Subject: search for conformers, empty column «minimization error»
Posted by nbehrnd on Thu, 17 Mar 2022 20:13:14 GMT
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Dear Thomas,

using DataWarrior to generate conformers (chemistry -> generate conformers), I notice the presence of a fifth column to report «minimization errors». So far, I did not met a run with a run where one of the entries were marked by a categorical warning, or a real number against a reference value (if the later, what would be the critical threshold). The chapter «Chemistry in 3D» of the help doesn't provide additional documentation about this. So, what is the anticipated user scenario where this assists the user?

The observation refers to DW 5.5.0 for Linux/Mac including the development updates by 2022-03-14.

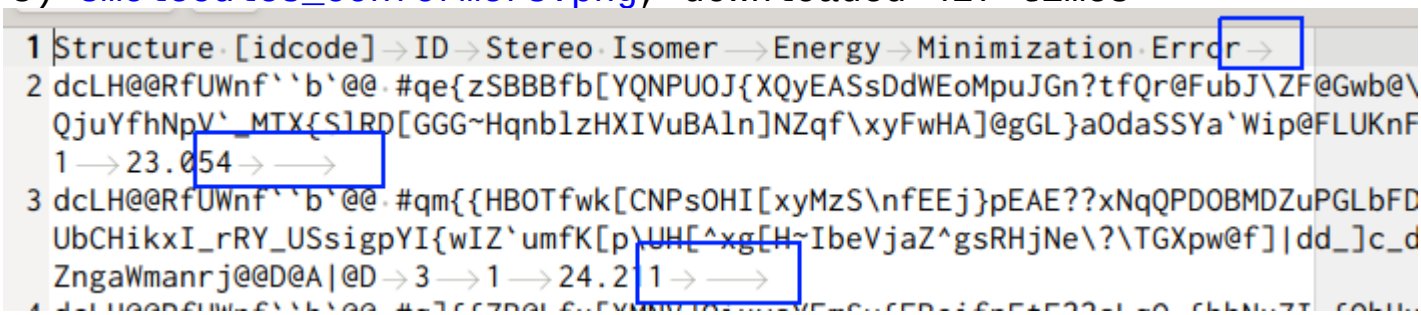
Thank you,

Norwid

(Exporting these results as a text file typically yields /two/ tabulators prior to the anticipated line feed, which once was unexpected for an AWK script down the road; one for the empty column, one for the general format of the record lines.)

File Attachments

1) 3molecules_conformers.dwar, downloaded 476 times
2) 3molecules_conformers.txt, downloaded 495 times
3) 3molecules_conformers.png, downloaded 427 times



Subject: Re: search for conformers, empty column «minimization error»
Posted by thomas on Wed, 06 Apr 2022 09:56:37 GMT
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Dear Norwid,

the minimization error column is populated in case the forcefield minimizer creates an error. A typical error would be a not supported atom type, because MMFF94 is limited to the usual organic atoms. I also noticed that if such an error occurrs, the energy field is empty and since there is an

active filter, rows with empty energy values are filtered out unless one disables the filter. I now changed that and disable the filter automatically, when the file is created and there are rows with minimization errors.

Best wishes,

Thomas