Subject: Re: Reaction enumeration with aromaticity
Posted by thomas on Tue, 01 Jun 2021 22:38:10 GMT
View Forum Message <> Reply to Message

Hi Mattia,

this was indeed a tricky one. I have checked and finally found that the problem was caused by the valence check after doing the substructure search of the generic in the real reactant. The check determines, whether all atoms in the real reactant have enough free valence needed for the reaction. For that it determines the delta between generic product and reactant atoms. Here was the problem: for the atoms with mapping numbers 4 and 9 it found the product atom valences to be +1 higher than their respective reactant valence. Since the real reactant valence atoms at the corresponding position had already the maximum valence of 4, they were sorted out after the substructure match. Calculating free valences with delocalized bonds is a tricky matter. It gets even worse, if multiple bond orders are allowed.

I have fixed this issue and deployed an update of DataWarrior. The dev patch is downloadable from the small print links on the download page after clicking the 'read and understood' checkbox. Some general tips: typically query features are only needed on the reactant side; delocalized bonds may be avoided by using the 'aromatic' query feature for bonds or atoms. A drawn double bond also matches a delocalized bond (in the reactor context). Thus, the following picture is equivalent to your generic reaction.

Hope, this solves it. Otherwise please let me know.

Thomas

File Attachments

1) reaction.png, downloaded 1271 times

