Subject: Molecule Displayed Incorrectly
Posted by sbembenek18 on Thu, 18 Jun 2020 20:48:49 GMT
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I've noticed in certain cases, DW will not correctly display the molecule. This appears to happen for 'non conventional' protomers mostly but not always. I've included an example. The attached molecule should appear as in the image. However, if you load the SDF in DW, you see that it does not appear this way.

File Attachments
1) mol.png, downloaded 365 times
2) mol_dw_error.sdf, downloaded 372 times

Subject: Re: Molecule Displayed Incorrectly
Posted by thomas on Sun, 21 Jun 2020 12:11:37 GMT
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Thank you for reporting this issue. There was indeed a bug in the charge neutralization part of the structure normalization, which takes place when importing structures from SD-Files or SMILES. This is fixed in the current development update. However, still DataWarrior doesn't show the structure as in mol.png, because DataWarrior normalizes and canonicalizes structures during the import. Part of the normalization is to neutralize charges as much as possible, meaning to move protons from protonated and positively charged atoms (e.g. ammonium) to negatively charged hetero atoms where possible.

Subject: Re: Molecule Displayed Incorrectly
Posted by sbembenek18 on Fri, 03 Jul 2020 21:26:14 GMT
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thanks. I appreciate why it is doing it. it could be useful to allow the user to change this default behavior so that DW displays the molecule "as is"