
Subject: Re: Faulty SDF import
Posted by [nbehrnd](#) on Wed, 21 Oct 2020 07:15:38 GMT
[View Forum Message](#) <> [Reply to Message](#)

My observation differs:

1) First I pasted the SMILES string into DW (5.2.1, natively Linux version [used in Debian 10 / unstable]) and obtained a pyridinium:

2) Then the .sdf provided by you (as generated by Marvin) was read by a separate, newly started instance of DW, again yielding a pyridinium:

which seems chemically plausible, matches (by constitution) both the former and the visual output when requesting OpenBabel (3.1.0) to visualize the .sdf as a .png:

File Attachments

- 1) [test.dwar](#), downloaded 240 times
 - 2) [test_in_DW.png](#), downloaded 560 times
 - 3) [untitled_molecule_file.dwar](#), downloaded 243 times
 - 4) [test_import.png](#), downloaded 434 times
 - 5) [untitled_molecule_file.png](#), downloaded 548 times
-