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.