Subject: V3000 input
Posted by bruno.b on Fri, 24 Oct 2014 07:54:15 GMT
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FYI, Data warrior cannot read the attached file. I think it is a valid V3000 file. Pubchem can read it.

Best regards,

Bruno

File Attachments
1) abs_stereo_index.v3000.sdf, downloaded 1410 times

Subject: Re: V3000 input
Posted by thomas on Sat, 25 Oct 2014 23:10:12 GMT
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After a quick check it seems that in a V3 molfile atoms have to be in order, which they are not.
In any case DataWarrior should throw a reasonable error message, or should be kind enough to accept
atoms in any order. I will check and let you know.

Thanks for the question and kind regards, Thomas

Subject: Re: V3000 input
Posted by bruno.b on Mon, 27 Oct 2014 15:00:24 GMT
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Hi Thomas,

according to the Symyx June 2010 documentation, the atom index can be any strictly positive number.

"Identifies atoms. The actual value of the index does not
matter as long as each index is unique to each atom. "

For the bonds:

"The actual value of the index does not matter as
long as all are unique."

I did not find comment about the order of the atom indices in the Symyx document.

Regards,

Bruno

Subject: Re: V3000 input
Posted by thomas on Wed, 05 Nov 2014 15:46:13 GMT
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Hi Bruno,

I checked myself and found the same thing. I will make sure, that this issue will be fixed in the next public DataWarrior release.

Kind regards,

Thomas
