

Additional Reading Material for Creating an Input File

Conversion of Mol file to XYZ file format.

Openbabel online interface can be used to convert a **MOL** file to **XYZ** file format.

Open a web browser and go to the **Openbabel** website as shown below.

<http://www.cheminfo.org/Chemistry/Cheminformatics/FormatConverter/index.html>

Openbabel website can also be used to convert other file formats to **xyz** file format.

Steps to convert a **mol file** to **xyz file**.

1. I will use the previously created and saved **water.mol** file as an example.
2. In the website we have a **drop or paste here your input file** box.
3. Click inside the box.
4. **File Upload** window opens.
5. Select the **water.mol** file from the folder.
6. Click the **Open** button at the top right corner of the window.
7. The **Input box** displays the information of the structure.
8. The **Options** panel has **Input format** and **Output format** drop downs.
9. From the options in the **Input format** dropdown, select **mol--MDL MOL** format.
10. From the options in the **Output format** dropdown, select **xyz--XYZ cartesian coordinates** format.
11. Leave the other options as such in the panel.
12. Below the **Options** box, click on the **Convert** button.
13. In the **OUTPUT** box, the xyz coordinates of water molecule will be displayed.
14. These coordinates can be copied and pasted to a text editor directly.
15. At the top right corner of the **Output** box we see **Download file** down arrow icon.
16. On clicking this icon, **Save** dialog box opens.
17. Type the Name as **water.xyz** and click on the **Save** button.
18. The XYZ file format can be used as an input file for ORCA.