

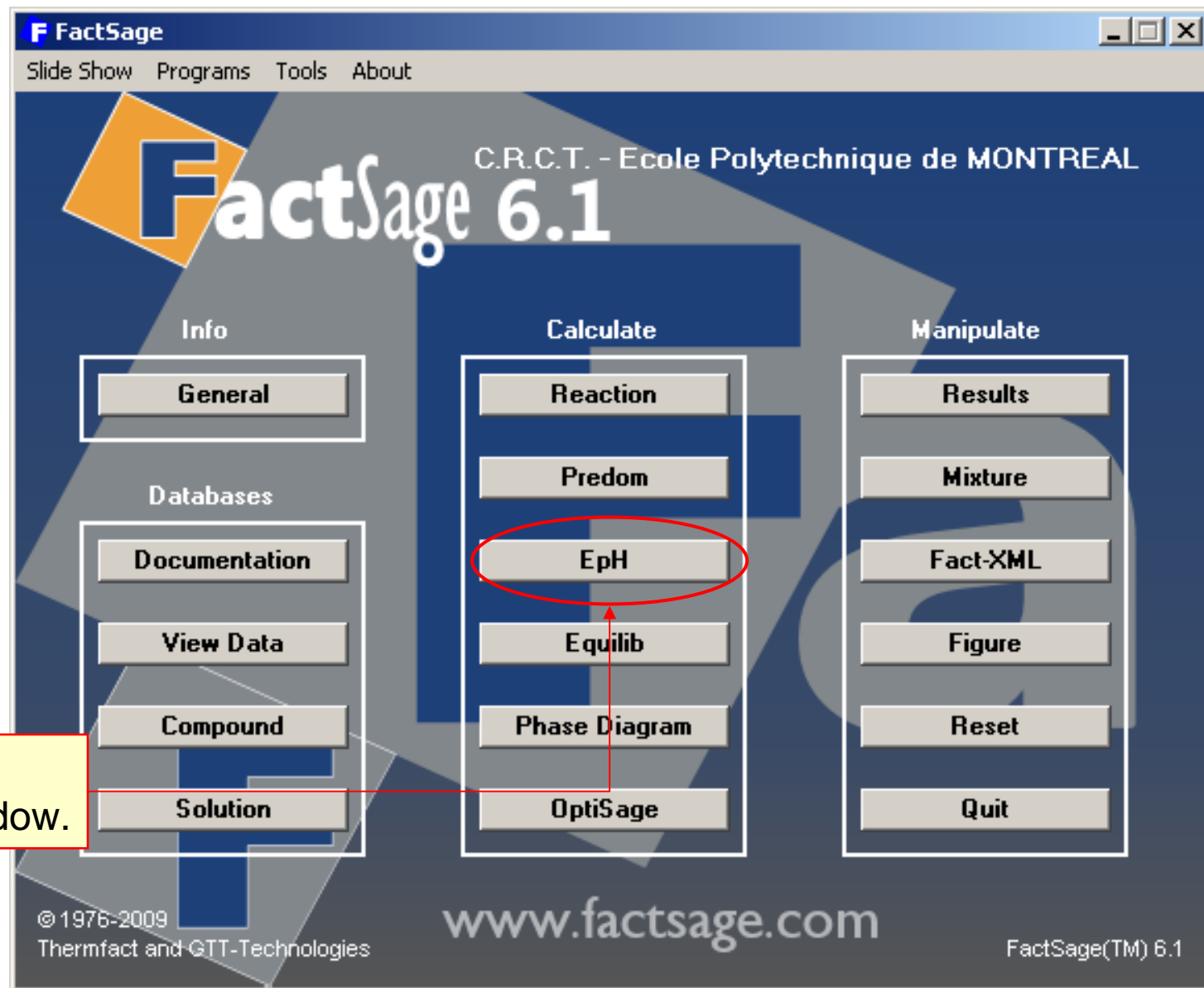
The *EpH* module

- *EpH* calculates and plots isothermal EpH (Pourbaix) diagrams.
- *EpH* accesses only compound databases and treats the aqueous phase as an ideal solution.

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The *EpH* module



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

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 screenshot shows the Eph software interface with the following components:

- Elements:** Radio buttons for 1-Metal (selected), 2-Metal, and 3-Metal. Below are input fields for Metals (Cu) and Non-metals (O, H). A "Next >>" button is circled in red.
- Parameters:** Includes Pressure (Isobar checked, P(atm): [no gas]), Constants (Temperature: 298.15, log10(Z): -10), Y-axis (log10(Y) with max: 1.8, min: -1.2, step: 0.1), and X-axis (log10(X) with max: 16, min: -2, step: 1).
- Metal Mole Fractions:** Sections for 2-Metal Diagram and 3-Metal Diagram.
- Species:** Checkboxes for gas, liquids, aqueous (checked), and solids. A "List" button is present.
- Labels and Display:** Radio buttons for chemical, number (selected), and none. Includes "full screen" and "titles" checkboxes.
- Calculate:** Radio buttons for diagram (selected), invariant point, and detailed point. A "Calculate >>" button is present.

At the bottom, it shows "FactSage" and "Compound: 1/27 databases".

When you **click** the **Next >>** button the pure substances databases are automatically scanned to find all the compounds and henrian solutes formed from the elements. When you make changes in the **Elements** frame 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 *E_pH* 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 later on.

Parameters

Pressure
Isobar: P(atm): (no gas)

Constants
Temperature
T(K): 298.15
log10(Z): -10

Y-axis
Y: Eh(volts)
max: 2.2
min: -1.8
step: 0.1

X-axis
X: pH
max: 16
min: -2
step: 1

Labels and Display
 chemical
 number
 none
size: 12
 full screen
 titles

Constants: 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: Eh(volts): -1.8 to 2.2, pH: -2 to 16.

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 type and size (8 – 20) and type of labels on the calculated diagram.

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, $m = 1 \times 10^{-6}$. To **examine** the species or to **add** or **remove** a particular species or **change** its activity, molality or partial pressure, **click** the "List" button.

Species

gas 0

liquids 0

aqueous 11 m: 1e-6

solids 5

List

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

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

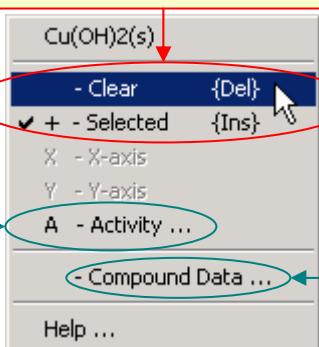
File Edit Help

+ 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, Pergamon 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**.



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.

+ 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			H2O(a)	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		298 - 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.

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

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

The screenshot shows the EpH software interface with the following settings:

- Elements:** 1-Metal selected, Metals: Cu, Non-metals: O, H.
- Parameters:** Temperature: 298.15 K, log10(Z): -10, Y-axis: Eh(volts), X-axis: pH.
- Species:** gas: 0, liquids: 0, aqueous: 11, solids: 4. m: 1e-6.
- Compound:** 1/27 databases.

Here, only the **FACT compound** database is included. See section 9 for **inclusion** or **exclusion** of a **database**.

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

- **Diagram:**
This calculates and plots the diagram.
- **Invariant Point:**
This gives the precise position of the triple points where three domains meet.
- **Detailed Point:**
This enables you to display the equilibrium activity or partial pressure of all species at a specified coordinate on the diagram.

The screenshot shows the FactSage EpH software interface. The 'Calculate' section is highlighted with a blue box, and the 'Species' section is highlighted with a red box. A red arrow points from the 'Species' section to a callout box.

Calculate

- diagram
- invariant point
- detailed point

Calculate >>

Species

<input type="checkbox"/>	gas	0		* - see List
<input type="checkbox"/>	liquids	0		
<input checked="" type="checkbox"/>	aqueous	11	m: 1e-6	List
<input checked="" type="checkbox"/>	solids	4		

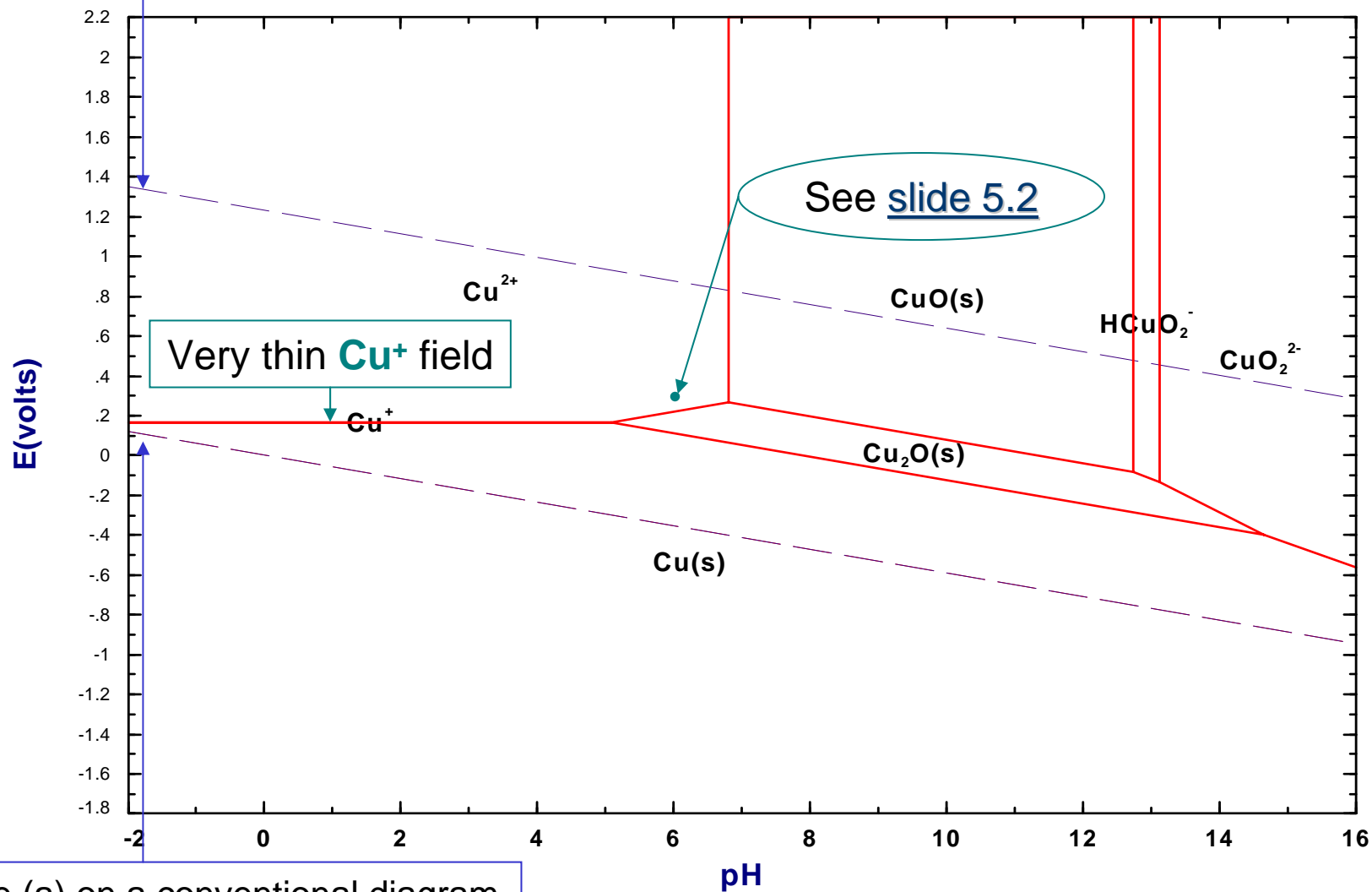
FactSage Compound: 1/27 databases

Note the **custom (*) selection** of **solid** species.

Cu-H₂O Eh-pH diagram: Graphical Output

O₂ (1 atm) line (b) on a conventional diagram

Cu-H₂O, 298.15 K
 $m = 1 \times 10^{-6}$



H₂ (1 atm) line (a) on a conventional diagram

Published Pourbaix diagram for **Cu-H₂O**

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

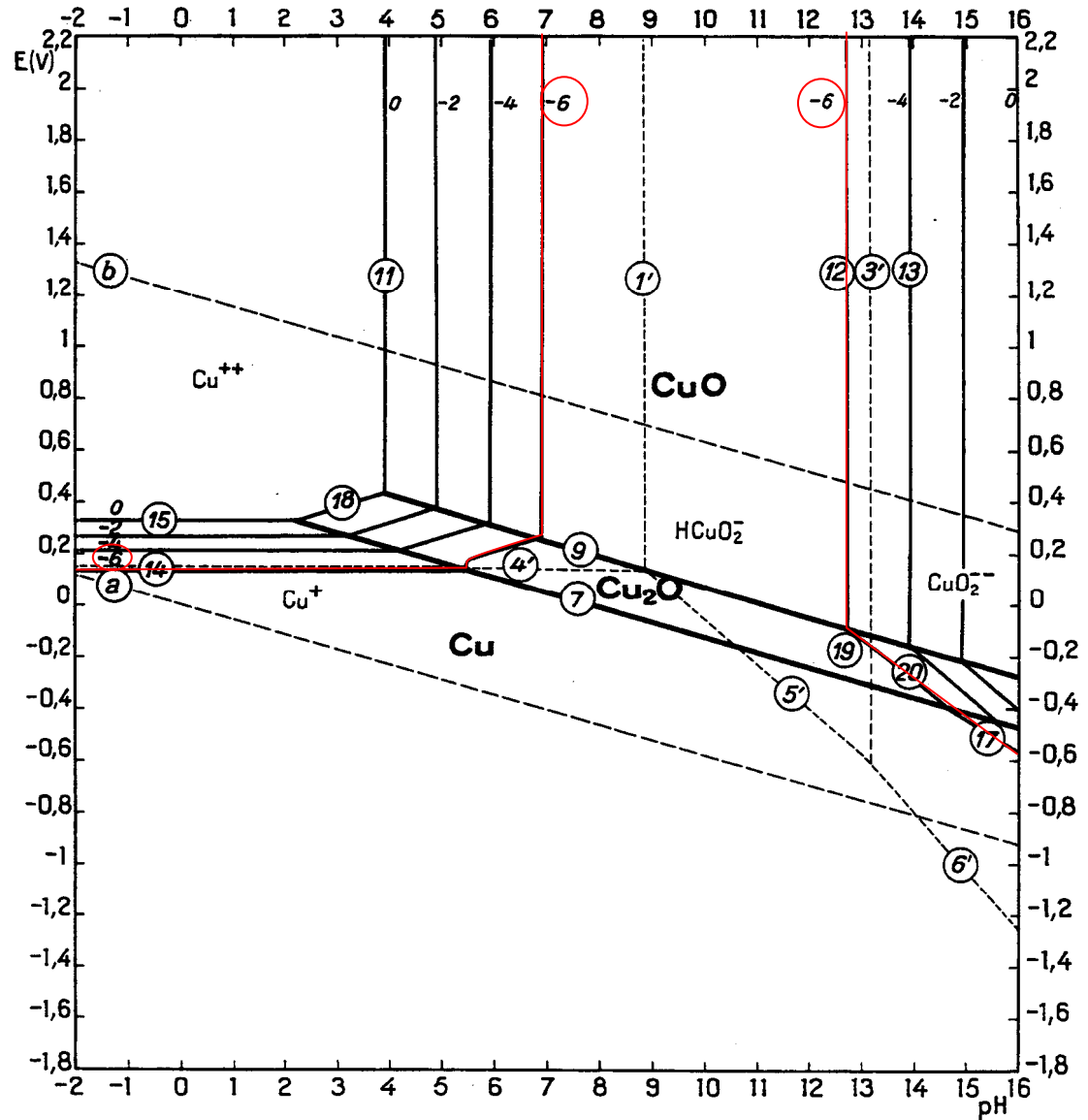


FIG. 1. Potential-pH equilibrium diagram for the system copper-water, at 25°C. [Considering the solid substances Cu, Cu₂O and CuO. Cu(OH)₂ is not considered.]

Cu-H₂O Eh-pH diagram: Computation of invariant points

Calculate

- diagram
- invariant point
- detailed point

Calculate >>

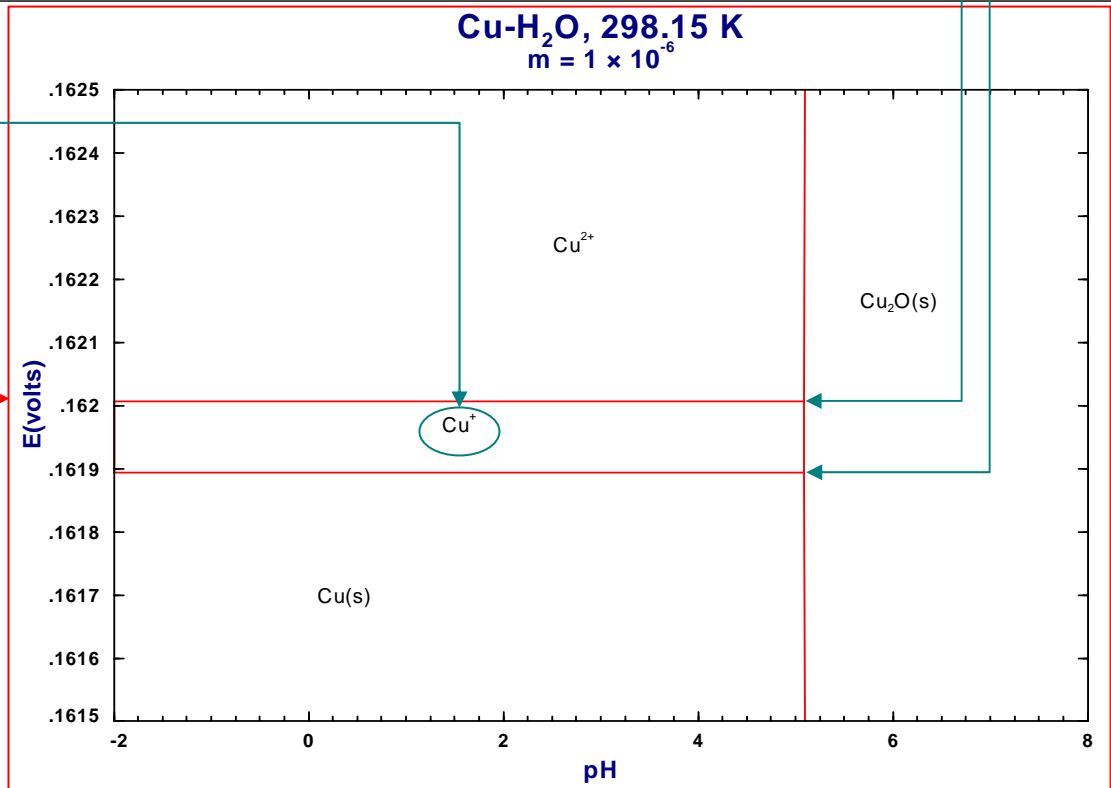
F Invariant Points - E(volts), pH, T(K) = 298.15

File Edit

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

A very thin **Cu⁺** field indeed!

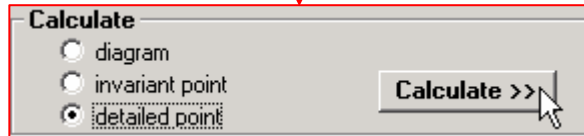
Enlargement of the previous diagram



Cu-H₂O Eh-pH diagram: Detailed Point Calculation

The point calculation gives activities and ideal concentrations for all metal-element containing species at the specified coordinate, E(volts), pH.

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.

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

File Edit Help

+	Code	T	Species	Data	A/P/M	Cp range
Cu gases:						
	1		Cu(g)	FACT	1.0000E+00	298 - 6000
	2		Cu ₂ (g)	FACT	1.0000E+00	298 - 6000
	3		CuO(g)	FACT	1.0000E+00	298 - 6000
Cu liquids:						
	4		Cu(l)	FACT	1.0000E+00	298 - 4000
	5		Cu ₂ O(l)	FACT	1.0000E+00	298 - 2000
Cu aqueous species:						
+	6		Cu(+)	FACT	1.0000E-06	298 - 573
+	7		Cu(2+)	FACT	1.0000E-06	298 - 573
+	8		CuO ₂ (2-)	FACT	1.0000E-06	298 - ****
+	9		HCuO ₂ (-)	FACT	1.0000E-06	298 - ****
Cu solids:						
+	10		Cu(s)	FACT	1.0000E+00	298 - 2001
+	11		CuO(s)	FACT	1.0000E+00	298 - 2000
+	12		Cu ₂ O(s)	FACT	1.0000E+00	298 - 2000
	13		Cu(OH) ₂ (s)	FACT	1.0000E+00	298 - 1500

Point Calculation

E(volts): 0.3

pH: 6

Calculate

The specified coordinate is in the **domain of Cu²⁺** set at **10⁻⁶** (the **green dot** on [slide 4.2](#)).

Cu-H₂O Eh-pH diagram: Detailed Point Calculation – Output

F List - Cu-H₂O, T = 298.15K

File Edit Help

Code	T	Species	Data	A/P/M	Cp range
Cu gases:					
1		Cu(g)	FACT	1.386E-57	298 - 6000
2		Cu ₂ (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		Cu ₂ O(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		CuO ₂ (2-)	FACT	3.519E-22	298 - ****
+ 9		HCuO ₂ (-)	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		Cu ₂ O(s)	FACT	1.464E-03	298 - 2000
13		Cu(OH) ₂ (s)	FACT	4.635E-01	298 - 1500

Domain: Cu(2+)

Point Calculation

E(volts): 0.3

pH: 6

Calculate

+	Code	T	Species	Data	A/P/M	Cp range
Cu gases:						
	1		Cu(g)	FACT	1.386E-57	298 - 6000
	2		Cu ₂ (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		Cu ₂ O(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			CuO ₂ (2-)	FACT	3.519E-22	298 - ****
+ 9			HCuO ₂ (-)	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			Cu ₂ O(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		H ₂ (g)	FACT	7.210E-23	298 - 6000
	16		O(g)	FACT	9.714E-61	298 - 6000
	17		O ₂ (g)	FACT	1.502E-39	298 - 6000
	18		O ₃ (g)	FACT	< 1.0E-70	298 - 6000
	19		OH(g)	FACT	3.252E-37	298 - 6000
	20		H ₂ O(g)	FACT	3.135E-02	298 - 6000
	21		H ₂ O ₂ (g)	FACT	3.808E-53	298 - 6000
	22		HO ₂ H(g)	FACT	3.263E-43	298 - 1500
Other liquids:						
	23		H ₂ O(l)	FACT	1.000E+00	298 - 500
	24		HO ₂ H(l)	FACT	1.107E-40	298 - 431
Other aqueous species:						
+ 25			H(+)	FACT	1.000E-06	298 - 500
+ 26			H ₂ (aq)	FACT	6.120E-26	298 - 573
+ 27			O ₂ (aq)	FACT	2.045E-42	298 - 400
+ 28			OH(-)	FACT	9.883E-09	298 - 573
+ 29			HO ₂ (-)	FACT	6.675E-44	298 - 573
+ 30			HO ₂ H(aq)	FACT	3.318E-38	298 - 473
+ 31			e(-)(aq)	ELEM	8.491E-06	298 - 6000
Other solids:						
+ 32	T		H ₂ O(s)	FACT	7.872E-01	250 - 273

Cu²⁺ is the stable species and its activity must be equal to the molality **m** specified for the aqueous species (here **1 × 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.

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 with **O**, **H** and **F** as non-metallic elements.

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

4° You must enter **2** constants.

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

5° Select the type of calculation and press **Calculate**.

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

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.

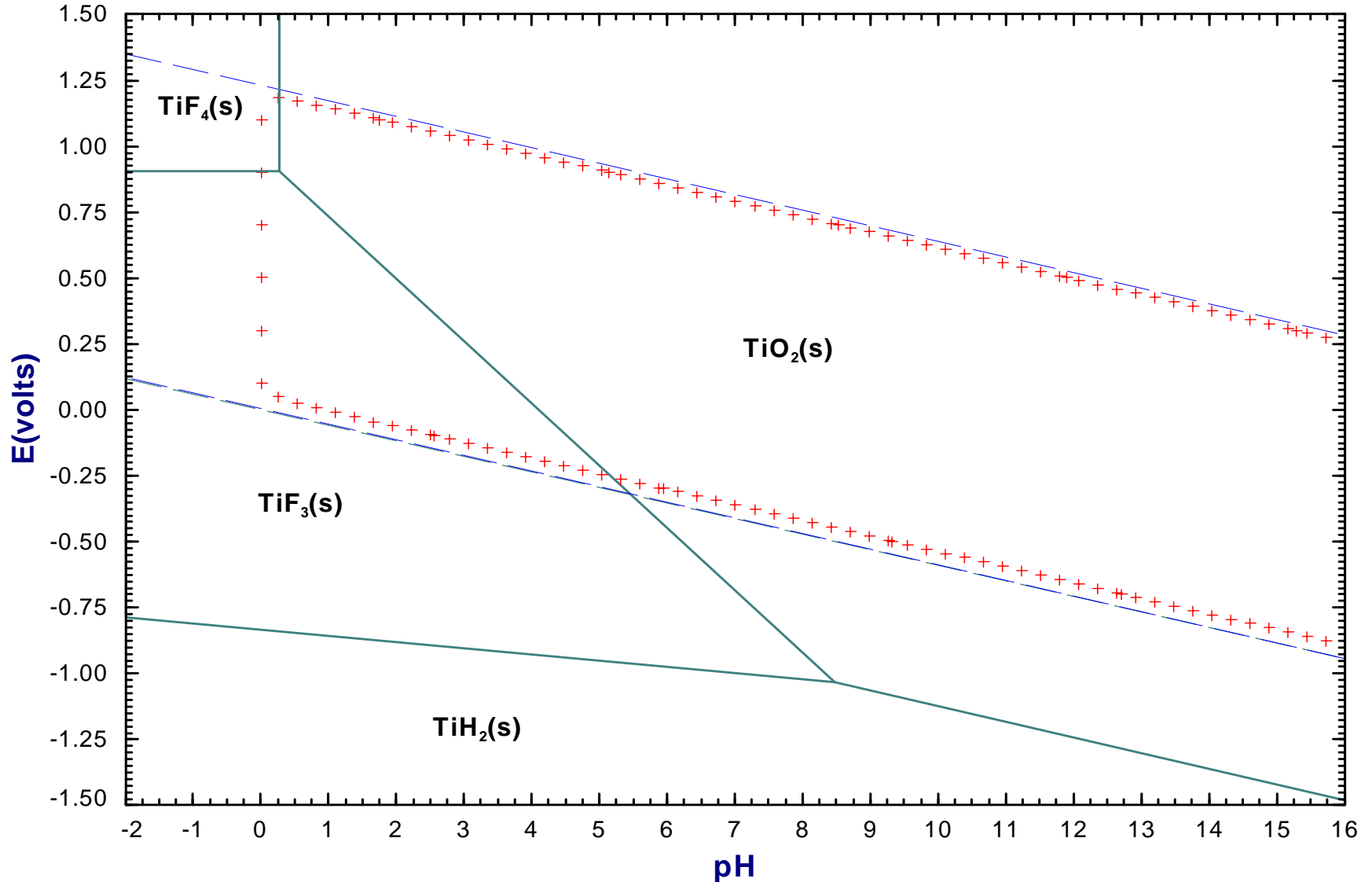
The screenshot shows the FactSage EpH software interface with the following settings:

- Elements:** 1-Metal selected. Metals: Ti. Non-metals: O, H, F. **Next >>** button is highlighted.
- Parameters:** Isobar checked, P(atm): 0.05. Constants: Temperature T(K): 298.15, Z: m[F(-)] (dropdown), log10(Z): -1.
- Y-axis:** Eh(volts), max: 1.5, min: -1.5, step: 0.2.
- X-axis:** pH, max: 16, min: -2, step: 1.
- Labels and Display:** chemical selected, full screen and titles checked, size: 12.
- Calculate:** diagram selected, **Calculate >>** button is highlighted.
- Species:** gas (30), liquids (0), aqueous (10), solids (11) are checked. m: 1. A red circle highlights the solids section.

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

Ti-F-H₂O, 298.15 K

$\log_{10}m(\text{F}^-) = -1, m = 1, '+' = 0.05 \text{ atm } P_{\text{total}}$ isobar



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 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 screenshot shows the FactSage EpH software interface. The 'Elements' section is set to '2-Metal' with 'Cu' and 'As' selected as metals and 'O' and 'H' as non-metals. The 'Next >>' button is highlighted. The 'Parameters' section shows 'Temperature' set to 298.15 K. The 'Metal Mole Fractions' section is enabled, showing a 2-Metal Diagram with the formula $R = \text{As}/(\text{Cu} + \text{As})$ and a range of (1) 0.0000 < R < 0.2500. The 'Species' section has checkboxes for 'gas', 'liquids', 'aqueous', and 'solids'. The 'Calculate' section has 'diagram' selected. The 'Y-axis' is set to 'Eh(volts)' and the 'X-axis' is set to 'pH'. The 'Labels and Display' section has 'chemical' selected and 'full screen' and 'titles' checked. The 'Calculate >>' button is highlighted.

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, $\text{Cu}_3(\text{AsO}_4)_2$ has a R value of 0.40 and Cu_3As has $R = 0.25$

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

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

- (1) $0.0000 < R < 0.2500$
- (2) $0.2500 < R < 0.4000$
- (3) $0.4000 < R < 1.0000$

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

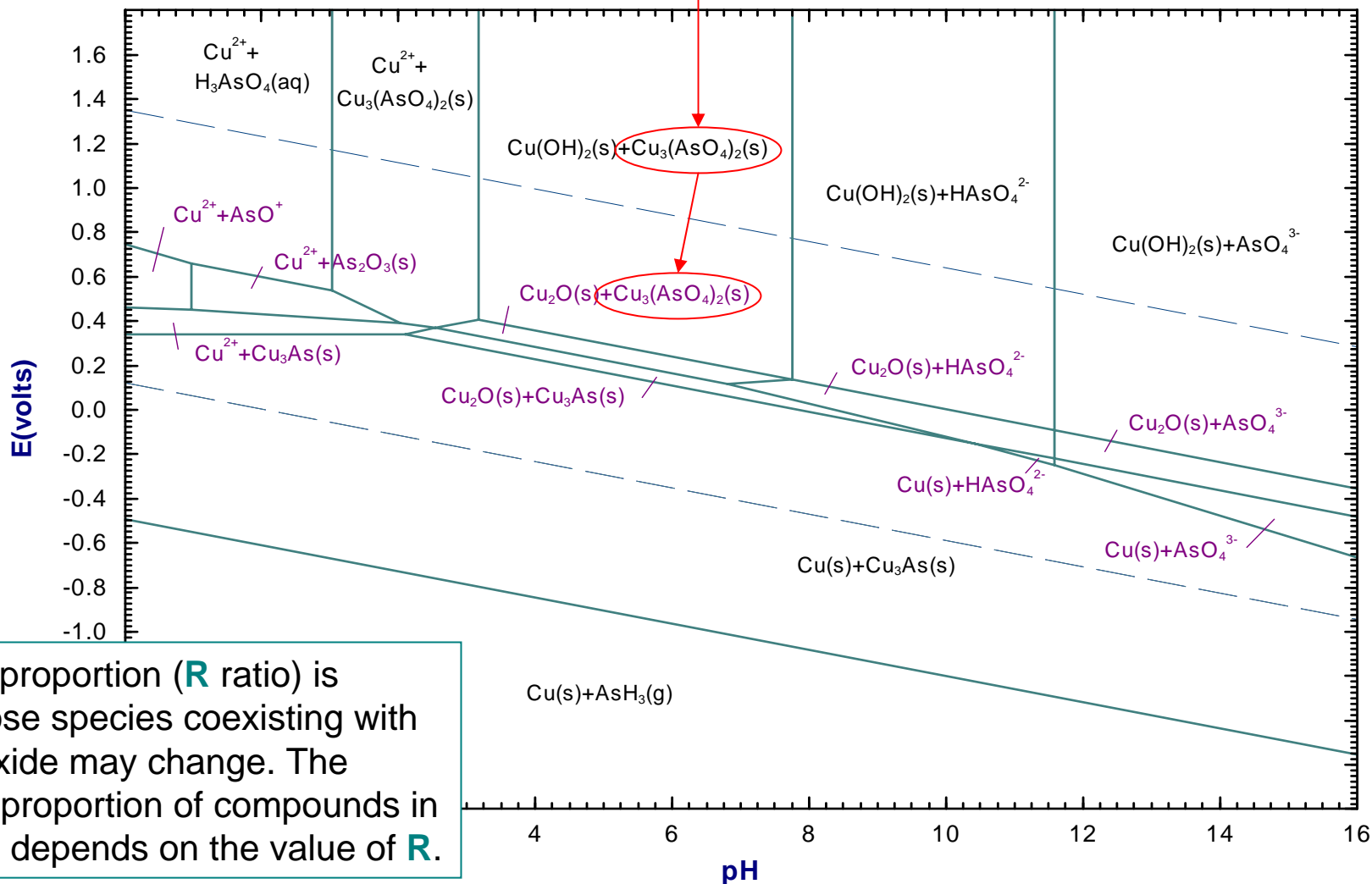
The screenshot shows the FactSage EpH software interface. The 'Metal Mole Fractions' section is highlighted with a red box, showing the '2-Metal Diagram' selected and the formula $R = \text{As}/(\text{Cu} + \text{As})$ circled. A dropdown menu is open, showing the selected range (1) $0.0000 < R < 0.2500$. The 'Parameters' section on the right shows 'Y-axis' set to 'Eh(volts)' and 'X-axis' set to 'pH'. The 'Calculate' section at the bottom right has 'diagram' selected. The 'Species' section at the bottom left shows 'liquids' suppressed (unchecked).

FactSage Compound: 1/27 databases

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

The mixed oxide $\text{Cu}_3(\text{AsO}_4)_2(\text{s})$ is shown – this species could not appear in the one-metal Cu or As Pourbaix diagrams.

Cu-As- H_2O , 298.15 K
 $0 < \text{As}/(\text{Cu}+\text{As}) < 0.25, m = 1$



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

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

File Edit

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-)

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-)

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

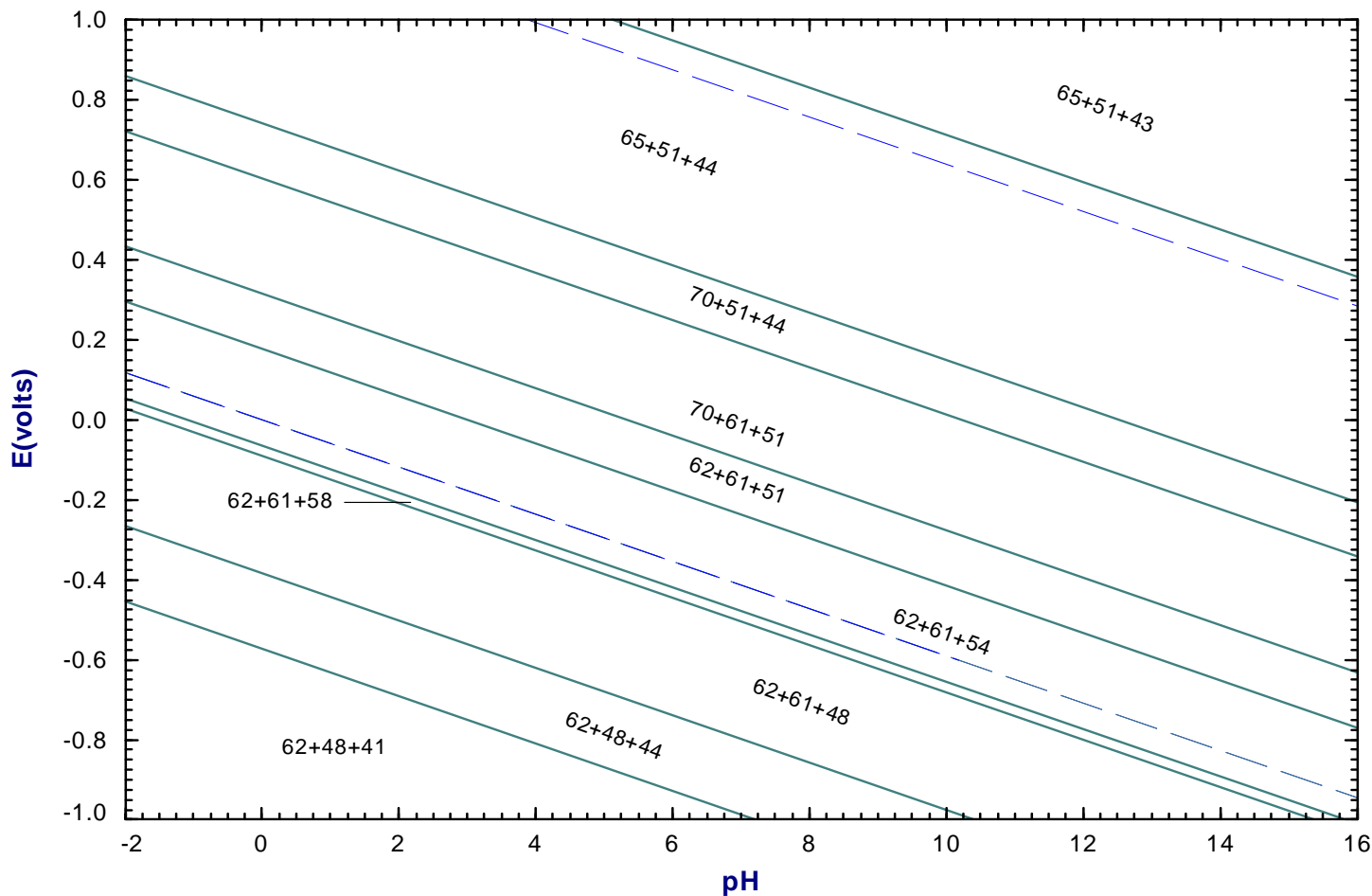
The screenshot shows the 'EPH' software window with the following settings:

- File Units Data Search Help**
- T(K) P(atm) Mass(mol)**
- Elements:** 1-Metal, 2-Metal, 3-Metal (selected). Metals: Fe, Cr, Cu. Non-metals: O, H. Buttons: Clear, optional, Next >>
- Metal Mole Fractions:** 2-Metal Diagram, 3-Metal Diagram. R1=Cr/(Fe+Cr+Cu), R2=Cu/(Fe+Cr+Cu). R1: 0.01, R2: 0.05.
- Species:** gas (0), liquids (0), aqueous (0), solids (32, checked). m: 1.0. Button: List.
- Parameters:** Pressure: Isobar (unchecked), P(atm): (no gas). Constants: Temperature: 298.15, Z: (dropdown), log10(Z): -10. Y-axis: Eh(volts), max: 1, min: -1, step: 0.1. X-axis: pH, max: 16, min: -2, step: 1. Labels and Display: chemical (unchecked), number (checked), none (unchecked), size: 12, full screen (checked), titles (checked).
- Calculate:** diagram (checked), invariant point (unchecked), detailed point (unchecked). Button: Calculate >>
- FactSage Compound: 1/27 databases**

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

Fe-Cr-Cu-H₂O, 298.15 K

Cr/(Fe+Cr+Cu) = 0.01, Cu/(Fe+Cr+Cu) = 0.05, m = 1



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 **Compound** database

Click on **Data Search** to **include** or **exclude** a **database** in the search. Here, only the **FACT** compound database is included.

The screenshot shows the FactSage EpH software interface. The 'Data Search' menu item is circled in red, with a red arrow pointing to it from the text box above. The interface is divided into several sections:

- File Units Data Search Help**: The menu bar.
- Elements**: Radio buttons for 1-Metal, 2-Metal, and 3-Metal. Example buttons for each. Metals: Cu. Non-metals: O, H. Buttons: Clear, optional, Next >>.
- Metal Mole Fractions**: 2-Metal Diagram and 3-Metal Diagram sections with dropdown menus.
- Species**: Checkboxes for gas, liquids, aqueous, and solids. Values: 0, 0, 11, 4. m: 1e-6. Button: List.
- Parameters**: Pressure (Isobar: , P(atm): [no gas]), Constants (Temperature: 298.15, Z: [dropdown], log10(Z): -10), Y-axis (Eh(volts), max: 2.2, min: -1.8, step: 0.1), X-axis (pH, max: 16, min: -2, step: 1), Labels and Display (chemical, number, none; size: 12; full screen, titles).
- Calculate**: Radio buttons for diagram, invariant point, detailed point. Button: Calculate >>.
- FactSage Compound: 1/27 databases**: Status bar at the bottom.

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

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

Data Search

Databases - 1/27 compound databases, 0/23 solution databases

FactSage[®] SGTE

ELEM FSopp BINS compounds only
 FACT FSlead SGPS solutions only
 Fact53 FSlite SGTE no data
 FToxid FSstel SGnobl Clear All
 FTsalt FSupsi SGsold Select All
 FTmisc FSnobl SGnucl Add/Remove Data
 FThall TDnucl RefreshDatabases
 FThelg OLIP OLIC
 FTpulp OLIG OLIL

Miscellaneous

COPP EXAM FTLI
 FTsalt* SGSL SGTE*

Information - EPH only accesses COMPOUND databases
If a database is stored on your PC but not listed here then it is not accessible to FactSage.
Click here to add the database to the list of files accessible to FactSage. You will be requested to identify the type (compound and/or solution) and the full file name of the database file.

Options

Default

Include

gaseous ions (plasmas)
 aqueous species
 limited data compounds (25C)

Limits

Organic species CxHy..., X(max) =
Minimum solution components: 1 2 cpts

Cancel Summary ... OK

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