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Subject: Re: Generate conformers - write to file does nothing

Posted by [nbehrnd](#) on Thu, 09 Jul 2020 08:10:08 GMT

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Hello Paul,

starting with the liquid\_crystal.dwar file attached below, and using the parameters shown in the screen photo below

the newly written conformers\_test.dwar contains multiple models. Not 16 which was set as the maximum number, but at least four. May you share a minimal example, including the parameters you use, leading to the empty .dwar file?

Norwid

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#### File Attachments

- 1) [liquid\\_crystal.dwar](#), downloaded 477 times
  - 2) [conformers\\_test.png](#), downloaded 1009 times
  - 3) [conformers\\_test.dwar](#), downloaded 516 times
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