Subject: V3000 export issue with long lines?
Posted by bruno.b on Mon, 06 Feb 2017 16:40:49 GMT
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Hi Thomas.

this is a part of a V3000 molfile I exported from DW:

M V30 END BOND
M V30 BEGIN COLLECTION
M V30 MDLV30/STEABS ATOMS=(18 5 8 11 14 18 32 33 37 39 73 76 79 82 86 100 101 105
107)
M V30 END COLLECTION
M V30 END CTAB
M END

The collection line has more than 80 characters.

From the CTfile document 2011 page 12 :

Each entry is one line of no more than 80 characters. To allow continuation when the
80-character line is too short, use a dash (-) as the last character. When read, the line is
concatenated with the next line by removing the dash and stripping the initial "M V30" from
the following line.

Best regards,

Bruno