
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 meet 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.

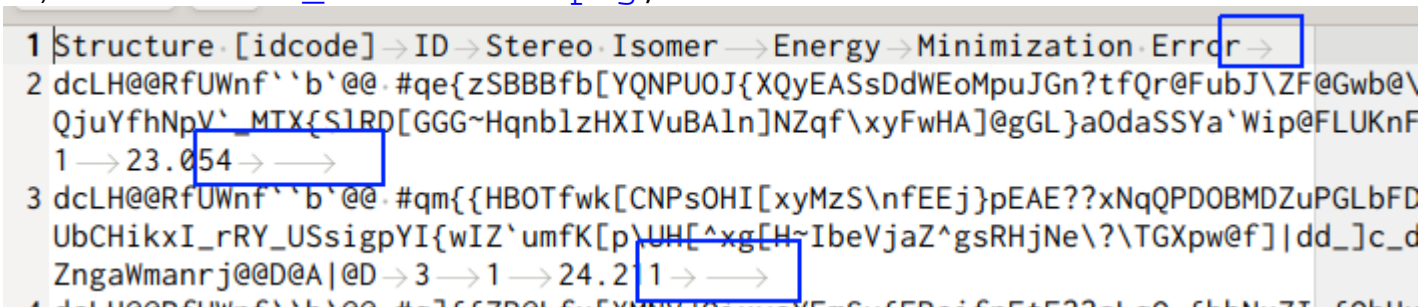
Thank you,

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 548 times
- 2) [3molecules_conformers.txt](#), downloaded 548 times
- 3) [3molecules_conformers.png](#), downloaded 594 times



The screenshot shows a table with the following columns: Structure, [idcode], ID, Stereo, Isomer, Energy, and Minimization Error. The first row is highlighted, and the 'Minimization Error' cell contains '1' with a blue box around it. The second row contains a long alphanumeric string followed by '1' in the 'Minimization Error' column, which is also boxed. The third row contains another long alphanumeric string followed by '1' in the 'Minimization Error' column, which is also boxed. The fourth row is partially visible at the bottom.

Structure	[idcode]	ID	Stereo	Isomer	Energy	Minimization Error
dcLH@@RfUWnf``b`@@. #qe{zSBBBfb[YQNPUOJ{XQyEASsDdWEoMpuJGn?tfQr@FubJ\ZF@Gwb@\ QjuYfhNpV`_MTX{S1RD[GGG~Hqnb1zHXIVuBA1n]NZqf\xyFwHA}@gGL}aOdaSSYa`Wip@FLUKnF		1				1
dcLH@@RfUWnf``b`@@. #qm{{HBOTfwk[CNPsoHI[xyMzS\nfEEj}pEAE??xNqQPDOBMDZuPGLbFD						1
ZngaWmanrj@@D@A @D		3		1	24.2	1