Chapter 2.7

DATABASE

Stored Elemental Data

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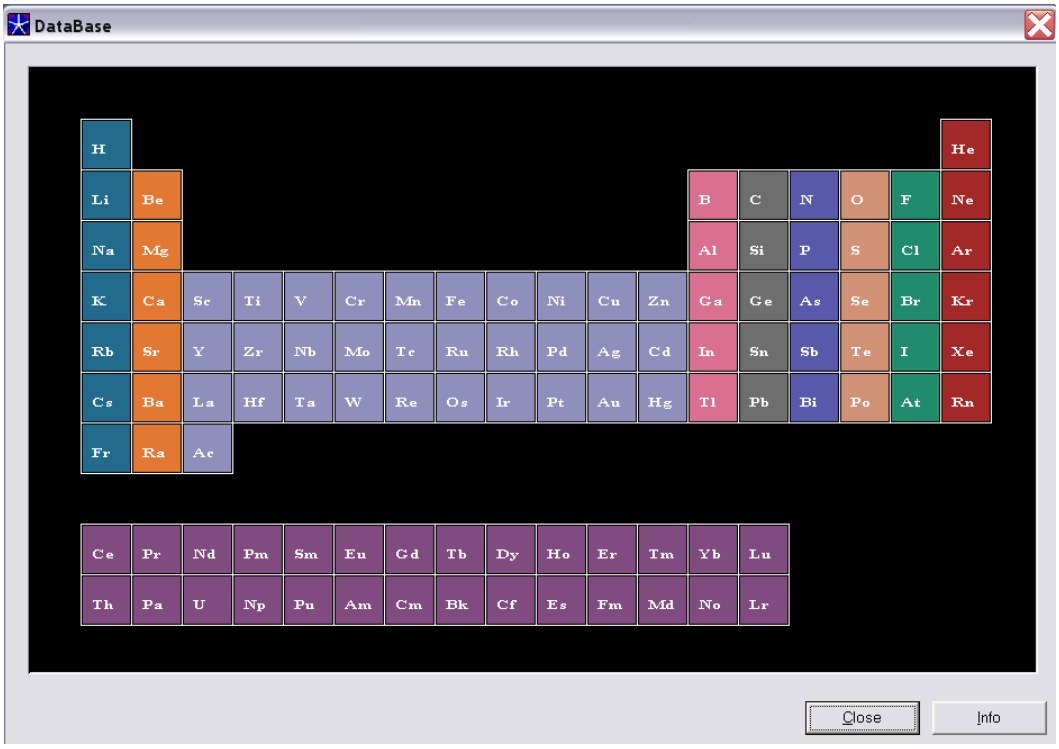
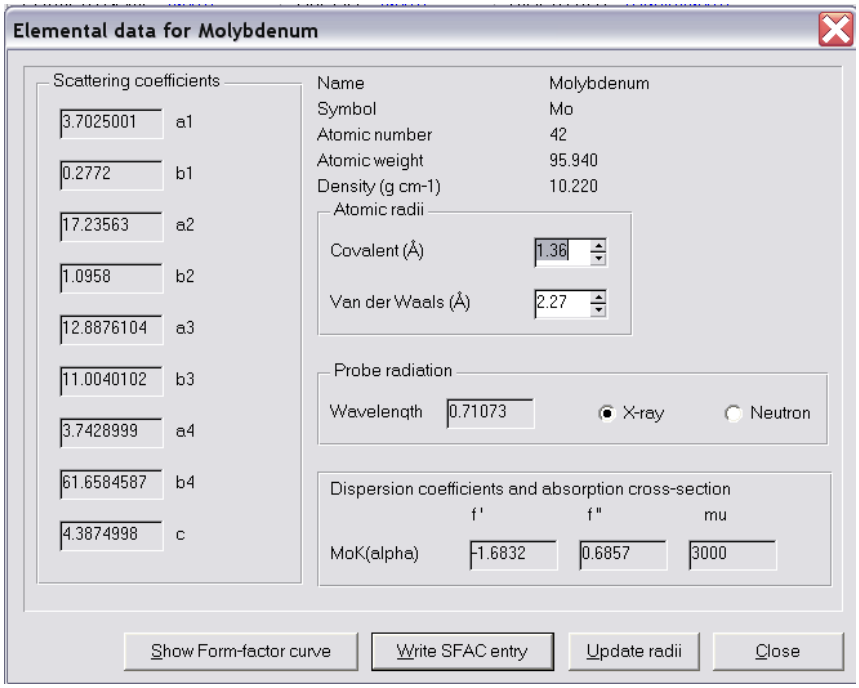
This menu item allows the user to view and adjust some of the elemental data stored in ***WinGX*** in the file *ELEMENT.DAT*. The following Periodic Table Window opens when this menu item is selected



Clicking on any element box, *e.g.* Mo gives the following Window :



This shows the scattering factors, dispersion and absorption coefficients and other data held on the element Molybdenum. It allows the user to change the covalent and van der Waals radii, which are used in other programs such as GEOM. In the present version of ***WinGX***, all other data are for information purposes only. Other options are :

- Clicking on the **OK** button saves the long form of the SHELX SFAC card into a file SFAC.OUT. These card images may be inserted in the .INS file to change the defaults for the SHELX programs.
- Clicking on the **Display SFAC** button gives a graphical display of the scattering factor as a function of $\sin(\theta)/\lambda$. The curves are shown with the *U* values of 0.0 (rest atom) and 0.03 and 0.05 $Å^2$