Subject: Re: Bug in how stereochemistry is reported
Posted by thomas on Thu, 27 Jul 2023 17:45:01 GMT
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Dear Tom,

molfiles V3000 don't use a 'chiral' flag. If you open your molfile in DataWarrior, you will notice that it shows an absolute stereo center. Of course, DataWarrior uses the correct Y-direction for molfiles, which is indeed inverted in comparison to most other xy-orientations. CFG=3 is a down bond and coordinates are correctly created leading to an R-isomer. ChemDraw does the same. I am afraid that ChemDoodle created the wrong CFG entry here.

Best wishes,

Thomas