Subject: 3D structure display is lost after hovering over certain structures
Posted by plkx on Mon, 26 Oct 2020 18:36:12 GMT
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Hello,

In either a DWAR or SDF file with 3D structures, the display window goes blank after certain structures are selected, or the mouse pointer is hovered over a row of the same (certain) structures.

Subsequently, 3D structures are not rendered for any other structures.

If the file is reopened (with or without quitting DataWarrior), 3D structure display returns, until the effect of a "deactivating structure" returns (e.g. by simply moving the mouse across the structure table pane).

The attached file contains examples of structures rendered properly, and those that deactivate 3D structure display. Methane, water, hydrogen sulfide, ammonia, and hydrogen halides cause the problem.

The file is not altered during the course of these glitches.

Best Regards,

Paul

File Attachments
1) Tests.dwar, downloaded 232 times

Subject: Re: 3D structure display is lost after hovering over certain structures
Posted by thomas on Tue, 27 Oct 2020 11:49:07 GMT
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Hello Paul,

thank you for that clear report and the sample file. With that I could quickly find the problem and fix it.
The issue was the following: The 3D-coordinate encoding includes a value for the 'average bond length' to properly scale
a molecule after decoding and assigning relative atom coordinates. In a special case, where hydrogen coordinates
are included in the encoding, the average bond length was still calculated from non-hydrogen atoms only, which failed
in molecules that have no bonds between non-hydrogen as HI. For these molecules H-I distance are still not correct, if
3D-coordinates are not freshly calculated. But they are displayed correctly now and don't crash

the 3D-viewer.

The bug is fixed in todays update of DataWarrior's development version.

Thomas

Subject: Re: 3D structure display is lost after hovering over certain structures
Posted by Paul on Tue, 27 Oct 2020 16:41:10 GMT
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Thank you, for providing the nice tool, and for such a quick fix.

Best Regards,

Paul