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Subject: Re: fragments

Posted by [thomas](#) on Sun, 14 Apr 2019 20:10:29 GMT

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Hi Patrick,

in DataWarrior the word fragment usually refers to a substructure fragment, which in contrast to a normal molecule is incomplete such open valences are not considered to be filled with hydrogen atoms. Fragments may also contains atom and bond query features.

In some cases, however, 'fragment' also refers to a molecule, e.g. the functionality 'Add largest fragment', which identifies all non-connected parts of a molecule (e.g. in salts) and just copies that one with the highest number of non-hydrogens atoms into a new column. This column then contains 'molecules', where all free atoms valences are implicitly considered to be filled with hydrogen atoms.

Finally it is a matter of the context. I assume this does not fully answer your question. What was the context in your case?

Thomas

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