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Subject: Re: Aromaticity perception

Posted by [nbehrnd](#) on Sun, 28 Jun 2020 21:57:00 GMT

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Hi Simon,

it was possible to replicate the problem with the .sdf shared by you. Tentatively, the problem is caused by the existence of multiple SMILES dialects by different programs which may be an obstacle for DW. I thus recommend to pass the .sdf to openbabel to pass the files' content into a new .sdf file to solve the issue. Here, DataWarrior (version 5.2.1, native installation in Linux Debian) and openbabel (version 3.1.0, June 9, 2020) were used.

Enter the directory containing the .sdf in question. From the terminal (Linux, Mac) or cmd.exe (Windows) provide a instruction in line of

```
obabel -isdf Aromatised.sdf -osdf -O Aromatised_passed_obabel.sdf
```

With only eight molecules, this is a quick operation. Comparing the original and the new / derived .sdf file with each other shows that the connection table in the files is adjusted, as shown in the screen photo below:

More importantly, the issues with tetravalent nitrogen atoms are resolved:

The .dwar eventually obtained is provided as an attachment of this answer.

Openbabel is a freely available program running on Windows, Mac, and Linux to interconvert chemical formats. Its code is open on GitHub, which equally hosts the executables. The documentation may be accessed online, or offline. If wanted, a GUI may provide you an easier entry into a selection of its functions, too.

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It is equally possible to convert the SMILES as provided into an .sdf, too. The command then would be

```
obabel -ismi probe.smi -osdf -O probe.sdf
```

to lead to the same result as above, or copy-pasting (without header row) the SMILES directly into DW. Both .smi and .sdf of this approach equally are provided here.

Norwid

<https://github.com/openbabel/openbabel>

<https://github.com/openbabel/openbabel/releases/tag/openbabel-3-1-1>

<https://open-babel.readthedocs.io/en/latest/>

[https://open-babel.readthedocs.io/\\_/downloads/en/latest/pdf/](https://open-babel.readthedocs.io/_/downloads/en/latest/pdf/)

## File Attachments

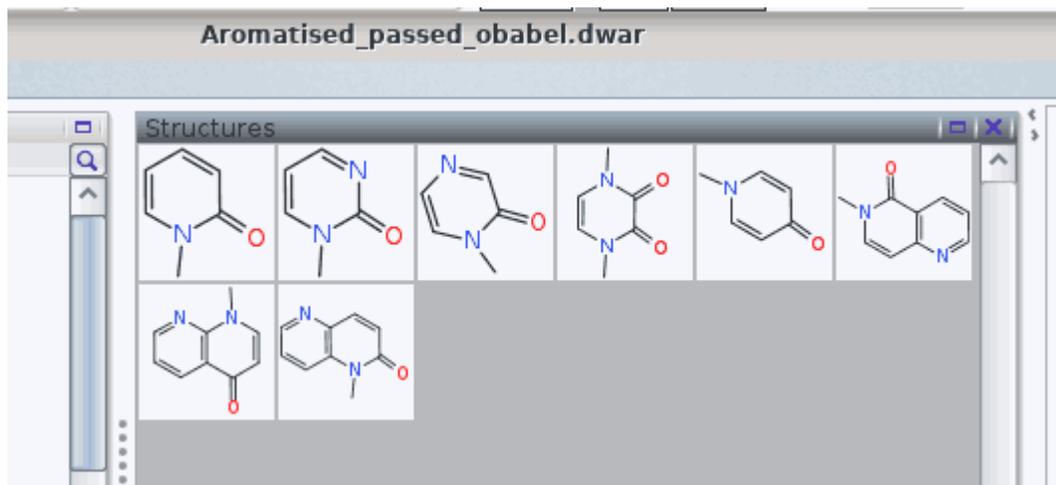
1) [diff\\_view.png](#), downloaded 1313 times

```
Terminal
1
1 Mrv1921 06272022562D
2
3 8 8 0 0 0 0 999 V2000
4 -1.4881 1.0829 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
5 -2.2025 0.6704 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
6 -2.2025 -0.1546 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
7 -1.4881 -0.5671 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0
8 -0.7736 -0.1546 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
9 -0.7736 0.6704 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
10 -0.0818 -0.6039 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0
11 -1.5744 -1.3876 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
12 1 2 4 0 0 0 0
13 1 6 4 0 0 0 0
14 2 3 4 0 0 0 0
15 3 4 4 0 0 0 0
16 4 5 4 0 0 0 0
17 4 8 1 0 0 0 0
18 5 6 4 0 0 0 0
19 5 7 2 0 0 0 0
20 M END
21 $$$$
22
23 Mrv1921 06272022562D
24
25 8 8 0 0 0 0 999 V2000
26 3.1151 1.0433 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
27 2.4006 0.6308 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
28 2.4006 -0.1942 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
29 3.1151 -0.6068 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0
30 3.8296 -0.1942 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
31 3.8296 0.6308 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0
32 4.5214 -0.6436 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0
33 3.0719 -1.4306 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
34 1 2 4 0 0 0 0

1
1 OpenBabel06282022212D
2
3 8 8 0 0 0 0 0 0 0
4 -1.4881 1.0829 0.0000
5 -2.2025 0.6704 0.0000
6 -2.2025 -0.1546 0.0000
7 -1.4881 -0.5671 0.0000
8 -0.7736 -0.1546 0.0000
9 -0.7736 0.6704 0.0000
10 -0.0818 -0.6039 0.0000
11 -1.5744 -1.3876 0.0000
12 1 2 1 0 0 0 0
13 1 6 2 0 0 0 0
14 2 3 2 0 0 0 0
15 3 4 1 0 0 0 0
16 4 5 1 0 0 0 0
17 4 8 1 0 0 0 0
18 5 6 1 0 0 0 0
19 5 7 2 0 0 0 0
20 M END
21 $$$$
22
23 OpenBabel06282022212D
24
25 8 8 0 0 0 0 0 0 0
26 3.1151 1.0433 0.0000
27 2.4006 0.6308 0.0000
28 2.4006 -0.1942 0.0000
29 3.1151 -0.6068 0.0000
30 3.8296 -0.1942 0.0000
31 3.8296 0.6308 0.0000
32 4.5214 -0.6436 0.0000
33 3.0719 -1.4306 0.0000
34 1 2 1 0 0 0 0

Aromatised.sdf 1,0-1 Top Aromatised_passed_obabel.sdf
"Aromatised_passed_obabel.sdf" 207L, 7858C
```

2) [Aromatised\\_passed\\_obabel-or8.png](#), downloaded 1341 times



- 3) [Aromatised\\_passed\\_obabel.dwar](#), downloaded 743 times
  - 4) [probe.sdf](#), downloaded 727 times
  - 5) [probe.smi](#), downloaded 796 times
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