

---

Subject: Datawarrior Protonates the Oxygen in a Phosphorous Oxygen Double Bond.

Posted by [SMolnar](#) on Wed, 22 May 2019 14:55:19 GMT

[View Forum Message](#) <> [Reply to Message](#)

---

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

[View Forum Message](#) <> [Reply to Message](#)

---

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

-----

Actelion Java MolfileCreator 1.0

```
7 6 0 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 0 0 0
 5.0579 -6.6301 -0.0000 C 0 0 0 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 0 0 0
 7.6304 -6.6301 -0.0000 O 0 0 0 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 0 0 0
 6.3442 -4.3584 -0.0000 O 0 0 0 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 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
$$$$
```

---