Subject: Re: Aromaticity perception
Posted by thomas on Thu, 02 Jul 2020 12:41:03 GMT
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many thanks Simon and Norwid for pointing to this issue suggesting work-arounds.

The problem was that DataWarrior didn't expect finding compounds with aromatic bond types in molfiles,
which are based on the Daylight aromaticity model into the bargain, e.g. having carbonyl carbon atoms being
maked as aromatic. This is unusual for two reasons: First, molfiles typically store alternating single and double bonds for aromatic rings rather than using the delocalized bond type, unless it encodes
a substructure with query features. Second, for the rare cases that the delocalized bond types may be used
one would expect an MDL/Symex/Hueckel aromaticity concept to be applied.

Nevertheless, since Marvin Sketch seems to read SMILES based atom aromaticity encodings and writes them directly into
written molfiles using aromatic bond types, I have updated DataWarrior to normalize this kind of encoding before
generating and writing idcodes (DataWarrior's canonical structure representation) into its native files.

The current developments version should not have this issue anymore.

Thomas