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 1109 times
- 2) both.dwar, downloaded 569 times
- 3) then 3D.png, downloaded 1222 times
- 4) both.sdf, downloaded 562 times