshot to highlight the issue.

Thanks!

File Attachments
1) , downloaded 582 times
2) 3dLostH_3D.sdf, downloaded 360 times
3) 3dLostH_3D.dwar, downloaded 366 times

Subject: Re: 3D coordinates of hydrogen atom lost for structures containing positive charged nitrogen
Posted by thomas on Tue, 24 Mar 2020 16:09:39 GMT
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thank you for sending the detailled description and the sample files. The problem is caused by a (probably) wrong interpretation of a field in the molfile part of your SD-file, that is meant to store (unusual) atom valences,
but is typically not used for atoms with usual valences. For charged atoms RDKit populates this value and DataWarrior
used to interpret this in a conflicting way causing wrong implicit hydrogen counts.
The issue is fixed now and you may download replacements files from
openmolecules.org/datawarrior/dw521x.zip (Linux or Mac) and
openmolecules.org/datawarrior/dw521win.zip (for Windows).

Thomas

Subject: Re: 3D coordinates of hydrogen atom lost for structures containing positive charged nitrogen
Posted by zhentg on Wed, 25 Mar 2020 08:50:30 GMT
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Thanks a lot, Thomas.
Just tested the new DataWarrior.exe, and the bug is fiexed.
With that, I can visualize 3D conformations better in DataWarrior.