Subject: Re: Incomplete SMILES related to double bonds
Posted by Christoph on Sun, 04 Jun 2017 11:39:28 GMT
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Hi Thomas,

Thank you very much for your answer and looking into this issue.

Saving the structures in DataWarrior in the SDF-format (2D) does preserve the stereocenters, is this correct? Then a workaround in the meantime until DataWarrior is updated would be to save the compounds as SDF-File and then convert it with obabel to obtain isomeric SMILES.

Best wishes,
Christoph