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