Subject: Re: Canonical codes do not distinguish stereoisomers
Posted by thomas on Thu, 04 Sep 2025 09:20:14 GMT
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I agree that this is disturbing at the first glance. However, here we have a situation, were the set of tautomers contain multiple stereo isomers. The canonical code of your different stereo isomers correctly differs for your different stereo isomers if it shall also distinguish tautomers. However, if you ask for different tautomers to create the same code, then this is what you get. The upper part of the image shows three tautomers of a part of your structure where from left to right a stereo center inverts its configuration, but all three structures are just different tautomers of the same thing. The bottom part of the image shows the same situation for the other stereo center.

File Attachments

1) tautomers.jpeg, downloaded 999 times

