Subject: Datawarrior Protonates the Oxygen in a Phosphorous Oxygen Double Bond.
Posted by SMolnar on Wed, 22 May 2019 14:55:19 GMT
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I have a series of organophosphorous compounds containing a Phosphorous-Oxygen double bond (pentavalent phosphorous). When I import the sdf file into Datawarrior (v-5.0.0) the the P=O bond is converted to a P-OH bond.

Subject: Re: Datawarrior Protonates the Oxygen in a Phosphorous Oxygen Double Bond.
Posted by thomas on Tue, 28 May 2019 09:02:34 GMT
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I tried with the following sdf example, which works fine. Can you send me an sdf record that does not work? Thanks in advance, Thomas

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Actelion Java MolfileCreator 1.0

```
  7  6  0  0  0  0  0  0  0  0999 V2000
    3.7717   -5.8584   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.0579   -6.6301   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.3442   -5.8584   -0.0000 P   0  0  0  0  0  0  0  0  0  0  0  0
    7.6304   -6.6301   -0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    8.9166   -5.8584   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.3442   -4.3584   -0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    7.6495   -5.1193   -0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  2  3  1  0  0  0  0
  3  4  1  0  0  0  0
  4  5  1  0  0  0  0
  3  6  2  0  0  0  0
  3  7  1  0  0  0  0
M  END
$$$$
```