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 983 times
2) 3dLostH_3D.sdf, downloaded 602 times
3) 3dLostH_3D.dwar, downloaded 593 times