Subject: Acidic oxygen
Posted by sansun on Fri, 05 Feb 2021 05:30:46 GMT
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While calculating 'Acidic oxygen', DW considers nitro group oxygen as acidic.

Is there a way to avoid this?

Subject: Re: Acidic oxygen
Posted by nbehrnd on Fri, 05 Feb 2021 06:53:14 GMT
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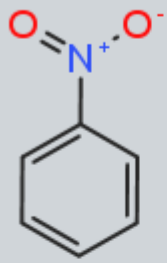
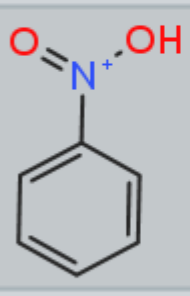
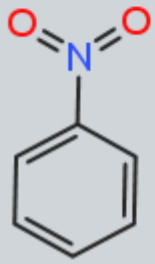
If the NO2 group is going to be exempt from this count because formally there is one positive charge on N and one negative on O, N-oxides (like in pyridine N-oxide) could be considered by analogy, too.

Subject: Re: Acidic oxygen
Posted by thomas on Fri, 05 Feb 2021 12:25:52 GMT
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When I tried to verify, I could confirm with version 5.2.1, but found also that this bug is fixed in the current development version. You may either wait for an official new release, or you may replace your executable with the downloadable patch file(s). You find the links in the small print on the DataWarrior download page after clicking the 'Read and understood' checkbox.

Current version result:

File Attachments
1) t.png, downloaded 1437 times

Structure	Acidic Oxygens
	0
	1
	0