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