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Subject: V3000 export issue

Posted by [bruno.b](#) on Tue, 31 Jan 2017 17:20:41 GMT

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Hi Thomas,

I think that there is a problem with DW (version 4.4.4) SDF V3000 export when there is a collection:

```
M V30 209 1 105 200
M V30 210 1 105 201
M V30 END BOND
M V30 BEGIN COLLECTION
M V30 MDLV30/STEABS ATOMS=(18 4 15 26 45 48 49 53 54 69 72 73 77 78 93 96 97 101 102)
M V30 END COLLECTION
M V30 END CTAB
M END
```

According to the documentation, the END CTAB must come before BEGIN COLLECTION:

```
M V30 BEGIN CTAB [ctabname]
counts-line
atom-block
[bond-block]
[sgroup-block]
[3d-block]
[link-line]*
M V30 END CTAB
[collection-block]
[rgroup-block]*
[template-block]
```

This would be the correct syntax:

```
M V30 209 1 105 200
M V30 210 1 105 201
M V30 END BOND
M V30 END CTAB
M V30 BEGIN COLLECTION
M V30 MDLV30/STEABS ATOMS=(18 4 15 26 45 48 49 53 54 69 72 73 77 78 93 96 97 101 102)
M V30 END COLLECTION
M END
```

Best regards,

Bruno

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Subject: Re: V3000 export issue  
Posted by [thomas](#) on Sun, 05 Feb 2017 21:39:04 GMT  
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Hi Bruno,

thank you for reporting this. I will check and correct immediately.

Thomas

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Subject: Re: V3000 export issue  
Posted by [thomas](#) on Mon, 06 Feb 2017 09:17:53 GMT  
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Hi Bruno,

my cfile formats document from 2005 does not seem to specify whether the collection block is part of the CTAB block or should start after the 'END CTAB' tag. However, the example molfile in the 'MDL's Enhanced Stereochemical Representation' document is conform with DataWarrior's way of producing molfiles. An up-to-date version of this document is online available:

<http://accelrys.com/products/pdf/enhanced-stereochemical-representation.pdf>

I also checked what ChemDraw Pro 15 is doing: Their molfiles have the collection block before 'END CTAB' as DataWarrior has.

I am currently waiting for a download link to the newest cfile document from biovia be sent to me. I assume that this is where you found the specification.

For now it seems that I am in good company, if I keep it as it is. Please let me know, if you come across any software that expects the format differently.

Thomas

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Subject: Re: V3000 export issue  
Posted by [bruno.b](#) on Mon, 06 Feb 2017 16:23:38 GMT  
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Hi Thomas,

I found the description I wrote above in the CT file format document from December 2011 at page 13. I don't have the 2005 CT file format document. The example from the white paper (from the link you posted) does not match the 2011 description. Both documents are coming from Accelrys. Since I don't know any software that produces molfiles that have the collection block after 'END CTAB' I agree that it might be better to keep it as it is.

Bruno

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