
Subject: Axial chirality

Posted by [zhentg](#) on Wed, 09 Sep 2020 00:46:29 GMT

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Hi DW developers,

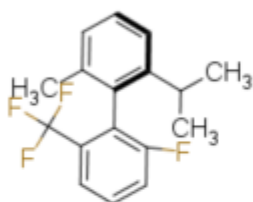
Axial chirality is not represented by most of encoding methods, e.g. SMILES, InChi.

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 1573 times



A screenshot of the 'Edit Structure of smiles' dialog box in DataWarrior. The dialog box has a toolbar on the left with various icons for editing, including 'Clear', 'Undo', 'Redo', 'Copy', 'Paste', 'Text', 'Line', 'Wedge', 'Arrow', 'Triangle', 'Square', 'Pentagon', 'Hexagon', 'Heptagon', 'Octagon', 'Benzene', '+', '-', 'C', 'Si', 'N', 'P', 'O', 'S', 'F', 'Cl', 'Br', 'I', 'H', and '?...'. The main area shows a chemical structure of the same biphenyl derivative as in the previous image. The structure is rendered with a 3D perspective, and the axial chirality is highlighted with a red 'abs' label and a red 'R' label. Below the structure, the text 'unknown chirality' is displayed in red. At the bottom of the dialog box, there are 'Help' and 'Cancel' buttons.