

HSC 8 – Geo - Mineralogical Calculations and Mineral Database November 19, 2014 14024-ORC-J

1 (26)

# 84. Geo Module - Mineralogical Calculations and Mineral Database

## 84.1. Introduction

The Geo module of HSC 8 is intended for:

- Studying mineral properties (Mineral database, Minerals: section 84.2)
- Finding minerals based on elements in the formula (Find mineral: 84.3)
- Identifying minerals based on the chemical composition (Identify mineral: 84.5)
- Calculating the modal composition (mineral composition) of samples based on chemical assays (Modal calculations: 84.6)
- Processing mineral liberation data (Mineral liberation: 85)





HSC 8 – Geo - Mineralogical Calculations and Mineral Database November 19, 2014 14024-ORC-J

2 (26)

## 84.2. Mineral database

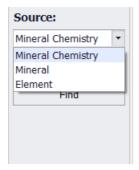
Press the Mineral database button to study the mineral database of HSC Chemistry.



### 84.2.1. Source

In "Source" select the source (table)

- Mineral Chemistry = Table of the chemical composition of minerals (different analyses of minerals from different locations)
- Mineral = Table of minerals, one row per mineral
- Element = Chemical elements



After selecting the source you can apply:

- Filter
- Search
- Edit



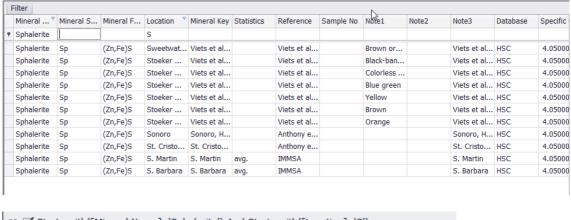
## HSC 8 – Geo - Mineralogical Calculations and Mineral Database November 19, 2014

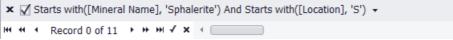
November 19, 2014 14024-ORC-J

3(26)

#### 84.2.2. Filter

In the Filter window, write text in any of the fields on the top row. For instance, in the example below Mineral Name = "Sphalerite" and the Location starts with S. There are a total of 11 records that fulfill the criteria. The criteria are shown below the table.





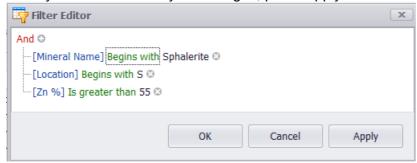
To edit the Filter, press Edit Filter on the right of the criteria panel.



In the Filter Editor window you can:

- · Edit the field by clicking the Field value given in blue
- Edit the operator by clicking the green operator and selecting a new one from the list, e.g. changing [Mineral Name] = Sphalerite
- Edit the value, e.g. by changing [Location] Begins with K
- Adding or deleting a condition

Once you have made all your changes, press Apply.

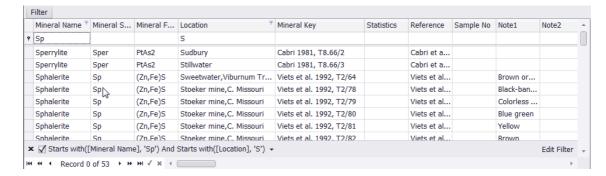




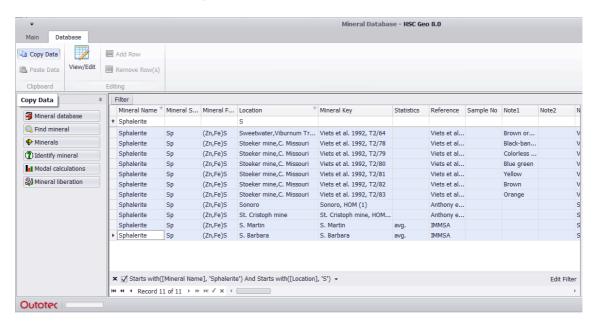
# HSC 8 – Geo - Mineralogical Calculations and Mineral Database

November 19, 2014 14024-ORC-J

4 (26)

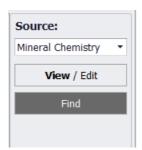


To copy data to the clipboard, select the rows you want to copy (use Ctrl or Shift to select several rows) and press Copy Data.



#### 84.2.3. Find

To start, press "Find" on the right panel. Find differs from Filtering in that it always searches all the fields and it always matches with any part of the field.



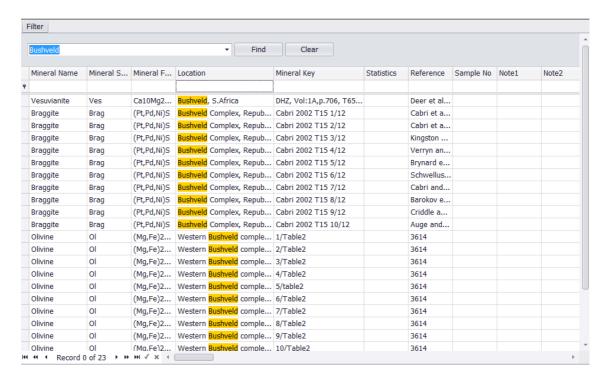
The Find box will appear. You can write any text (or number) in the Find box and press "Find". Geo will filter to show only fields where the text is found.



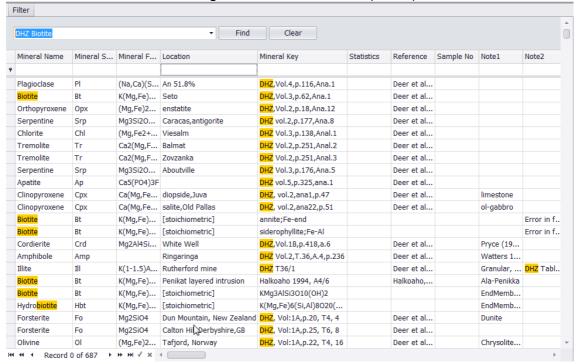
## HSC 8 – Geo - Mineralogical Calculations and Mineral Database

November 19, 2014 14024-ORC-J

5 (26)



You can write several searches by separating them with a space, e.g. writing DHZ biotite will show all the fields containing the text DHZ or biotite (below).





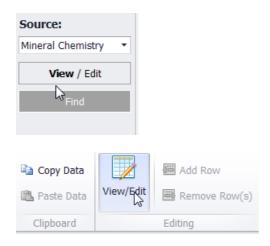
## **HSC 8 – Geo - Mineralogical Calculations and Mineral Database** November 19, 2014

14024-ORC-J

6(26)

#### 84.2.4. **Edit**

To edit the database, press View / Edit on the right panel or in the ribbon (top).



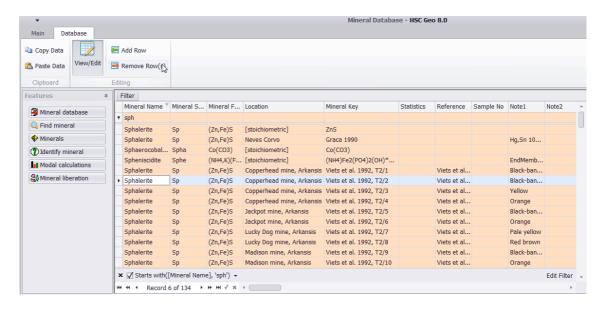
The database view color will change to pink, indicating that the database is in edit mode. Pressing the View/Edit button again will change the database to the view mode and the color white.

## Editing a content of a row

Activate the row and cell you want to edit and just type the new value in the cell. Change the cursor position and the value will be automatically saved in the database.

#### Deleting a row

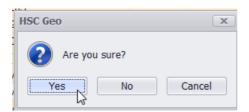
Select the row you want to delete and press Remove Row. Geo will ask you to confirm the removal.





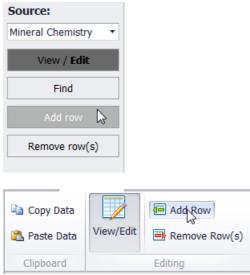
## HSC 8 – Geo - Mineralogical Calculations and Mineral Database November 19, 2014

14024-ORC-J 7 (26)

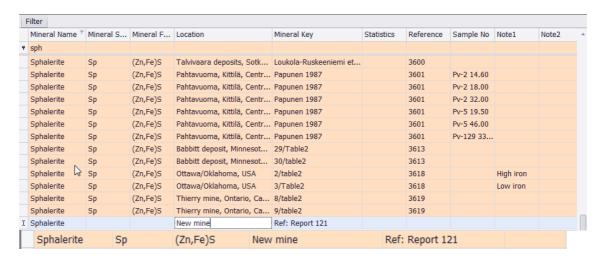


## Adding a new row by manually typing

Press Add Row on the right panel or in the ribbon.



Geo creates a new row at the end of the table. Type in the appropriate values. When ready, change the cursor and Geo will automatically fill in the Mineral Symbol and Mineral Formula fields.



### Adding a new row by pasting

The easiest way of adding new mineral rows to the Geo mineral database is to organize the table (e.g. in Microsoft Excel) and paste it into Geo.

When organizing the data, you need to comply with the following rules:

- · Data must be horizontal, one record on a row
- The first row must give the field (column) names



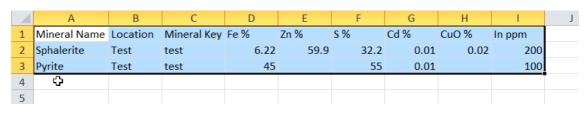
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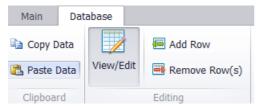
November 19, 2014 14024-ORC-J

8 (26)

- · The column names must be exactly as in the Geo mineral database
- Information is required for at least the Mineral Name, Location and Mineral Key columns

Select the data in Excel and in Geo select Paste Data.





Geo will advise how many rows were added and how many columns were identified. For example, the columns CuO % and In ppm were not identified and the data were not entered into the database. Copper values should have been given as Cu % and indium as In % for a successful paste.





HSC 8 – Geo - Mineralogical Calculations and Mineral Database November 19, 2014 14024-ORC-J

9 (26)

#### 84.3. Find mineral

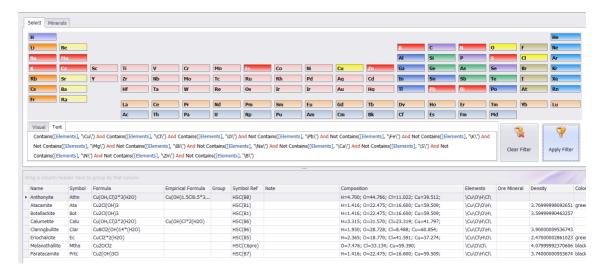
Find mineral is used to find minerals based on elements in their formula.

#### Press Find mineral



In the periodic table, click once the elements which are found in the mineral (shown in yellow) and twice for elements which are not in the mineral (shown in red). Pressing Apply Filter will make a query in the mineral database and show the ones which pass the criteria. The query conditions can be seen either in visual or text output below the periodic table.

An example of the minerals containing Cu, Cl and O but not B, N, Na, Mg, S, K, Ca, Fe, Zn, Pb and Bi is shown below.



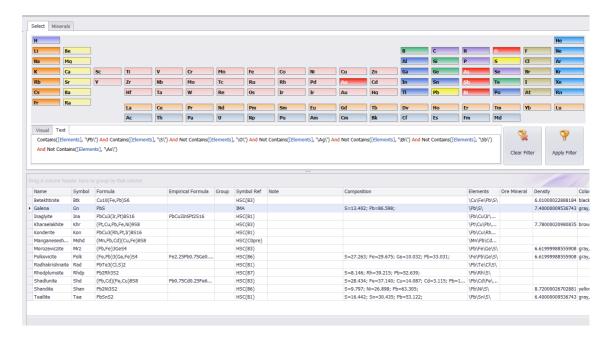
Another example of search for lead-bearing sulfides is shown below.



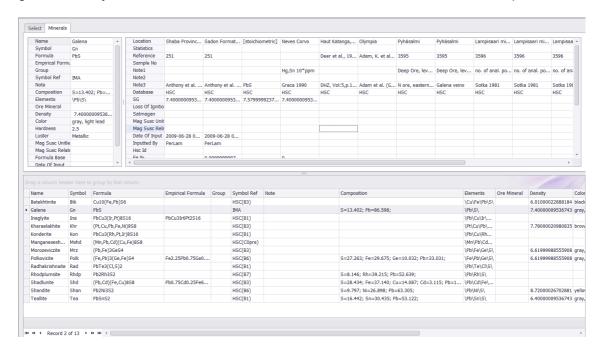
## HSC 8 – Geo - Mineralogical Calculations and Mineral Database

November 19, 2014 14024-ORC-J

10 (26)



To see more details on one of the minerals on the list, select the row and click the "Minerals" tab. An example concerning Galena is shown below. On the left, the general properties of the mineral (galena) are listed and on the right there is a table of different galenas analyzed from different localities are shown with their chemical composition.





HSC 8 – Geo - Mineralogical Calculations and Mineral Database November 19, 2014 14024-ORC-J

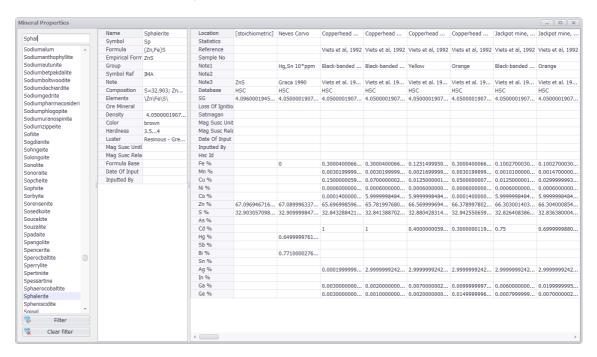
11 (26)

## 84.4. Minerals – Mineral properties

The Minerals button gives access to mineral properties by name.



In the Mineral Properties window, type the names of the mineral of interest (e.g. sphal... for sphalerite) and Geo will select the first mineral which matches the text you typed. On the left-hand side, there are the general properties of minerals and on the right-hand side, there is a table with different analyses of the selected mineral from different locations shown.



To study the chemical composition in the XY graph, press XY in the ribbon (group Mineral Graphs).



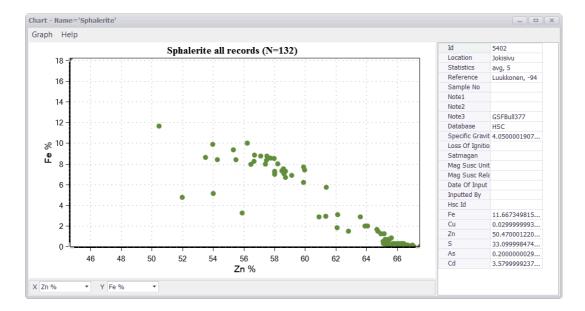
You can change the elements shown on the X and Y axis from the combo boxes below the graph.



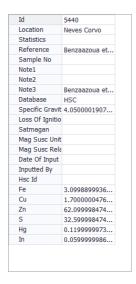
## HSC 8 – Geo - Mineralogical Calculations and Mineral Database

November 19, 2014 14024-ORC-J

12 (26)



When double-clicking any of the points on the graph, a table on the right-hand side of the graph will be updated to show the mineral analysis in question.



Another graph type available is Line Chart.



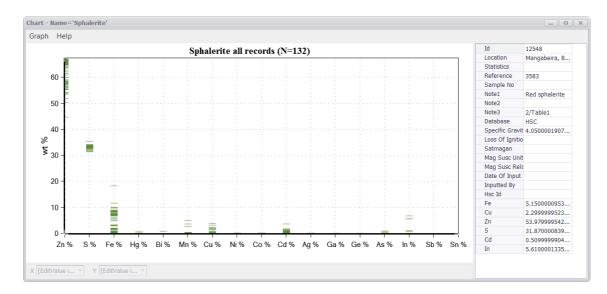
Pressing Line will summarize the variation in the chemical composition of the selected minerals in a line chart where each analyzed element is shown on the X axis and the narrow horizontal line represents one record in the database. More information on each point can be received when double- clicking: a table on the right-hand side will show the properties of the selected mineral analysis (i.e. record in the database).



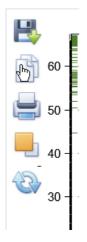
## HSC 8 – Geo - Mineralogical Calculations and Mineral Database

November 19, 2014 14024-ORC-J

13 (26)



To save, copy, or print, move the mouse on the picture and select the appropriate option in the floating menu.



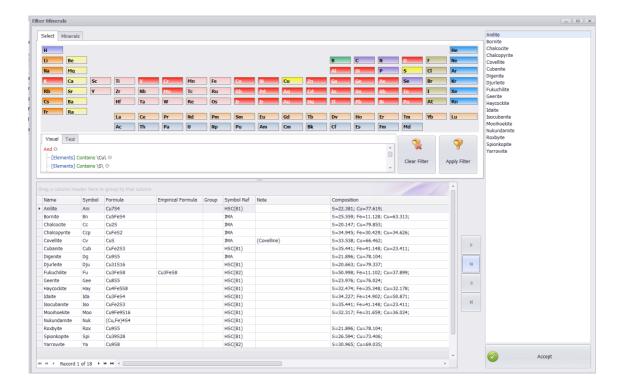
You can also use Filter by pressing the Filter in the lower left corner of the Mineral Properties window. In the Filter window, you can filter the minerals by the elements found in the formula (see the previous chapter on Find mineral). Move the desired minerals to the selected ones with and buttons (move selected, move all, respectively). When ready, press Accept.



# HSC 8 – Geo - Mineralogical Calculations and Mineral Database

November 19, 2014 14024-ORC-J

14 (26)



In the Mineral Properties window, select the minerals you want to study further and press XY.



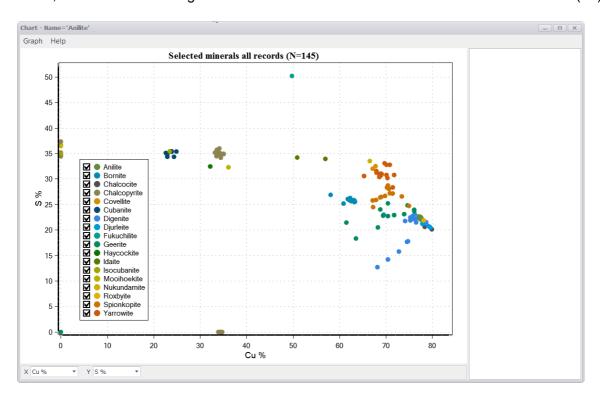
In the XY graph, you can select which minerals are shown by checking or unchecking them in the legend.



## HSC 8 – Geo - Mineralogical Calculations and Mineral Database

November 19, 2014 14024-ORC-J

15 (26)





## HSC 8 – Geo - Mineralogical Calculations and Mineral Database November 19, 2014

November 19, 2014 14024-ORC-J

16 (26)

## 84.5. Identify mineral

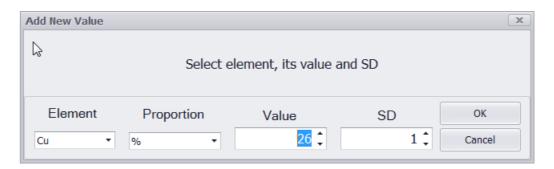
Identify Mineral is used to find a name for a mineral based on its chemical composition. Typically, this kind of question is faced when studying samples with scanning electron microscope (SEM) and EDS (or WDS) analysis is collected from a mineral grain.

Press Identify mineral in the left panel.

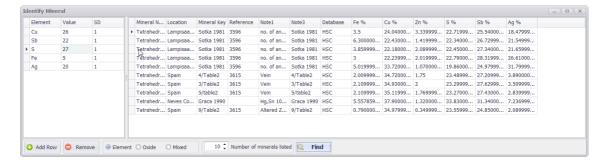


Let us propose that the EDS analysis gave 26% Cu, 22% Sb, 27% S, 5% Fe and 20% Ag.

To start with, press the Add button and select Cu for the element, % for the proportion, 26 for the value. SD is a standard deviation and you can obtain this information by analyzing the same grain several times and calculating the value of the standard deviation. You can use a default value of 1%. Press OK and add the next elements.



Finally, when adding all the conditions to be identified, press \_\_\_\_\_ Find\_\_\_



Geo will show you the 10 best matching minerals. Matching is done by calculating the Weighed Sum of Squares according to the following function:

$$SSQ = \sum_{E=1}^{n} \left( \frac{Database_{E} - Given_{E}}{SD_{E}} \right)^{2}$$

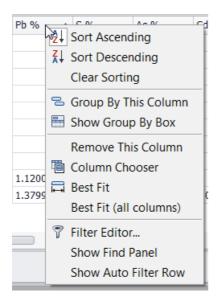


## HSC 8 – Geo - Mineralogical Calculations and Mineral Database November 19, 2014

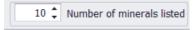
14024-ORC-J 17 (26)

The lower the SSQ, the better the match. The rows are displayed in the order of increasing SSQ. This time all the 10 best matches are for tetrahedrite and the identification can be regarded as reliable.

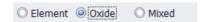
The table can be organized right-clicking on the columns and for example hiding it (Remove This Column).



The number of minerals listed can be changed in the lower part of the window.



It is also possible to change the give assays (composition) to an oxide form.





HSC 8 – Geo - Mineralogical Calculations and Mineral Database November 19, 2014

November 19, 2014 14024-ORC-J

18 (26)

## 84.6. Modal calculations – mass proportion of minerals in samples

## 84.6.1. Background and theory

Modal calculation means converting the elemental grades of a sample to mineral grades (Whiten, 2007)<sup>6</sup>. This is also called element to mineral conversion. The method is traditional and provides a simple way to estimate modal mineralogy (i.e. mass proportion of minerals in a sample) by solving simultaneously a set of mass balance equations formulated between chemical elements and minerals. The method is restricted to relatively simple mineralogy where the number of minerals is not larger than the number of analyzed components and the chemical composition of minerals (mineral matrix) is known. Mathematically, this can be written as follows:

$$A \times X = b$$

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \times \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

Where A is the matrix on the chemical composition of minerals (Mineral Matrix), x is the vector including the unknown mass proportion of minerals (modal mineralogy) in the sample and b is the vector on the analyzed chemical composition of the sample. The unknown x can be found e.g. using the non-negative least square method (Lawson & Hanson, 1995)<sup>2</sup>.

Element to mineral conversion can be improved by also using, in addition to conventional whole rock analysis, mineral selective methods like bromine-methanol leaching for nickel ores (Penttinen, Palosaari, & Siura, 1977)<sup>4</sup>, copper phase analysis for copper ores (Lamberg, Hautala, Sotka, & Saavalainen, 1997)<sup>1</sup> and Satmagan analysis for iron ores (Stradling, 1991, Lund et al., 2013)<sup>5,3</sup>.

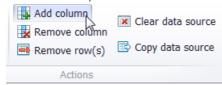
## 84.6.2. Simple calculation

#### **Manual input**

To give the chemical assays of samples manually, select Modal calculations



In the ribbon, select Add column



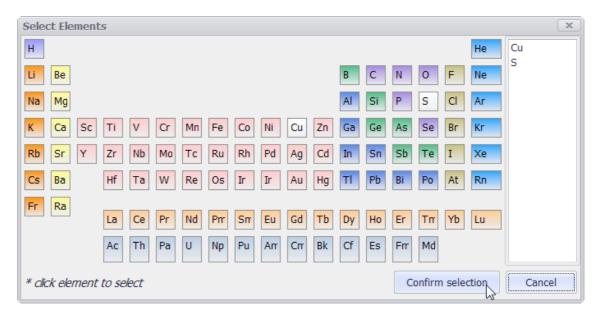


## HSC 8 – Geo - Mineralogical Calculations and Mineral Database November 19, 2014

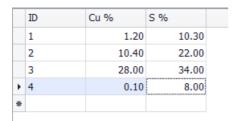
November 19, 2014 14024-ORC-J

19 (26)

In the Select Elements window, select the elements the assays are for. In this example, assays are available for Cu and S. Click on Cu and S and then Confirm selection.



Type in the sample ID and assays in the grid, for example as follows:



#### **Calculation Rules**

Press Rules to define the calculation rules



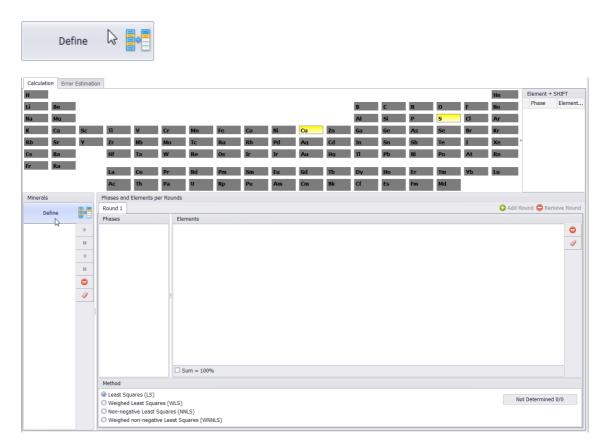
In the Modal Calculation window, the Periodic Table on the top shows the analyzed elements. The next step is to define the minerals. Press Define on the left side of the window.



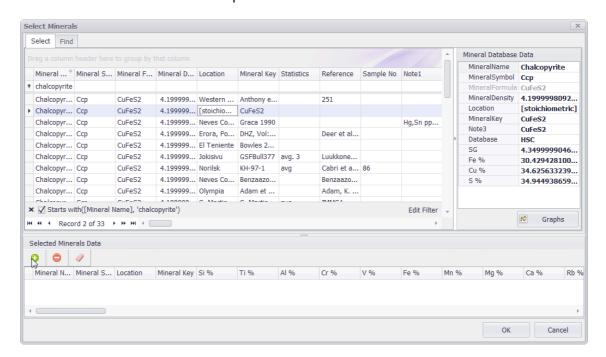
# HSC 8 – Geo - Mineralogical Calculations and Mineral Database

November 19, 2014 14024-ORC-J

20 (26)



In the Select Minerals type for instance the mineral name or other search criteria in the first row. Here chalcopyrite is written and Geo shows all the chalcopyrite records existing in the database. Select the record and press Add



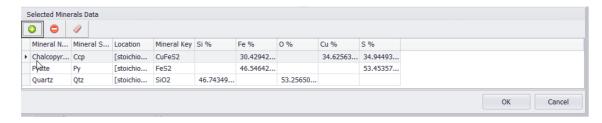
Continue until all the minerals existing in the samples are selected. In this example, the minerals are chalcopyrite, pyrite and quartz. Press OK when ready.



# HSC 8 – Geo - Mineralogical Calculations and Mineral Database

November 19, 2014 14024-ORC-J

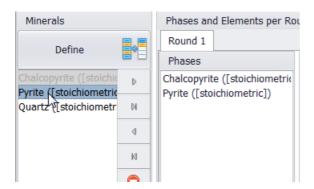
21 (26)



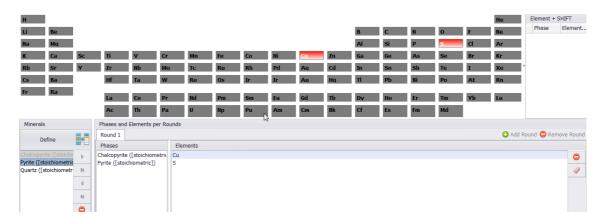
The next step is to define the rules for calculations. In this case, the rules are as follows:

- Chalcopyrite and Pyrite are calculated from Cu and S assays
- · Quartz is the remaining

Select the minerals (Chalcopyrite and Pyrite) and press to move them to the list of Phases (on Round 1).



Now select the elements, i.e. click on Cu and S to move them to the list of Elements. The color of Cu and S changes to red indicating that they have been used in the calculations.



Press Add Round to add another round for Quartz.



Select and move Quartz to the list of Phases and check the Sum = 100% option.



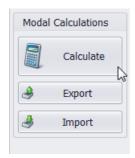
## **HSC 8 – Geo - Mineralogical Calculations and Mineral Database** November 19, 2014

14024-ORC-J

22 (26)



#### **Press Calculate**



## Studying the calculation result

The result is shown on seven tabs:

- Modal gives the mineral mass proportions (wt %)
- Distribution is to calculate the distribution of elements between the minerals
- Fraction is to calculate the composition of a given mineral fraction
- Residual gives the residue of the calculation
- Bulk Ch. gives the back-calculated chemical composition of the samples
- Notes/Statistics is for error estimation
- Initial values show the sample analyses and mineral matrix

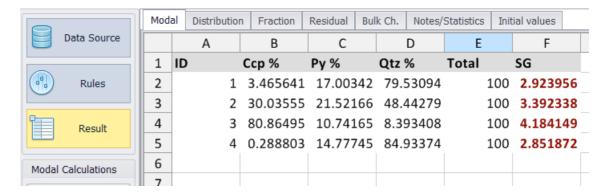
In the Modal sheet, each sample is listed horizontally, mineral grades are given as wt %, the total is displayed and SG is the calculated specific gravity (density) of the sample. Please note that when calculating density, the missing part (i.e. if the sum is below 100) is not regarded. The calculation is made as if the modal mineralogy would be normalized to 100%.



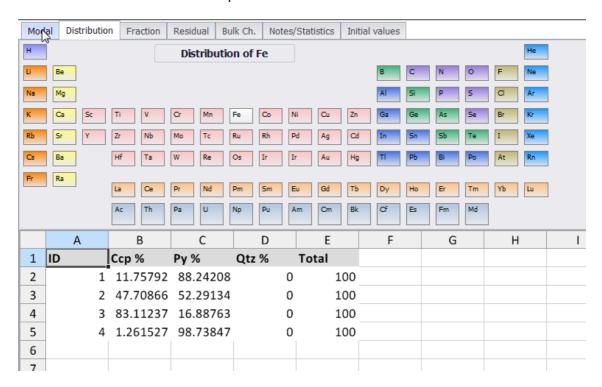
## HSC 8 – Geo - Mineralogical Calculations and Mineral Database

November 19, 2014 14024-ORC-J

23 (26)



To calculate the Distribution of any element between minerals, select the Distribution tab and select the element from the periodic table.



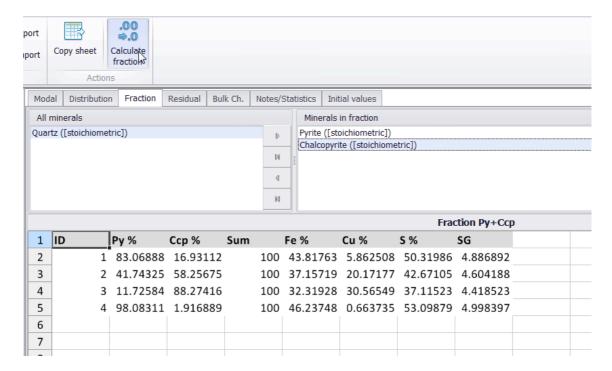
To calculate the composition of a mineral fraction select the Fraction tab, select and move the minerals to the list of Minerals in the fraction and press Calculate Fraction. Minerals in the fraction are normalized to 100% and the chemical composition of the mineral fraction is displayed. The fraction is used to estimate the composition of bulk sulfide concentrate, for example.



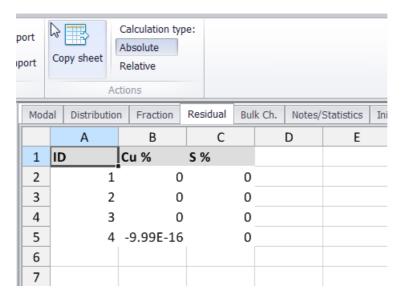
## HSC 8 – Geo - Mineralogical Calculations and Mineral Database

November 19, 2014 14024-ORC-J

24 (26)



Residual (in the Residual tab) shows the residue of the calculation. You can display the result either on an Absolute or Relative base.



Bulk Chemistry (on the Bulk Ch. Tab) shows the chemical composition of the sample when back- calculated from the modal composition (x) and chemical composition of minerals (A matrix).



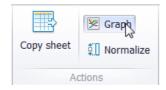
HSC 8 – Geo - Mineralogical Calculations and Mineral Database November 19, 2014

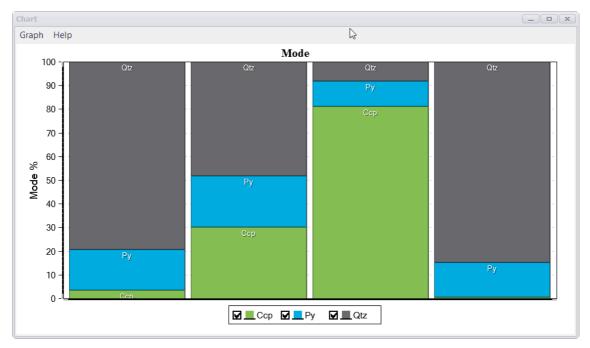
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14024-ORC-J 25 (26)

Mod	al Distribution	n Fraction	Residual Bul	k Ch. Notes/	Statistics Init	tial values	
	А	В	С	D	Е	F	G
1	ID	Si %	Fe %	0 %	Cu %	S %	SG
2	1	37.17554	8.969056	42.3554	1.2	10.3	2.923956
3	2	22.64385	19.15721	25.79894	10.4	22	3.392338
4	3	3.923372	29.60659	4.470036	28	34	4.184149
5	4	39.701	6.966257	45.23275	0.1	8	2.851872
6							
7							

Pressing the Graph on different sheets will show the result in a graphical format.







## HSC 8 – Geo - Mineralogical Calculations and Mineral Database November 19, 2014 14024-ORC-J

26 (26)

#### 84.7. References

- 1. Lamberg, P., Hautala, P., Sotka, P., & Saavalainen, S. (1997). Mineralogical balances by dissolution methodology, (1992), 1–29.
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