19. H, S, C AND G DIAGRAMS

The diagram module presents the basic thermochemical data for the given species in graphical format. Eight different diagram types can be drawn as a function of temperature:

- H Enthalpy (total)
- H Enthalpy (latent)
- S Entropy
- Cp Heat Capacity
- G Gibbs Energy
- DH
- DS
- DG (Ellingham diagrams)

The basic steps for drawing a diagram for all types is quite the same, except the small difference with the DG-diagrams. These steps are described in more detail in following lines, see example in Fig. 1:

1. Type the **species** formulae to the first column of the **X-data** sheet. There is no need to open the other sheets, because these are in the programs internal use only.
2. Select the diagram type from **Diagram Type** list, in this example H Enthalpy (latent) has been selected, see Fig. 1.
3. **DG-diagrams only**: Select an element from the list (for example: O for oxides, S for sulfides, Cl for chlorides, etc.) and press **Balance Element Amount**.
4. Press **Read Data from Database**. This will search the data from the database for the given ranges. You can force the HSC to use its own or main database by setting 1 or 2 to the **Database No** column. Without this setting, the diagram module looks for the data first from HSC own database and then from the main database.
5. Press **Diagram** to draw the diagram. You can also modify all the default settings such as x- and y-axis ranges and units. However, you must always press **Read Data from Database** after these modifications before you can press the **Diagram**.

An example of a diagram is shown in Fig. 2. The **solid lines** show the values, which are based on data in the database, and the **dotted lines** show the extrapolated values. Sometimes the extrapolated data may behave irregularly because the Cp-function extrapolates incorrectly outside the given range. The scales, lines and labels can be edited in the same manner as in the other graphics routines.

The DG-diagrams (Ellingham) show the relative stability of various oxides, sulfates, chlorides etc. These diagrams must contain only the same type of substances, such as oxides, sulfides, chlorides, etc. The species amounts must be balanced to contain exactly the same amount of the main element, such as oxygen in oxides and sulfur in sulfides.

An example of Ellingham diagram settings is given in Fig. 3. The results in Fig. 4 show, for example, that iron oxides can be reduced with carbon at higher temperatures than 700 °C, i.e. FeO + C -> Fe + CO(g). Metals whose oxide DG is smaller at a selected temperature, Fig. 4, can be used to reduce those oxides where the DG is higher. The most stable oxides (Cr_2O_3, MgO) are located at the bottom of the diagram.

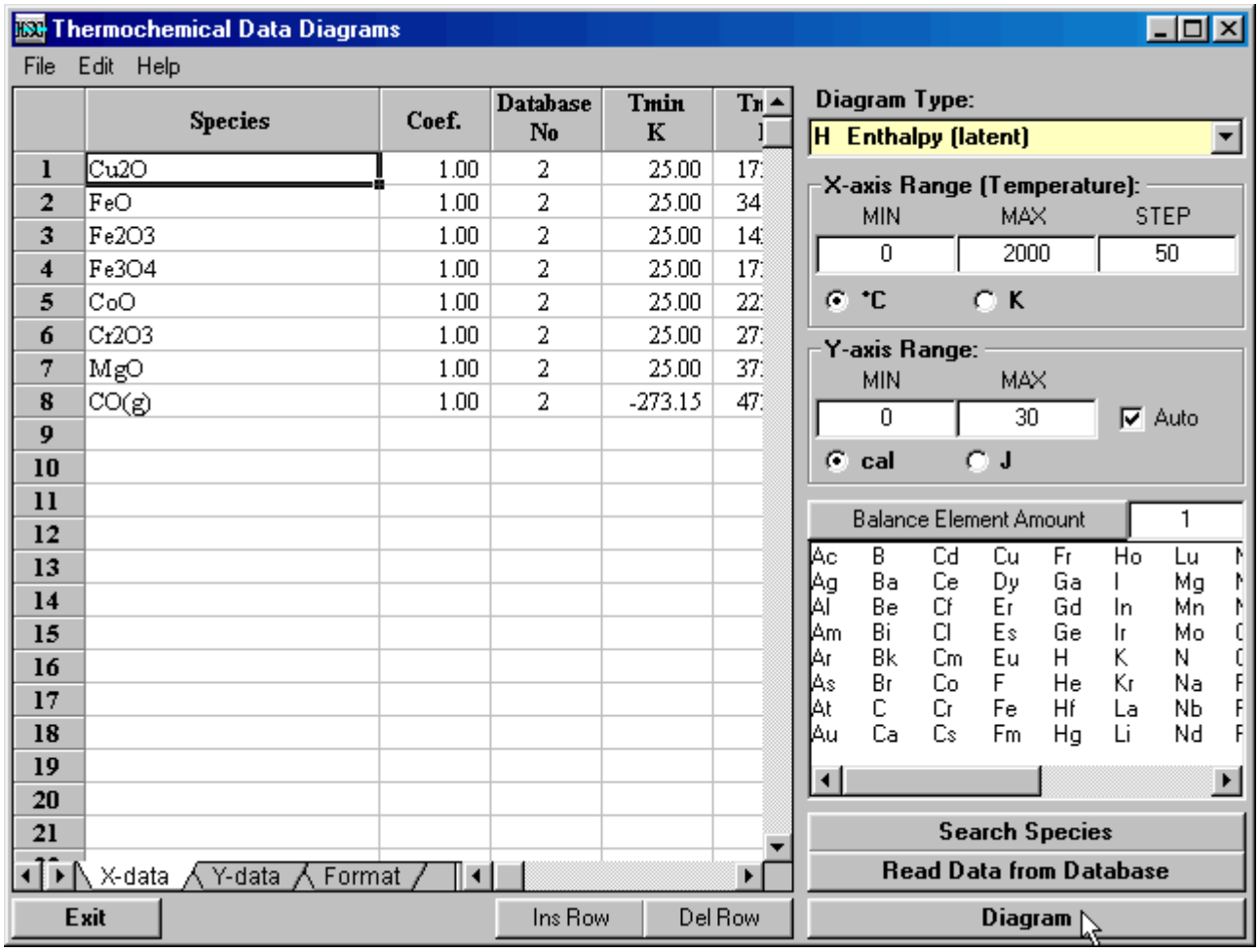

Fig. 1. The diagram menu. Enthalpy diagram type selected.

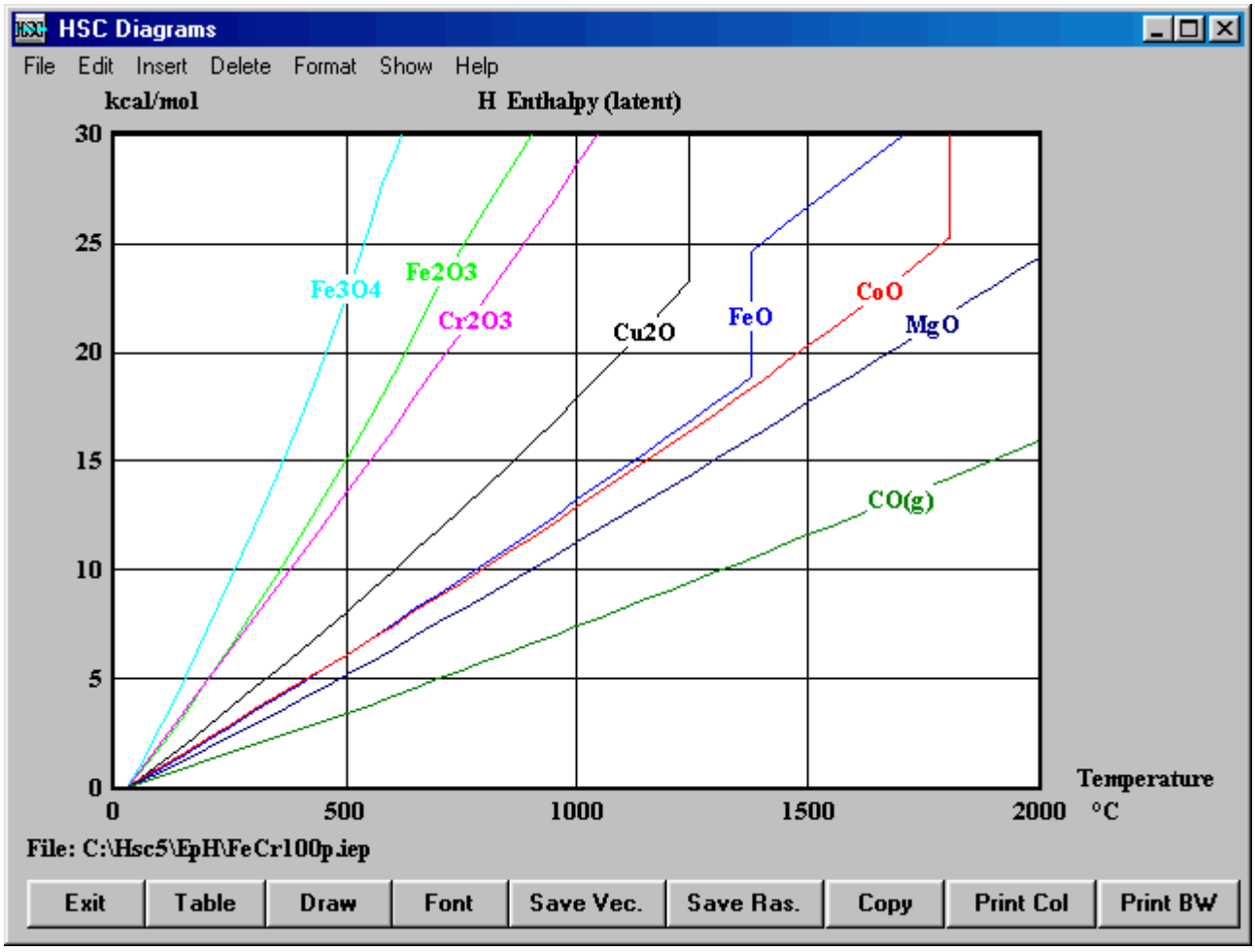

Fig. 2. The Enthalpy (latent) diagram based on the settings in Fig. 1.

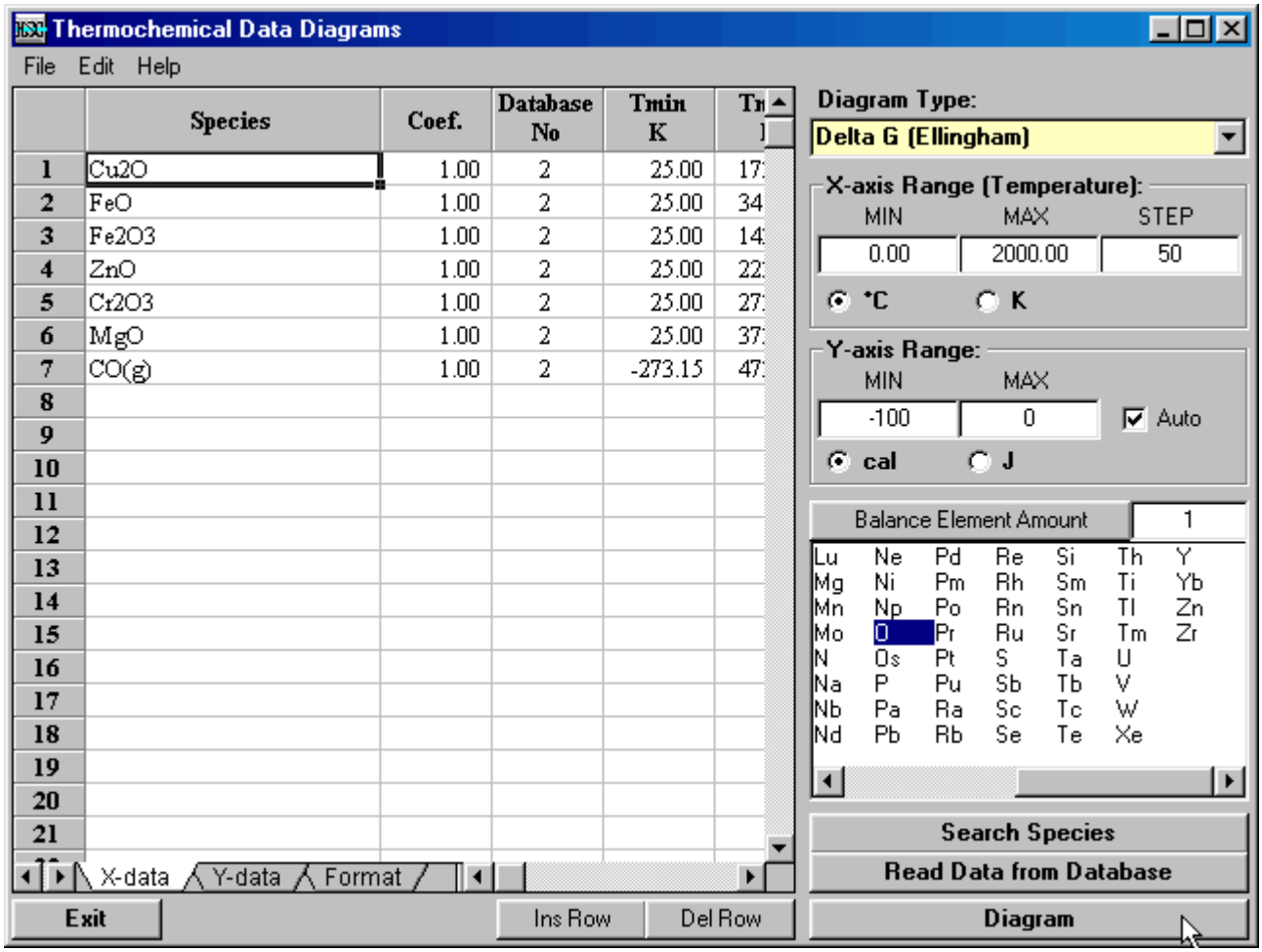

Fig. 3. Diagram settings of the Ellingham diagram for oxides.

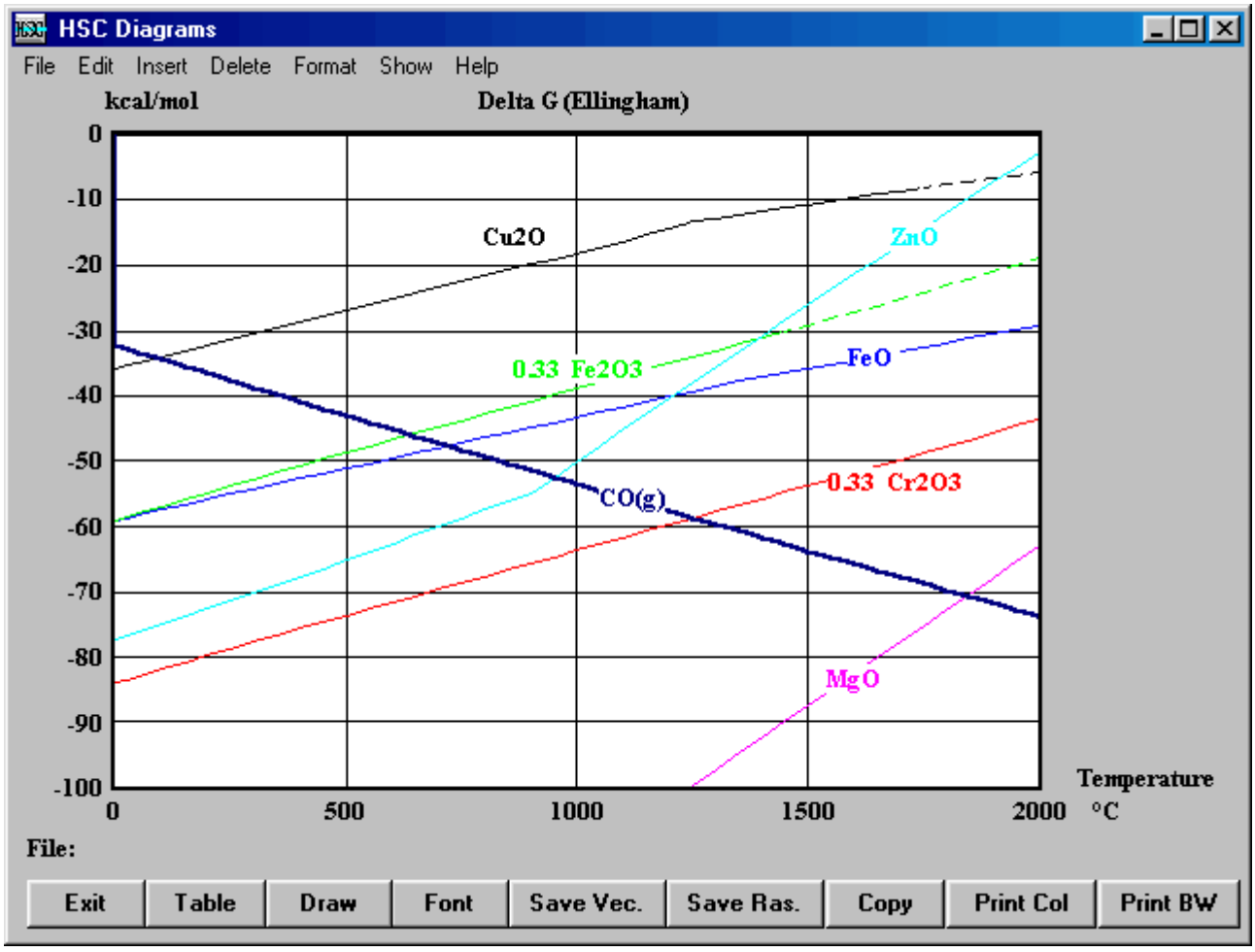

Fig. 4. Ellingham diagram of oxides based on the settings in Fig. 3.