Subject: Re: sp3 count
Posted by thomas on Thu, 19 Aug 2021 19:23:57 GMT
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Dear Mvamos,

DataWarrior considers C,N,O,P,S as potential sp3 atoms. In your case the 2 oxygen atoms are considered to be sp3 in addition to the 3 obvious carbon atoms. I agree that an ether-oxygen doesn't contribute much to the 3D-shape of a molecule, but the same is true for an (sp3) methyl group. It is a formal number. sp3 fraction in carbon atoms is simple and I will add it...

Thomas