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Subject: Re: Chemistry in 3D

Posted by [nbehrnd](#) on Thu, 17 Mar 2022 21:34:52 GMT

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Dear Christophe,

do you refer to one of the two videos mirrored on youtube?[1,2]

May you specify if your interest concerning «conformers and 3D chemistry» is about the theory behind the scenes, or the choice of one of the algorithms available? For the later, it would help to know what you want to do once the conformers are in obtained. The force-fields offered by DW strive for affordable results in obtained short delay, they may serve as a starting point for computations at higher level of theory with other programs.

(Inferring from the context set above:) The addition of an empty row will fail if the .dwar in question is about conformers already generated and is a container of these (newly generated) 3D coordinates. At stage where the molecules are «only 2D sketches» like on paper, the addition of rows will work.

The red frame is visual aid. To define e.g., the deletion of rows, the range is defined by the cells with the toggled background color (e.g. from default light to dark); this selection moves independently from the red frame.

Norwid

[1] <https://www.youtube.com/watch?v=mQCf9GakQW0>

[2] <https://www.youtube.com/watch?v=ls2hLqqSFvM>

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