# The *EpH* module

- Use ***EpH*** to calculate and plot isothermal EpH (Pourbaix) diagrams.
- ***Note:*** ***EpH*** accesses compound databases, i.e. treats the aqueous phase as an ideal solution.

Table of Contents

# The *EpH* module

**1° Click** on ***EpH*** in the main ***FactSage*** window.

# Preparing a calculation

The following five slides show how a simple metal-water Pourbaix diagram is generated.

The type of system is selected, the desired element(s) is (are) entered, the axes ranges are defined, the type of output is selected.

# Specifying the Cu-water Eh-pH diagram: the Elements frame

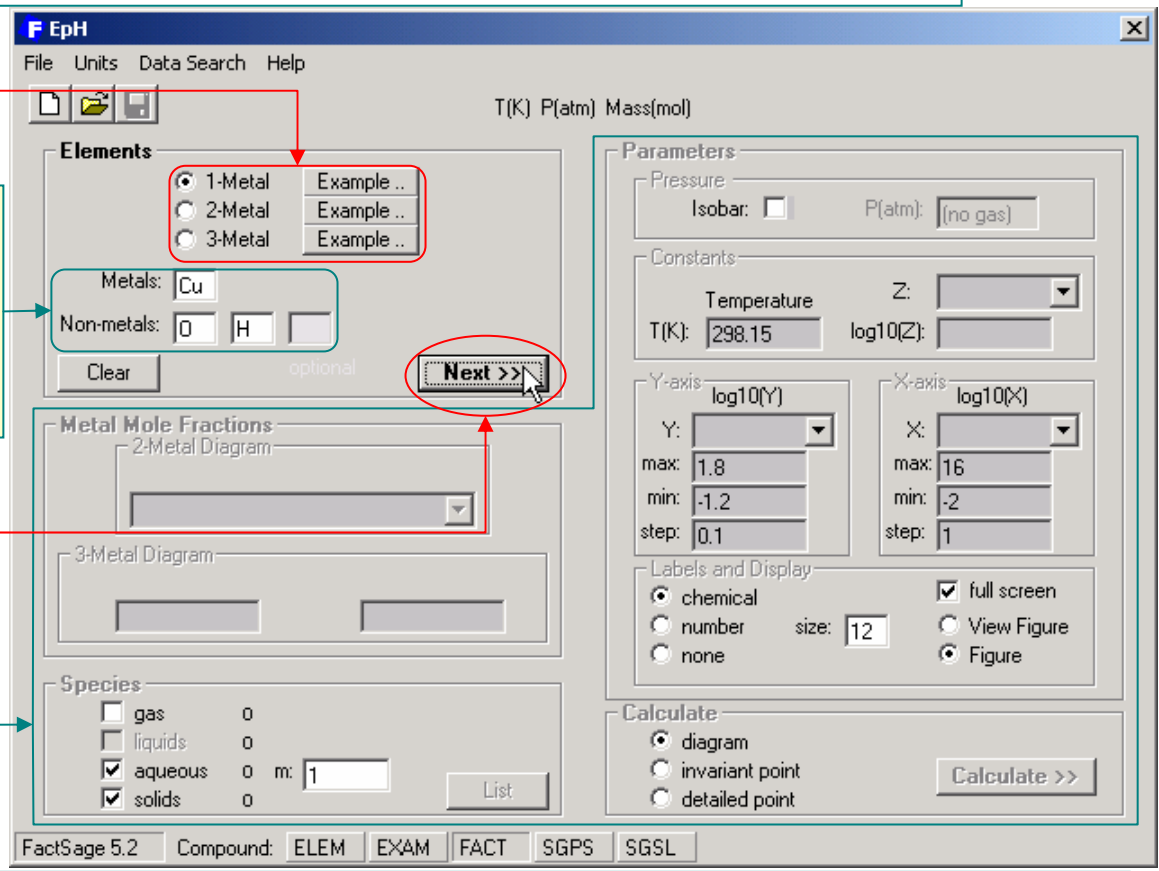
***EpH*** generates redox **potential-pH** (**Pourbaix**) **diagrams** using data from the **compound databases** that include **dilute Henrian solutes**.

**1°** **Specify** the type of Pourbaix diagram (**1-**, 2- or 3-Metal)

**2°** **Enter** the elements: **Cu**, **O**, **H** (**O** and **H** are **automatically** entered). **Cu-based species will appear in all domains**.

**3°** **Click** the **Next >>** button to initiate the **data search**.

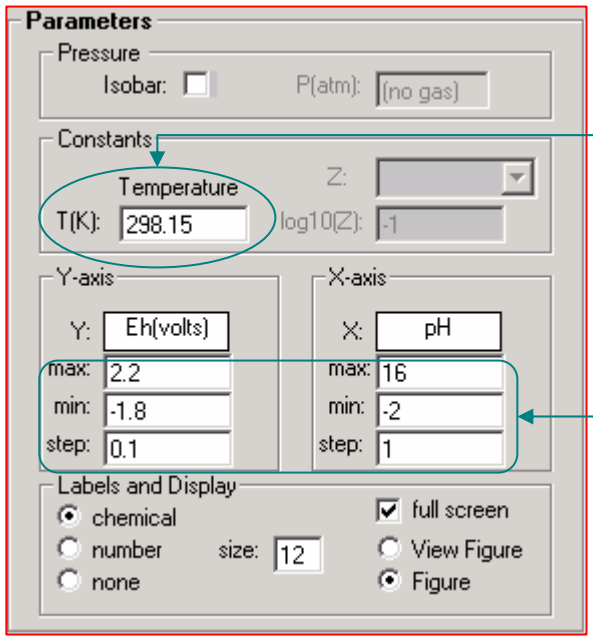
The other frames are activated when the **data search** is completed.




When you **click** the **Next >>** button the pure substances databases are automatically searched to find all the compounds (and henrian solutes) involving the indicated elements. Any time you make changes in the **Elements** frame all other frames are deactivated and it is necessary to **click** the **Next >>** button to **refresh** the system.

# Specifying the Cu-water Eh-pH diagram: the Parameters frame

**Pressure:** The total pressure has no effect upon the ***EpH*** diagram. If you specify a total pressure isobar, this will appear as a series of '**+**'s on the calculated diagram. The total pressure is the sum of partial pressures of all gaseous species and is only computed after the diagram has been calculated. For example, see the **Ti-H-O-F** diagram on slides 6.0 to 6.2. Note that the calculation of the isobar for a large system can be time consuming.



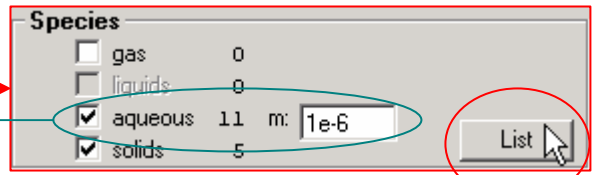

**Constants: Here, T = 298.15 K.**
For a diagram with a non metallic element other than H and O (Ti-H-O-F for example), it is necessary to specify an additional thermodynamic variable, Z.

**Axes: Here,** the limits are: **-1.8** to **2.2** for the **potential** and **-2** to **16** for the **pH.**
The axes are alwaysEh(volts) and pH. The step size determines the axis «ticks» and labels on the diagram and the density of characters '**+**' for the total pressure isobar. A step of **0.1** for the Y-axis and **1** for the X-axis is typical.

**Labels and Display:** Here you can control the size (8 – 20) and type of labels on the calculated diagrams. ***View Figure*** produces a crude ***EpH*** diagram that can not be edited. However it is a very efficient module that only requires a small amount of computer memory. ***Figure*** creates an ***EpH*** diagram that can be **edited**, **manipulated** and **stored** in a variety of ways. However, ***Figure*** requires a lot of computer memory and may overwhelm the resources of the PC.

# Specifying the Cu-water Eh-pH diagram: the Species frame

Here you **select** the species to be used in calculation. You may **include** or **exclude** all the **gases**, all the **solids** or all the **liquids**. Unless indicated otherwise, metallic species are assumed to be pure and at unit activity, molality or partial pressure. You can also use the input box "**m:**" to set a common value to all **aqueous** species. For example, **m = 1×10$^{-6}$**. To **examine** the species or to **add** or **remove** a particular species or **change** its activity, molality or partial pressure, **click** the "**List**" button.




The **concentration** of ions provides the **standard** **Pourbaix** diagram used in **corrosion** application.

List - P(atm), T(K) = 298.15

File Edit Help

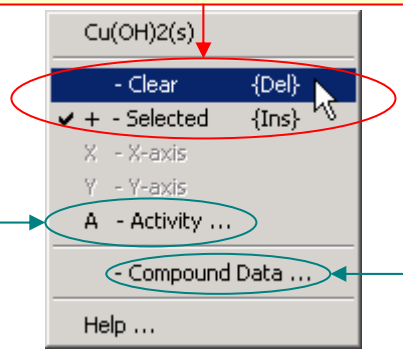
| + | Code | A | T | Species | Data | A/P/M | Cp range | G(KJ) | G(Kcal) |
|---|---|---|---|---|---|---|---|---|---|
| | | | | Cu gases: | | | | | |
| | 1 | | | Cu(g) | FACT | 1.0000E+00 | 298 - 6000 | 288.021 | 68.839 |
| | 2 | | | Cu2(g) | FACT | 1.0000E+00 | 298 - 6000 | 413.308 | 98.783 |
| | 3 | | | CuO(g) | FACT | 1.0000E+00 | 298 - 6000 | 236.351 | 56.489 |
| | | | | Cu liquids: | | | | | |
| | 4 | | | Cu(l) | FACT | 1.0000E+00 | 298 - 4000 | -0.552 | -0.132 |
| | 5 | | | Cu2O(l) | FACT | 1.0000E+00 | 298 - 2000 | -150.740 | -36.028 |
| | | | | Cu aqueous species: | | | | | |
| + | 6 | A | | Cu[+] | FACT | 1.0000E-06 | 298 - 573 | 59.446 | 14.208 |
| + | 7 | A | | Cu[2+] | FACT | 1.0000E-06 | 298 - 573 | 94.542 | 22.596 |
| + | 8 | A | | CuO2[2-] | FACT | 1.0000E-06 | 298 - **** | -183.678 | -43.900 |
| + | 9 | A | | HCuO2[-] | FACT | 1.0000E-06 | 298 - **** | -258.571 | -61.800 |
| | | | | Cu solids: | | | | | |
| + | 10 | | | Cu(s) | FACT | 1.0000E+00 | 298 - 2001 | -9.888 | -2.363 |
| + | 11 | | | CuO(s) | FACT | 1.0000E+00 | 298 - 2000 | -168.762 | -40.335 |
| + | 12 | | | Cu2O(s) | FACT | 1.0000E+00 | 298 - 2000 | -198.244 | -47.381 |
| + | 13 | | | Cu(OH)2(s) | FACT | 1.0000E+00 | 298 - 1500 | -482.675 | -115.362 |
| | | | | | | | | | |
| | | | | Other gases: | | | | | |
| | 14 | | | H(g) | FACT | | 298 - 6000 | 183.829 | 43.936 |
| | 15 | | | H2(g) | FACT | | 298 - 6000 | -38.930 | -9.304 |
| | 16 | | | O(g) | FACT | | 298 - 6000 | 201.186 | 48.085 |
| | 17 | | | O2(g) | FACT | | 298 - 6000 | -61.132 | -14.611 |
| | 18 | | | O3(g) | FACT | | 298 - 6000 | 71.469 | 17.082 |

# Specifying the Cu-water Eh-pH diagram: the List window

We **suppress** species 13: **$Cu(OH)_2$** in order to compare the calculated diagram with one published in the «**Atlas of Electrochemical Equilibria in Aqueous Solution**» (M. Pourbaix, Pergammon Press, 1966)

**Click** in the **+** to **remove** species **13**. You can also **right-click** on the «+» column to access an extended menu and **select clear**.

| + | Code | A | T | Species | Data | A/P/M | Cp range | G(KJ) | G(Kcal) |
|---|---|---|---|---|---|---|---|---|---|
| | | | | Cu gases: | | | | | |
| | 1 | | | Cu(g) | FACT | 1.0000E+00 | 298 - 6000 | 288.021 | 68.839 |
| | 2 | | | Cu2(g) | FACT | 1.0000E+00 | 298 - 6000 | 413.308 | 98.783 |
| | 3 | | | CuO(g) | FACT | 1.0000E+00 | 298 - 6000 | 236.351 | 56.489 |
| | | | | Cu liquids: | | | | | |
| | 4 | | | Cu(l) | FACT | 1.0000E+00 | 298 - 4000 | -0.552 | -0.132 |
| | 5 | | | Cu2O(l) | FACT | 1.0000E+00 | 298 - 2000 | -150.740 | -36.028 |
| | | | | Cu aqueous species: | | | | | |
| + | 6 | A | | Cu[+] | FACT | 1.0000E-06 | 298 - 573 | 59.446 | 14.208 |
| + | 7 | A | | Cu[2+] | FACT | 1.0000E-06 | 298 - 573 | 94.542 | 22.596 |
| + | 8 | A | | CuO2[2-] | FACT | 1.0000E-06 | 298 - ***** | -183.678 | -43.900 |
| + | 9 | A | | HCuO2[-] | FACT | 1.0000E-06 | 298 - ***** | -258.571 | -61.800 |
| | | | | Cu solids: | | | | | |
| + | 10 | | | Cu(s) | FACT | 1.0000E+00 | 298 - 2001 | -9.888 | -2.363 |
| + | 11 | | | CuO(s) | FACT | 1.0000E+00 | 298 - 2000 | -168.762 | -40.335 |
| + | 12 | | | Cu2O(s) | FACT | 1.0000E+00 | 298 - 2000 | -198.244 | -47.381 |
| | 13 | | | Cu(OH)2(s) | FACT | 1.0000E+00 | 298 - 1500 | -482.675 | -115.362 |
| | | | | Other gases: | | | | | |
| | 14 | | | H(g) | FACT | | 298 - 6000 | 183.829 | 43.936 |
| | 15 | | | H2(g) | FACT | | 298 - 6000 | -38.930 | -9.304 |
| | 16 | | | O(g) | FACT | | 298 - 6000 | 201.186 | 48.085 |
| | 17 | | | O2(g) | FACT | | 298 - 6000 | -61.132 | -14.611 |
| | 18 | | | O3(g) | FACT | | 298 - 6000 | 71.469 | 17.082 |
| | 19 | | | OH(g) | FACT | | 298 - 6000 | -15.753 | -3.765 |
| | 20 | | | H2O(g) | FACT | | 298 - 6000 | -298.102 | -71.248 |
| | 21 | | | HO2(g) | FACT | | 298 - 6000 | -66.183 | -15.818 |
| | | | | | | | 298 - 1500 | -205.540 | -49.125 |
| | | | | | | | 298 - 500 | -306.686 | -73.300 |
| | | | | | | | 298 - 431 | -219.984 | -52.577 |
| | | | | | | | 298 - 500 | 0.000 | 0.000 |
| + | 26 | A | | H2(aq) | FACT | | 289 - 573 | -21.399 | -5.114 |
| + | 27 | A | | O2(aq) | FACT | | 298 - 400 | -44.773 | -10.701 |
| + | 28 | A | | OH[-] | FACT | | 298 - 573 | -226.744 | -54.193 |
| + | 29 | A | | HO2[-] | FACT | | 298 - 573 | -167.358 | -39.999 |
| + | 30 | A | | HOOH(aq) | FACT | | 298 - 473 | -234.122 | -55.956 |
| + | 31 | A | | e[-](aq) | ELEM | | 298 - 6000 | -19.465 | -4.652 |
| | | | | Other solids: | | | | | |
| + | 32 | | T | H2O(s) | FACT | | 250 - 273 | -306.093 | -73.158 |

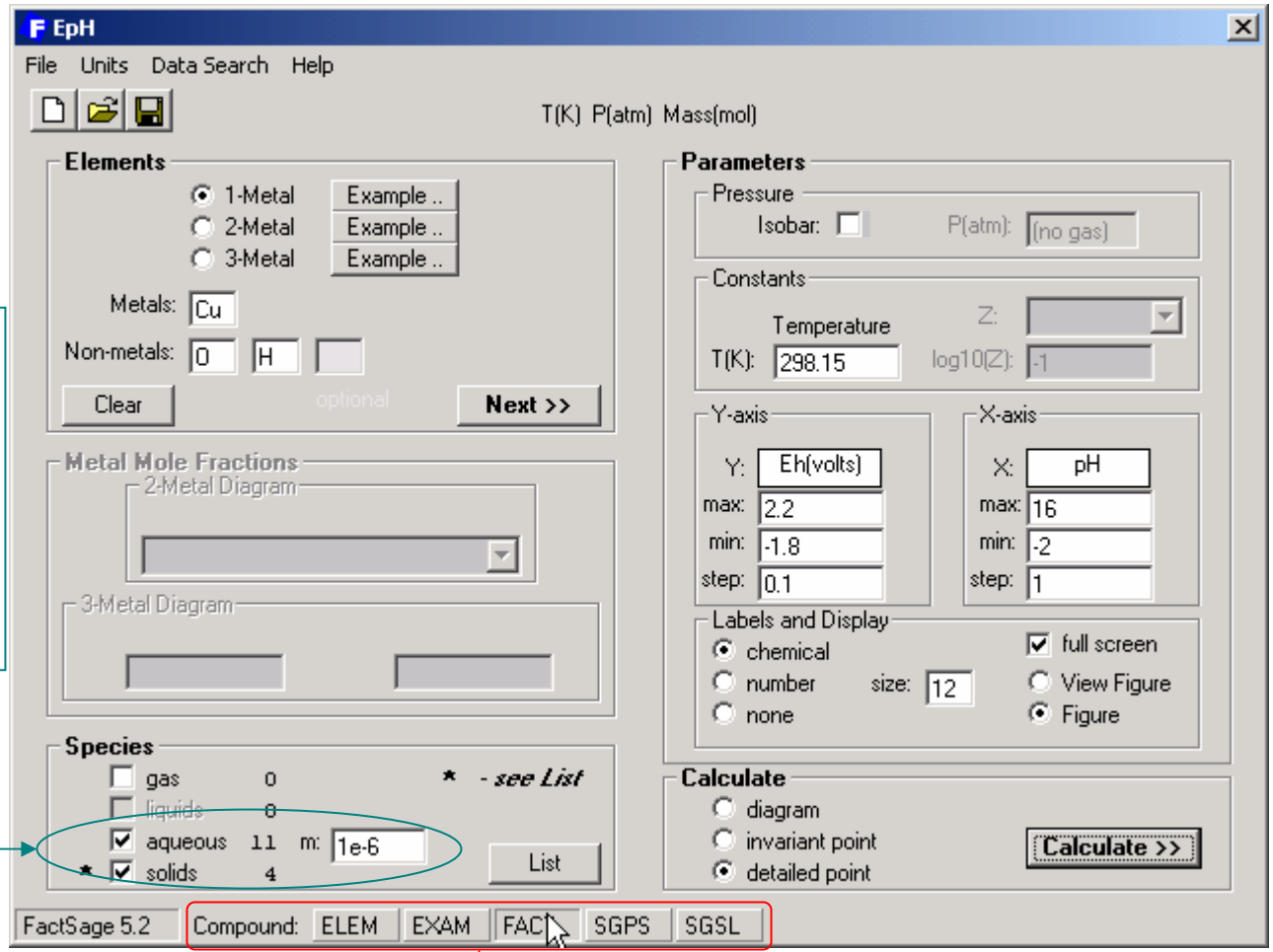



**Select** – Compound Data… or **double-click** on the species to **view** it's compound data.

You can **select** A – Activity… or **double-click** in the A/P/M column to **change** the activity (partial pressure or molality) of a species.

# Specifying the Cu-water Eh-pH diagram: Compound selection

**11 aqueous** species and **4 solids** species were selected in the ***FACT*** **compound** database containing **Cu**, **O** and/or **H**.




Here, only the ***FACT*** **compound** database is included.
See slides 9.0 to 9.2 for **inclusion** or **exclusion** of a **database**.

# Executing the calculation and generating a diagram

In the following three slides is shown how the Pourbaix diagram for the Cu-O-H system is generated.

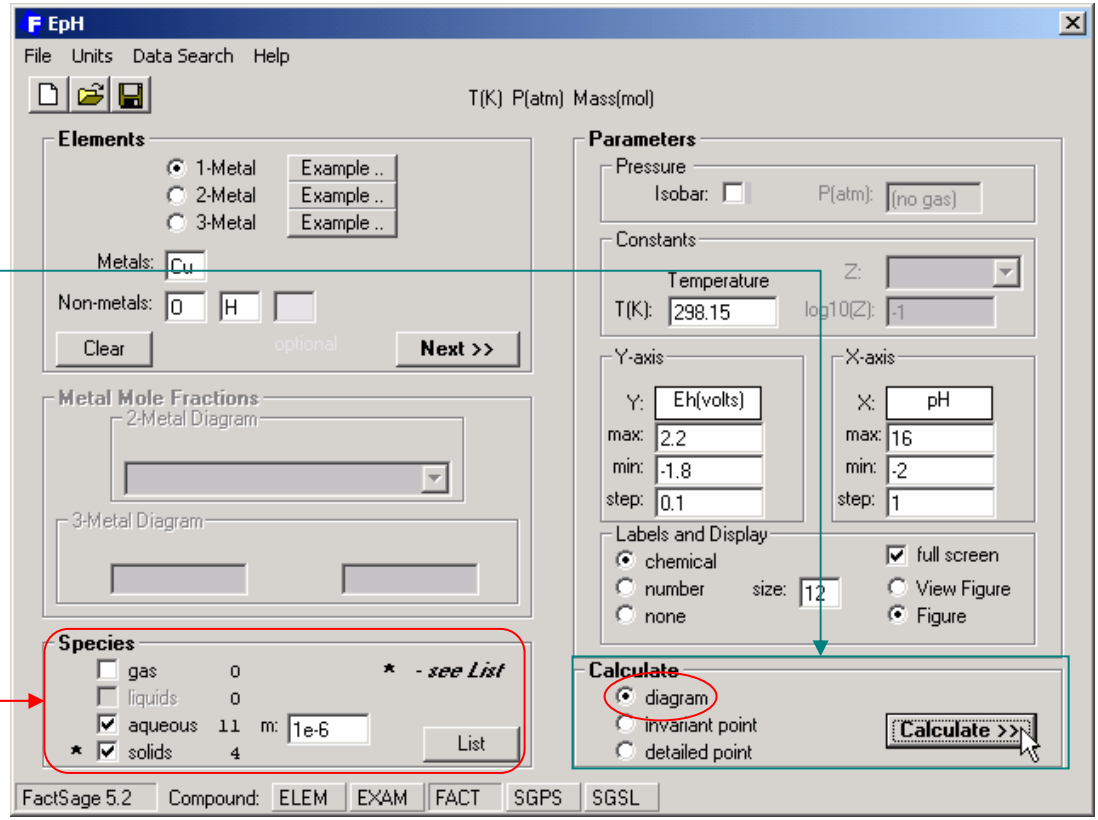
The diagram is compared with the appropriate diagram from the Pourbaix Atlas.

Furthermore explanations are given on the non-graphical types of output which can be generated with ***EpH*** calculations.

# Specifying the Cu-water Eh-pH diagram: the Calculate frame

- **Diagram:**
  Here the diagram is calculated and plotted. It may then be stored as a *.fig file or other graphics format.
- **Invariant Point:**
  This gives the precise position of the triple points as shown in slide 5.1 where three domains meet.

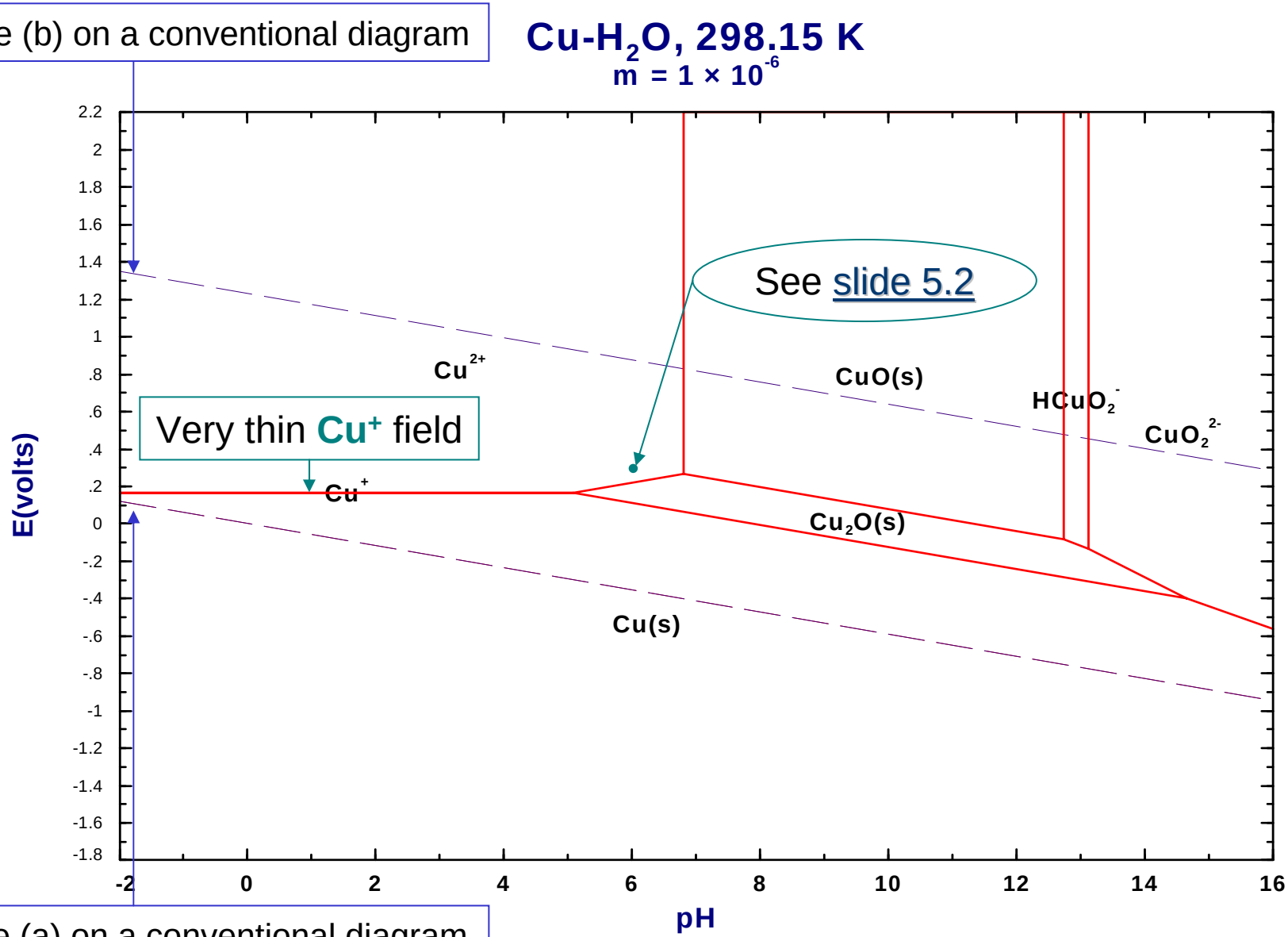
Please note the **custom** (*) **selection** of **solid** species.




- **Detailed Point:**
  This enables you to display the equilibrium activity or partial pressure of all species at a specified coordinate on the diagram. In the output shown in Slide 5.3, the specified coordinate falls in the field of $Cu^{2+}$. That is $Cu^{2+}$ is the stable species and its activity must be equal to the molality m specified for the aqueous species (here $1 \times 10^{-6}$) – the activities of the other Cu-bearing species are less than 1.0 for the solids and $1 \times 10^{-6}$ for the other aqueous species. The further the field of a species is from the specified coordinate the lower its activity.

# Cu-$H_2O$ Eh-pH diagram: Graphical Output

$O_2$ (1 atm) line (b) on a conventional diagram




$H_2$ (1 atm) line (a) on a conventional diagram

# Published **Pourbaix** diagram for **Cu-$H_2O$**

Lines for **m = 1 × $10^{-6}$** are highlighted in red.

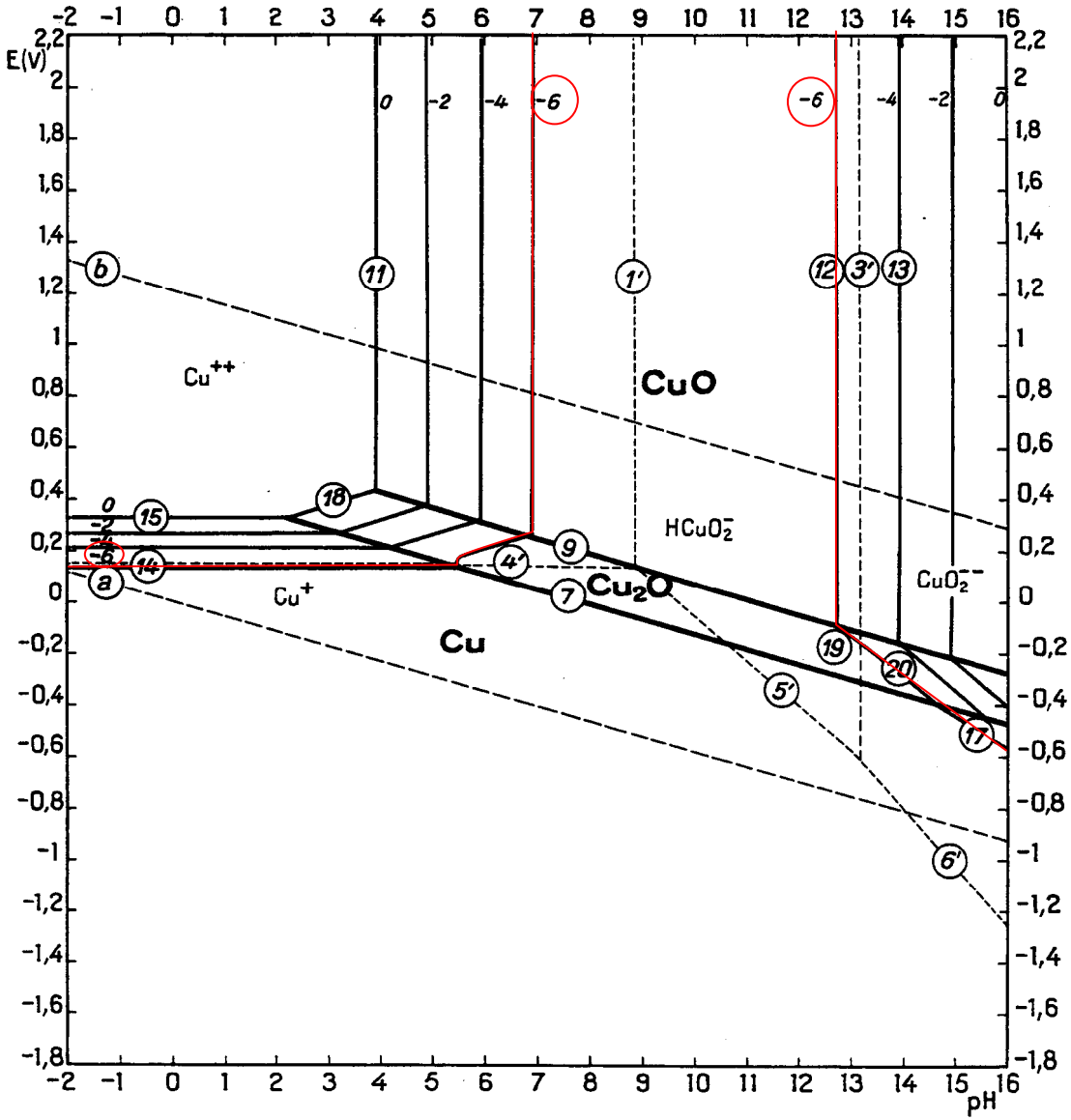



FIG. 1. Potential–pH equilibrium diagram for the system copper–water, at 25°C.
[Considering the solid substances Cu, $Cu_2O$ and CuO. $Cu(OH)_2$ is not considered.]

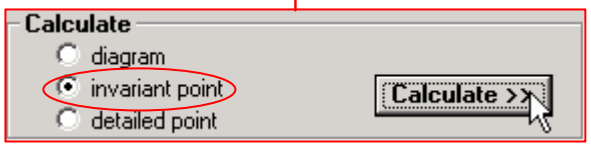
# Output options to obtain numerical results

The following three slides show the type of numerical/tabular result that is also possible with EpH.

Tables of invariant points and of a point calculation are shown for the system Cu-O-H.

# $Cu\text{-}H_2O$ Eh-pH diagram: Computation of invariant points

**Select invariant point** in the **Calculate frame** to **calculate invariant points**.



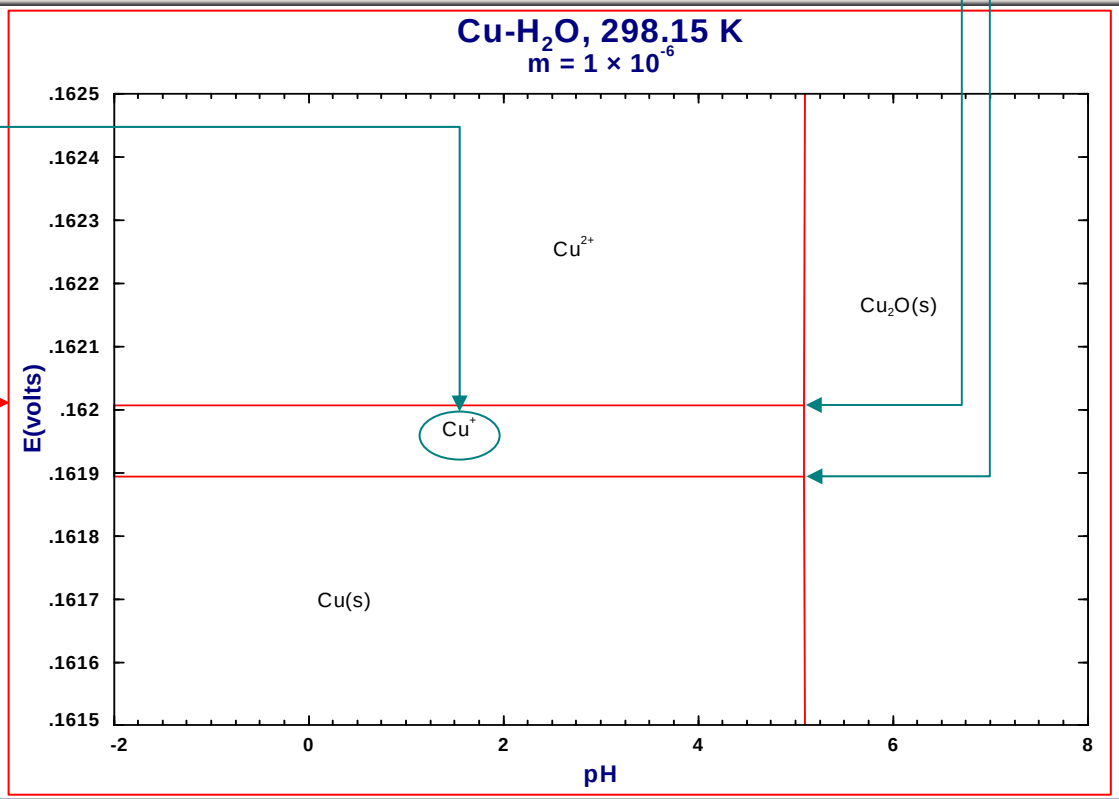

Invariant Points - E(volts), pH, T(K) = 298.15

File Edit

| E(volts) | pH | | Species A | | Species B | | Species C |
|---|---|---|---|---|---|---|---|
| 0.1619 | 5.0847 | 10 | Cu[s] | 6 | Cu[+] | 12 | Cu2O[s] |
| -0.4036 | 14.6431 | 10 | Cu[s] | 8 | CuO2[2-] | 12 | Cu2O[s] |
| 0.1620 | 5.0847 | 6 | Cu[+] | 7 | Cu[2+] | 12 | Cu2O[s] |
| 0.2635 | 6.8000 | 7 | Cu[2+] | 11 | CuO[s] | 12 | Cu2O[s] |
| -0.0875 | 12.7328 | 11 | CuO[s] | 12 | Cu2O[s] | 9 | HCuO2[-] |
| -0.1334 | 13.1207 | 8 | CuO2[2-] | 12 | Cu2O[s] | 9 | HCuO2[-] |

A very thin $Cu^+$ field indeed!

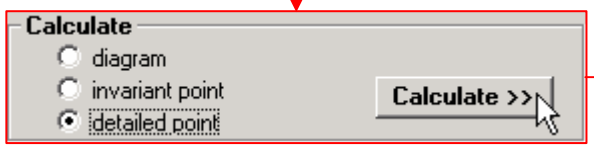
Enlargement of the previous diagram



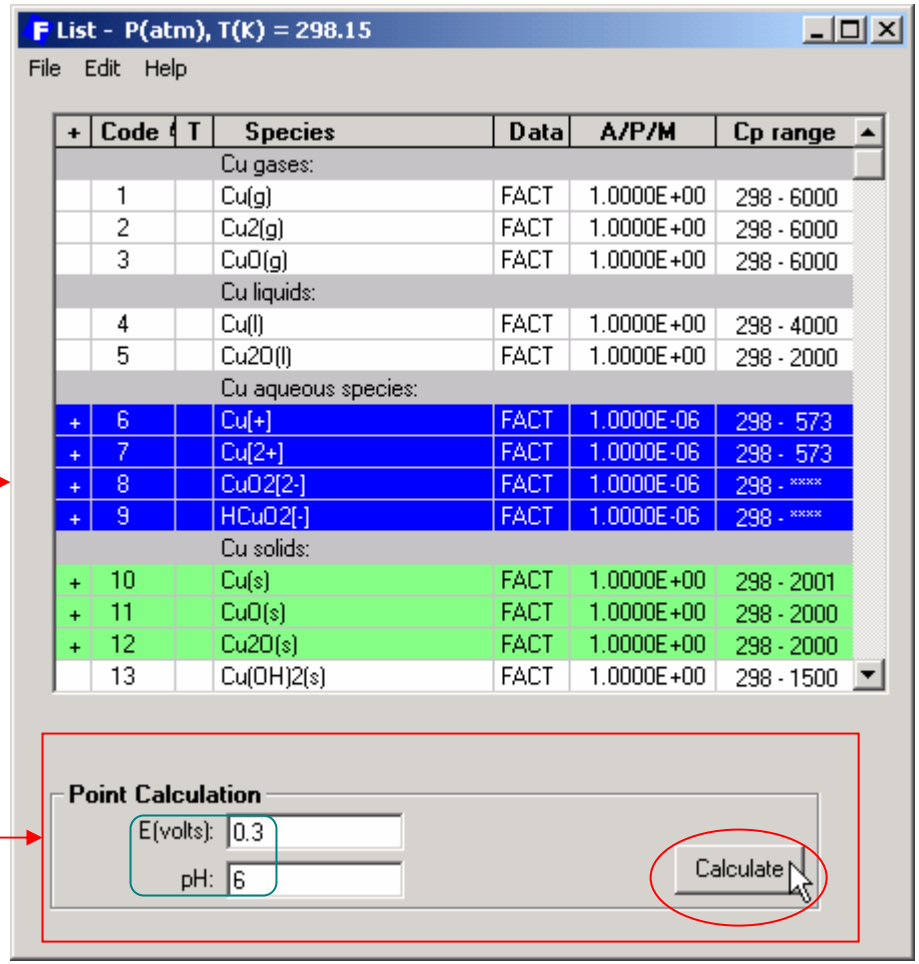
# $Cu\text{-}H_2O$ Eh-pH diagram: Detailed Point Calculation

The point calculation gives activities and ideal concentrations for all metal-element containing species at the specified coordinate.

**1° Select detailed point in the Calculate frame to open a Point Calculation dialog box.**

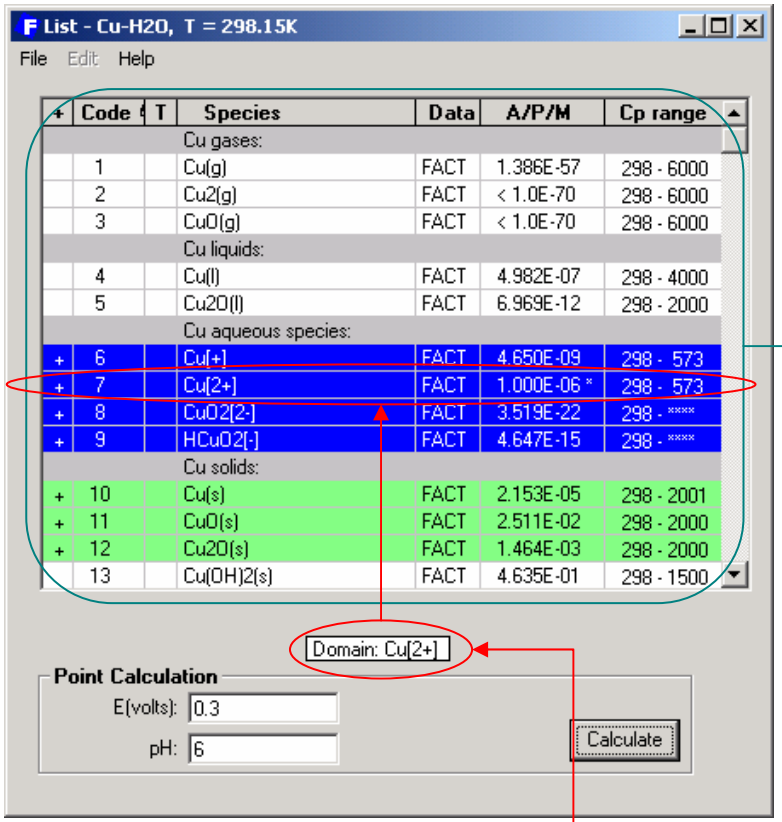



**2° Enter the coordinate of interest and press the Calculate button.**




**The specified coordinate is in the domain of $Cu^{2+}$ set at $10^{-6}$ (the green dot on slide 4.2).**

# Cu-$H_2O$ Eh-pH diagram: Detailed Point Calculation – Output




| + | Code | T | Species | Data | A/P/M | Cp range |
|---|---|---|---|---|---|---|
| | | | Cu gases: | | | |
| | 1 | | Cu(g) | FACT | 1.386E-57 | 298 - 6000 |
| | 2 | | Cu2(g) | FACT | < 1.0E-70 | 298 - 6000 |
| | 3 | | CuO(g) | FACT | < 1.0E-70 | 298 - 6000 |
| | | | Cu liquids: | | | |
| | 4 | | Cu(l) | FACT | 4.982E-07 | 298 - 4000 |
| | 5 | | Cu2O(l) | FACT | 6.969E-12 | 298 - 2000 |
| | | | Cu aqueous species: | | | |
| + | 6 | | Cu[+] | FACT | 4.650E-09 | 298 - 573 |
| + | 7 | | Cu[2+] | FACT | 1.000E-06 * | 298 - 573 |
| + | 8 | | CuO2[2-] | FACT | 3.519E-22 | 298 - ***** |
| + | 9 | | HCuO2[-] | FACT | 4.647E-15 | 298 - ***** |
| | | | Cu solids: | | | |
| + | 10 | | Cu(s) | FACT | 2.153E-05 | 298 - 2001 |
| + | 11 | | CuO(s) | FACT | 2.511E-02 | 298 - 2000 |
| + | 12 | | Cu2O(s) | FACT | 1.464E-03 | 298 - 2000 |
| | 13 | | Cu(OH)2(s) | FACT | 4.635E-01 | 298 - 1500 |
| | | | | | | |
| | | | Other gases: | | | |
| | 14 | | H(g) | FACT | 2.059E-47 | 298 - 6000 |
| | 15 | | H2(g) | FACT | 7.210E-23 | 298 - 6000 |
| | 16 | | O(g) | FACT | 9.714E-61 | 298 - 6000 |
| | 17 | | O2(g) | FACT | 1.502E-39 | 298 - 6000 |
| | 18 | | O3(g) | FACT | < 1.0E-70 | 298 - 6000 |
| | 19 | | OH(g) | FACT | 3.252E-37 | 298 - 6000 |
| | 20 | | H2O(g) | FACT | 3.135E-02 | 298 - 6000 |
| | 21 | | HOO(g) | FACT | 3.808E-53 | 298 - 6000 |
| | 22 | | HOOH(g) | FACT | 3.263E-43 | 298 - 1500 |
| | | | Other liquids: | | | |
| | 23 | | H2O(l) | FACT | 1.000E+00 | 298 - 500 |
| | 24 | | HOOH(l) | FACT | 1.107E-40 | 298 - 431 |
| | | | Other aqueous species: | | | |
| + | 25 | | H[+] | FACT | 1.000E-06 | 298 - 500 |
| + | 26 | | H2(aq) | FACT | 6.120E-26 | 289 - 573 |
| + | 27 | | O2(aq) | FACT | 2.045E-42 | 298 - 400 |
| + | 28 | | OH[-] | FACT | 9.883E-09 | 298 - 573 |
| + | 29 | | HO2[-] | FACT | 6.675E-44 | 298 - 573 |
| + | 30 | | HOOH(aq) | FACT | 3.318E-38 | 298 - 473 |
| + | 31 | | e[-](aq) | ELEM | 8.491E-06 | 298 - 6000 |
| | | | Other solids: | | | |
| + | 32 | T | H2O(s) | FACT | 7.872E-01 | 250 - 273 |

**$Cu^{2+}$** is the stable species and its activity must be equal to the molality **m** specified for the aqueous species (here **$1 \times 10^{-6}$**) – the activities of the other Cu-bearing species are less than 1.0 for the solids and than $m = 1 \times 10^{-6}$ in our case for the other aqueous species. The further the field of a species is from the specified coordinate the lower its activity.

# A metal-water-gas system: Ti-O-H-F

The following two slides show the input and calculated diagram for a metal-water-gas system.

The results are for the Ti-O-H-F system.

# One-metal Eh-pH diagram with four elements: Ti-O-H-F

**Specifying** the Eh-pH diagram for: **Ti-O-H-F** at 298.15 K and m [$F^-$] = 0.1 (i.e. $\log_{10}$ (m [$F^-$]) = -1).

**1° Enter** the elements. This is a **1-metal Ti** system as metal with **O**, **H** and **F** as non-metallic elements.

**2° Press Next** to search the compound databases.

**3° To Calculate** an isobar, **Check** Isobar and **enter** a value (**here, 0.05 atm**).

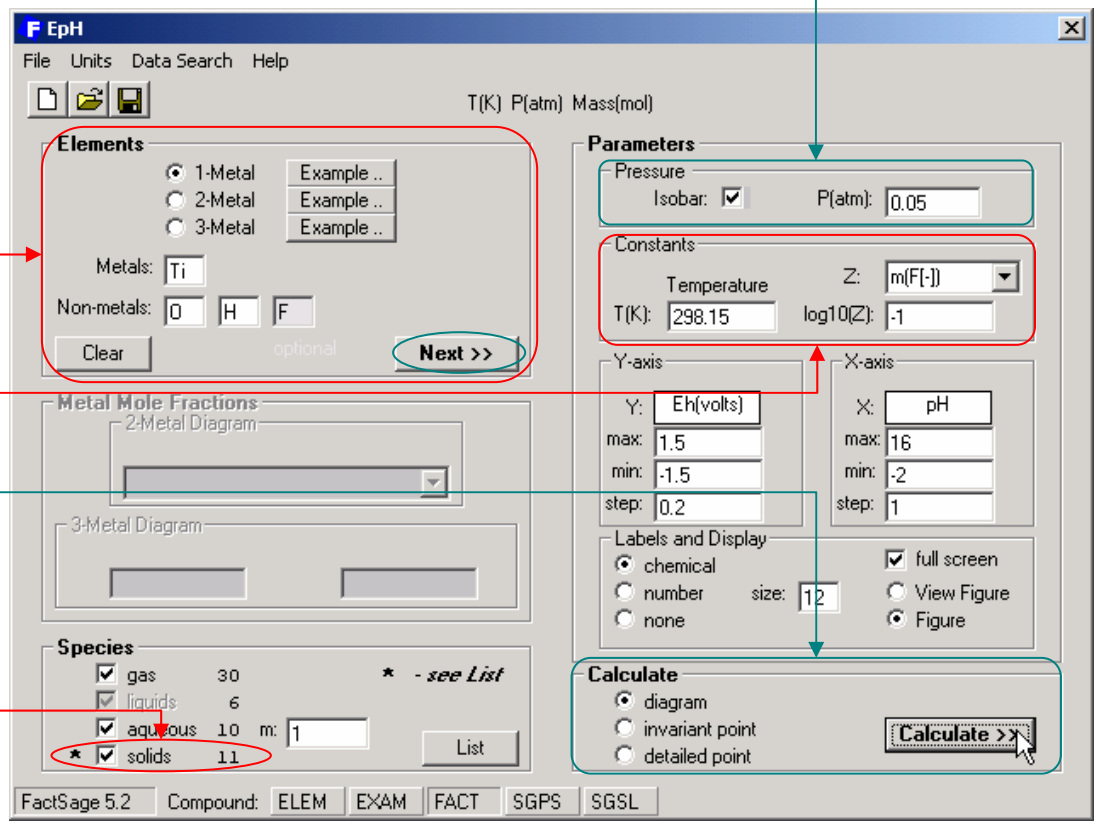
**Note**: to activate the Pressure frame, select gaseous species in the Species frame.

**4°** You must **enter 2** constants.

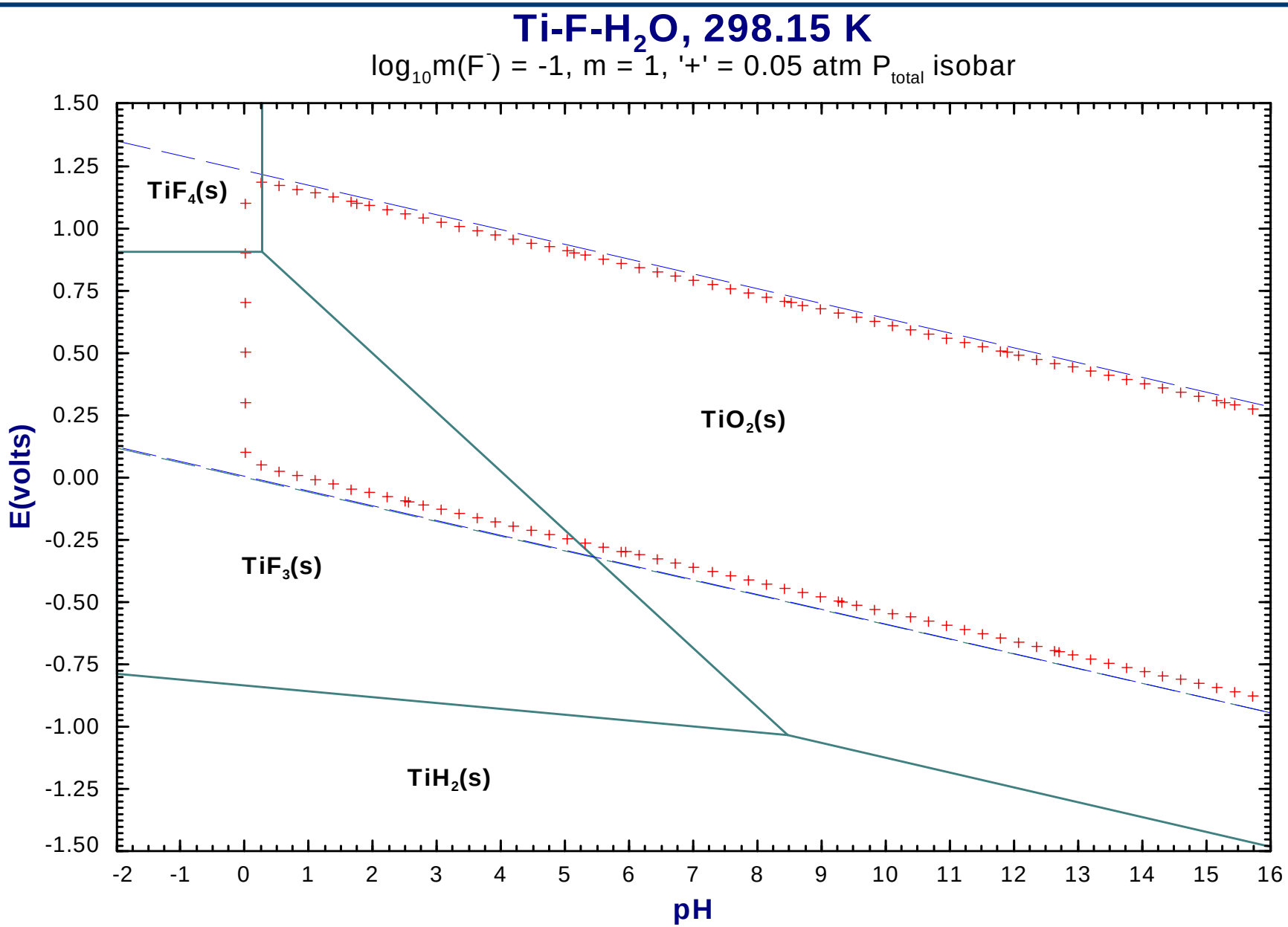
- **T = 298.15 K**
- **Z = m [$F^-$] = $10^{-1}$**

**5° Select** what you want to calculate and press **Calculate**.

**Note**: For diagram clarity, we remove all solid titanium oxides $Ti_xO_y$ with x > 1 and y > 2.



# One-metal Eh-pH diagram with four elements: Output



# Two metals and water: Cu-As-O-H

The following four slides show how the input is prepared for a two-metal water system.

Note the additional selection of the $Me_1/Me_2$ ratio that is required in order to find proper results according to the intermetallic compounds and the double oxides and their respective $Me_1/Me_2$ ratios.

As an example the system Cu-As-O-H is chosen.

# **Two-metal** Pourbaix diagram for Cu-As – formation of mixed oxides

We calculate the diagram in the usual manner except we specify two metal elements **Cu** and **As** since we wish to study the formation of mixed oxides.

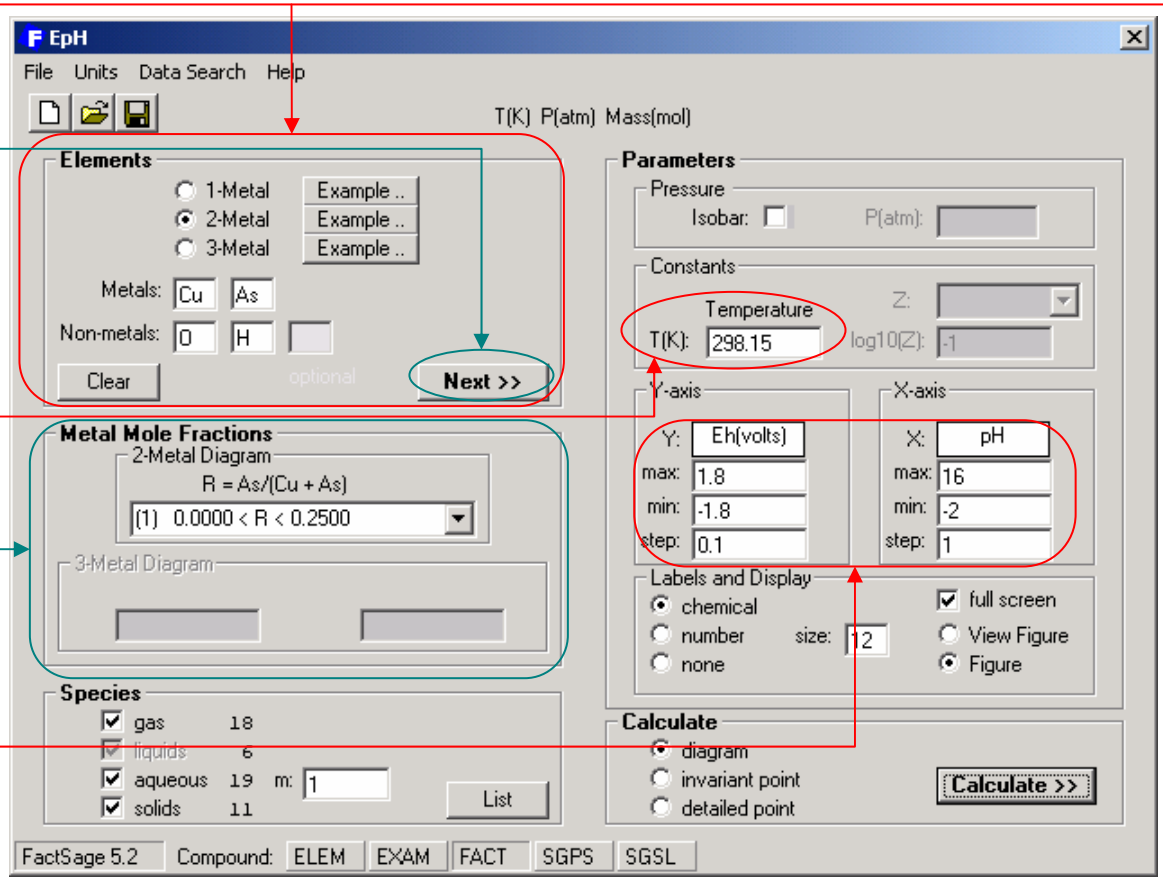
**1° Enter** the elements. This is a **2-metal Cu-As** system as metals with **O** and **H** as non-metallic elements. **We wish to see if Cu and As form intermediate compounds. Each domain will contain a Cu-bearing and an As-bearing species.**

**2° Press Next** to search the compound databases.

**3° Enter** the temperature: **T = 298.15 K**

**Note** that the **Metal Mole Fractions** frame is **enabled**.

**4° Enter** the limits of the axes.

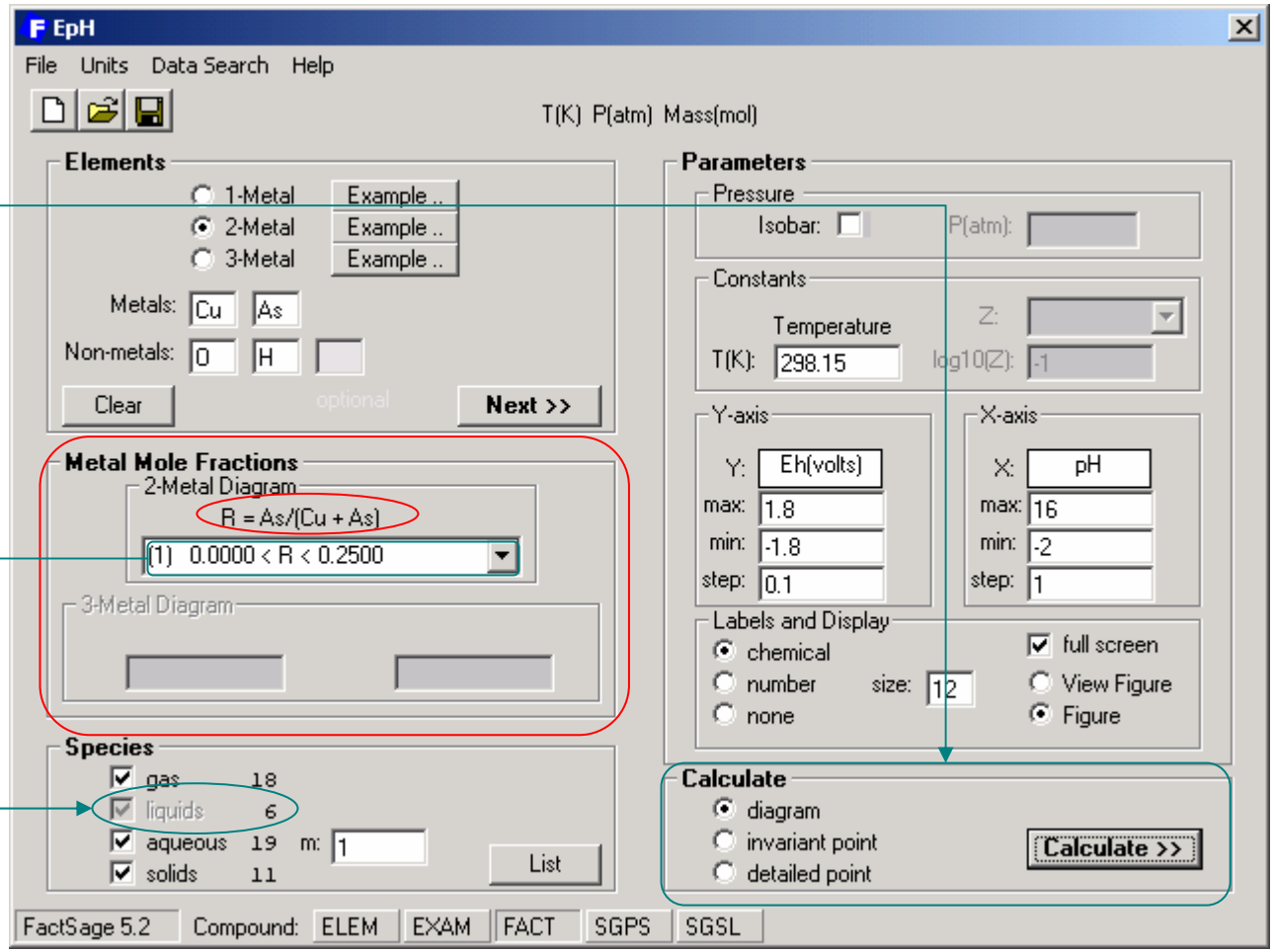


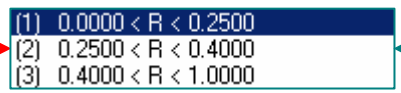
# The Cu-As-water Eh-pH diagram: the **Metal Mole Fraction** frame

The values 0.25 and 0.40 are the **As/(Cu+As)** compositions of the Cu-As intermediate compounds. For example, $Cu_3(AsO_4)_2$ has a R value of 0.40 and $Cu_3As$ has R = 0.25

**5° Select** the range of atomic ratio **R = As/(Cu+As)**. **A Cu-rich-alloy is assigned**.

**6° Select diagram and press Calculate.**

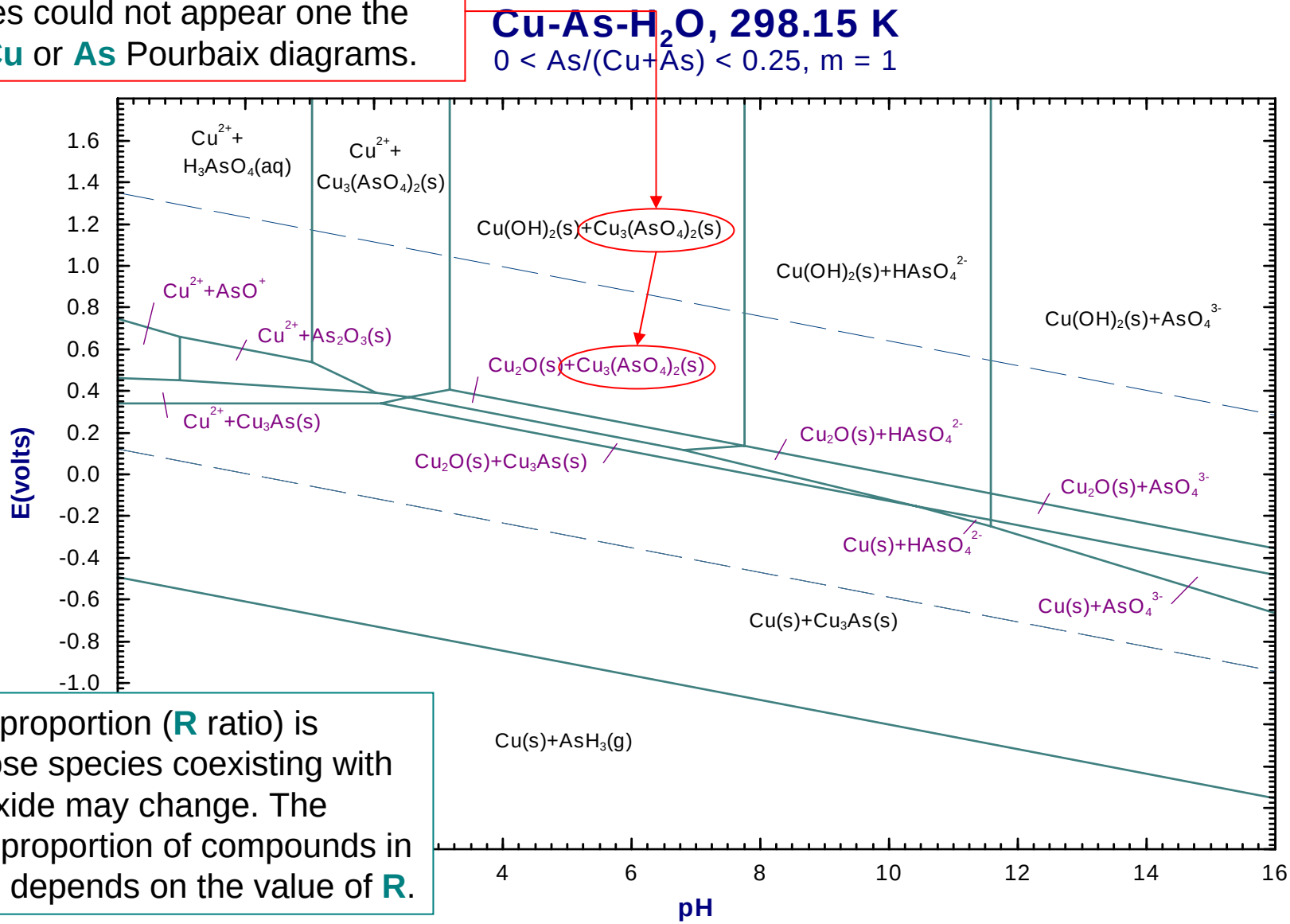



**Note** that the **all liquid (non-aqueous) base metal species are suppressed**.

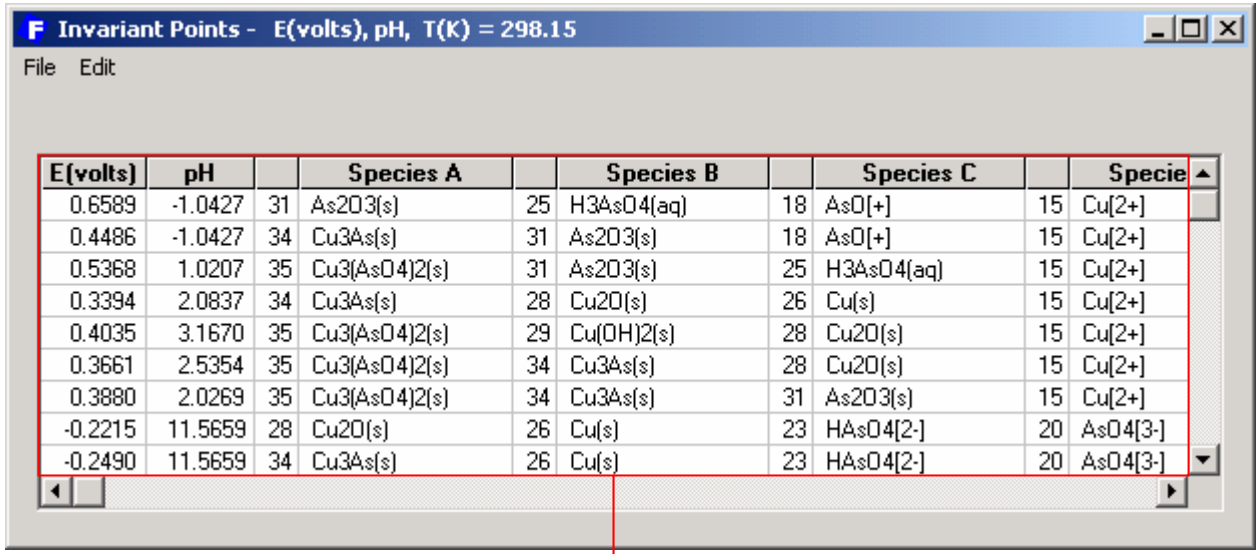
# The Cu-As-water Eh-pH diagram: graphical output

The mixed oxide $Cu_3(AsO_4)_2(s)$ is shown – this species could not appear one the one-metal **Cu** or **As** Pourbaix diagrams.




If the **Cu/As** proportion (**R** ratio) is changed, those species coexisting with the double oxide may change. The actual molar proportion of compounds in each domain depends on the value of **R**.

# The Cu-As-water Eh-pH diagram: **invariant points**




| E(volts) | pH | | Species A | | Species B | | Species C | | Specie |
|---|---|---|---|---|---|---|---|---|---|
| 0.6589 | -1.0427 | 31 | As2O3(s) | 25 | H3AsO4(aq) | 18 | AsO[+] | 15 | Cu[2+] |
| 0.4486 | -1.0427 | 34 | Cu3As(s) | 31 | As2O3(s) | 18 | AsO[+] | 15 | Cu[2+] |
| 0.5368 | 1.0207 | 35 | Cu3(AsO4)2(s) | 31 | As2O3(s) | 25 | H3AsO4(aq) | 15 | Cu[2+] |
| 0.3394 | 2.0837 | 34 | Cu3As(s) | 28 | Cu2O(s) | 26 | Cu(s) | 15 | Cu[2+] |
| 0.4035 | 3.1670 | 35 | Cu3(AsO4)2(s) | 29 | Cu(OH)2(s) | 28 | Cu2O(s) | 15 | Cu[2+] |
| 0.3661 | 2.5354 | 35 | Cu3(AsO4)2(s) | 34 | Cu3As(s) | 28 | Cu2O(s) | 15 | Cu[2+] |
| 0.3880 | 2.0269 | 35 | Cu3(AsO4)2(s) | 34 | Cu3As(s) | 31 | As2O3(s) | 15 | Cu[2+] |
| -0.2215 | 11.5659 | 28 | Cu2O(s) | 26 | Cu(s) | 23 | HAsO4[2-] | 20 | AsO4[3-] |
| -0.2490 | 11.5659 | 34 | Cu3As(s) | 26 | Cu(s) | 23 | HAsO4[2-] | 20 | AsO4[3-] |

**Note** the **4 coexisting species** at **each invariant point** which is consistent with the **Gibbs Phase Rule**.

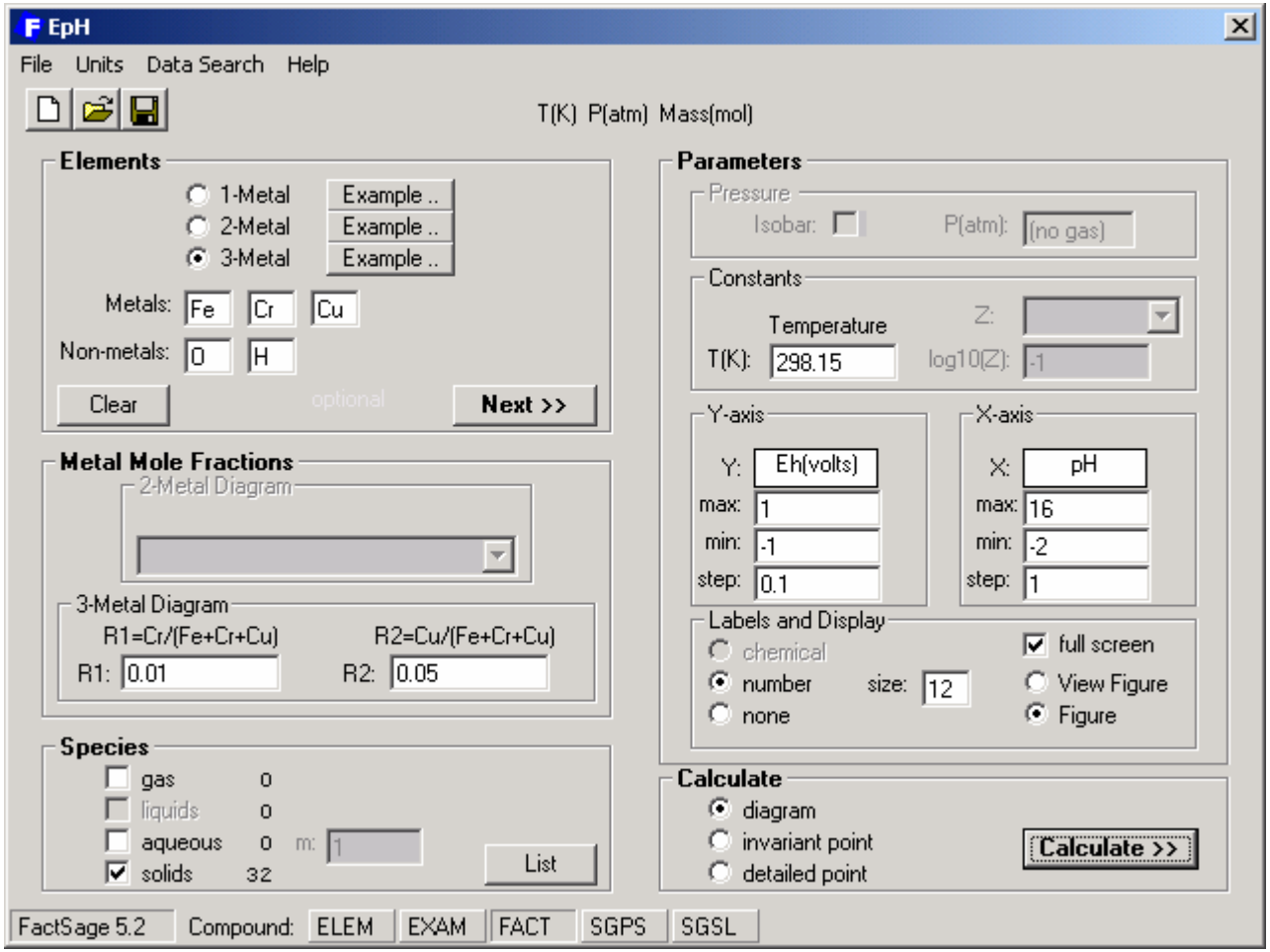
| E(volts) | pH | | Species A | | Species B | | Species C | | Species D |
|---|---|---|---|---|---|---|---|---|---|
| 0.6589 | -1.0427 | 31 | As2O3(s) | 25 | H3AsO4(aq) | 18 | AsO[+] | 15 | Cu[2+] |
| 0.4486 | -1.0427 | 34 | Cu3As(s) | 31 | As2O3(s) | 18 | AsO[+] | 15 | Cu[2+] |
| 0.5368 | 1.0207 | 35 | Cu3(AsO4)2(s) | 31 | As2O3(s) | 25 | H3AsO4(aq) | 15 | Cu[2+] |
| 0.3394 | 2.0837 | 34 | Cu3As(s) | 28 | Cu2O(s) | 26 | Cu(s) | 15 | Cu[2+] |
| 0.4035 | 3.1670 | 35 | Cu3(AsO4)2(s) | 29 | Cu(OH)2(s) | 28 | Cu2O(s) | 15 | Cu[2+] |
| 0.3661 | 2.5354 | 35 | Cu3(AsO4)2(s) | 34 | Cu3As(s) | 28 | Cu2O(s) | 15 | Cu[2+] |
| 0.3880 | 2.0269 | 35 | Cu3(AsO4)2(s) | 34 | Cu3As(s) | 31 | As2O3(s) | 15 | Cu[2+] |
| -0.2215 | 11.5659 | 28 | Cu2O(s) | 26 | Cu(s) | 23 | HAsO4[2-] | 20 | AsO4[3-] |
| -0.2490 | 11.5659 | 34 | Cu3As(s) | 26 | Cu(s) | 23 | HAsO4[2-] | 20 | AsO4[3-] |
| -0.0934 | 11.5659 | 29 | Cu(OH)2(s) | 28 | Cu2O(s) | 23 | HAsO4[2-] | 20 | AsO4[3-] |
| -0.1530 | 10.4070 | 34 | Cu3As(s) | 28 | Cu2O(s) | 26 | Cu(s) | 23 | HAsO4[2-] |
| 0.1329 | 7.7413 | 35 | Cu3(AsO4)2(s) | 29 | Cu(OH)2(s) | 28 | Cu2O(s) | 23 | HAsO4[2-] |
| 0.1142 | 6.7938 | 35 | Cu3(AsO4)2(s) | 34 | Cu3As(s) | 28 | Cu2O(s) | 23 | HAsO4[2-] |

# Three metals and water: Fe-Cr-Cu-O-H

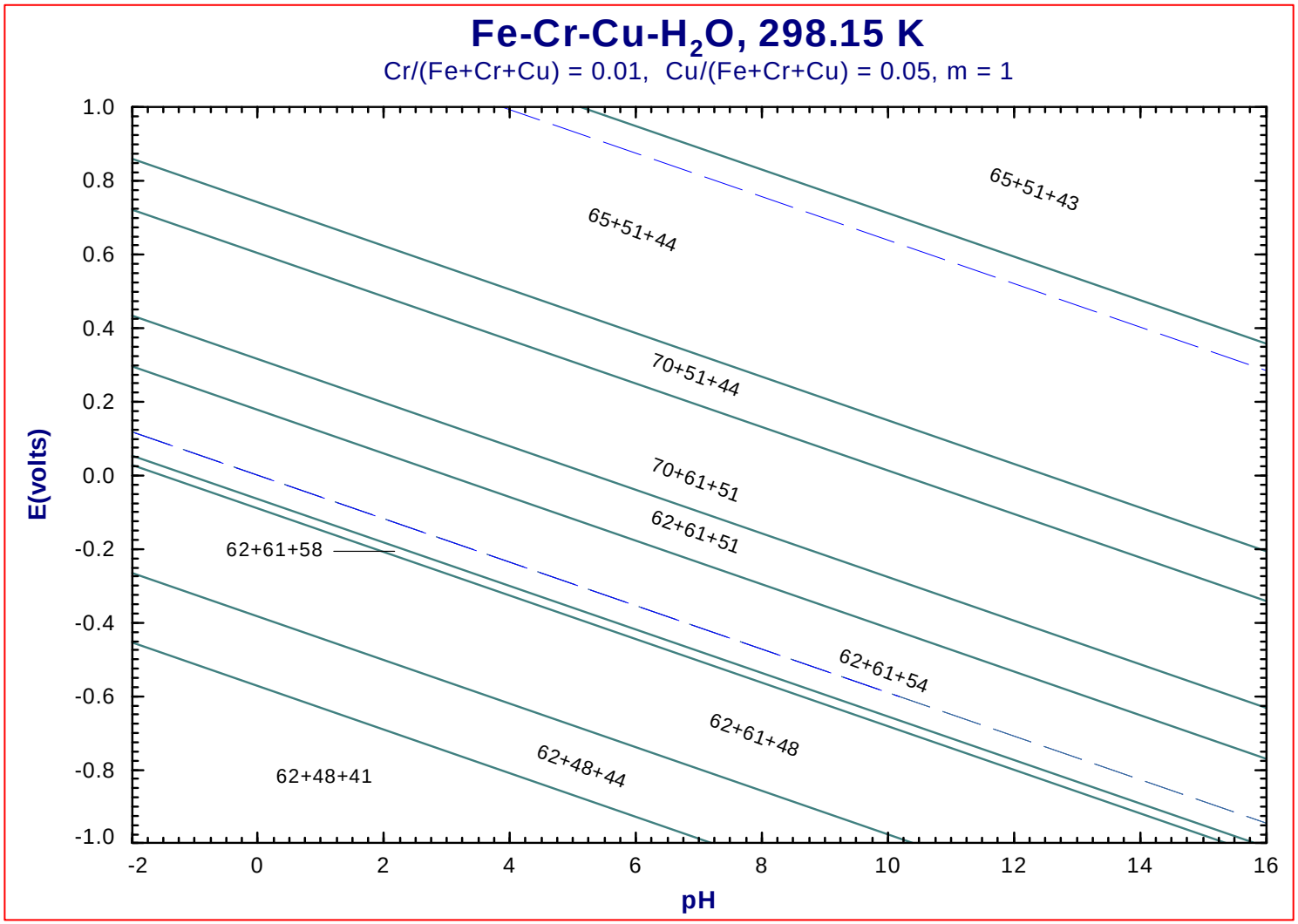
The following two slides show a three-metal water system.

Note the use of numerical labels and a legend in the resulting Pourbaix diagram.

# The Fe-Cr-Cu-water Eh-pH diagram: input



# The Fe-Cr-Cu-water Eh-pH diagram: graphical output and list



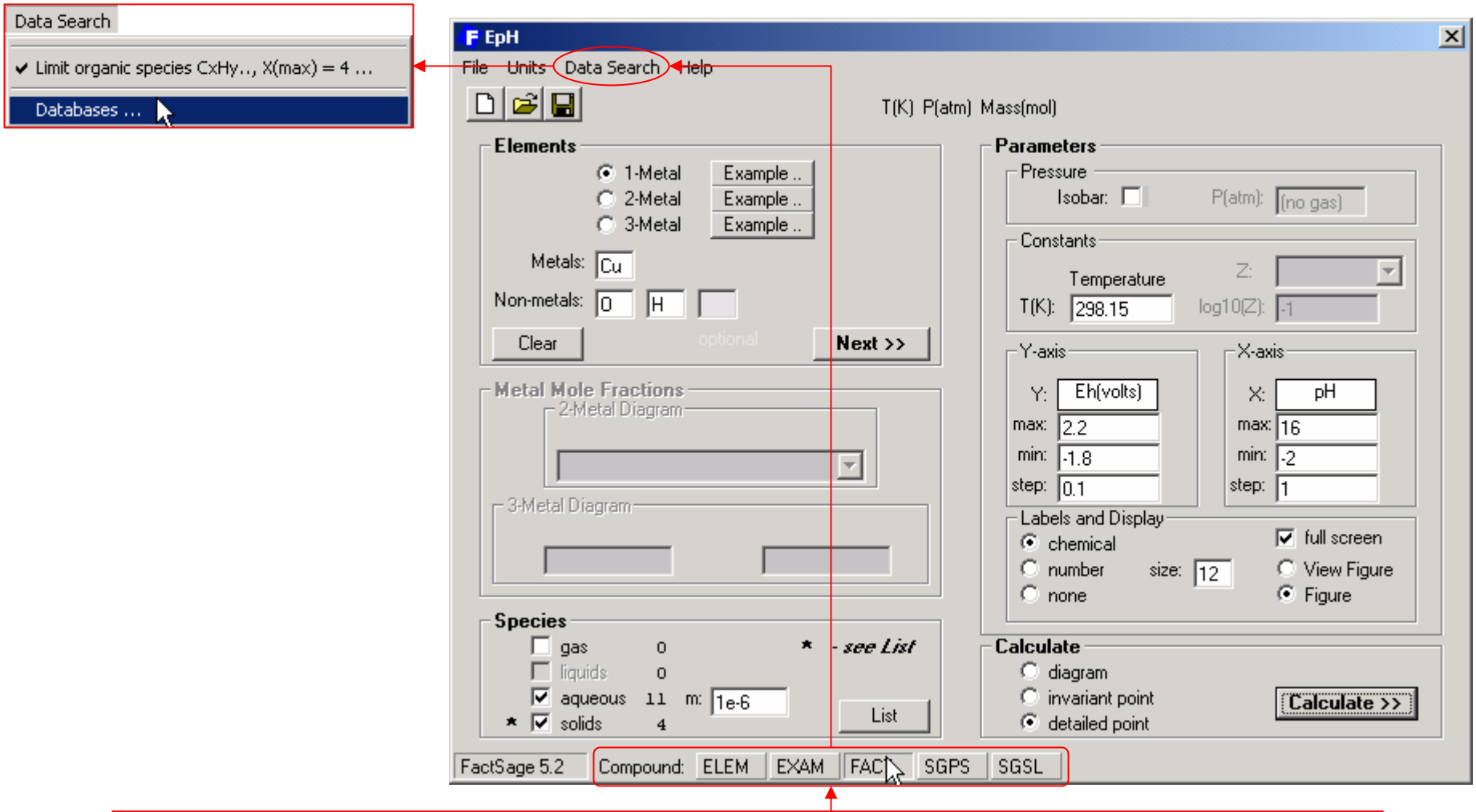

| | | Fe, Cr, Cu solids: |
|---|---|---|
| 41 | | Cr(s) |
| 42 | | CrO2(s) |
| 43 | | CrO3(s) |
| 44 | | Cr2O3(s) |
| 45 | T | Cr3O4(s) |
| 46 | | Cr5O12(s) |
| 47 | | Cr8O21(s) |
| 48 | | Fe(s) |
| 49 | | Fe(s2) |
| 50 | | FeO(s) |
| 51 | | Fe2O3(s) |
| 52 | | Fe2O3(s2) |
| 53 | T | Fe2O3(s3) |
| 54 | | Fe3O4(s) |
| 55 | T | Fe3O4(s2) |
| 56 | | Fe3O4(s3) |
| 57 | T | Fe3O4(s4) |
| 58 | | Fe(OH)2(s) |
| 59 | | Fe(OH)3(s) |
| 60 | | Fe2O3(H2O)(s) |
| 61 | | FeCr2O4(s) |
| 62 | | Cu(s) |
| 63 | | CuO(s) |
| 64 | | Cu2O(s) |
| 65 | | Cu(OH)2(s) |
| 66 | | CuFeO2(s) |
| 67 | | (CuO)(Fe2O3)(s) |
| 68 | T | (CuO)(Fe2O3)(s2) |
| 69 | T | (CuO)(Fe2O3)(s3) |
| 70 | | (Cu2O)(Fe2O3)(s) |
| 71 | T | (Cu2O)(Fe2O3)(s2) |

# Loading another database

In the following two slides is shown how another database of the Compound type can be loaded in order to perform calculations with the ***EpH*** module.

Note that the appropriate database would have to contain data for aqueous species according to the dilute solution approach. Non-ideal aqueous solution using for example the Pitzer model or the OLI model are not permitted in the ***EpH*** module.

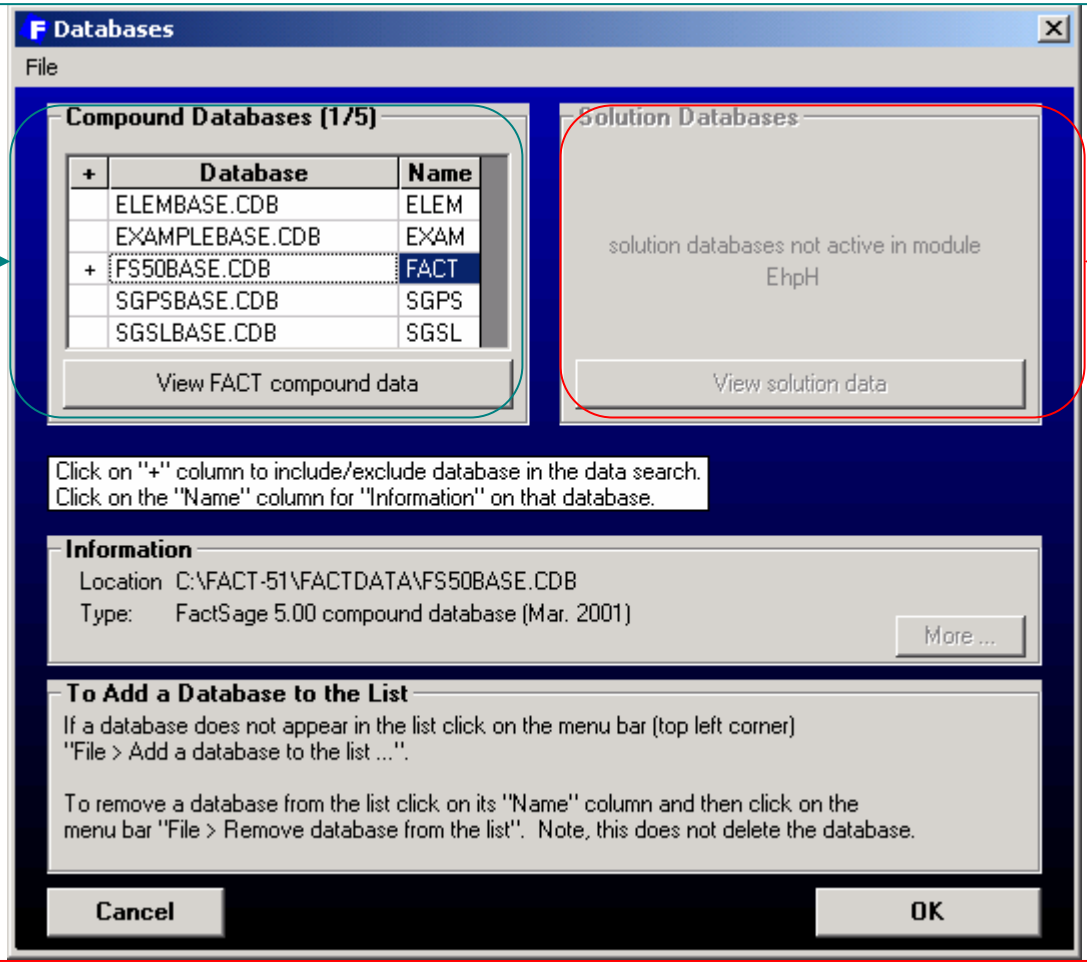
# Loading another Compound database




**Click** here (or, from the menu bar, **select** **Data Search > Databases…**) to **include** or **exclude** a **database** in the search. Here, only the ***FACT*** **compound** database is included.

# Specifying the Cu-water Eh-pH diagram: Databases window

***EpH*** can only access the compound databases – these databases include **dilute Henrian solute data**.




**Concentrated** aqueous solutions (for example: ***FACT***, **OLI Solutions**) are not accessible to ***EpH***.