Subject: Axial chirality
Posted by zhentg on Wed, 09 Sep 2020 00:46:29 GMT
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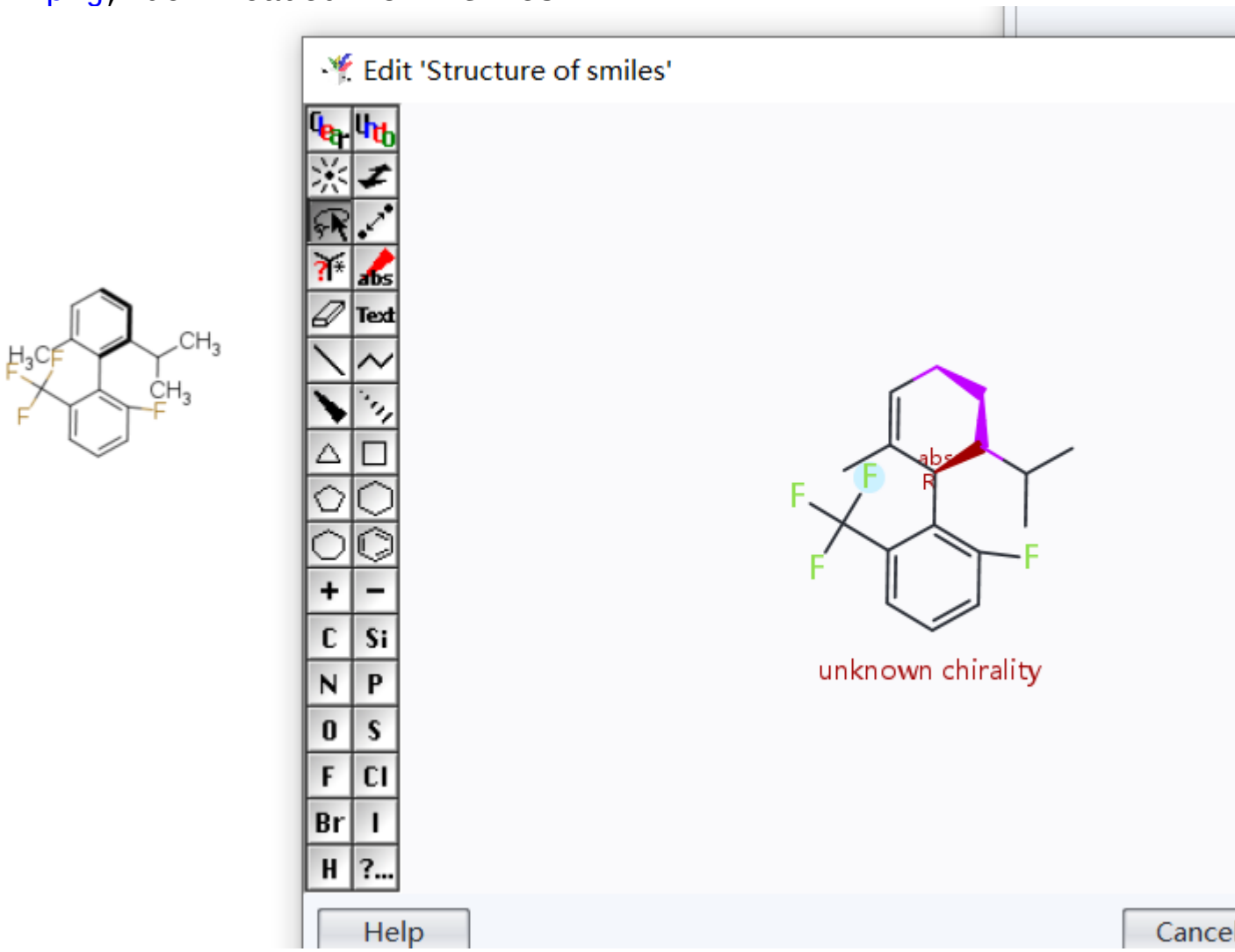
Hi DW developers,

Axial chirality is not represented by most of encoding methods, e.g. SMILES, InChi.
Axial chirality can be drawn in ChemDraw and MarvinSketch, but it seems not supported by the built-in sketcher of DataWarrior.

Can you please provide more details on this topic?

File Attachments

1) dw1.png, downloaded 1571 times



Subject: Re: Axial chirality

Posted by nbehrnd on Fri, 11 Sep 2020 09:37:45 GMT
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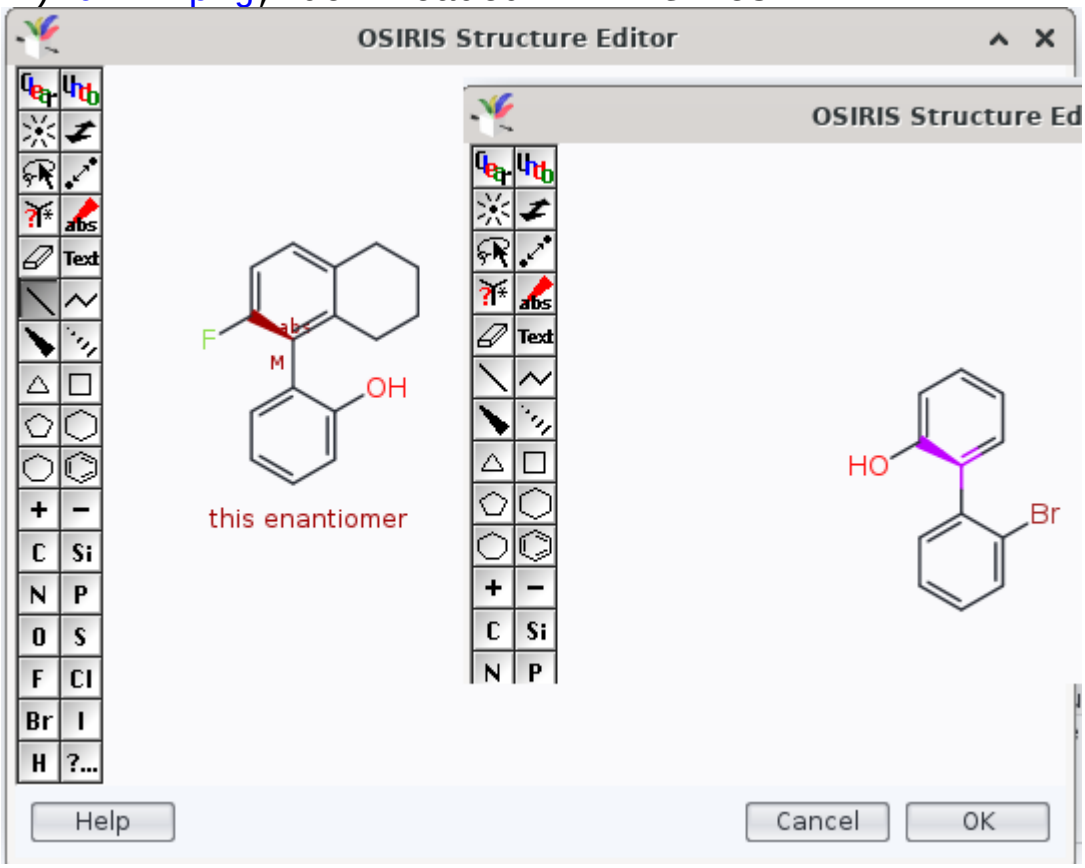
Possibly the scrutiny for P/M in simpler biphenyls differs from the one in larger systems with axial chirality when structures are drawn in the sketcher from scratch:

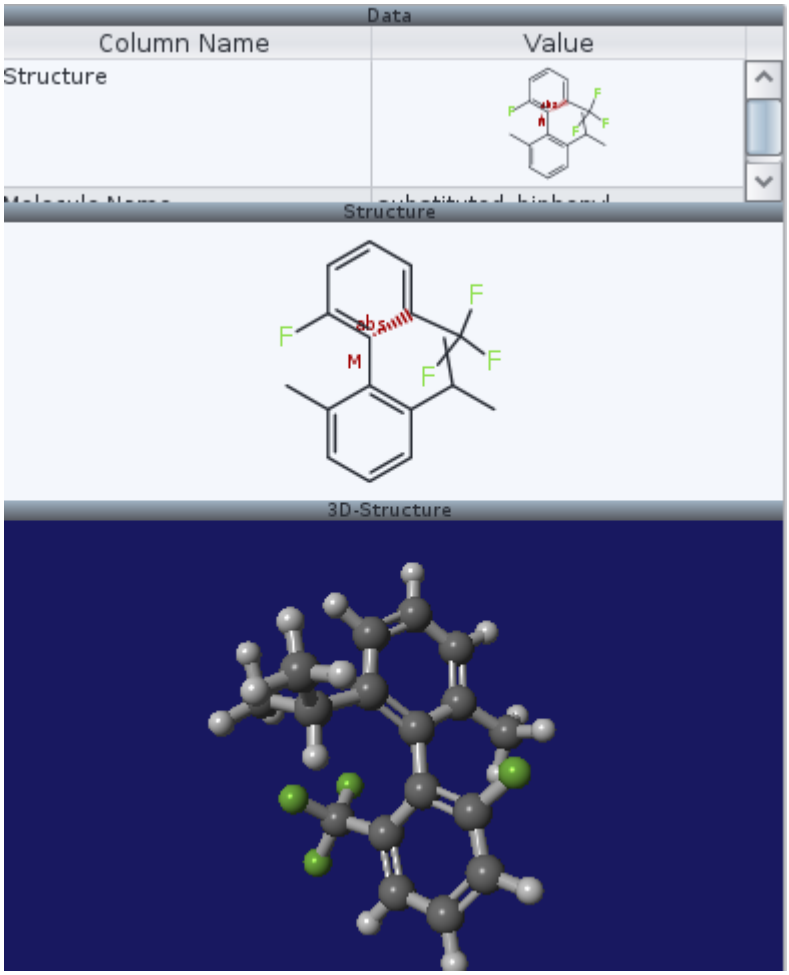
As a bit lengthy work-around: I redrew two structures like the one drawn by you outside DW. After their export as .mol (including 3D coordinates), they were converted with openbabel into an .sdf in common. DW apparently recognized the chirality (both.dwar, attached):

File Attachments

1) diff.png, downloaded 1441 times



2) both.dwar, downloaded 694 times
3) then3D.png, downloaded 1601 times



4) both.sdf, downloaded 691 times

Subject: Re: Axial chirality
Posted by thomas on Sun, 13 Sep 2020 10:04:05 GMT
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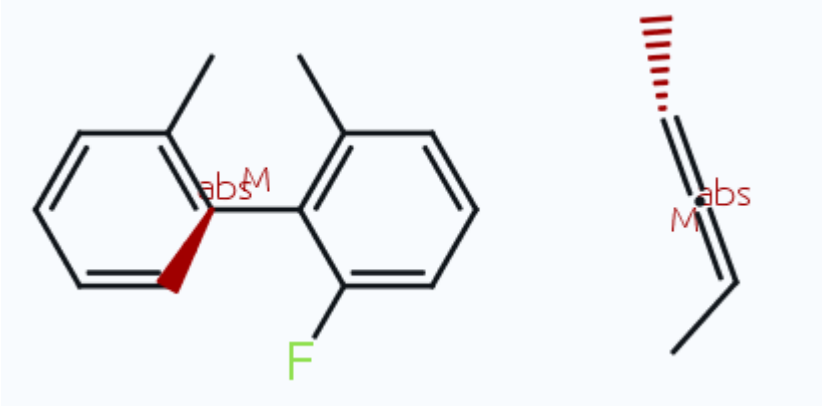
Axial chirality (indicated as M or P) is covered to some extend:

- For allenes the configuration is assigned to the central atom.
- In case of atropisomers only bi-phenyls with at least three ortho substituents are considered because of the reliably hindered rotation. Here the central bond carries the configuration information.

File Attachments

1) axialChirality.png, downloaded 1475 times



Subject: Re: Axial chirality
Posted by zhentg on Wed, 16 Sep 2020 00:03:45 GMT
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Thanks for your comprehensive answer.
I did not know the P/M definition before, and assigning P/M in DW really works.

However, in terms of data exchange feasibility, axial chirality can be represented in MOL format, but not in SMILES. Here you used MOL to transfer data from SDF to DW. That is a nice solution.

Subject: Re: Axial chirality
Posted by zhentg on Wed, 16 Sep 2020 00:07:54 GMT
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Thanks Thomas. Is this Axial chirality introduction covered in the online help of DW?
It will be helpful to add.

By the way, the online Help is not searchable. It would be nice to make it searchable, so that keywords like "axial chirality" will be located easier.

Subject: Re: Axial chirality
Posted by thomas on Fri, 02 Oct 2020 09:37:19 GMT
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Thanks for the recommendation. I will look into search functionality. I know and regret that online help is always much behind the actual functionality. I could need some support here...