

---

Subject: Chiral drawn structures in dwar / sdf different

Posted by [Dennis](#) on Tue, 05 Jun 2018 11:15:14 GMT

[View Forum Message](#) <> [Reply to Message](#)

---

I have a question about the way a structure is presented in a dwar file compared to a sdf file. When I draw a chiral structure with unknown chirality and save this as a dwar file and open it again, I see the structure drawn as in 1.png:

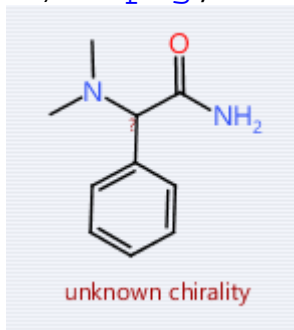
When I save this file as sdf file and open this sdf file, the drawn structure is different, see 2.png:

Why is the chirality presented differently for these files? You would expect the same presentation.

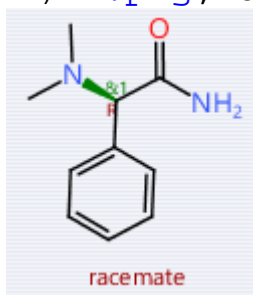
### File Attachments

---

1) [1.png](#), downloaded 2305 times



2) [2.png](#), downloaded 2209 times



---

Subject: Re: Chiral drawn structures in dwar / sdf different

Posted by [thomas](#) on Tue, 12 Jun 2018 21:47:24 GMT

[View Forum Message](#) <> [Reply to Message](#)

---

In principle you are right. DataWarrior and SD-Files, both distinguish unknown chirality from a racemic.

In molfiles stereo centers are usually represented by an up- or down-bond at the stereo center. In addition the wide-spread molfile version 2 has one flag (wrongly called 'chiral' flag), which defines,

whether the molecule is racemic (flag=0) or the drawn enantiomer (flag=1). Correctly, a racemate would have a down- or up-bond and the chiral flag would be 0. The molfile also allows an 'either' bond, which

would describe a mixture and thus supposedly also a racemic situation.

When DataWarrior writes an unknown stereo center into the molfile, it doesn't write any stereo information making the stereo center effectively unknown.

The problem starts when the molfile is read again. If you get SD-files from chemicals' providers, they often encode racemates of molecules with one stereo center the same way, i.e. they don't use one of the two proper methods described above to define the racemate. They just don't write any stereo information. Therefore, molecules with one stereo center, which have no information, are usually meant to be racemates. For this reason DataWarrior also treats them as racemate. Another ugly example is that many software packages read molecules as pure enantiomers if a stereo center has an up- or down-bond, even if the chiral flag is not set. This means, encoding a racemate the right way often creating a wrong result. This may also be the reason for many software providers to rather write no stereo information in case of racemates.

If you need to write structure files with DataWarrior to read them again from DataWarrior I strongly suggest to use the native format, because the conversion to and from molfiles is not guaranteed to give the same result. This is especially true for substructures, which contain query features.

Thomas

---

---

Subject: Re: Chrial drawn structures in dwar / sdf different  
Posted by [Dennis](#) on Wed, 20 Jun 2018 09:30:42 GMT  
[View Forum Message](#) <> [Reply to Message](#)

---

Thank you for the explanation

---