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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

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