
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

[View Forum Message](#) <> [Reply to Message](#)

Dear developers,

When I load SDF with 3D coordinates, I found if a structure contains positively charged nitrogen, then its hydrogen atom will disappear 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) [3dLostH_3D.dwar](#), downloaded 708 times
 - 2) [3dLostH_3D.sdf](#), downloaded 425 times
 - 3) [3dLostH_3D.dwar](#), downloaded 424 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

[View Forum Message](#) <> [Reply to Message](#)

thank you for sending the detailed 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

[View Forum Message](#) <> [Reply to Message](#)

Thanks a lot, Thomas.

Just tested the new DataWarrior.exe, and the bug is fixed.

With that, I can visualize 3D conformations better in DataWarrior.
