Subject: Re: Bug in how stereochemistry is reported
Posted by thomas on Fri, 12 Mar 2021 14:34:22 GMT
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I just updated the dev version such that when loading an sd-file, then it interprets the content:
If all entries are V2000 and if zero entries have the chiral flag set and if some entries have stereo centers,
then the user is asked, whether entries with stereo centers shall be interpreted as pure enantiomers.
The macro task 'Open File' also got an option to assume the chiral flag to be set for such cases.