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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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