Subject: Re: Visualising SMILES string
Posted by thomas on Sat, 20 Mar 2021 14:07:46 GMT
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Hi Angus,

if you replace [*:1] by *, then the atom is interpreted as wildcard query feature, which is drawn as a '?'.
In this case the new molecule is considered as sub-structure rather than as normal structure. The difference is
that a sub-structure may have query features and all unspecified atom valences are not implicitly considered
to be blocked by hydrogen atoms. Therefore, a single bonded oxygen is shown as -O in contrast to -OH in a normal molecule.

DataWarrior makes this distinction, which is not made by most other software, possibly, because the SMILES definition itself does not distinguish between these two structure flavors.

Thomas