Subject: tautomer & protomer display
Posted by sbembenek18 on Mon, 02 Mar 2020 00:02:41 GMT

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I notice that sometimes DW will display a given tautomer/protomer different than what was written to the SDF file.

For example, I have the canonical smiles:

Nc1nc([O-])c2[nH]c[nH+]c2n1

which DW will display as:

Nc(nc1O)nc2c1[nH]cn2

I seem to be able to prevent this by adding explicit Hs when writing the SDF. I'd just like to have a clearer picture of what it is doing.

thanks!