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Subject: Re: TFA salts

Posted by [nbehrnd](#) on Mon, 15 Jun 2020 20:50:09 GMT

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Thus, DataWarrior's approach to neutralize charges yields to the same results as the --neutralize instruction added by Noel O'Boyle to openbabel (version 3.1.0, by 2020-05-05)?

Norwid

<https://open-babel.readthedocs.io/en/latest/ReleaseNotes/ob3>

[10.html?highlight=neutralize#new-features-and-improvements](https://open-babel.readthedocs.io/en/latest/ReleaseNotes/ob3)

<https://baoilleach.blogspot.com/2019/12/no-charge-simple-app> roach-to.html

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