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Subject: Re: Aromaticity perception

Posted by [richards99](#) on Sat, 27 Jun 2020 22:09:10 GMT

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Hi Norwid,

I cannot find a way to attach an SDF file, but basically this set of smiles below causes a problem.

If you create a CSV/TXT file of these and import them into DW, then all is fine.

But if you create an SDF file of these smiles using Marvin Sketch for example (kept as aromatised), and then import them into DW, then all the double bonds are messed up!

Other programmes such as Marvin, RDKit do not seem to have issues with these.

```
Cn1cccc1=O
Cn1cccnc1=O
Cn1ccncc1=O
Cn1ccn(C)c(=O)c1=O
Cn1ccc(=O)cc1
Cn1ccc2ncccc2c1=O
Cn1ccc(=O)c2cccnc12
Cn1c2cccnc2ccc1=O
```

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