Subject: Re: Export of Chiral compounds
Posted by thomas on Fri, 02 Oct 2020 09:00:21 GMT
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DataWarrior and OpenChemLib don't use the 'either' bond, but uses the 'chiral flag' to specify whether the molecule is racemic or not. For molecules with one racemic stereo center DataWarrior writes a V2000 molfile with up or down bond (1 or 6) and chiral flag = 0, which makes it a racemic molecule. If you have multiple racemic stereo centers all in the same group, that is with given relative configuration, then up/down bonds are necessary to not loose the relative stereo information. Still the chiral flag defines, whether we have a racemate or a pure diastereomer. If multiple racemic stereocenters are in independent groups, then the molfile V2000 cannot represent this anymore. I can only suggest using V3000 when you need to export and only use software that supports MDL's concept of 'enhanced stereo representation'. In this context SMILES are even worse, because they cannot even distinguish relative from absolute stereo centers, i.e. racemates from pure diastereomers.

The molfile bond stereo value 4 seems to leave room for interpretation and does not necessarily mean racemic. The MDL ctfiles specification says for the bond stereo field:
"Single bonds: 4 = Either, Double bonds: 3 = Cis or trans (either) double bond"
From this I conclude that 4 for single bonds may means (or at least may mean) up or down.

Hope this explains it,

Thomas