winmostar tutorial

Modeling Crystal Adsorption Model

V11.5.6

11 January, 2024 X-Ability Co., Ltd.

About This Document

- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult Beginner's Guide.
- For those who wish to explore the details of each feature, please refer to Winmostar User Manual.
- If you are unable to proceed with the operations as outlined in this manual, please first consult Frequently asked questions.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us from Contact. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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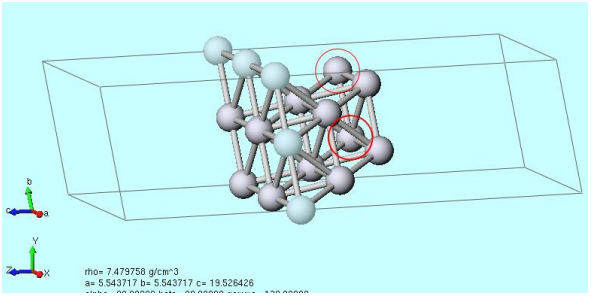
A. Creation of Slab

For detailed methods of creating a slab, please refer to Crystal Modeling Slab Model Edition tutorial.

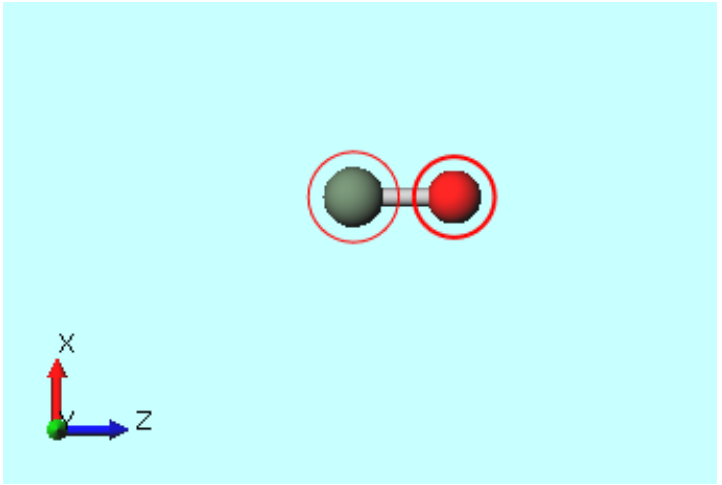
A. Click **File | New File**, **New Project**, or **Edit | Reset Structure**.
B. Click **File** | **Import** | **Sample File** | **pt.cif**, then click **Discard and import**.
   – If you wish to load a specific file, use **File | Import File** at this stage instead.
C. Click **Solid** | **Slab Builder**.
D. Change **Miller indices** to '1', '1', '1', set **a-axis** of **Supercell** to '2', and **b-axis** to '2', then click **Generate Slab**.
   – Adjust the thickness (**Minimum slab size**) and size in the x and y directions (**Supercell**) as needed. In this manual, we create it with the minimal size as an example.
E. Change **Vacuum** to '15' and click **OK**. If 'Successfully generated slab' is displayed, click **OK** again.
   – Adjust **Vacuum** as necessary.
F. Click  **Export File** and save as 'pt111.mol2'.



B. Creation of Adsorbed Molecule

For detailed methods on creating molecular structures, please refer to Molecular Modeling Organic Molecules Edition tutorial.

A. Click **Edit** | **Reset Structure**.
B. Click  **Align View to Y-Axis**
C. Right-click on a hydrogen atom (yellow) and click **Change Element to | O 8**.
D. Rotate the molecule as needed so that the Z-direction becomes the adsorption direction. In this manual, we click **Edit | Adjust Axes | Swap Axes (XYZ to ZXY)**.
E. Click  **Export File** and save as 'co.mol2'.



C. Creation of ontop/fcc/hcp Adsorption Models

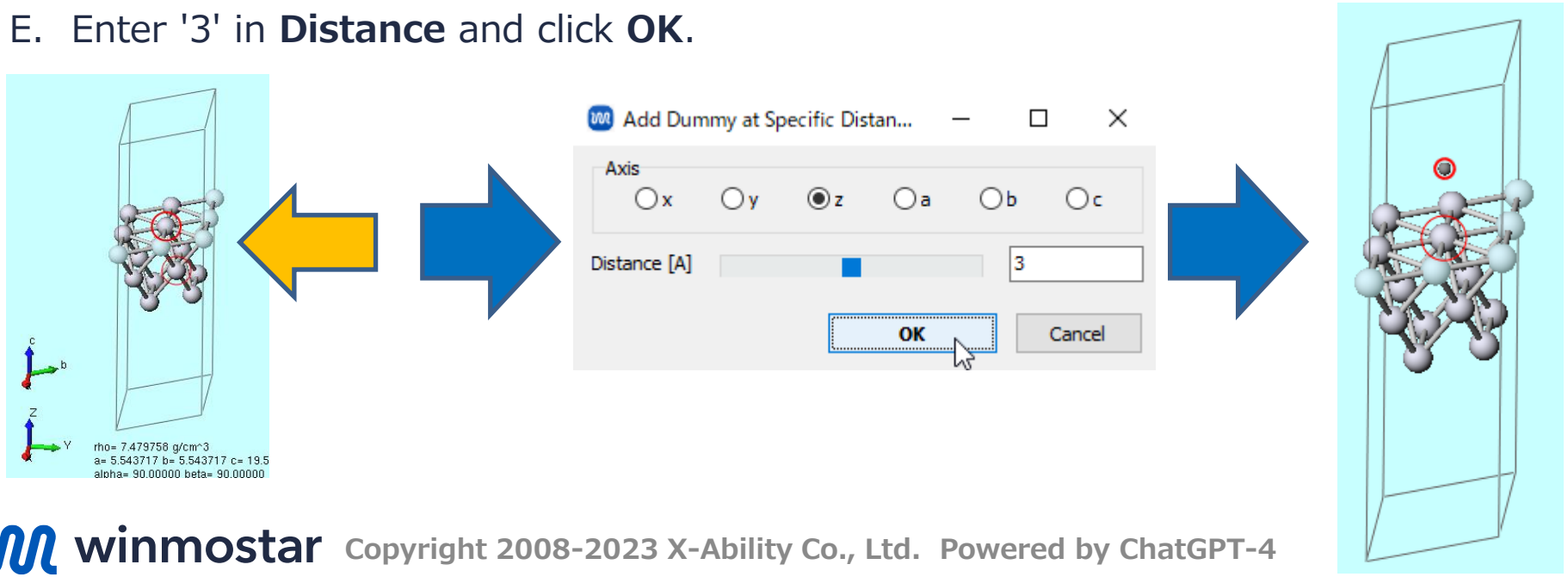
A. Click **Import File** and open the pt111.mol2 file saved on page 3, then click **Discard and import**.

B. Click **Align View to X-Axis**.

C. Adjust the view so that the Z-axis is upwards and the surface is visible, and click on the atom directly below the adsorbed molecule (ontop: first layer, hcp: second layer, fcc: third layer) as shown in the diagram below.

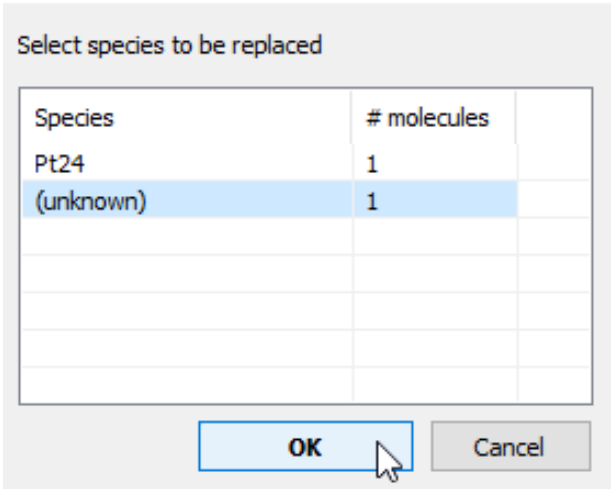
D. Click **Edit** | **Add Atom** | **Add Dummy Atom at Specific Distance from Marked Atom**.

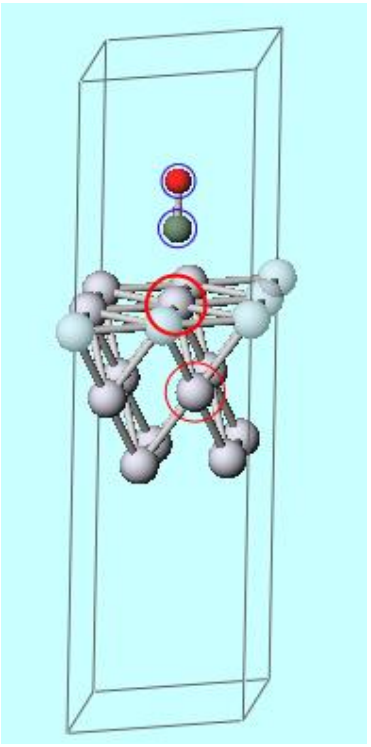
E. Enter '3' in **Distance** and click **OK**.



C. Creation of ontop/fcc/hcp Adsorption Models

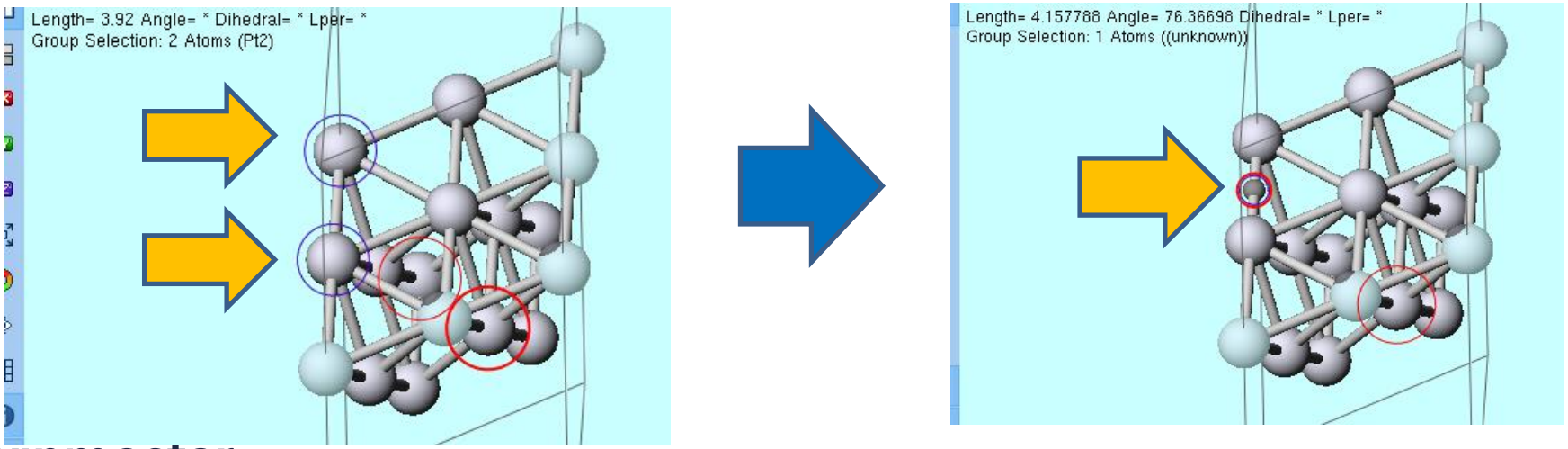
A. Click **MD | Replace Molecules**, click on the row labeled '(unknown)', and then click **OK**.
B. When the dialog 'Select file to be inserted' opens, open the co.mol2 file saved on page 4. Click **OK** when 'Successfully replaced molecules' is displayed.
C. If you need to adjust the position of the adsorbed molecule, proceed to page 9.





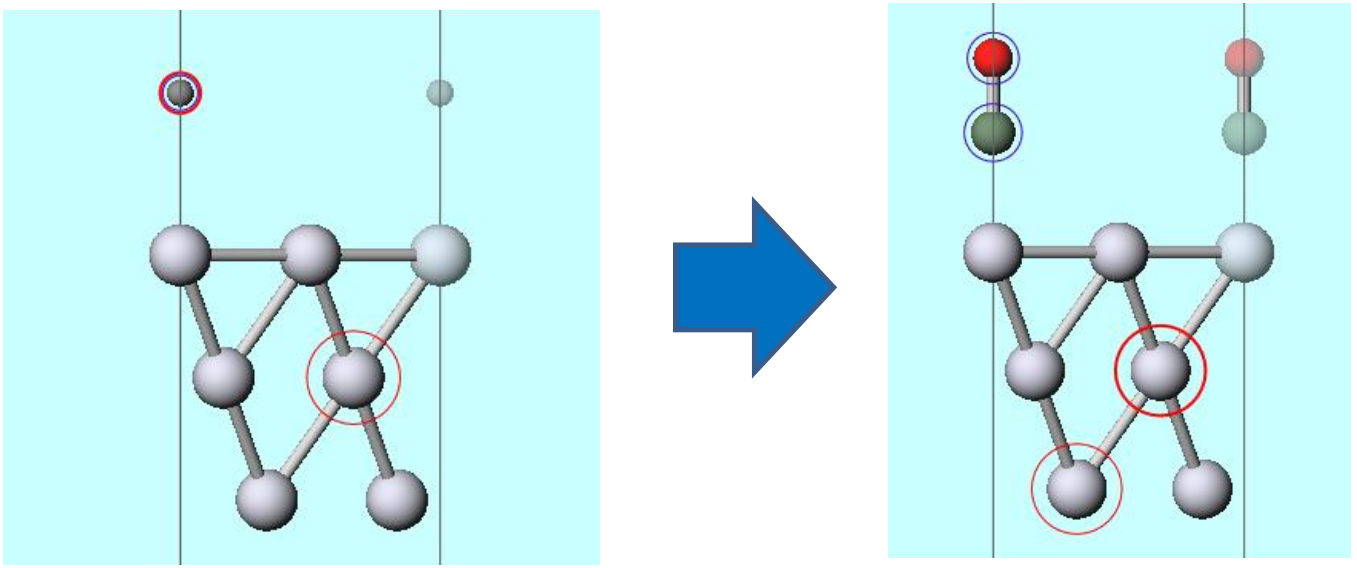
C. Creation of Bridge Adsorption Model

A. Click **Import File** and open the pt111.mol2 file saved on page 3, then click **Discard and import**.
B. Click **Align View to X-Axis**.
C. Adjust the view so that the Z-axis is upwards and the surface is visible, and then sequentially Ctrl+click on two adjacent atoms in the first layer of the surface that are not displayed semi-transparently, as shown in the diagram below.
D. Click **Edit | Add Atom | Add Dummy Atom To Center of Geometry of Selected Gtoup**.
E. Click **Select | Select None**.
F. Ctrl+click on the dummy atom added in step D.



C. Creation of Bridge Adsorption Model

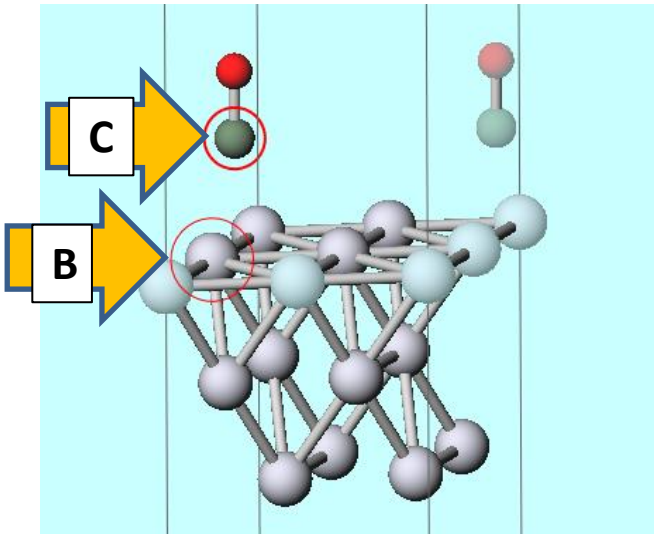
A. Click **Align View to X-Axis**.
B. Click **Modify Selected Group** | **Translate (Numerical)**, change Z to '3', and click **OK**.
C. Click **MD** | **Replace Molecules**, select the '(unknown)' row, and click **OK**.
D. When the dialog 'Select file to be inserted' opens, open the co.mol2 file saved on page 4. If 'Successfully replaced molecules' is displayed, click **OK**.
E. If you need to adjust the position of the adsorbed molecule, proceed to page 9.

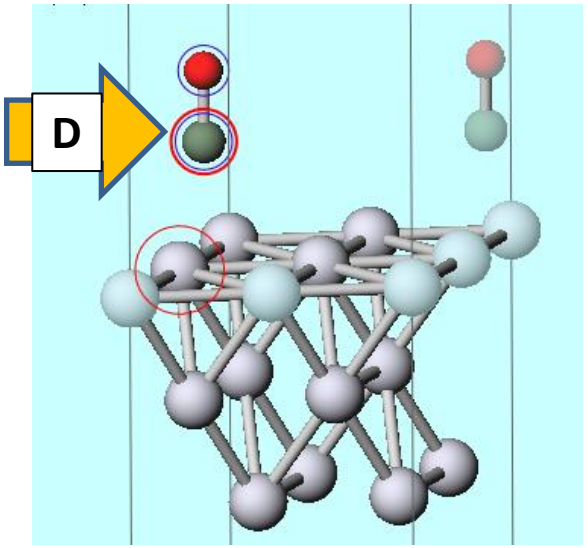


D. Adjusting the Position of Adsorbed Molecules

Here, we demonstrate how to adjust the distance between the C atom of the adsorbed molecule and the first layer of the Pt slab surface to 2 Å.

A. Click **Select | Select None**.
B. Click on any Pt atom in the first layer of the surface (a thick red circle will move to the Pt atom).
C. Click on the C atom of the adsorbed molecule (a thick red circle will move to the C atom).
D. Shift+click on the C atom of the adsorbed molecule to group select the adsorbed molecule.

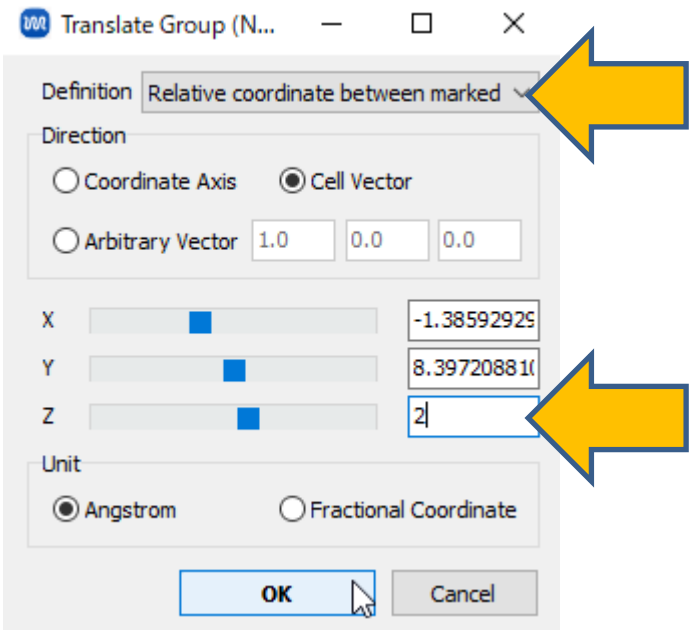


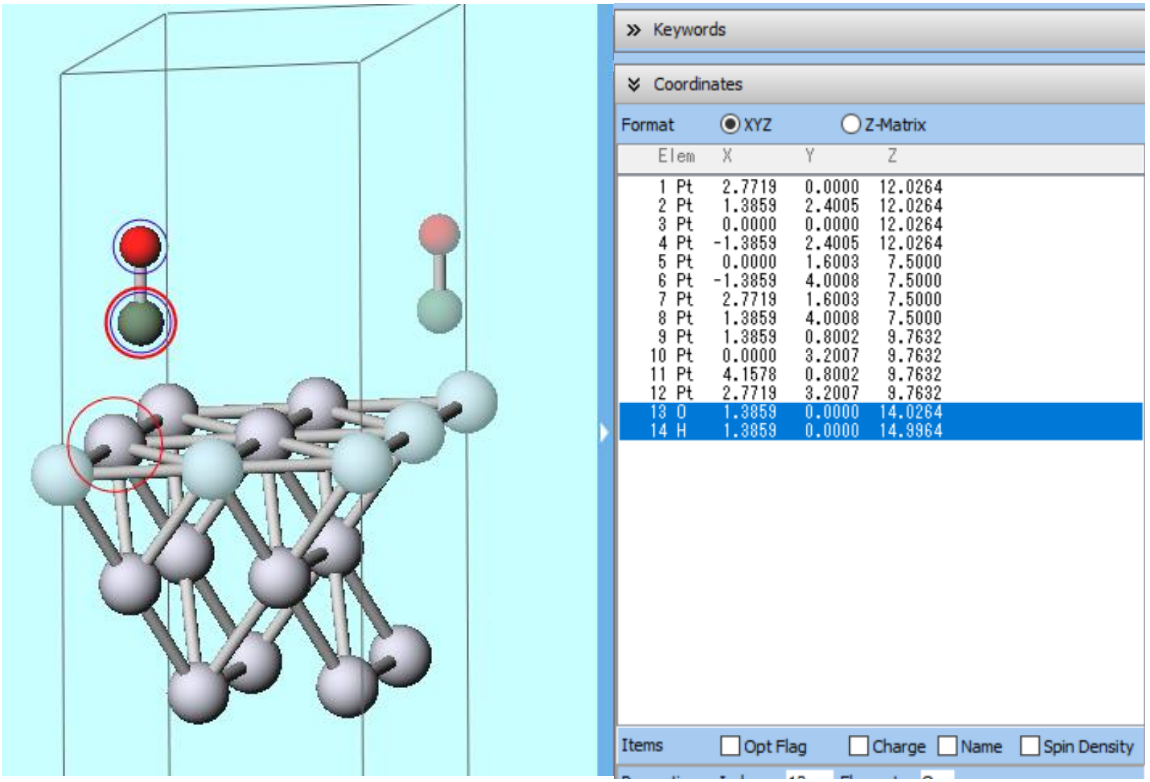


D. Adjusting the Position of Adsorbed Molecules

A. Click  **Modify Selected Group** | **Translate (Numerical)**を, and change **Definition** to 'Relative coordinate between marked atoms'.

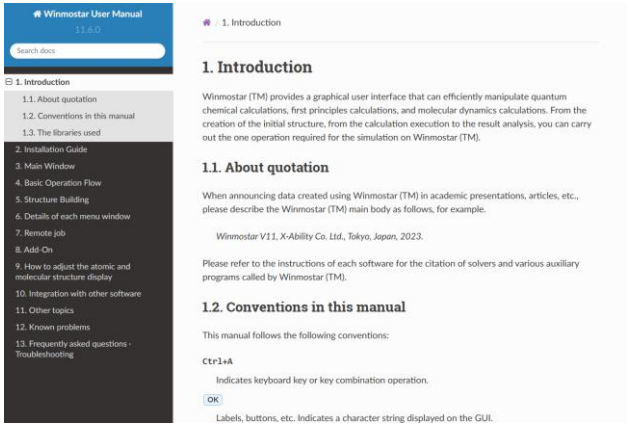
B. Change the value of **Z** to '2' and click 'OK'.





Troubleshooting and Additional Resources

- For detailed information on each feature, please refer to Winmostar User Manual.



Winmostar User Manual

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