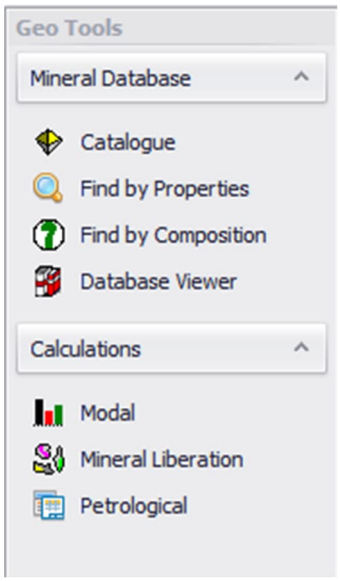
84. Geo Module - Mineralogical Calculations and Mineral Database

84.1. Introduction

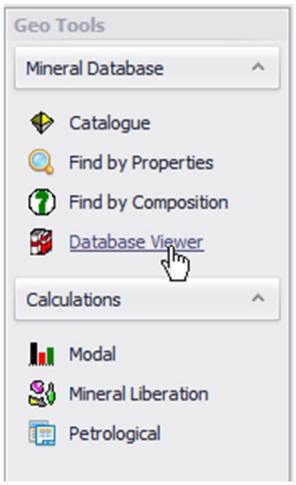
The Geo module of HSC is intended for:

- Studying mineral properties (Database Viewer, Catalogue: section 84.2, 84.4)
- Finding minerals based on elements in the formula (Find by Properties: 84.3)
- Identifying minerals based on the chemical composition (Find by Composition: 84.5)
- Performing petrological calculations (Petrological: 84.6)
- Calculating the modal composition (mineral composition) of samples based on chemical assays (Modal : 84.7)
- Processing mineral liberation data (Mineral liberation: 85)



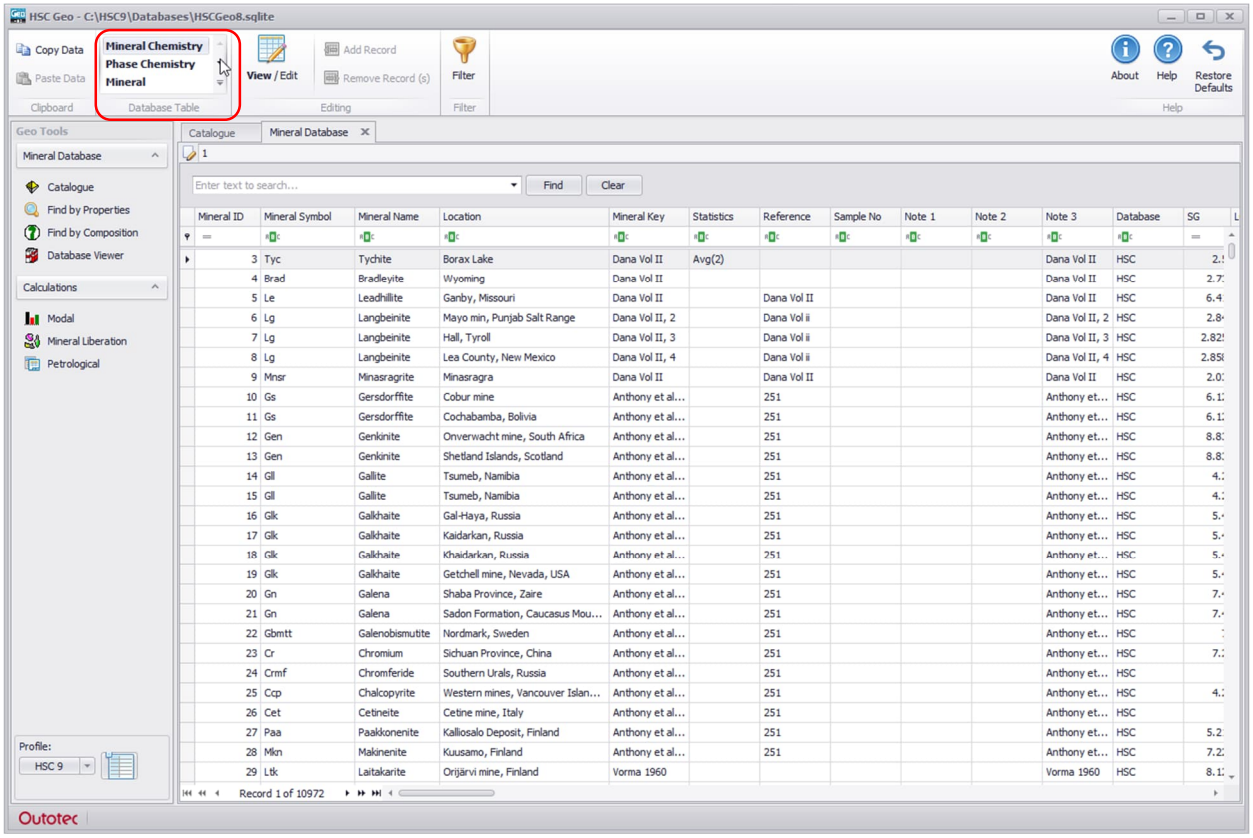
84.2. Mineral database

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



84.2.1. Source

There are different sources for the mineral database. These can be selected as in figure below



- Mineral Chemistry = Table of the chemical composition of minerals (different analyses of minerals from different locations)
- Phase Chemistry = Table of chemical compositions of different compounds

- Mineral = Table of minerals, one row per mineral
- Element = Chemical elements
- Mineral Dissolution = Table of mineral dissolutions alongside with method of analysis and the fraction extracted

After selecting the source you can apply:

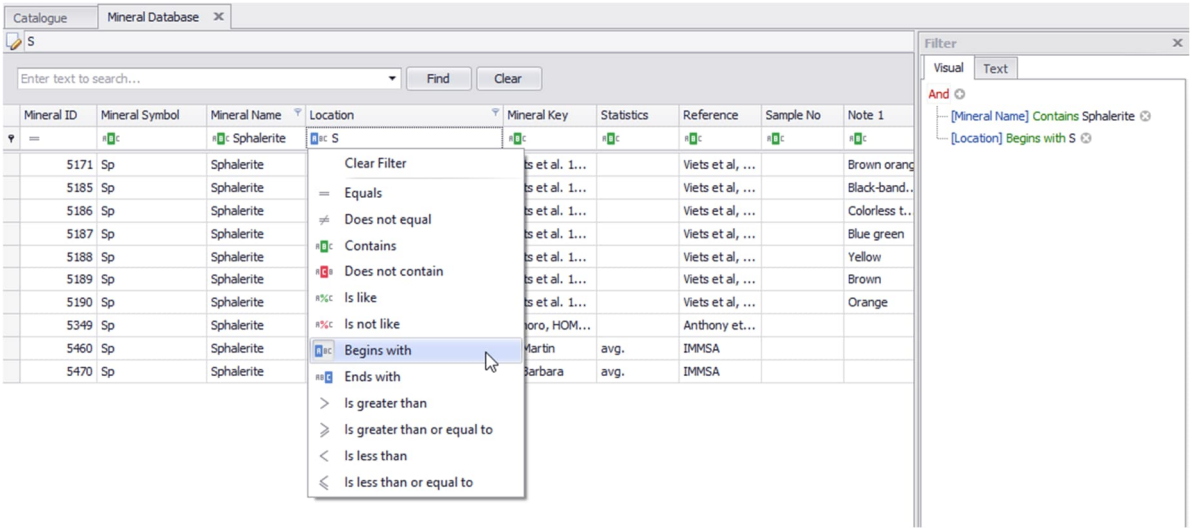
- Filter
- Search
- Edit

84.2.2. Filter

By clicking the filter icon 

, a new “Filter” window will appear in the right hand panel. You can then write a text in any of the fields in the top row. The small green “ABC” icon  beside the text can be pressed to choose the search criteria. The resulting search criteria will be shown in the “Filter” window.

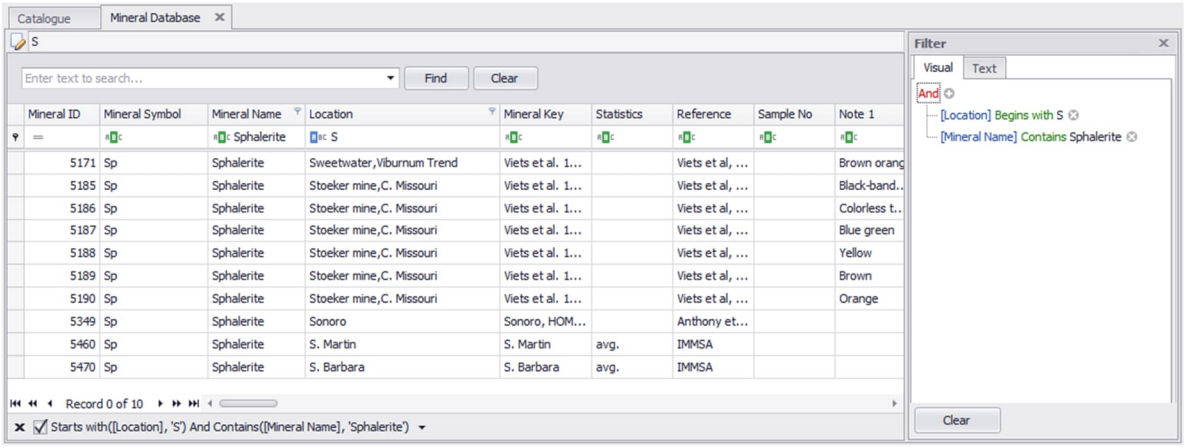
For instance, we want to search sphalerite minerals in all locations starting with the letter “S”. Type the Mineral Name = “Sphalerite” and the Location = “S”. By default the search criteria will then be all mineral names containing the word “Sphalerite” in all locations containing the letter “S”. To change this click the “ABC” icon under the Location column to define the criteria as “Begins with” the letter “S”. The search criteria is visualized in the Filter Window. There are a total of 10 records that fulfill the search criteria



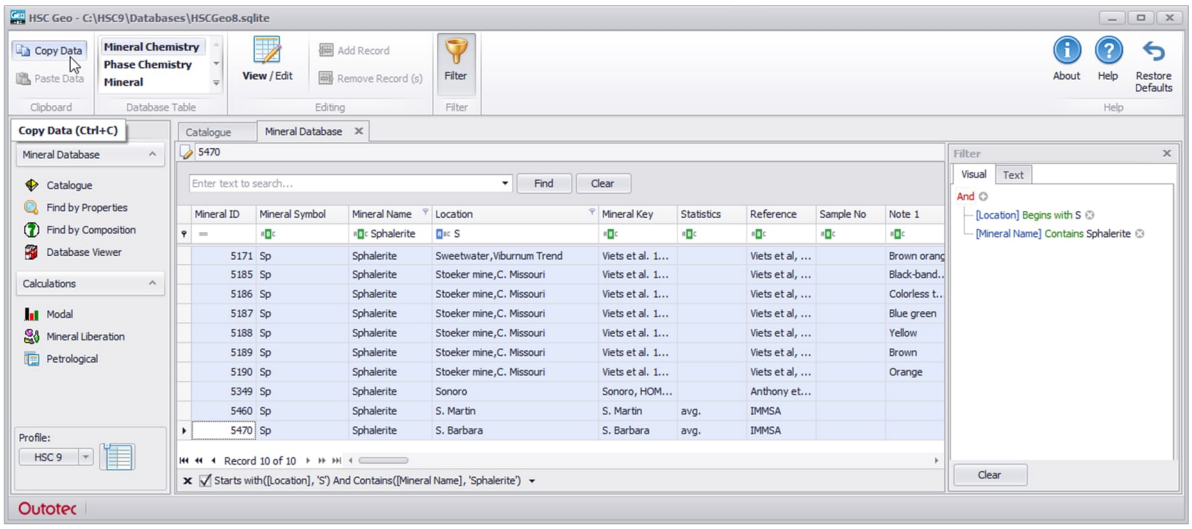
In the Filter Window you can:

- Edit the field by clicking the Field value given in blue and selecting a new one from the list, e.g. changing [Mineral Name] to [Mineral Symbol].
- Edit the condition given in green and selecting a new one from the list, e.g. changing “Contains” to “Begin With”
- Edit the operator given in red and selecting a new one from the list, e.g. changing “And” to “Or”

- Adding or deleting a search criteria. Alternatively you can clear all search criteria at once by pressing clear.

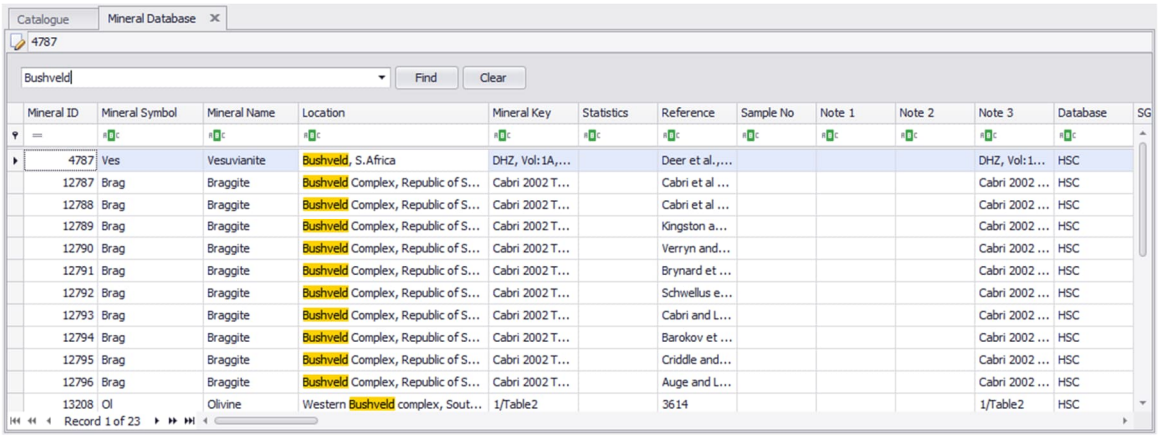


To copy data to the clipboard, select the rows you want to copy (use Ctrl or Shift to select several rows) and press “Copy Data.” Alternatively you can press the keyboard shortcut Ctrl + C.

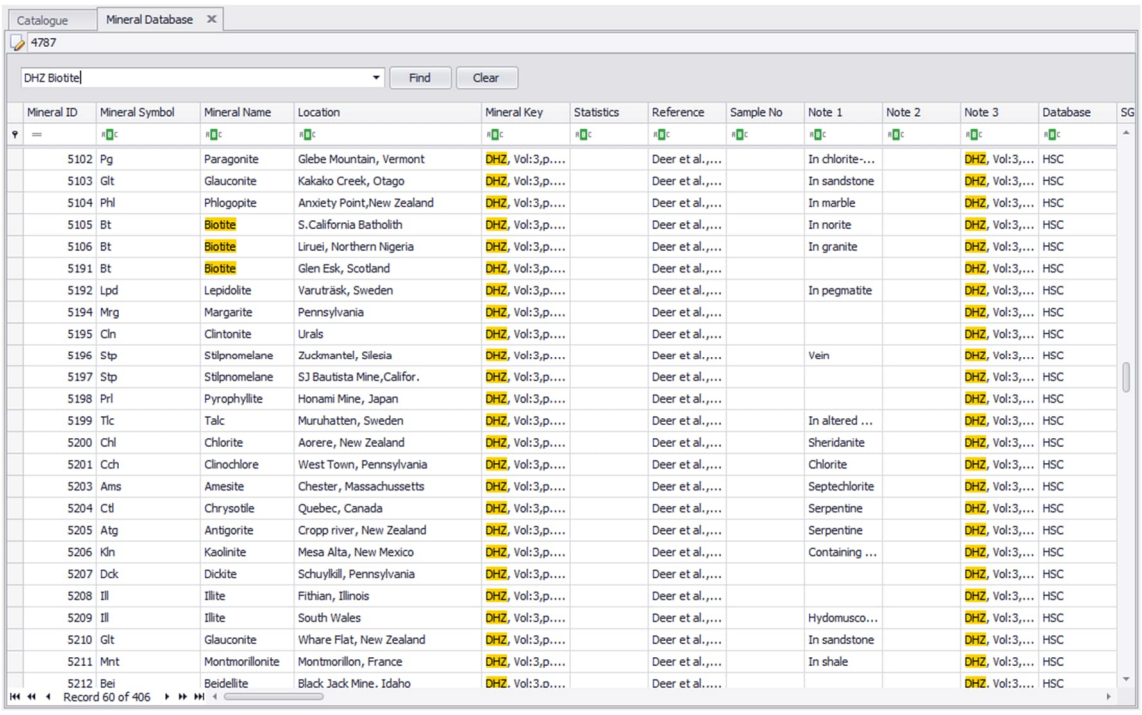


84.2.3. Find

You can search through the database by entering the keyword and clicking Find. Find differs from Filtering in that it always searches all the fields and it always seeks matches with any part of the field.

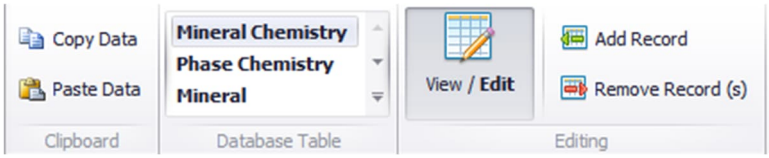


You can write several searches by separating them with a space, e.g. writing DHZ biotite will show all the fields containing the text DHZ or biotite (see below).



84.2.4. Edit

To edit the database, press View / Edit in the ribbon (top).



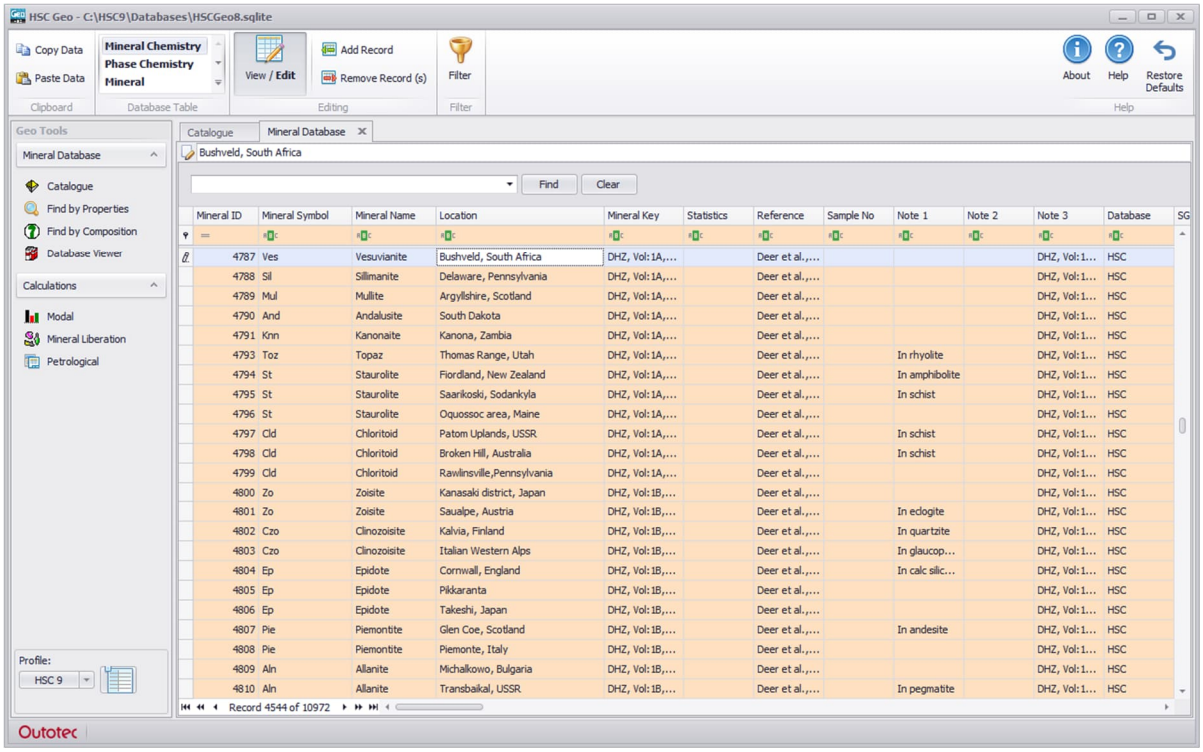
The database view color will change to orange, indicating that the database is in edit mode. Pressing the View/Edit button again will change the database to the view mode and the color to white.

Editing the 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.

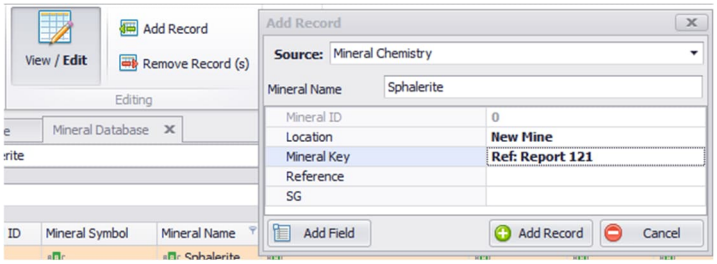
Deleting a row

Select the row you want to delete and press “Remove Record(s)”. Geo will ask you to confirm the removal.



Adding a new row by manually typing

Press “Add Record” on the right panel or in the ribbon. A new window will show in which you can enter the new record. You can add new field for the new record by pressing “Add Field”.



Geo creates a new row at the end of the table. Geo will also automatically fill in the Mineral Symbol fields.

Mineral ID	Mineral Symbol	Mineral Name	Location	Mineral Key	Statistics	Reference	Sample No	Note 1	Note 2	Note 3	Database
12625	Sp	Sphalerite	Pyhäsalmi	E corner		3595		Deep Ore, l...		E corner	HSC
12626	Sp	Sphalerite	Pyhäsalmi	W ore		3595		Deep Ore, l...		W ore	HSC
12627	Sp	Sphalerite	Pyhäsalmi	Galena veins		3595		Deep Ore, l...		Galena veins	HSC
12666	Sp	Sphalerite	Lampisaari mine, Vihanti	Lampinsaari, ...		3596		no. of anal...		Lampinsaar...	HSC
12667	Sp	Sphalerite	Lampisaari mine, Vihanti	Sotka 1981		3596		no. of anal...		Sotka 1981	HSC
12668	Sp	Sphalerite	Lampisaari mine, Vihanti	Sotka 1981		3596		no. of anal...		Sotka 1981	HSC
12685	Sp	Sphalerite	Talvivaara deposits, Sotkamo, Ka...	Törnroos 1982		3598				Törnroos 1...	HSC
12715	Sp	Sphalerite	Talvivaara deposits, Sotkamo, Ka...	Loukola-Rusk...		3600				Loukola-Ru...	HSC
12722	Sp	Sphalerite	Pahtavuoma, Kittilä, Central Lapl...	Papunen 1987		3601	Pv-2 14.60			Papunen 1...	HSC
12723	Sp	Sphalerite	Pahtavuoma, Kittilä, Central Lapl...	Papunen 1987		3601	Pv-2 18.00			Papunen 1...	HSC
12724	Sp	Sphalerite	Pahtavuoma, Kittilä, Central Lapl...	Papunen 1987		3601	Pv-2 32.00			Papunen 1...	HSC
12725	Sp	Sphalerite	Pahtavuoma, Kittilä, Central Lapl...	Papunen 1987		3601	Pv-5 19.50			Papunen 1...	HSC
12726	Sp	Sphalerite	Pahtavuoma, Kittilä, Central Lapl...	Papunen 1987		3601	Pv-5 46.00			Papunen 1...	HSC
12727	Sp	Sphalerite	Pahtavuoma, Kittilä, Central Lapl...	Papunen 1987		3601	Pv-129 33.50			Papunen 1...	HSC
13206	Sp	Sphalerite	Babbitt deposit, Minnesota, USA	29/Table2		3613				29/Table2	HSC
13207	Sp	Sphalerite	Babbitt deposit, Minnesota, USA	30/table2		3613				30/table2	HSC
13281	Sp	Sphalerite	Ottawa/Oklahoma, USA	2/table2		3618		High iron		2/table2	HSC
13282	Sp	Sphalerite	Ottawa/Oklahoma, USA	3/Table2		3618		Low iron		3/Table2	HSC
13300	Sp	Sphalerite	Thierry mine, Ontario, Canada	8/table2		3619				8/table2	HSC
13301	Sp	Sphalerite	Thierry mine, Ontario, Canada	9/table2		3619				9/table2	HSC
13336	Sp	Sphalerite	New Mine	Ref: Report ...							

Adding a new row by pasting

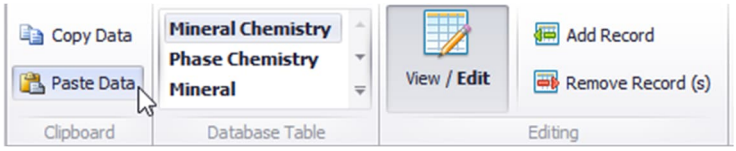
The easiest way of adding new mineral rows to the Geo mineral database is to organize the table (e.g. in Microsoft Excel) and paste it into Geo.

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

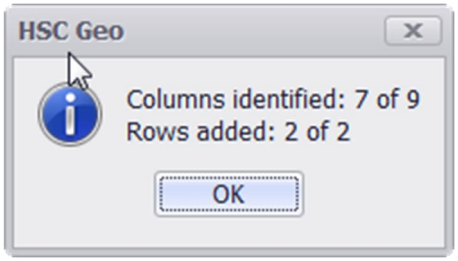
- Data must be horizontal, one record per row
- The first row must give the field (column) names
- The column names must be exactly the same as in the Geo mineral database
- Information is required for at least the Mineral Name, Location, and Mineral Key columns

Select the data in Excel and in Geo select Paste Data. Alternatively, the keyboard shortcut Ctrl + V can be used

	A	B	C	D	E	F	G	H	I	J
1	Mineral Name	Location	Mineral Key	Fe %	Zn %	S %	Cd %	CuO %	In ppm	
2	Sphalerite	Test	test	6.22	59.9	32.2	0.01	0.02	200	
3	Pyrite	Test	test	45		55	0.01		100	
4										
5										



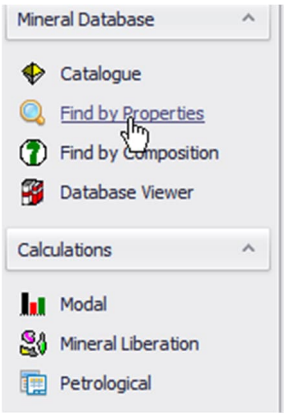
Geo will advise how many rows were added and how many columns were identified. For example, the columns CuO % and In ppm were not identified and the data were not entered into the database. Copper values should have been given as Cu % and indium as In % for a successful paste.



84.3. Find by Properties

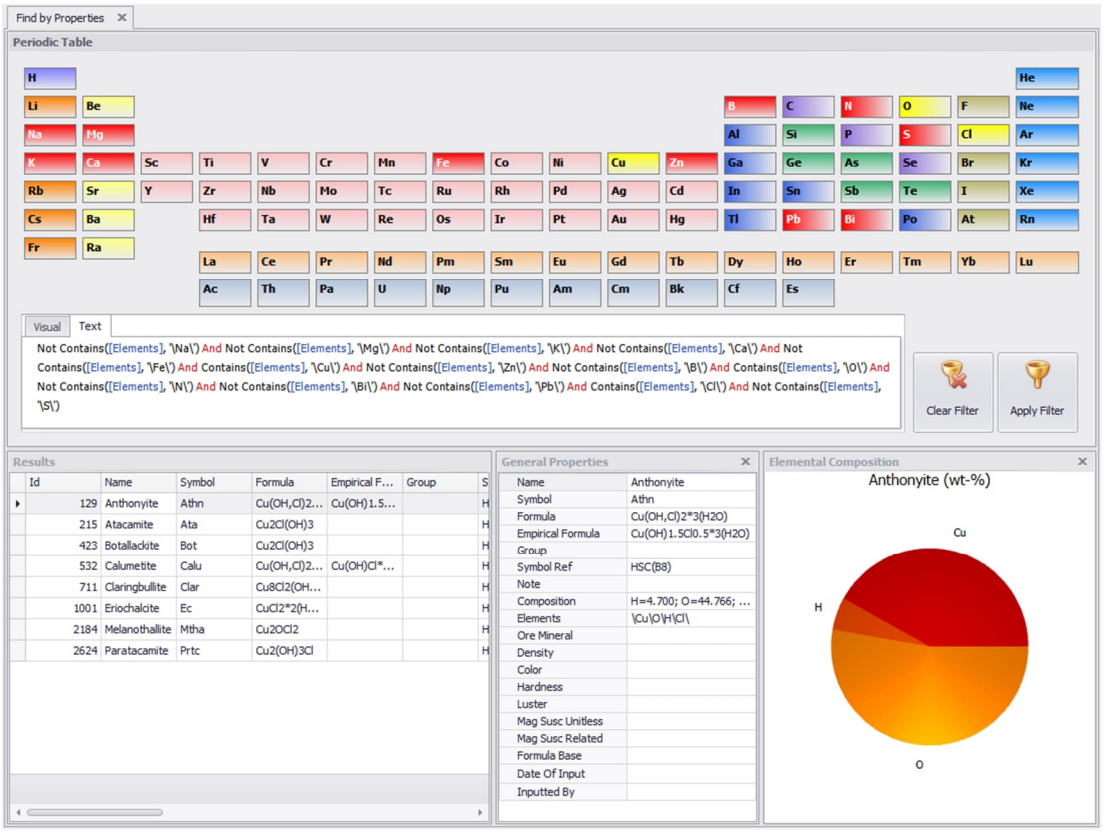
“Find by Properties” is used to find minerals based on elements in their formula.

Press “Find by Properties”

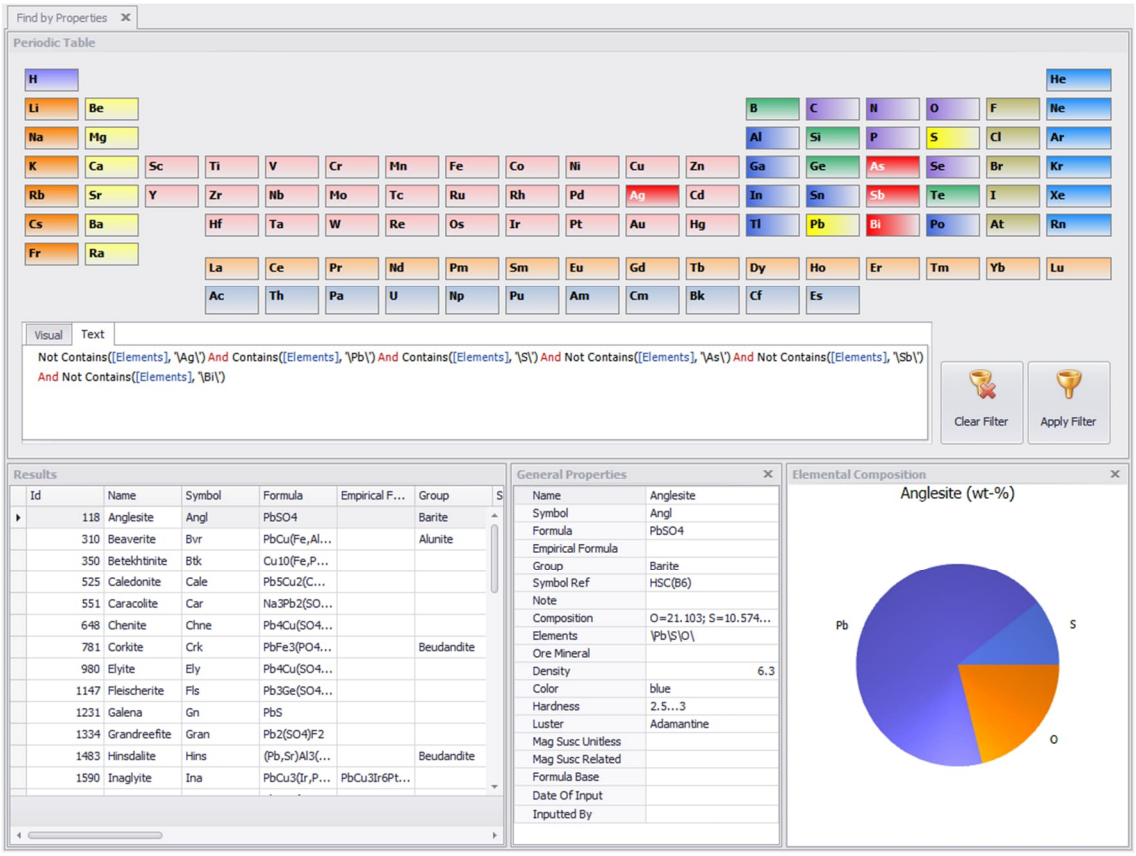


In the periodic table, click once on the elements that are found in the mineral (shown in yellow) and twice for elements that are not in the mineral (shown in red). Pressing Apply Filter will make a query in the mineral database and show those that pass the criteria. The query conditions can be seen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

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



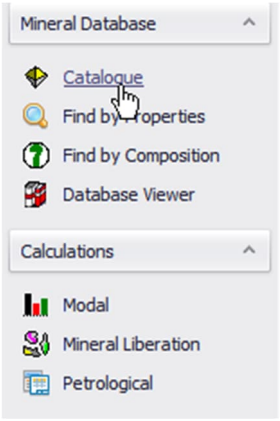
Id	Name	Symbol	Formula	Empirical F…	Group
118	Anglesite	Angl	PbSO4		Barite
310	Beaverite	Bvr	PbCu(Fe,Al…		Alunite
350	Betekhtinite	Btk	Cu10(Fe,P…		
525	Caledonite	Cale	Pb5Cu2(C…		
551	Caracolite	Car	Na3Pb2(SO…		
648	Chenite	Chne	Pb4Cu(SO4…		
781	Corkite	Crk	PbFe3(PO4…		Beudandite
980	Elyite	Ely	Pb4Cu(SO4…		
1147	Fleischerite	Fls	Pb3Ge(SO4…		
1231	Galena	Gn	PbS		
1334	Grandreefite	Gran	Pb2(SO4)F2		
1483	Hinsdalite	Hins	(Pb,Sr)Al3(…		Beudandite
1590	Inaglyite	Ina	PbCu3(Ir,P…	PbCu3Ir6Pt…	

Name	Anglesite
Symbol	Angl
Formula	PbSO4
Empirical Formula	
Group	Barite
Symbol Ref	HSC(B6)
Note	
Composition	O=21.103; S=10.574…
Elements	\Pb\S\O\
Ore Mineral	
Density	6.3
Color	blue
Hardness	2.5…3
Luster	Adamantine
Mag Susc Unitless	
Mag Susc Related	
Formula Base	
Date Of Input	
Inputted By	

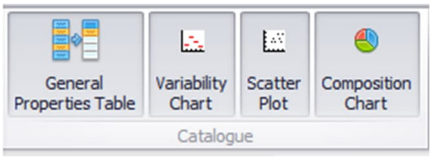
The details of the resulting minerals are readily available in the lower panels. By selecting one row, the general properties of that mineral can be seen, alongside with the chemical composition graph. Example here is shown for Anglesite.

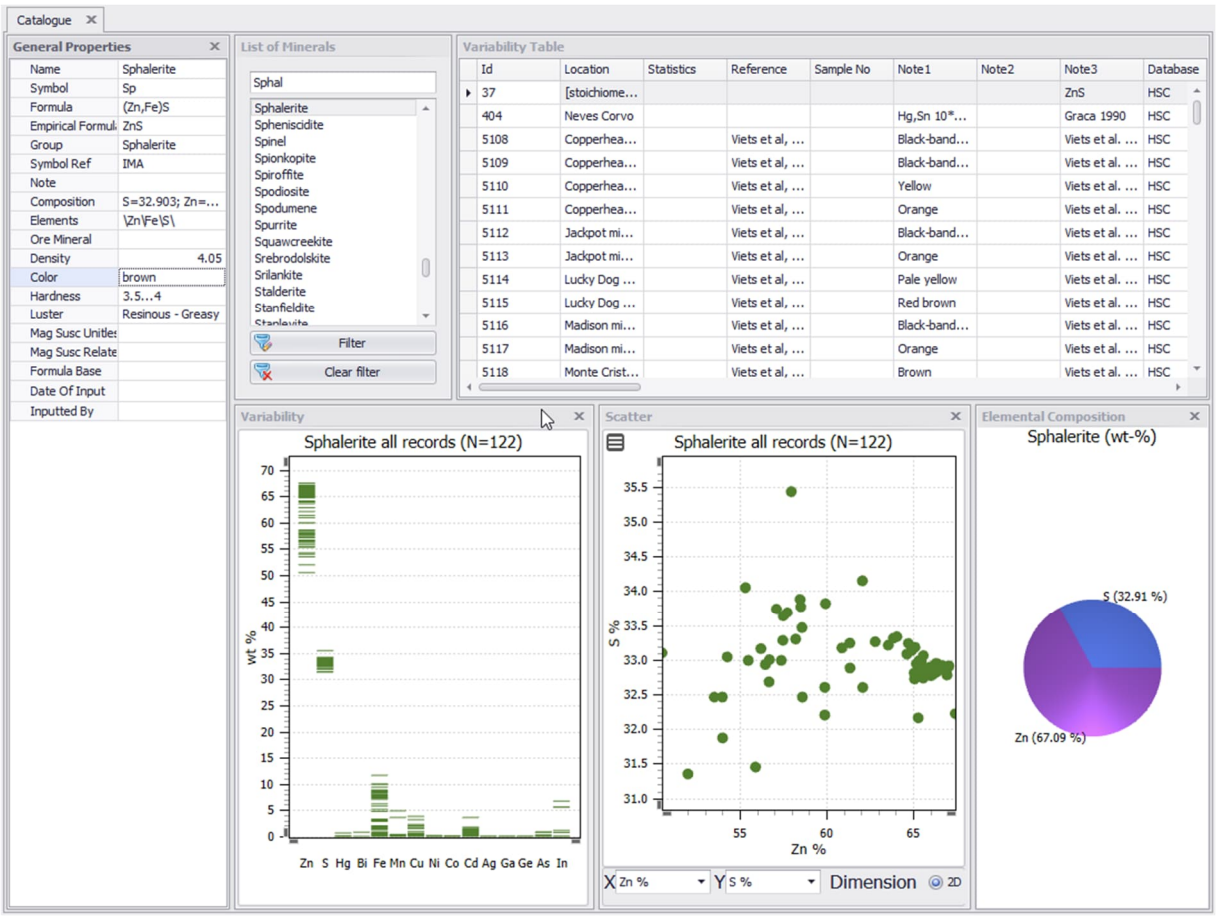
84.4. Catalogue

The Catalogue button gives access to mineral properties by name.

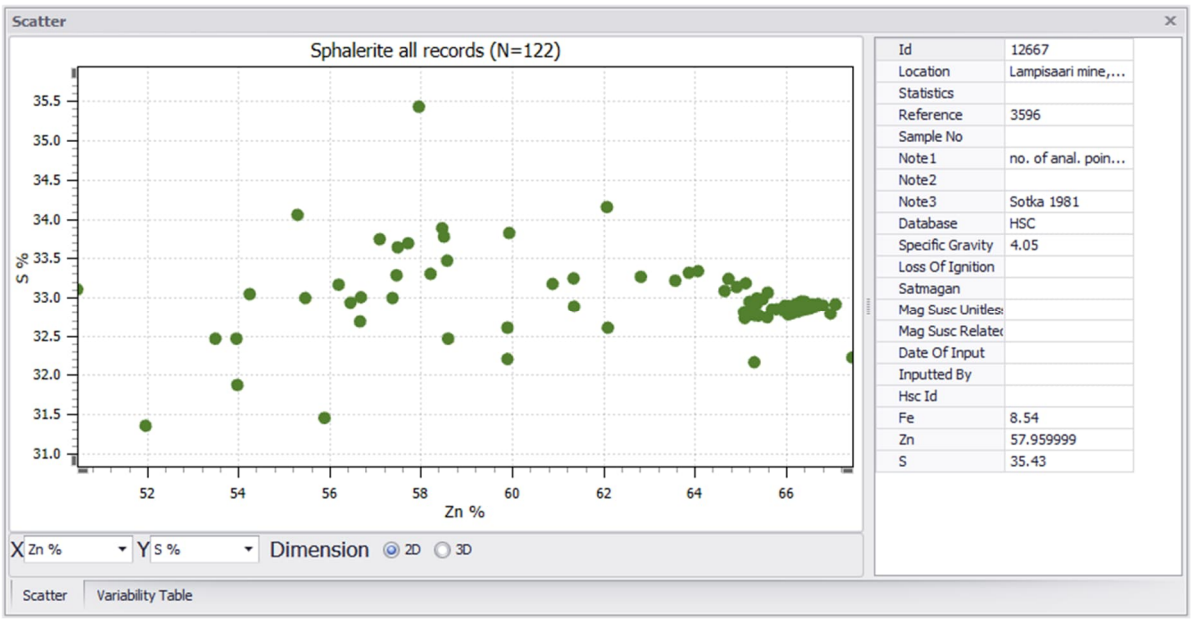


In the List of Minerals window, type the names of the mineral of interest (e.g. sphal… for sphalerite) and Geo will select the first mineral that matches the text you typed. The general properties of minerals are on the left and there is a table with different analyses of the selected mineral from the different locations shown on the right. By default, three graphs are given: elemental composition pie chart, scatter plot between different elements, and variability of the elements. This can be turned on and off in the top ribbon





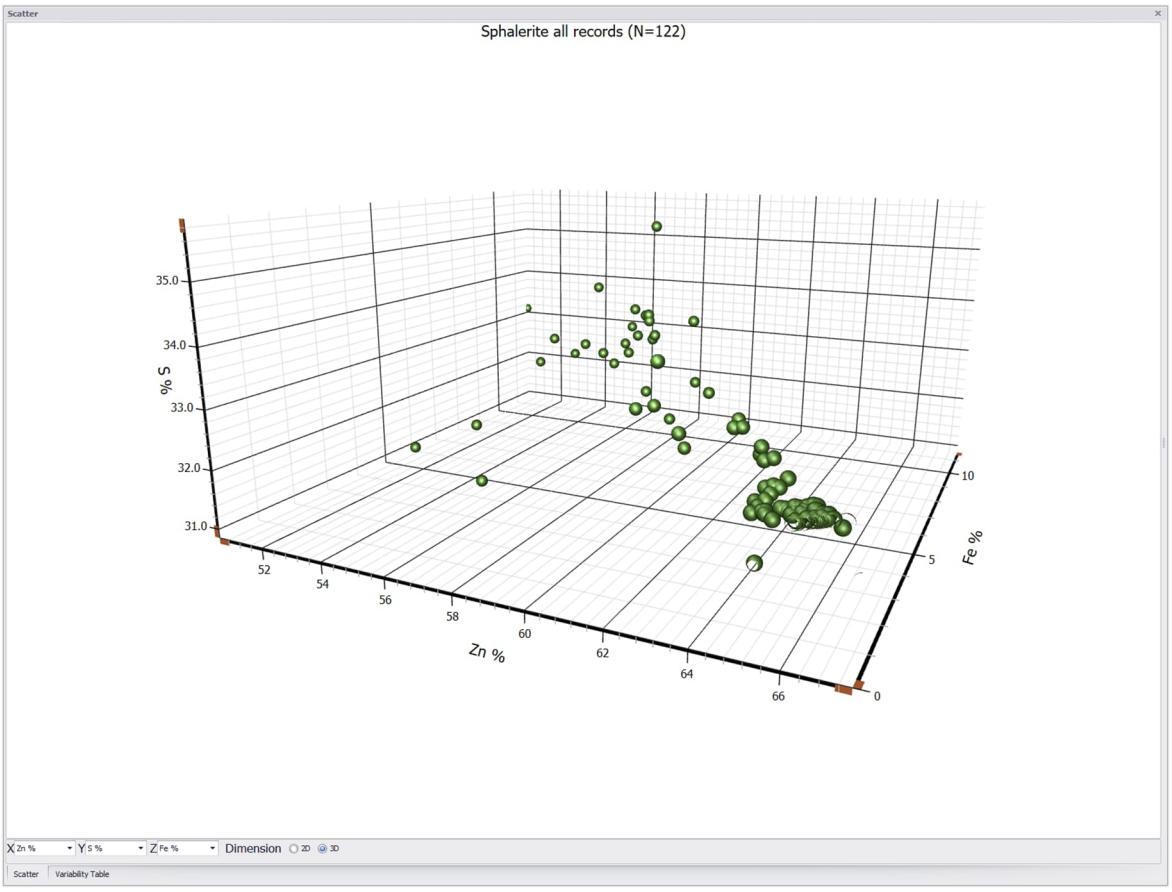
In the scatter plot, you can change the elements shown on the X and Y axis from the combo boxes below the graph.



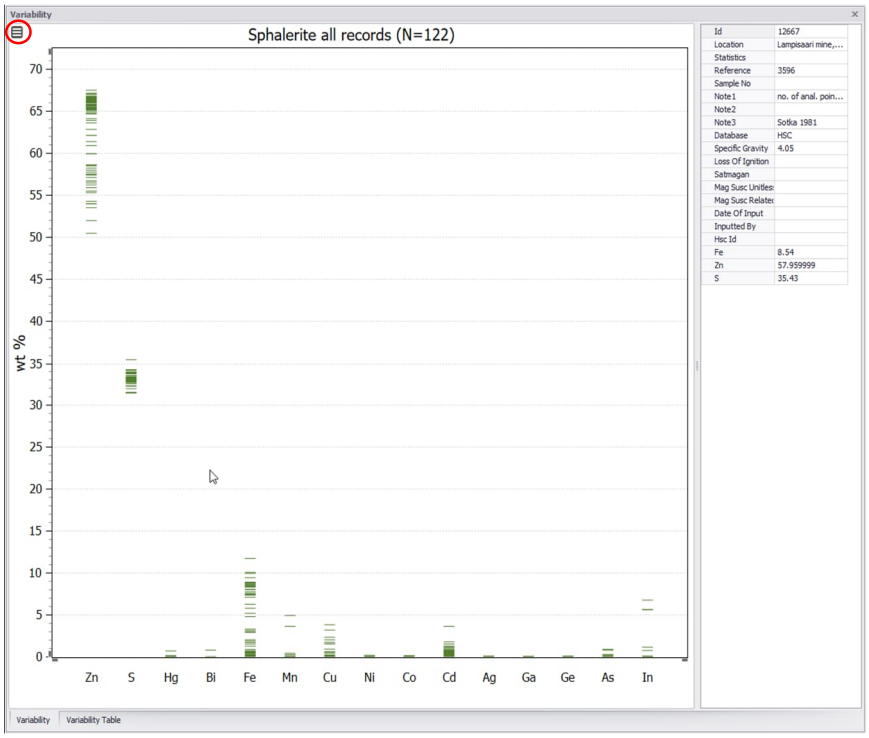
When double-clicking any of the points on the graph, the table on the right-hand side of the graph will be updated to show the mineral analysis in question.

Id	13300
Location	Thierry mine, On...
Statistics	
Reference	3619
Sample No	
Note1	
Note2	
Note3	8/table2
Database	HSC
Specific Gravity	4.05
Loss Of Ignition	
Satmagan	
Mag Susc Unitles:	
Mag Susc Relatec	
Date Of Input	
Inputted By	
Hsc Id	
Fe	6.22
Cu	1.5
Ni	0.15
Co	0.12
Zn	59.900002
S	32.200001

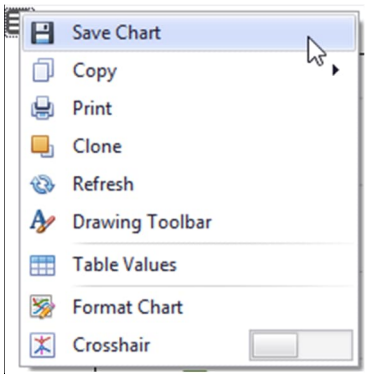
Additionally, an additional Z-axis could also be made for making 3D scatter plot.



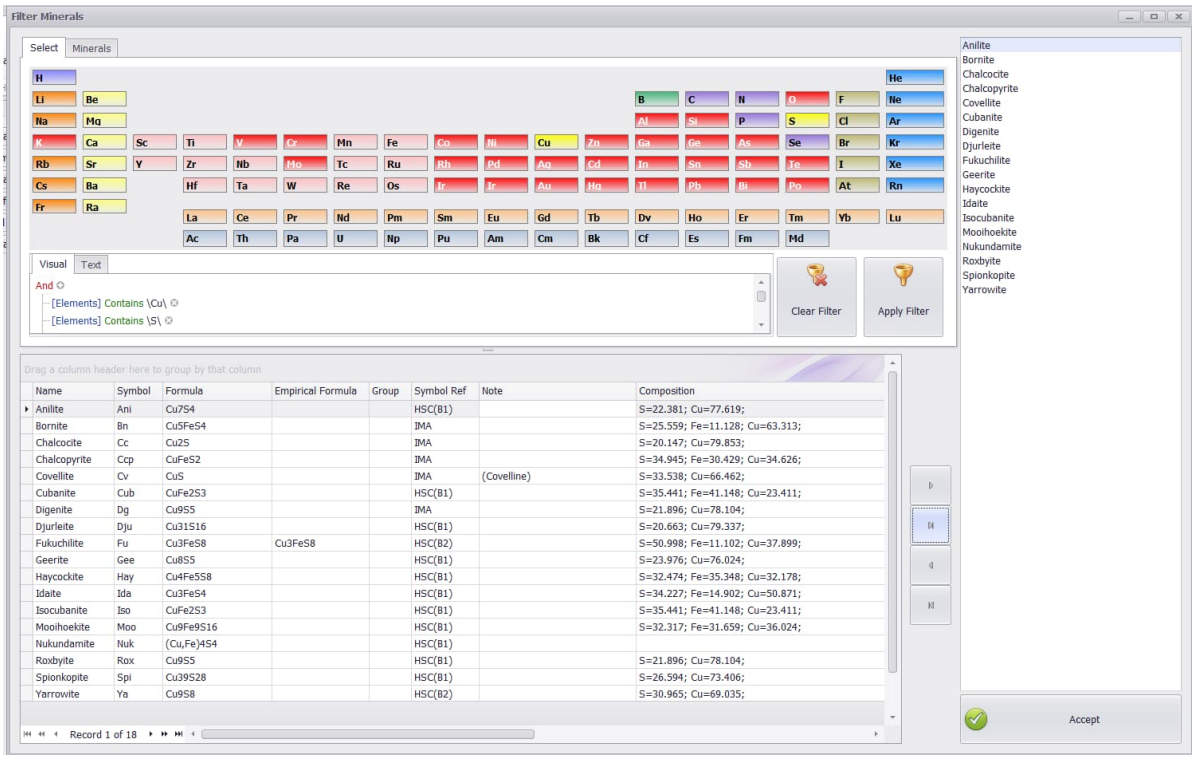
The variability chart summarizes the variation in the chemical composition of the selected minerals in a line chart, where each analyzed element is shown on the X axis and the narrow horizontal line represents one record in the database. More information on each point can be received when double-clicking: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



To save, copy, or print, select the three rows icon in the top left corner of the chart.



You can also use a filter by pressing “Filter” in the lower left corner of the List of Minerals 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 the  and  buttons (move selected, move all, respectively). When ready, press “Accept”.

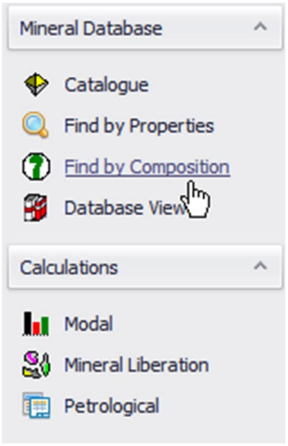


In the List of Minerals window, select the mineral that you want to study further.

84.5. Find by Composition

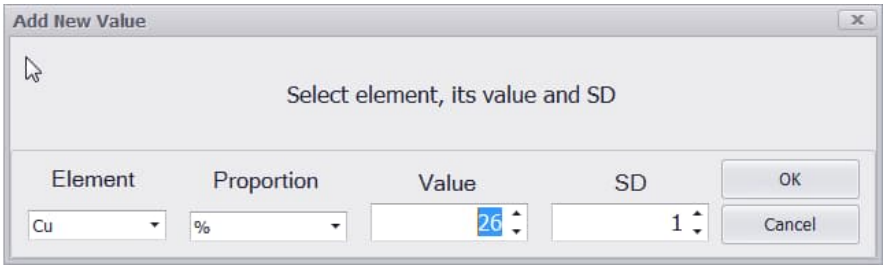
“Find by Composition” is used to find a name for a mineral based on its chemical composition. Typically, this kind of question is faced when studying samples with scanning electron microscope (SEM) and EDS (or WDS) and an analysis is collected from a mineral grain.

Press “Find by Composition” in the left panel.

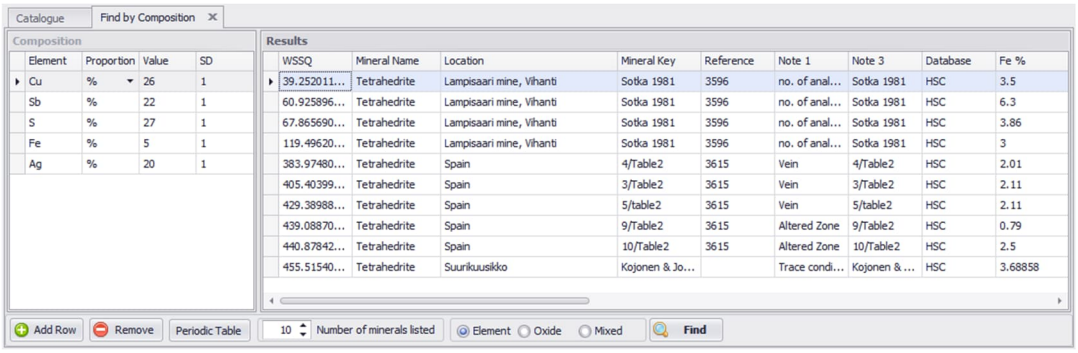


Let us propose that the EDS analysis gave 26% Cu, 22% Sb, 27% S, 5% Fe, and 20% Ag. To start with, press the Add button 

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. Alternatively, the elements can be added by choosing from the periodic table 



Finally, when you have added all the conditions to be identified, press 

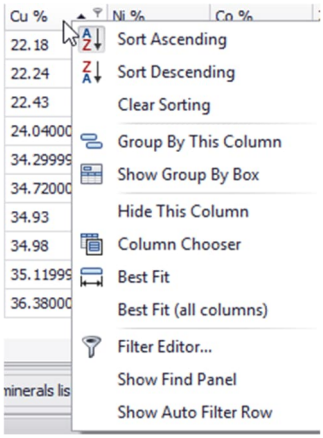


Geo will show you the 10 best matching minerals. Matching is done by calculating the Weighed Sum of Squares according to the following function:

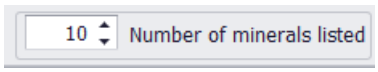
$$WSSQ = \sum_{E=1}^{n} \left(\frac{Database_E - Given_E}{SD_E} \right)^2$$

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

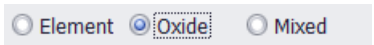
The table can be organized by right-clicking on the columns and for example hiding it (Hide This Column).



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



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



84.6. Petrological calculations

84.6.1. General procedure

The general procedure of HSC Geo in working with rock and mineral analyses is as follows:

1) Prepare the data e.g. in Excel and save using Excel file format.
2) Open the files in HSC Geo or paste to HSC Geo
3) Run the identification routine
4) Customize the calculation routines, if required
5) Do the calculations
6) Check and recalculate, if necessary
7) Save the result

84.6.2. Preparing the data

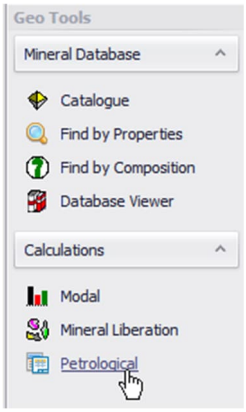
To ease and quicken the data processing in HSC Geo, prepare your data to satisfy the following requirements:

- Data should be row-wise; one observation or measurement per line, i.e. each sample has its own row.
- Place each data type in its own file or own sheet. For example, one sheet/file has the header information of samples, one sheet includes XRF analyses, another REE analyses, and one PGE assays
- Place the header in the first row and ID column in the first column
- In the header row or rows you should specify the element in analysis, the analysis method, and the unit, e.g. SiO2/XRF/%. The following options exist:
    - Place the element, method and unit in individual rows:
        - Place the element in the first row and name this row ELEMENT
        - Place the method in the second (or third) row and name it METHOD
        - Place the unit in its own row and name it UNIT. HSC Geo understands the following units: wt%, %, ppm, g/t, ppb
    - Place the element, method and unit in the first row and separate them with a space or / (e.g. Cr XRF ppm, Cr/XRF/ppm)
    - Name the file or sheet according to the method and then there is no need to repeat it. On the XRF sheet, the header gives the element and method, for example, Cr ppm.
- The decimal separator should be a point (e.g. 21.34)
- Save data as an Excel file (version 5) or as a tab-separated text file

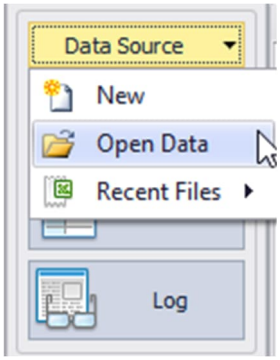
84.6.3. Tutorial Data in Excel File with Multiple Sheets – Step-by-step

This tutorial guides you through the HSC Geo steps where you open the dataset, perform the calculations, and save the result in the database.

1. Run HSC Geo, Choose Petrological



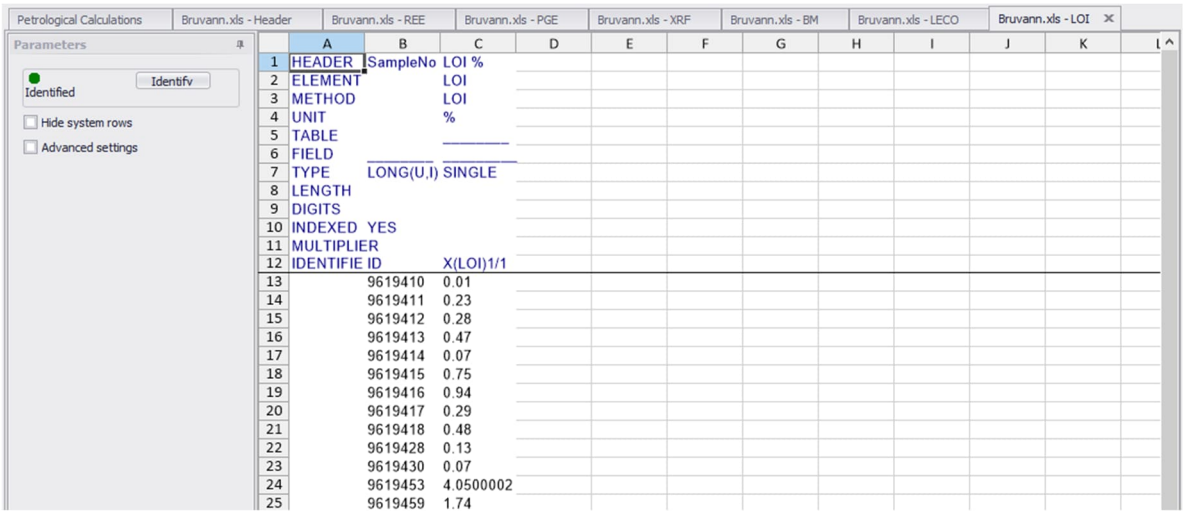
2. Select Data Source, then Open Data from the left button list



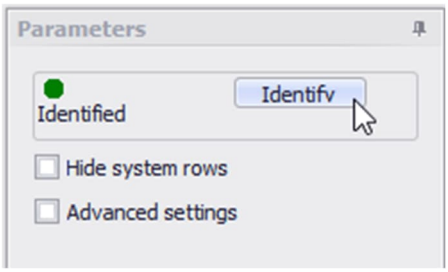
3. Select from the data folder (C:\Program Files (x86)\HSC10\Geo\Data) example file Bruvann.xls
4. HSC Geo opens the Excel file and places each sheet as its own source window. A total of seven sources are visible:

- Bruvann / Header (header data, location data)
- Bruvann / LOI (loss of ignition analyses)
- Bruvann / LECO (Leco analyses)
- Bruvann / BM (bromine-methanol analyses)
- Bruvann / XRF (X-ray fluorescence analyses)
- Bruvann / PGE (PGE analyses)
- Bruvann / REE (REE analyses)

In each source (Excel sheet) the data is row-wise, the first row includes the header, and the sample ID is placed in each file in the first column. For the chemical elements, both the element name and unit are given in the first row separated by a space, e.g. Al2O3 %. Each source (i.e. Excel sheet) has been named according to the assay method. Please follow this procedure with your own data. Do not leave empty columns or rows.

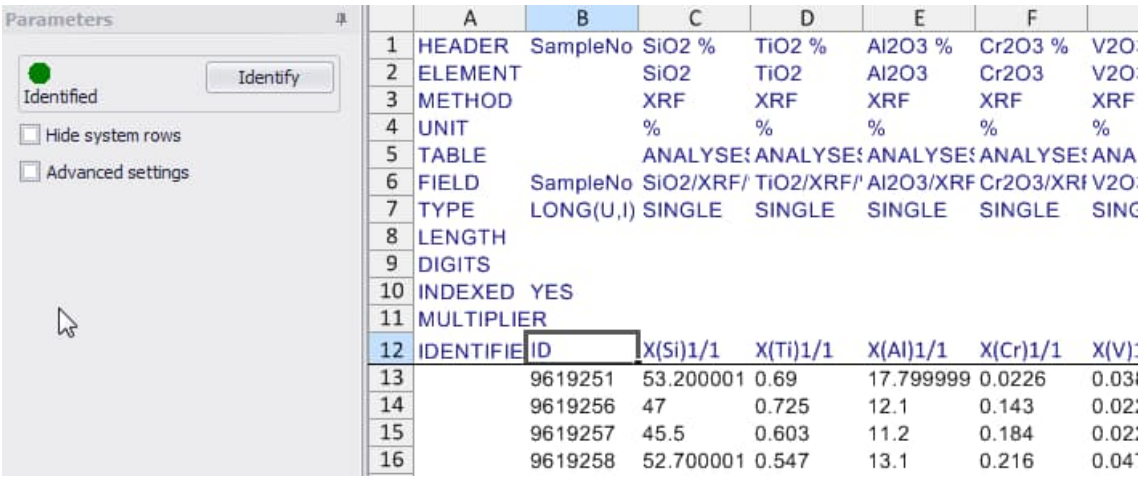


5. If the excel data fulfil the format requirements, HSC Geo would automatically identify the structure when opening the data. Otherwise, click identify in the Parameters window. If identified correctly the status would turn from red dot “Not Identified” to green dot “Identified”



6. HSC Geo identifies the structure of each source and, to indicate the result, each source includes **header rows** (blue text on gray background) as follows:

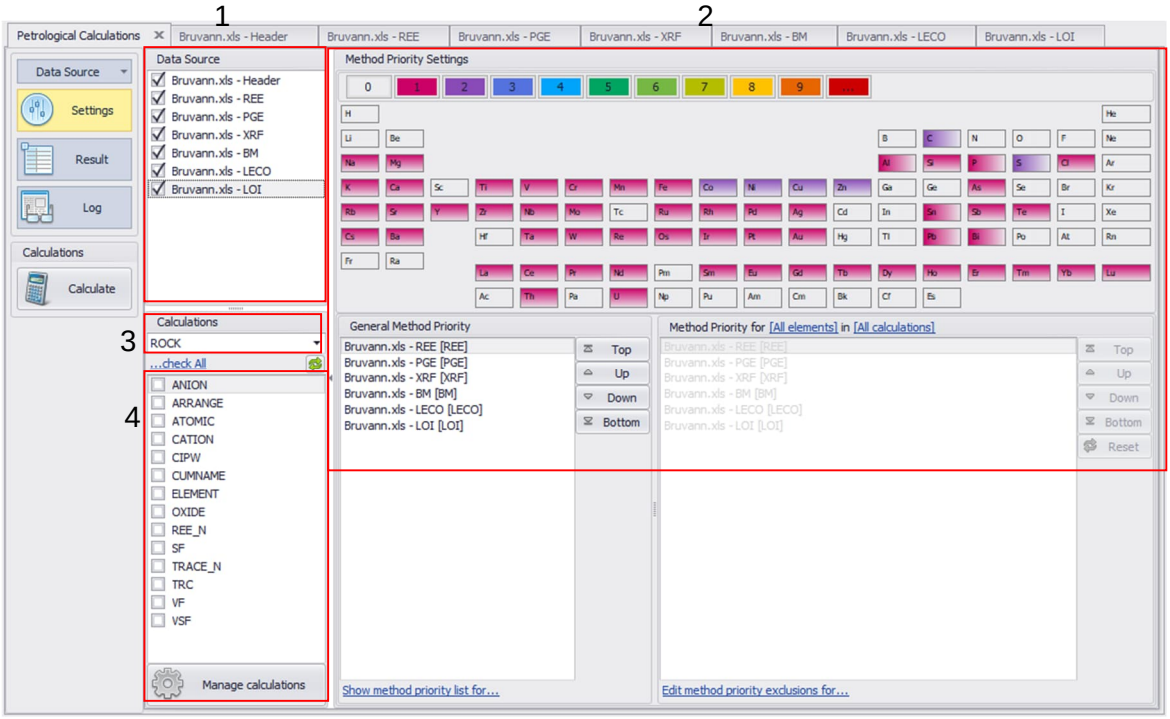
- -Hdr- HEADER: is the original header of the data
- -Ele- ELEMENT: is the name of the chemical element if HSC Geo has identified the column as a chemical element
- -Met- METHOD: indicates the method of the analysis (e.g. XRF)
- -Uni- UNIT: unit of the assay (e.g. ppm)
- -Tab- TABLE: name of the table where the data will be stored, for analysis ANALYSIS is default
- -Fld- FIELD: name of the field in the table, e.g. SiO2/XRF/% in the table ANALYSIS
- -Typ- TYPE: field type, e.g. SINGLE
- -Len- LENGTH: length of the character field
- -Dig- DIGITS: number of digits in the numeric fields
- -Idx- INDEXED: Yes, if the field is indexed. Key and ID fields are indexed
- -Mul- MULTIPLIER: The multiplier if the data has been multiplied to reach a uniform structure, e.g. Fe-> FeO
- -Idf- IDENTIFIED: X and name of the chemical element and the total number of the element in the source, e.g. X(Si)1/2 indicates that the field is silica and there are also silica analyses with possible different analysis methods in the same file



	A	B	C	D	E	F
1	HEADER	SampleNo	SiO2 %	TiO2 %	Al2O3 %	Cr2O3 %
2	ELEMENT		SiO2	TiO2	Al2O3	Cr2O3
3	METHOD		XRF	XRF	XRF	XRF
4	UNIT		%	%	%	%
5	TABLE		ANALYSES	ANALYSES	ANALYSES	ANALYSES
6	FIELD	SampleNo	SiO2/XRF/	TiO2/XRF/	Al2O3/XRF	Cr2O3/XRF
7	TYPE	LONG(U,I)	SINGLE	SINGLE	SINGLE	SINGLE
8	LENGTH					
9	DIGITS					
10	INDEXED	YES				
11	MULTIPLIER					
12	IDENTIFIE	ID	X(Si)1/1	X(Ti)1/1	X(Al)1/1	X(Cr)1/1
13		9619251	53.200001	0.69	17.799999	0.0226
14		9619256	47	0.725	12.1	0.143
15		9619257	45.5	0.603	11.2	0.184
16		9619258	52.700001	0.547	13.1	0.216

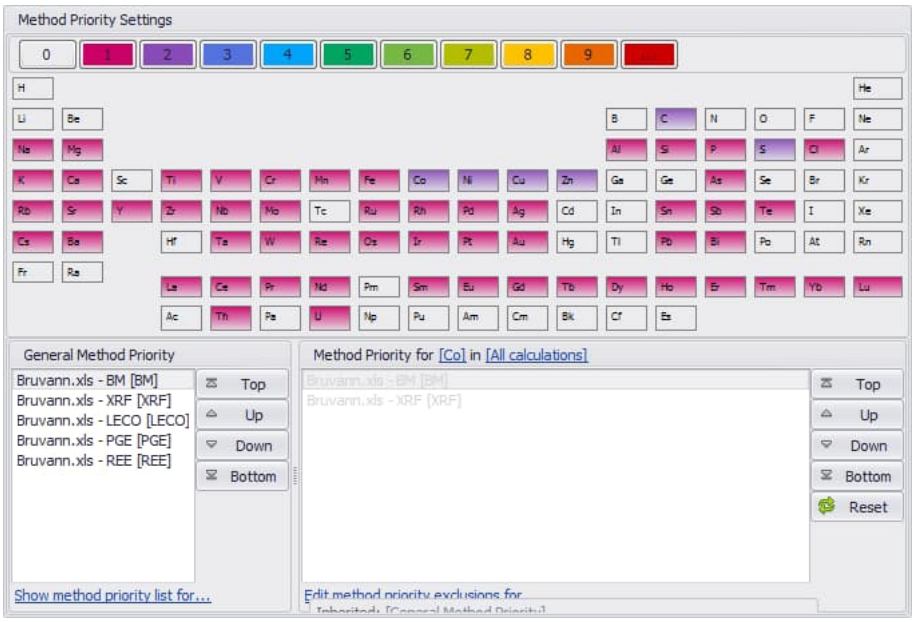
7. In the calculation window you can define settings to include:

- Data source (check the sources you want to use) (1)
- Priority order for methods for each element (2)
- Calculation group selected (3)
- Calculations to be performed (4)

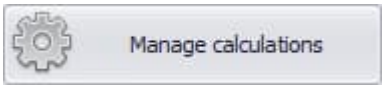


In order to edit the priority order (the order of methods used in calculations):

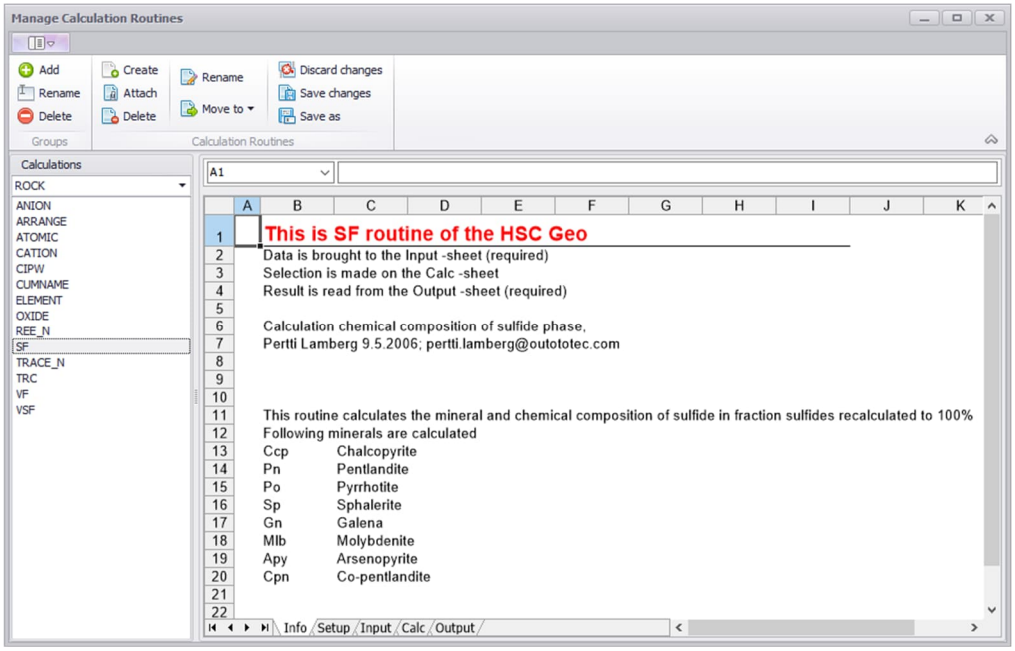
- Click the element of interest, the color code shows where the data sources (methods) of the element can be found. For example, in the figure below, cobalt can be found in two data sources: [BM] and [XRF]. Use the Top, Up, Down, and Bottom buttons to move the methods in the desired order.



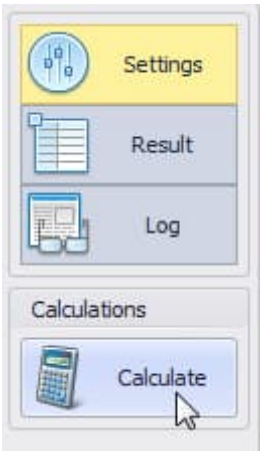
- The calculation options can be edited by pressing “Manage Calculation.”

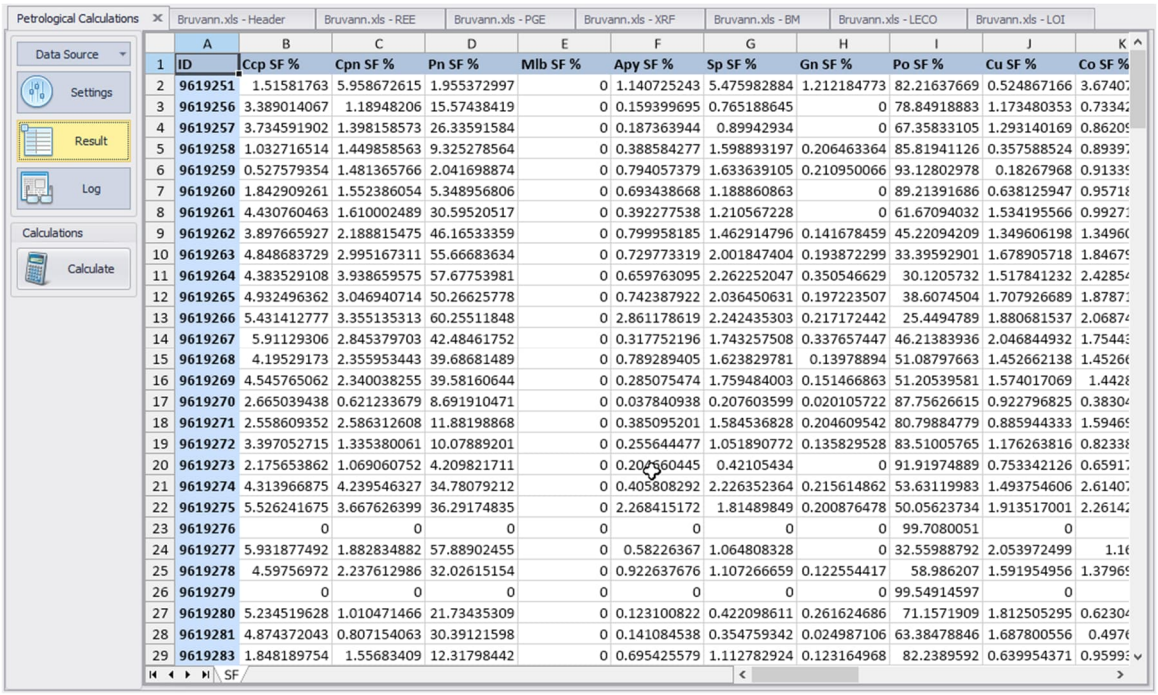


and by selecting the appropriate method. For more details on calculation routines and how to modify them, see the following chapters.



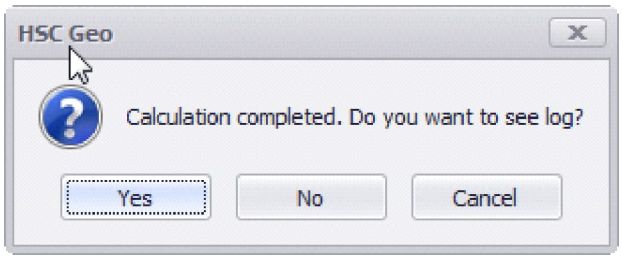
9. When the identification is ready, you can progress to calculations. Check the calculations you want to do for the samples by checking and unchecking the calculations in the list box. The calculations listed below are done by default. When ready, press “CALCULATE”



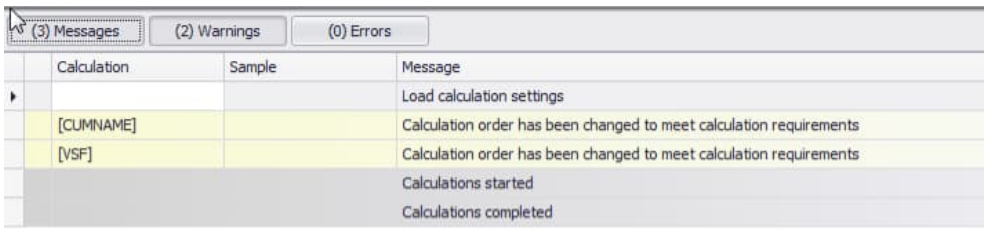


	A	B	C	D	E	F	G	H	I	J	K
1	ID	Ccp SF %	Cpn SF %	Pn SF %	Mlb SF %	Apy SF %	Sp SF %	Gn SF %	Po SF %	Cu SF %	Co SF %
2	9619251	1.51581763	5.958672615	1.955372997	0	1.140725243	5.475982884	1.212184773	82.21637669	0.524867166	3.6740
3	9619256	3.389014067	1.18948206	15.57438419	0	0.159399695	0.765188645	0	78.84918883	1.173480353	0.7334
4	9619257	3.734591902	1.398158573	26.33591584	0	0.187363944	0.89942934	0	67.35833105	1.293140169	0.8620
5	9619258	1.032716514	1.449858563	9.325278564	0	0.388584277	1.598893197	0.206463364	85.81941126	0.357588524	0.8939
6	9619259	0.527579354	1.481365766	2.041698874	0	0.794057379	1.633639105	0.210950066	93.12802978	0.18267968	0.9133
7	9619260	1.842909261	1.552386054	5.348956806	0	0.693438668	1.188860863	0	89.21391686	0.638125947	0.9571
8	9619261	4.430760463	1.610002489	30.59520517	0	0.392277538	1.210567228	0	61.67094032	1.534195566	0.9927
9	9619262	3.897665927	2.188815475	46.16533359	0	0.799958185	1.462914796	0.141678459	45.22094209	1.349606198	1.3496
10	9619263	4.848683729	2.995167311	55.66683634	0	0.729773319	2.001847404	0.193872299	33.39592901	1.678905718	1.8467
11	9619264	4.383529108	3.938659575	57.67753981	0	0.659763095	2.262252047	0.350546629	30.1205732	1.517841232	2.4285
12	9619265	4.932496362	3.046940714	50.26625778	0	0.742387922	2.036450631	0.197223507	38.6074504	1.707926689	1.8787
13	9619266	5.431412777	3.355135313	60.25511848	0	2.861178619	2.242435303	0.217172442	25.4494789	1.880681537	2.0687
14	9619267	5.91129306	2.845379703	42.48461752	0	0.317752196	1.743257508	0.337657447	46.21383936	2.046844932	1.7544
15	9619268	4.19529173	2.355953443	39.68681489	0	0.789289405	1.623829781	0.13978894	51.08797663	1.452662138	1.4526
16	9619269	4.545765062	2.340038255	39.58160644	0	0.285075474	1.759484003	0.151466863	51.20539581	1.574017069	1.4428
17	9619270	2.665039438	0.621233679	8.691910471	0	0.037840938	0.207603599	0.020105722	87.75626615	0.922796825	0.3830
18	9619271	2.558609352	2.586312608	11.88198868	0	0.385095201	1.584536828	0.204609542	80.79884779	0.885944333	1.5946
19	9619272	3.397052715	1.335380061	10.07889201	0	0.255644477	1.051890772	0.135829528	83.51005765	1.176263816	0.8233
20	9619273	2.175653862	1.069060752	4.209821711	0	0.204560445	0.42105434	0	91.91974889	0.753342126	0.6591
21	9619274	4.313966875	4.239546327	34.78079212	0	0.405808292	2.226352364	0.215614862	53.63119983	1.493754606	2.6140
22	9619275	5.526241675	3.667626399	36.29174835	0	2.268415172	1.81489849	0.200876478	50.05623734	1.913517001	2.2614
23	9619276	0	0	0	0	0	0	0	99.7080051	0	
24	9619277	5.931877492	1.882834882	57.88902455	0	0.58226367	1.064808328	0	32.55988792	2.053972499	1.16
25	9619278	4.59756972	2.237612986	32.02615154	0	0.922637676	1.107266659	0.122554417	58.986207	1.591954956	1.3796
26	9619279	0	0	0	0	0	0	0	99.54914597	0	
27	9619280	5.234519628	1.010471466	21.73435309	0	0.123100822	0.422098611	0.261624686	71.1571909	1.812505295	0.6230
28	9619281	4.874372043	0.807154063	30.39121598	0	0.141084538	0.354759342	0.024987106	63.38478846	1.687800556	0.497
29	9619283	1.848189754	1.55683409	12.31798442	0	0.695425579	1.112782924	0.123164968	82.2389592	0.639954371	0.9599

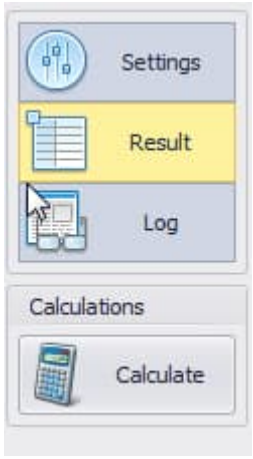
10. When completed, Geo asks if you want to see the log.



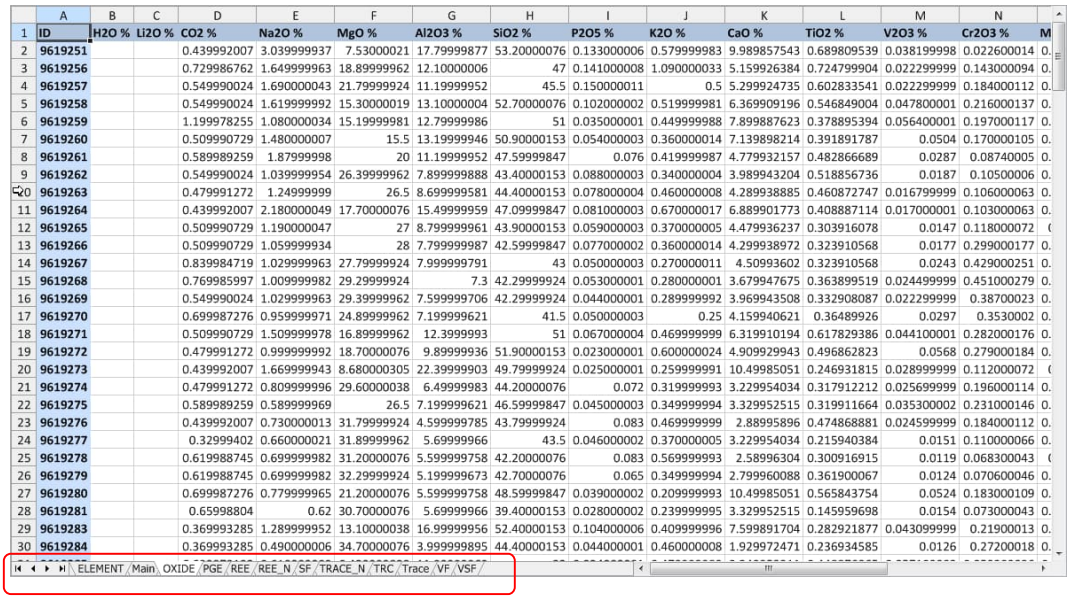
11. If there are errors you can see them in the Log window.



12. Calculation results are calculated in the “Calculation Result” window,



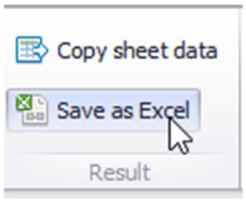
which is similar in structure to the input files. The result of each of the calculation routines is shown on its own page.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	
1	ID	H2O %	Li2O %	CO2 %	Na2O %	MgO %	Al2O3 %	SiO2 %	P2O5 %	K2O %	CaO %	TiO2 %	V2O3 %	Cr2O3 %	M
2	9619251			0.439992007	3.039999937	7.53000021	17.79999877	53.20000076	0.133000006	0.579999983	9.989857543	0.689809539	0.038199998	0.022600014	0.
3	9619256			0.729986762	1.649999963	18.89999962	12.10000006	47	0.141000008	1.090000033	5.159926384	0.724799904	0.022299999	0.143000094	0.
4	9619257			0.549990024	1.690000043	21.79999924	11.19999952	45.5	0.150000011	0.5	5.299924735	0.602833541	0.022299999	0.184000112	0.
5	9619258			0.549990024	1.619999992	15.30000019	13.10000004	52.70000076	0.102000002	0.519999981	6.369909196	0.546849004	0.047800001	0.216000137	0.
6	9619259			1.199978255	1.080000034	15.19999981	12.79999986	51	0.035000001	0.449999988	7.899887623	0.378895394	0.056400001	0.197000117	0.
7	9619260			0.509990729	1.480000007	15.5	13.19999946	50.90000153	0.054000003	0.360000014	7.139898214	0.391891787	0.0504	0.170000105	0.
8	9619261			0.589989259	1.87999998	20	11.19999952	47.59999847	0.076	0.419999987	4.779932157	0.482866689	0.0287	0.08740005	0.
9	9619262			0.549990024	1.039999954	26.39999962	7.899999888	43.40000153	0.088000003	0.340000004	3.989943204	0.518856736	0.0187	0.10500006	0.
10	9619263			0.479991272	1.24999999	26.5	8.699999581	44.40000153	0.078000004	0.460000008	4.289938885	0.460872747	0.016799999	0.106000063	0.
11	9619264			0.439992007	2.180000049	17.70000076	15.49999959	47.09999847	0.081000003	0.670000017	6.889901773	0.408887114	0.017000001	0.103000063	0.
12	9619265			0.509990729	1.190000047	27	8.799999961	43.90000153	0.059000003	0.370000005	4.479936237	0.303916078	0.0147	0.118000072	(
13	9619266			0.509990729	1.059999934	28	7.799999987	42.59999847	0.077000002	0.360000014	4.299938972	0.323910568	0.0177	0.299000177	0.
14	9619267			0.839984719	1.029999963	27.79999924	7.999999791	43	0.050000003	0.270000011	4.50993602	0.323910568	0.0243	0.429000251	0.
15	9619268			0.769985997	1.009999982	29.29999924	7.3	42.29999924	0.053000001	0.280000001	3.679947675	0.363899519	0.024499999	0.451000279	0.
16	9619269			0.549990024	1.029999963	29.39999962	7.599999706	42.29999924	0.044000001	0.289999992	3.969943508	0.332908087	0.022299999	0.38700023	0.
17	9619270			0.699987276	0.959999971	24.89999962	7.199999621	41.5	0.050000003	0.25	4.159940621	0.36489926	0.0297	0.3530002	0.
18	9619271			0.509990729	1.509999978	16.89999962	12.3999993	51	0.067000004	0.469999999	6.319910194	0.617829386	0.044100001	0.282000176	0.
19	9619272			0.479991272	0.999999992	18.70000076	9.89999936	51.90000153	0.023000001	0.600000024	4.909929943	0.496862823	0.0568	0.279000184	0.
20	9619273			0.439992007	1.669999943	8.680000305	22.39999903	49.79999924	0.025000001	0.259999991	10.49985051	0.246931815	0.028999999	0.112000072	(
21	9619274			0.479991272	0.809999996	29.60000038	6.49999983	44.20000076	0.072	0.319999993	3.229954034	0.317912212	0.025699999	0.196000114	0.
22	9619275			0.589989259	0.589999969	26.5	7.199999621	46.59999847	0.045000003	0.349999994	3.329952515	0.319911664	0.035300002	0.231000146	0.
23	9619276			0.439992007	0.730000013	31.79999924	4.599999785	43.79999924	0.083	0.469999999	2.88995896	0.474868881	0.024599999	0.184000112	0.
24	9619277			0.32999402	0.660000021	31.89999962	5.69999966	43.5	0.046000002	0.370000005	3.229954034	0.215940384	0.0151	0.110000066	0.
25	9619278			0.619988745	0.699999982	31.20000076	5.599999758	42.20000076	0.083	0.569999993	2.58996304	0.300916915	0.0119	0.068300043	(
26	9619279			0.619988745	0.699999982	32.29999924	5.199999673	42.70000076	0.065	0.349999994	2.799960088	0.361900067	0.0124	0.070600046	0.
27	9619280			0.699987276	0.779999965	21.20000076	5.599999758	48.59999847	0.039000002	0.209999993	10.49985051	0.565843754	0.0524	0.183000109	0.
28	9619281			0.65998804	0.62	30.70000076	5.69999966	39.40000153	0.028000002	0.239999995	3.329952515	0.145959698	0.0154	0.073000043	0.
29	9619283			0.369993285	1.289999952	13.10000038	16.99999956	52.40000153	0.104000006	0.409999996	7.599891704	0.282921877	0.043099999	0.21900013	0.
30	9619284			0.369993285	0.490000006	34.70000076	3.999999895	44.40000153	0.044000001	0.460000008	1.929972471	0.236934585	0.0126	0.27200018	0.

ELEMENT | Main | OXIDE | PGE | REE | REE_N | SF | TRACE_N | TRC | Trace | VF | VSF

13. To save the results, press Save as Excel and give the file a name.

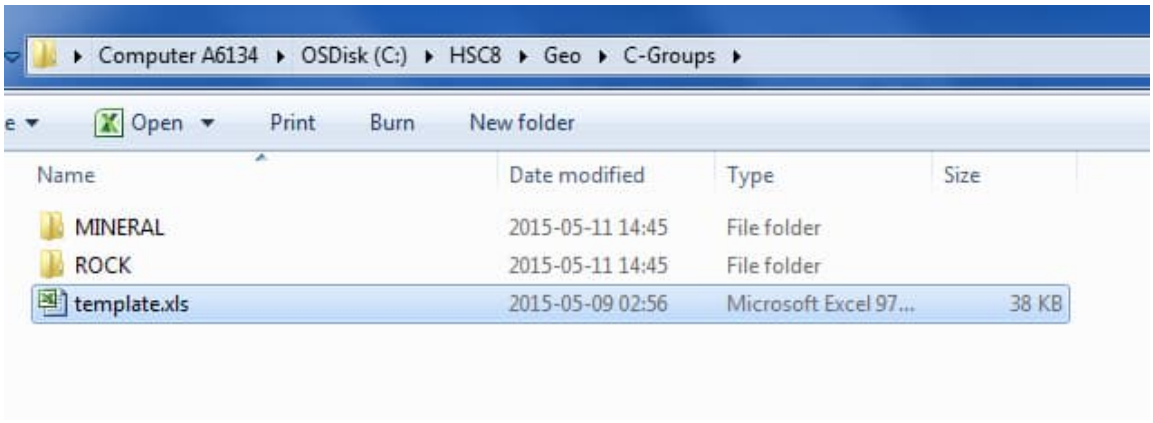


84.6.4. Calculation routines

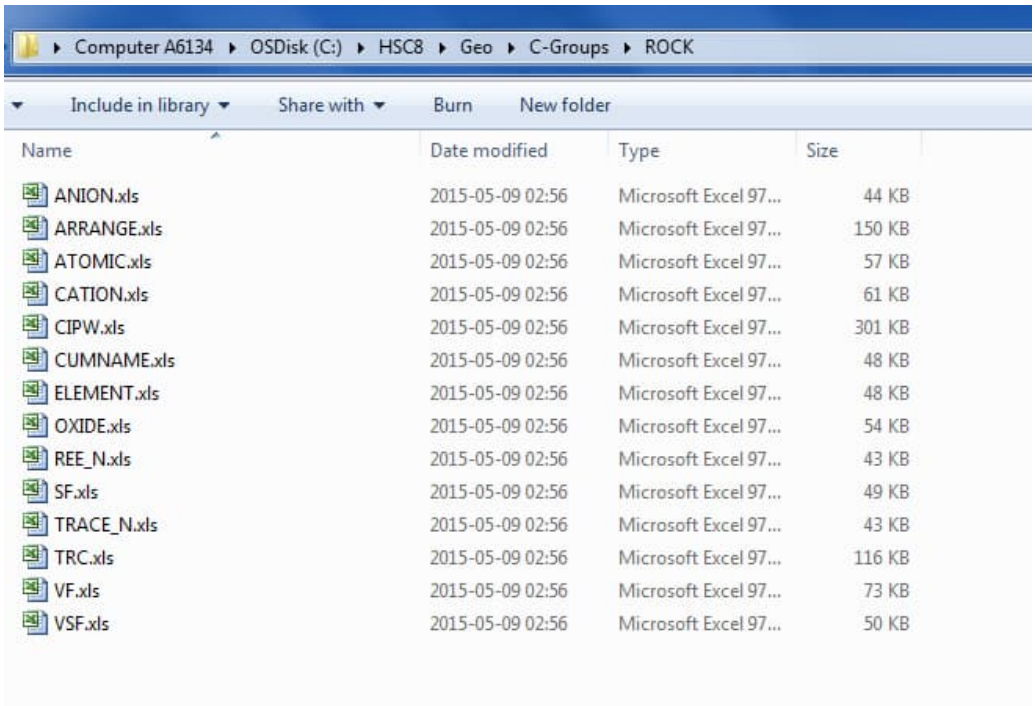
HSC Geo allows you to calculate certain frequently used routines in the same way, although the input format may change from one data source to another. HSC Geo includes a number of petrological calculation routines but since the actual calculations are carried out in Microsoft Excel, it is quite easy for users to make their own routines as well.

General structure

In HSC Geo, the calculation routines are actually Microsoft Excel files. Files must be located in folders under C:\Program Files (x86)\HSC10\Geo\C-Groups. In the example below, there are two different sets of calculations: “ROCK” and “MINERAL.”

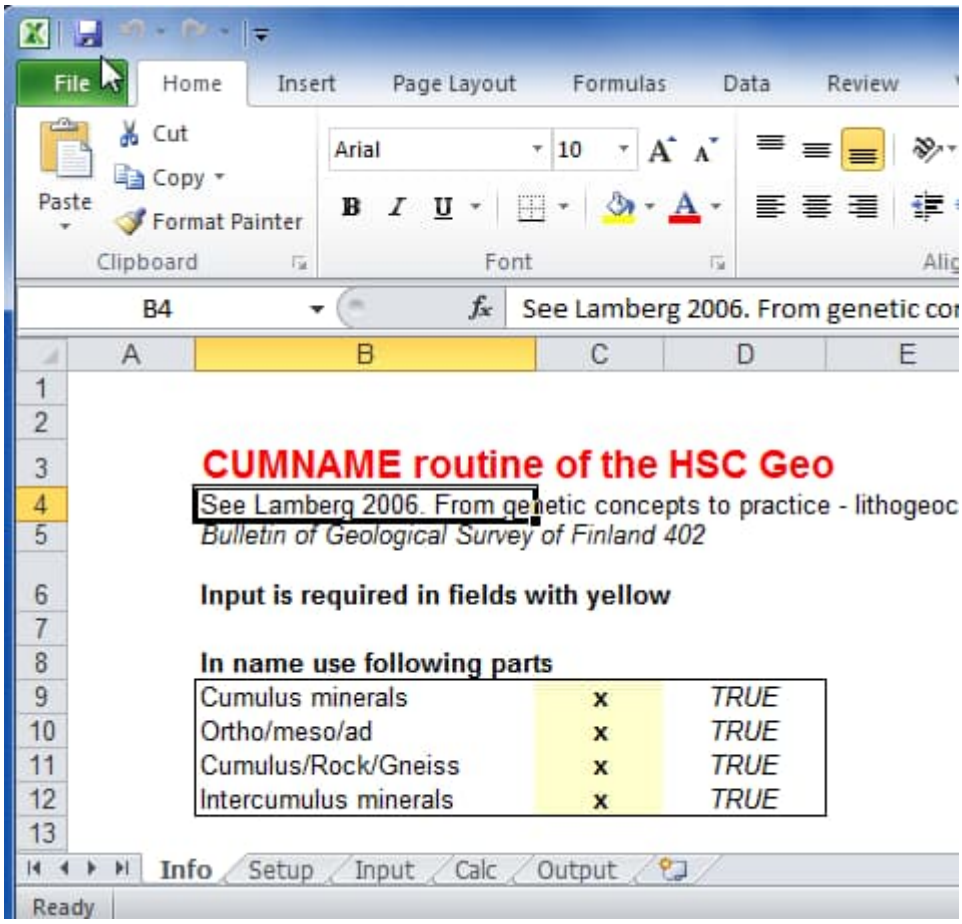


Under the ROCK folder (i.e. C:\Program Files (x86)\HSC10\Geo\C-Groups\ROCK) there are Excel files, all of which have their own individual calculation routines.

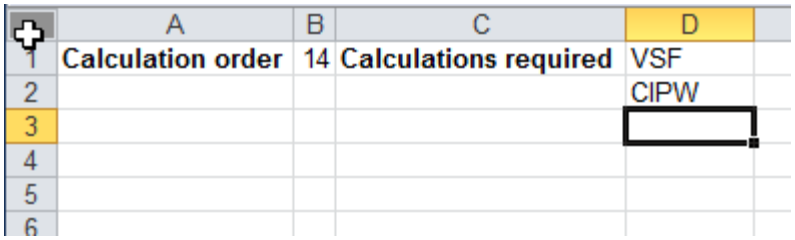


The calculation file consists of five worksheets.

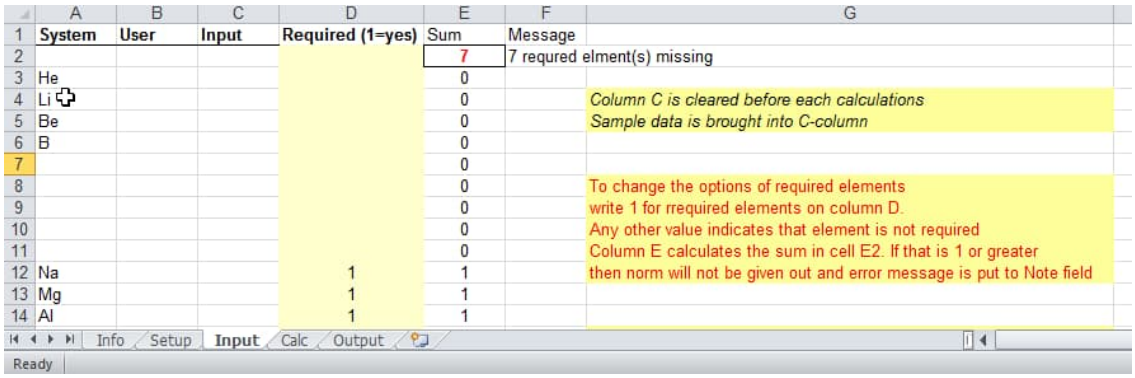
1. The first worksheet (Info) is for information.
2. The second worksheet (Setup) gives the ordinal number of the routine and defines which routines should be done before the calculation in question is run.
3. The third worksheet is the Input sheet, i.e. data from HSC Geo to Excel.
4. The fourth worksheet (Calc) is reserved for calculations done in Excel.
5. The fifth worksheet (Output) is for output data, i.e. data from Excel to HSC Geo.



In the Setup worksheet, the ordinal number is given in cell B1. If the number is missing, HSC Geo adds the routine last in the list. The routines which should be run before the routine in question are listed in the D column from D1 downwards.



The Input sheet lists the input values required for the calculations. Column A is for the system name. If the input is a chemical analysis, then HSC Geo inputs the assay according to the element's number in the periodic table, i.e. if the input value is for example carbon, then its number is 6 and it will be brought to one row below, i.e. row 7 (the row 1 is for headers; see figure below). The assay will always be transformed to **ELEMENT WEIGHT PERCENTAGES**. For example, if the assay is 1000 ppm CO2, then HSC Geo will change it to 0.0273 % C and send the value 0.0273 to cell C7.

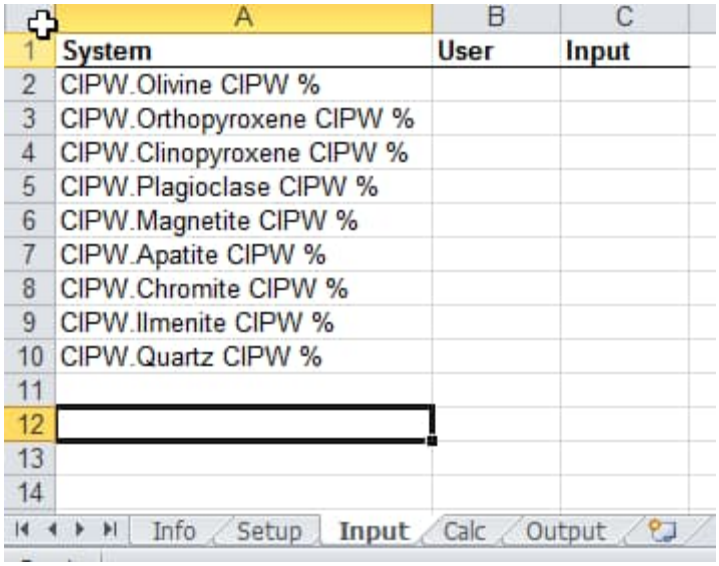


	A	B	C	D	E	F	G
1	System	User	Input	Required (1=yes)	Sum	Message	
2					7	7 requred element(s) missing	
3	He				0		
4	Li				0		*Column C is cleared before each calculations*
5	Be				0		*Sample data is brought into C-column*
6	B				0		
7					0		
8					0		To change the options of required elements
9					0		write 1 for rrequired elements on column D.
10					0		Any other value indicates that element is not required
11					0		Column E calculates the sum in cell E2. If that is 1 or greater
12	Na			1	1		then norm will not be given out and error message is put to Note field
13	Mg			1	1		
14	Al			1	1		

Info | Setup | **Input** | Calc | Output

Ready

If the input value is not a chemical assay, then the full name of the value in question has to be written. For example, the CUMNAME routine uses among others the CIPW normative olivine as an input value. Then value “CIPW.Olivine CIPW %” stands for the input value in cell A2 (see below).

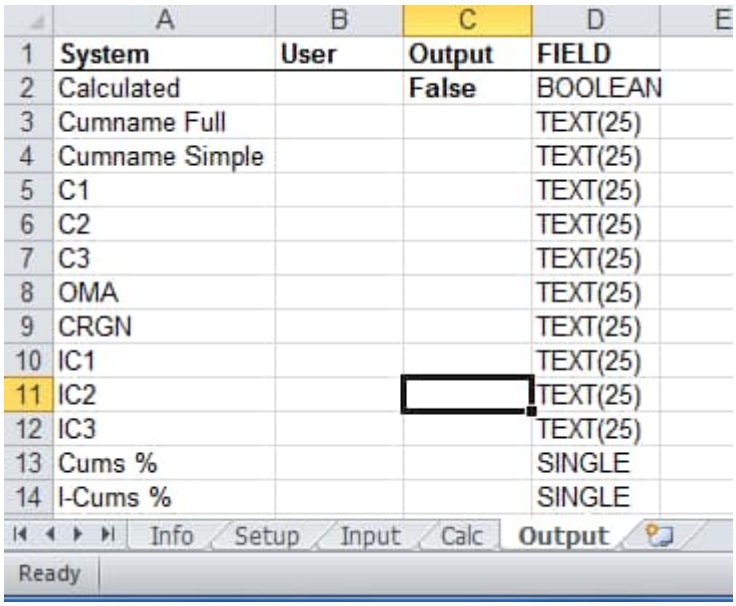


	A	B	C
1	System	User	Input
2	CIPW.Olivine CIPW %		
3	CIPW.Orthopyroxene CIPW %		
4	CIPW.Clinopyroxene CIPW %		
5	CIPW.Plagioclase CIPW %		
6	CIPW.Magnetite CIPW %		
7	CIPW.Apatite CIPW %		
8	CIPW.Chromite CIPW %		
9	CIPW.Ilmenite CIPW %		
10	CIPW.Quartz CIPW %		
11			
12			
13			
14			

Info | Setup | **Input** | Calc | Output

The Calc. sheet is an independent calculation sheet not affected by HSC Geo.

The Output sheet has field names in the first column starting from row 2. If the user wishes to change the name, it is better to type the desired name in the column B. If text appears in the column B, that name will be used. Column C is the output value. In most of the built-in routines column C refers to the calculation page. Column D gives the data type for the database.



	A	B	C	D	E
1	**System**	**User**	**Output**	**FIELD**	
2	Calculated		**False**	BOOLEAN	
3	Cumname Full			TEXT(25)	
4	Cumname Simple			TEXT(25)	
5	C1			TEXT(25)	
6	C2			TEXT(25)	
7	C3			TEXT(25)	
8	OMA			TEXT(25)	
9	CRGN			TEXT(25)	
10	IC1			TEXT(25)	
11	IC2			TEXT(25)	
12	IC3			TEXT(25)	
13	Cums %			SINGLE	
14	I-Cums %			SINGLE	

Info | Setup | Input | Calc | **Output**

Ready

HSC Geo actions in calculation

The calculations in HSC Geo will take place as follows:

1. After the input format has been identified and the user presses the Calculate button, HSC Geo will make a list of the calculation routines according to user selections, the ordinal number on the Setup pages and other required calculation routines on the Setup page.
2. Before each sample HSC Geo will empty column C on the Input sheet.
3. HSC Geo inputs the data in the Input page. For chemical elements the format is ELEMENT WEIGHT PERCENTAGES.
4. HSC Geo calls the Recalculate routine.
5. HSC Geo reads the calculation results on the Output page and writes the values in the “Calculation Results” window on the page named according to the routine.
6. HSC Geo performs steps 2-5 for the next sample.

Routines included

HSC Geo includes the following petrological and mineralogical calculation routines:

- ARRANGE – Arrange routine
- ANION – Anion proportions
- CATION – Cation proportions
- VF – Volatile free composition
- SF – Composition of the sulfide fraction
- VSF – Volatile and sulfide free composition
- CIPW – CIPW normative mineral composition
- REE_N – Normalization for rare earth elements
- CUMNAME – Normative cumulus name for ultramafic-mafic igneous rocks
- TRC – Calculate the normative trace element content in igneous minerals of ultramafic-mafic rocks.
- TRACE_N – Normalization for trace elements
- ELEMENT – Elemental composition
- OXIDE – Oxide composition

SF – Sulfide fraction

Normative minerals of the SF, i.e. sulfide fraction, are: pyrrhotite (FeS), pyrite (FeS_2), pentlandite ($Ni_{4.76}Fe_{4.24}S_8$), chalcopyrite ($CuFeS_2$), Co-pentlandite (Co_9S_8), arsenopyrite (FeAsS), sphalerite (ZnS), molybdenite (MoS_2) and galena (PbS). In calculation, all of the sulfidic base metals are allotted in a single phase as follows: lead in galena, molybdenum in molybdenite, zinc in sphalerite, arsenic in arsenopyrite, cobalt in Co-pentlandite, copper in chalcopyrite, and nickel in pentlandite. The remaining sulfur and iron are balanced between pyrrhotite and pyrite. The equations and chemical composition of normative sulfide minerals are given in the table below.

When the weight percentages of normative sulfides have been calculated, trace elements bound in sulfides: i.e. Os, Ir, Ru, Rh, Pt, Pd, Au, Re, Ag, Cd, Sn, Sb, Bi, Se, Te and Hg, if analyzed, are added to the sulfides. Recalculation to 100% gives the mineral composition and trace element content of the sulfide fraction. The chemical composition of the sulfide fraction is calculated from mineral abundances as given in the table below (step 8).

If only bulk assays are available, the chemical composition of a sulfide fraction is calculated by setting the pyrite to zero and by following the guidelines given in the table below. Since nickel and cobalt are also bound in non-sulfides, the calculation gives either too high a pentlandite and cobalt pentlandite and consequently Ni and Co content of the sulfide fraction, or residual sulfur ends up negative. In the latter case, all normative sulfides are set to zero and S is allotted to pyrrhotite.

Although the sulfides of a sample may also contain other sulfides than those listed in the table below, such as cubanite, gersdorffite, and various pyrrhotites (troilite, monoclinic and hexagonal), the result of the chemical composition of the sulfide fraction is more accurate and reliable than if a fixed sulfur content were used. If the sulfide fraction is calculated from total analyses, then samples containing less than 2% sulfides must be treated with caution for the above-mentioned reasons.

Calculation of the sulfide fraction and normative sulfide minerals.

(1) Weight percentages of chalcopyrite, pentlandite, cobalt pentlandite, sphalerite, galena, molybdenite and arsenopyrite are calculated as given below in the Equation column. Content of elements in equations are weight percentages in the sample.
(2) Residual sulfur content is calculated. If it is negative, then all sulfides except pyrrhotite are set to zero, and pyrrhotite is calculated according to step 4.
(3) If Fe analysis is carried out by the bromine-methanol method, then the amounts of pyrite and pyrrhotite are solved as follows: writing in matrix format the mass balance: $\begin{bmatrix} 36.48 & 53.45 \\ 63.52 & 0.07\times 46.55 \end{bmatrix} \cdot \begin{bmatrix} Po \\ Py \end{bmatrix} = \begin{bmatrix} S \\ Fe \end{bmatrix}$, where S and Fe are residual sulfur and iron contents after removing S and Fe bond in previously calculated sulfides. Po and Py are solved by the non-negative least square method.
(4) If Fe bromine-methanol analysis is not available, or the only Fe sulfide is pyrrhotite, then pyrite is set to zero and the pyrrhotite is calculated according to the equation: Po=100*S/36.48.
(5) Trace elements in sulfides: Os, Ir, Ru, Rh Pt, Pd, Au, Re, Ag, Cd, Sn, Sb, Bi, Se, Te and Hg are added to the previously calculated sulfides.
(6) Sum of minerals and trace elements is the *normative sulfide content* (the word normative may be left out)
(7) Minerals and trace elements are recalculated to 100%
(8) Normalization gives the trace element content in the sulfide fraction directly. The Cu, Ni, Co, Zn, Pb, Mo, and As content of the sulfide fraction is back-calculated from the normative minerals. E.g. The Ni tenor: Ni_SF%=Pn_SF%*36.16/100. The iron and sulfur contents are calculated by totaling the sulfur and iron content bound in each normative mineral.

Mineral	Symbol	Formula used	Element	wt.%	Fe wt.%	S wt.%	Equation
Chalcopyrite	Ccp	$CuFeS_2$	Cu=	34.63	30.43	34.94	Ccp=100*Cu/34.63
Pentlandite	Pn	$Ni_{4.76}Fe_{4.24}S_8$	Ni=	36.16	30.64	33.20	Pn=100*Ni/36.16
Cobalt pentlandite	Cpn	Co_9S_8	Co=	67.40	0.00	52.94	Cpn=100*Co/67.40
Sphalerite	Sp	ZnS	Zn=	67.10	0.00	32.90	Sp=100*Zn/67.10
Galena	Ga	PbS	Pb=	86.60	0.00	13.40	Ga=100*ga/86.60
Molybdenite	Mb	MoS_2	Mo=	59.94	0.00	40.06	Mb=100*Mo/59.94
Arsenopyrite	Apy	FeAsS	As=	46.01	34.30	19.69	Apy=100*As/46.01
Pyrrhotite	Po	FeS			63.52	36.48	(3) or (4)
Pyrite	Py	FeS_2			46.55	53.45	(3) or (4)

VF and VSF

The calculation of volatile-free (anhydrous) composition is a common practice in petrological studies of mafic-ultramafic rocks and is a simple recalculation of selected elements to 100%. The main problem is the distribution of total iron between sulfides and the divalent and trivalent states in the rock, forming silicates and oxides. Iron incorporated in sulfides can be solved as described above in the SF routine. The proportion of ferric iron in mafic and ultramafic cumulates is normally low. This only has to be taken into account when chromite, magnetite or ilmenite are present as a cumulus mineral. In this study all non-sulfidic iron was calculated as total FeO in both volatile and volatile- and sulfide-free calculations.

Volatile- and sulfide-free composition (VSF) is the anhydrous chemical composition of the rock where the sulfides have been removed. When the composition of the sulfide fraction has been calculated and the portion of base metals in the sulfides is known, the calculation of volatile- and sulfide-free composition is a simple recalculation of selected elements to 100%. If the composition of the sulfide fraction was determined from the bromine-methanol leach, the recalculation is reliable even for samples rich in sulfides.

The volatile- and sulfide-free composition (VSF) is very useful for Ni-Cu sulfide-bearing samples: it can be applied to compare the host rocks of sulfide-rich samples with ordinary cumulates and country rocks.

TRC

By mass balance, the concentration of an element E in a multi-phase mineral assemblage can be expressed as the sum of the products of the molar proportions X (as mass fractions of 1) times the concentrations W, of element E, in a mineral phase Ma (Bedard 1994). The weight fraction of element E in a sample is
$W_{E,T} = \sum_{a=1}^{n} W_{E,Ma} * X_{Ma}$,
where $W_{E,Ma}$ is the weight fraction of element E in mineral Ma and X_{Ma} is the weight fraction of mineral Ma in a sample. When the bulk composition ($W_{E,T}$) and weight fractions of minerals (X_{Ma}) are known, one can estimate the weight fraction of the element in mineral $W_{E,Ma}$ by
applying the elemental partition coefficients between the minerals.

CUMNAME

To give the proper cumulus name for an igneous rock is often time-consuming. Thin and polished sections of representative samples have to be studied. However, it has been found that B-normative compositions are in good harmony with the actual primary igneous mineralogy. Consequently, a cumulus naming procedure has been developed on the basis of the CIPW norm.

A comparison of the CIPW norm with the cumulus name defined by microscopy names made it possible to determine the threshold abundances above which minerals belong to a cumulus phase. For normative orthopyroxene, clinopyroxene, and plagioclase it was found to be roughly 25% and for normative olivine 10% (see table below). The sum of the normative cumulus minerals identified in this way is higher than 50% in cumulates, but less than 50% in non-cumulate rocks such as volcanites.

Automated cumulus naming procedure

A cumulus name consists of four parts; the naming rules in each part are as follows:

1 Cumulus minerals	**2** Cumulus type	**3** Cumulus/rock index	**4** Intercumulus minerals
Listed in the order of abundance using the following abbreviations. The normative abundance must be above the given boundary. o=olivine (>10%) b=orthopyroxene (>25%) a=clinopyroxene (>25%) p=plagioclase (>25%) m=magnetite (>10%) c=chromite (>0.6%) t=apatite(>1%) $=sulfides (>0.3%)	If the rock is a cumulate, one of the following symbols is used to describe the amount of cumulus minerals. A=adcumulate (cumulus minerals>93%) M=mesocumulate (cumulus minerals 75-93%) O=orthocumulate (cumulus minerals 50-75%)	To distinguish if a rock is cumulate or non-cumulate: C=cumulate (cumulus minerals >50%) R=non-cumulate rock (cumulus minerals <50%)	Listed in the order of abundance using the following abbreviations. The normative abundance must be between the given boundaries. b=orthopyroxene (10-25%) a=clinopyroxene (10-25%) p=plagioclase (10-25%)

e.g. oMCa=olivine mesocumulate with clinopyroxene as intercumulus mineral; bRpa=non-cumulate rock where the main phase is orthopyroxene and the other significant phases are, in the order of abundance, plagioclase and clinopyroxene

84.7. Modal calculations – mass proportion of minerals in samples

84.7.1. Background and theory

Modal calculation means converting the elemental grades of a sample to mineral grades (Whiten, 2007)[6]. 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:

$$A \times x = b$$

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

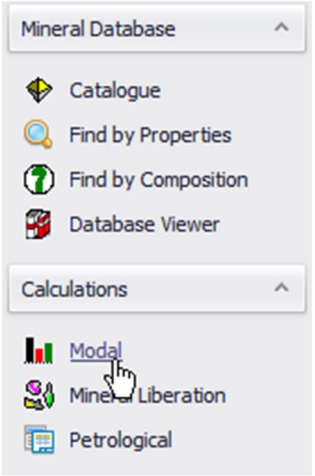
Where A is the matrix on the chemical composition of minerals (Mineral Matrix), x is the vector including the unknown mass proportion of minerals (modal mineralogy) in the sample and b is the vector on the analyzed chemical composition of the sample. The unknown x can be found e.g. using the non-negative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

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)[4], copper phase analysis for copper ores (Lamberg, Hautala, Sotka, & Saavalainen, 1997)[1] and Satmagan analysis for iron ores (Stradling, 1991, Lund et al., 2013)[5,3].

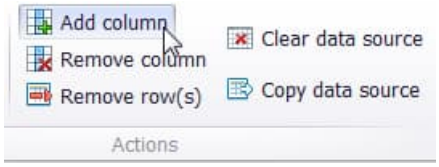
84.7.2. Simple calculation

Manual input

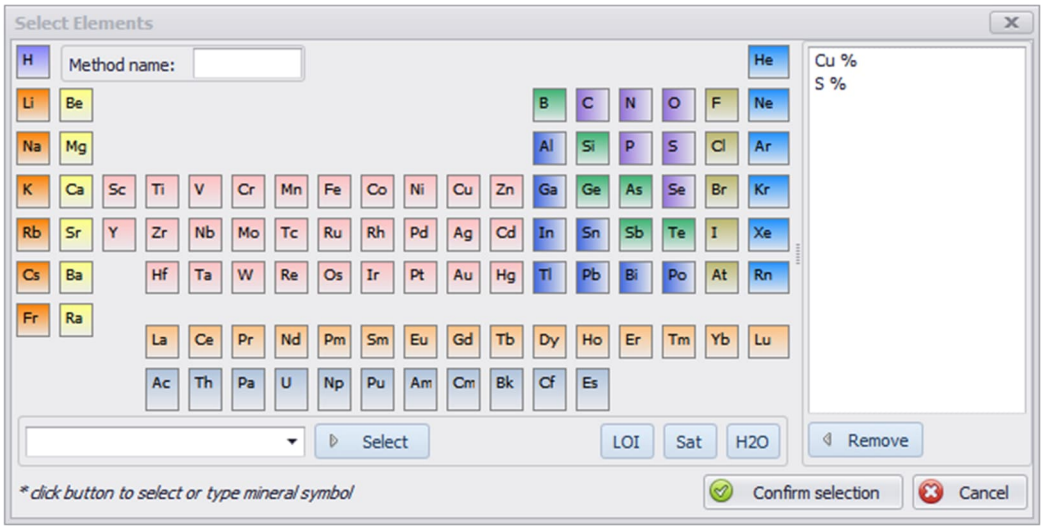
To give the chemical assays of samples manually, select Modal calculations.



In the ribbon, select Add column.



In the Select Elements window, select the elements the assays are for. Additionally, you can also choose other type of analysis such as Satmagan (Sat), Loss of Ignition (LOI), and moisture content (H2O). Alternatively you can also select mineral assays (example: XRD Rietveld results) using the drop down in the bottom left corner. In this example, assays are available for Cu and S. Click on Cu and S and then "Confirm selection."



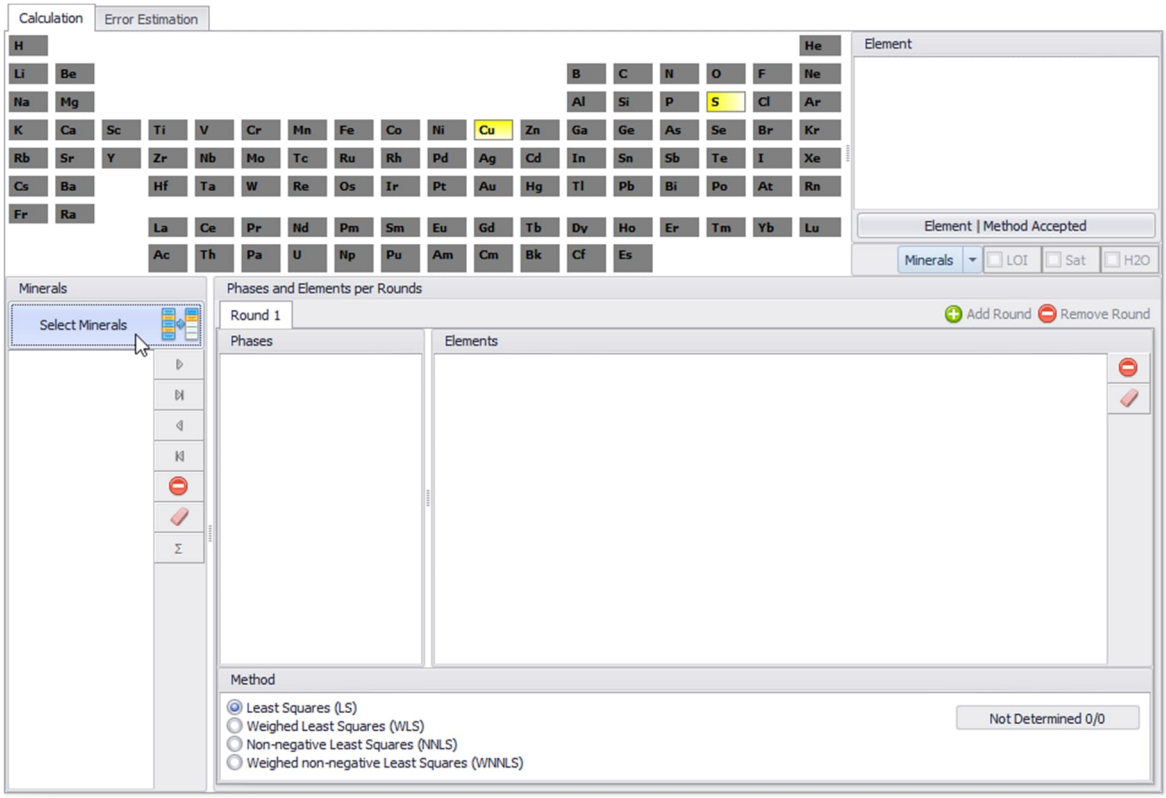
Type in the sample ID and assays in the grid, for example as follows:

	ID	Cu %	S %
	1	1.20	10.30
	2	10.40	22.00
	3	28.00	34.00
▸	4	0.10	8.00
*			

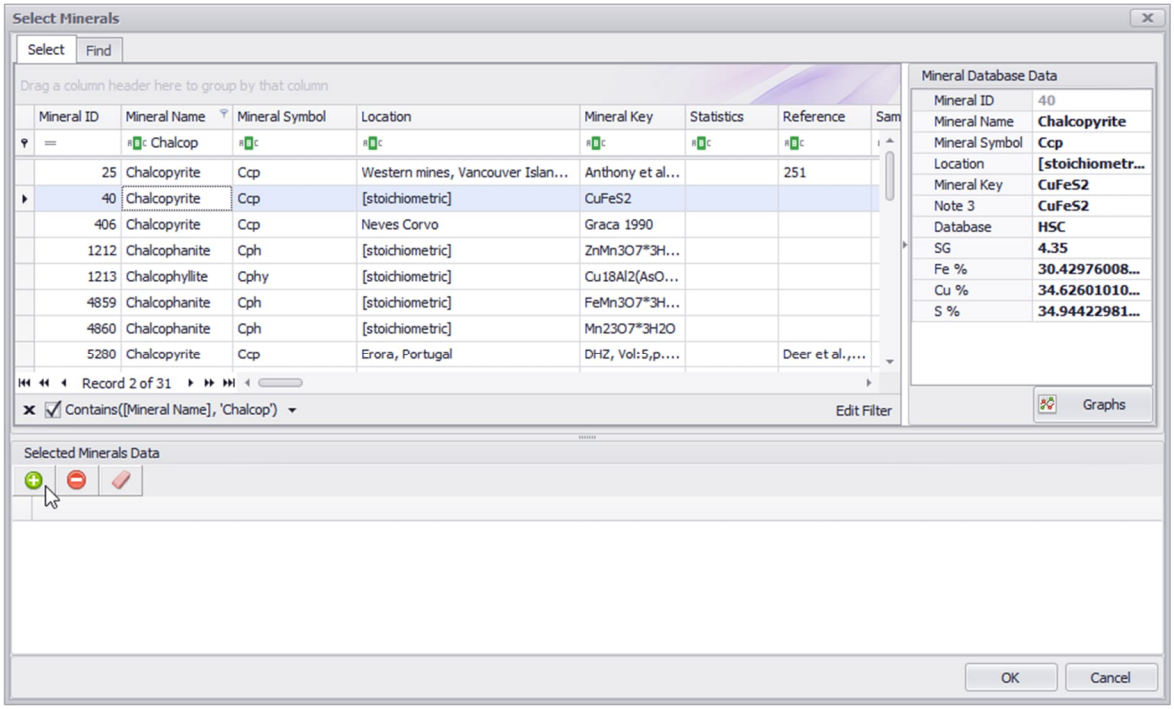
Calculation Rules

Press “Rules” to define the calculation rules.

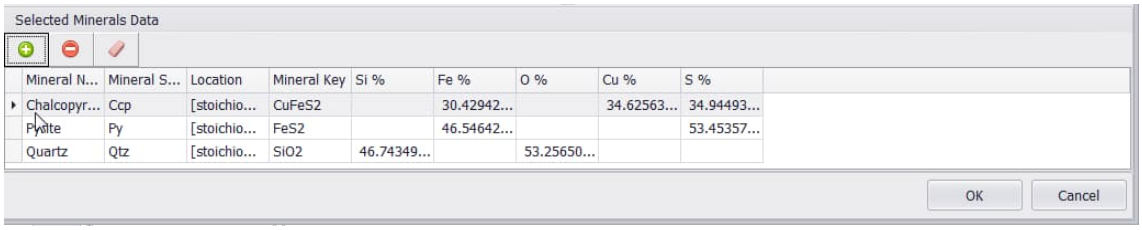
In the Calculation window, the periodic table on the top shows the analyzed elements. The next step is to define the minerals. Press Select Minerals on the left side of the window.



In 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  or double click the record.



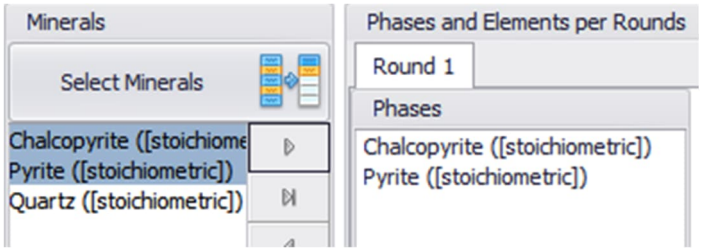
Continue until all the minerals existing in the samples have been selected. In this example, the minerals are chalcopyrite, pyrite and quartz. Press OK when ready.



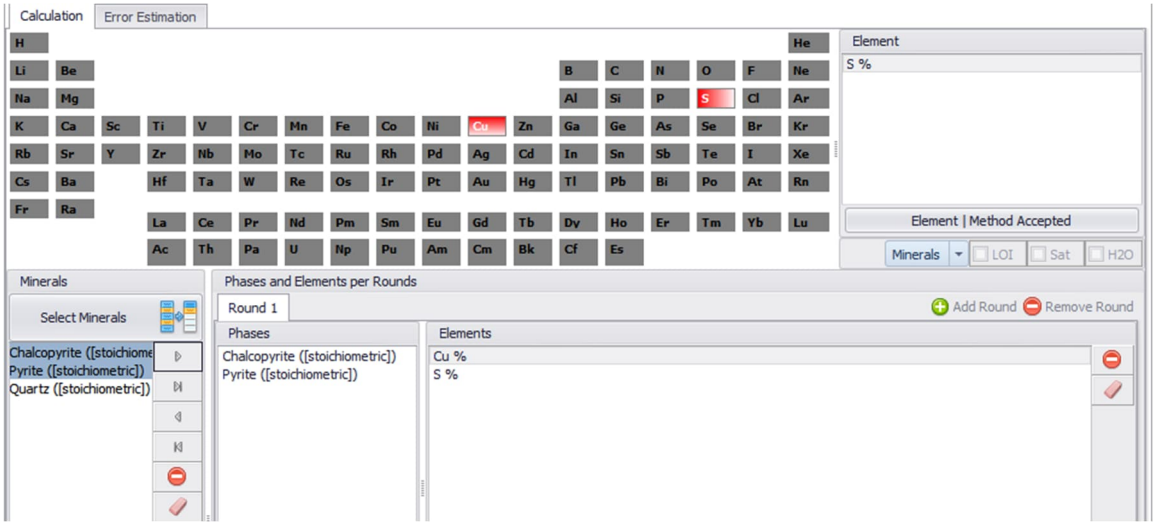
The next step is to define the rules for calculations. In this case, the rules are as follows:

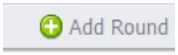
- Chalcopyrite and pyrite are calculated from the Cu and S assays
- Quartz is the remaining, i.e. 100-others

Select the minerals (chalcopyrite and pyrite) and press  to move them to the list of phases (in Round 1).

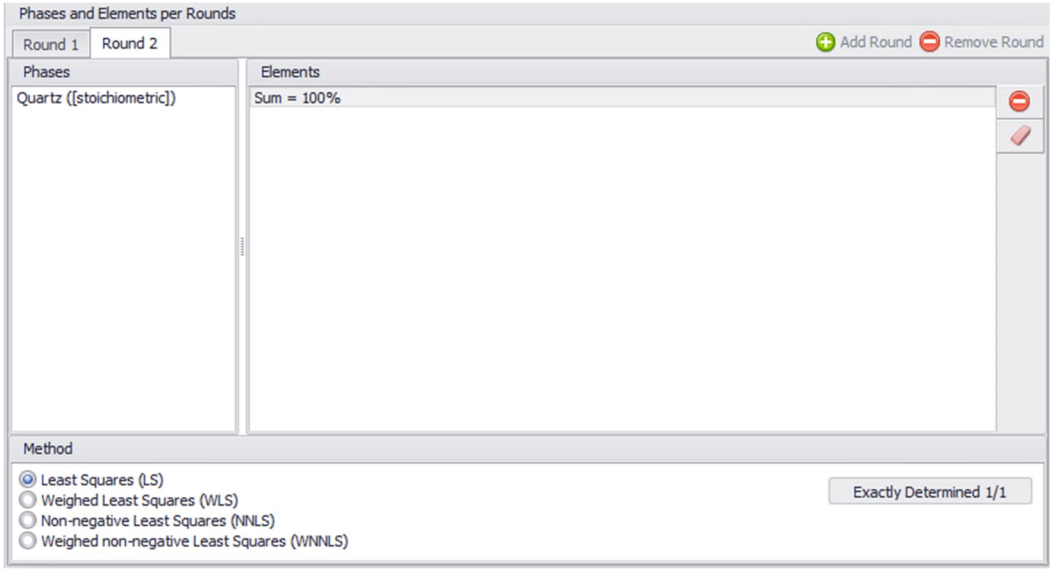


Now select the elements, i.e. click on Cu and S to move them to the list of elements. The color of Cu and S changes to red indicating that they have been used in the calculations.

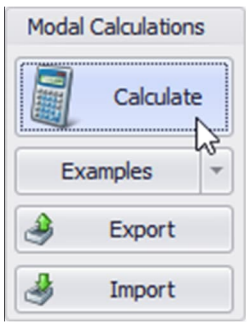


Press “Add Round”  to add another round for quartz.

Select and move quartz to the list of phases and press  to set quartz as the remaining, i.e., 100 – (Chalcopyrite + Pyrite). The calculation rules are now defined. In case you want to reset these rules, you can press Reset 



Press Calculate

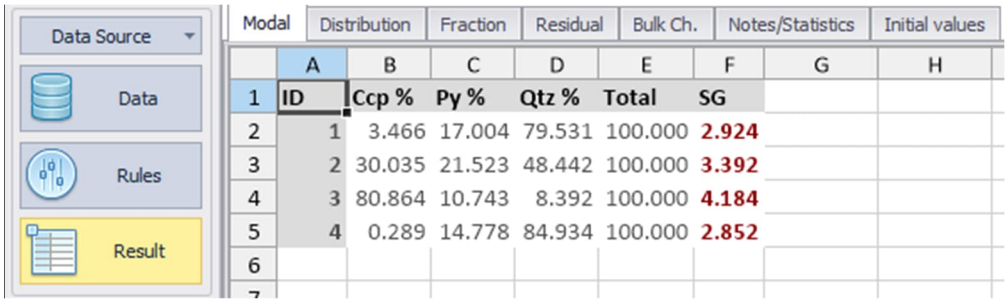


Studying the calculation result

The result is shown in seven tabs:

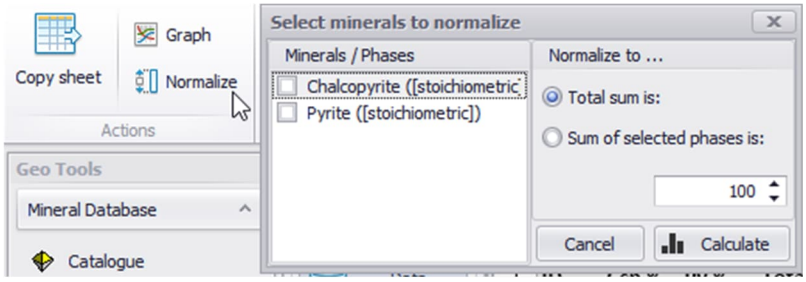
- Modal gives the mineral mass proportions (wt%)
- Distribution is for calculating the distribution of elements between the minerals
- Fraction is for calculating the composition of a given mineral fraction
- Residual gives the residue of the calculation
- Bulk Ch. gives the back-calculated chemical composition of the samples
- Notes/Statistics is for error estimation
- “Initial values” shows 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 taken into account. The calculation is made as if the modal mineralogy were normalized to 100%.



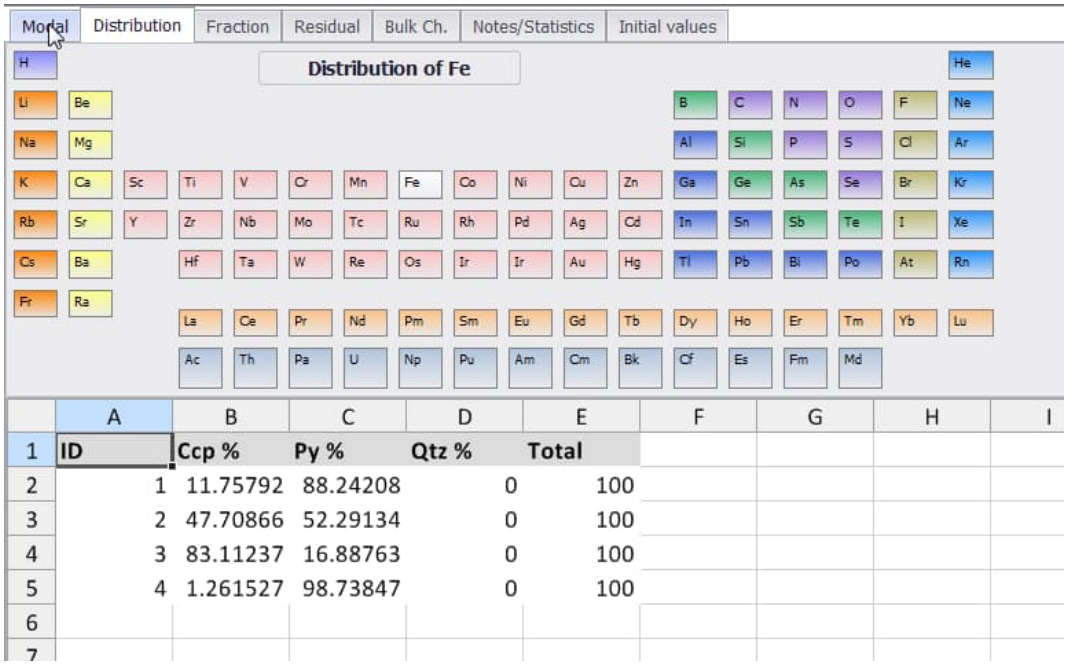
	A	B	C	D	E	F	G	H
1	ID	Ccp %	Py %	Qtz %	Total	SG		
2	1	3.466	17.004	79.531	100.000	2.924		
3	2	30.035	21.523	48.442	100.000	3.392		
4	3	80.864	10.743	8.392	100.000	4.184		
5	4	0.289	14.778	84.934	100.000	2.852		
6								

Instead of selecting one mineral to be the remaining (as quartz in this example), the modal result can also be normalized proportionally so that the sum of all minerals become 100%. This is done by selecting normalize in the top ribbon.



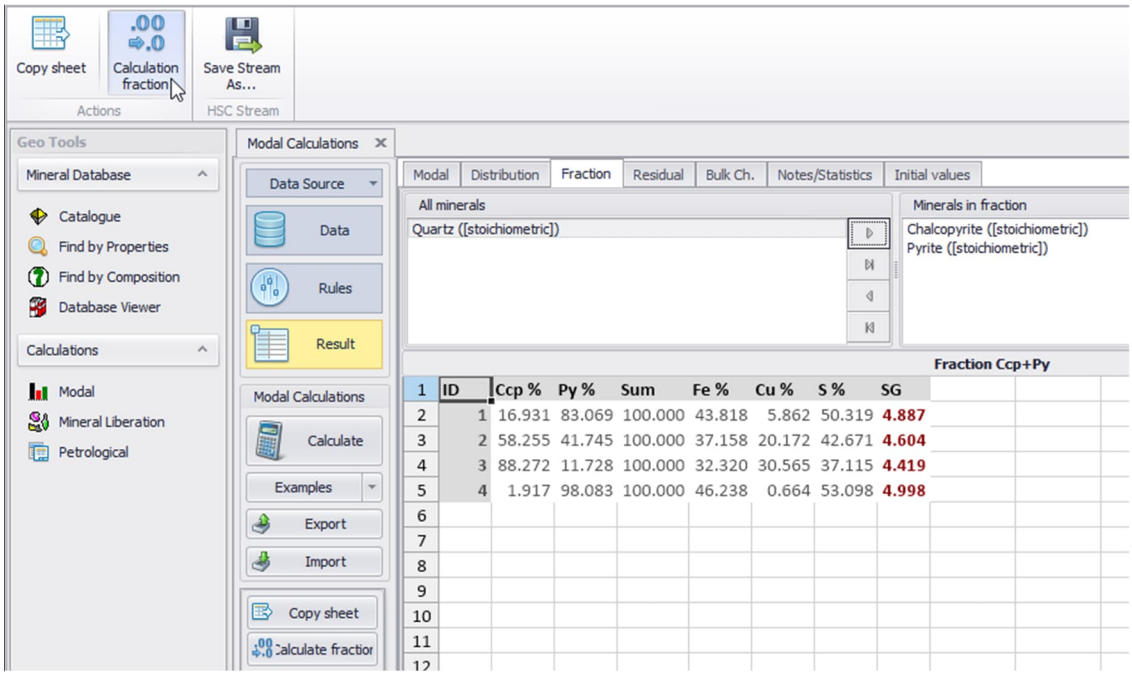
In the pop up window, you can select on how the result should be normalized. You can either select the total sum of the minerals to be 100 (adjustable) or select phases to sum up to a certain amount.

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



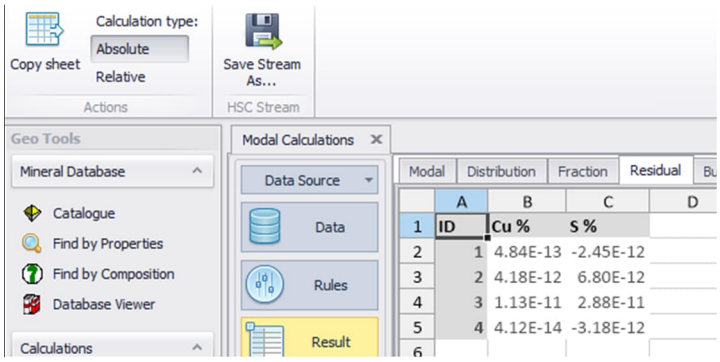
	A	B	C	D	E	F	G	H	I
1	ID	Ccp %	Py %	Qtz %	Total				
2	1	11.75792	88.24208	0	100				
3	2	47.70866	52.29134	0	100				
4	3	83.11237	16.88763	0	100				
5	4	1.261527	98.73847	0	100				
6									
7									

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 for estimating the composition of bulk sulfide concentrate, for example.

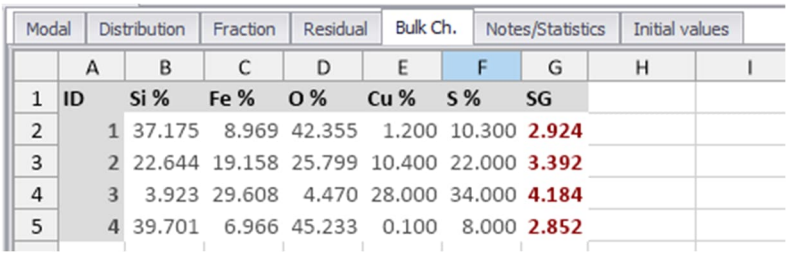


	ID	Ccp %	Py %	Sum	Fe %	Cu %	S %	SG
2	1	16.931	83.069	100.000	43.818	5.862	50.319	4.887
3	2	58.255	41.745	100.000	37.158	20.172	42.671	4.604
4	3	88.272	11.728	100.000	32.320	30.565	37.115	4.419
5	4	1.917	98.083	100.000	46.238	0.664	53.098	4.998

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

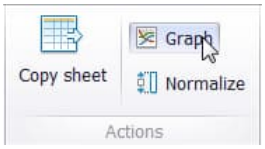


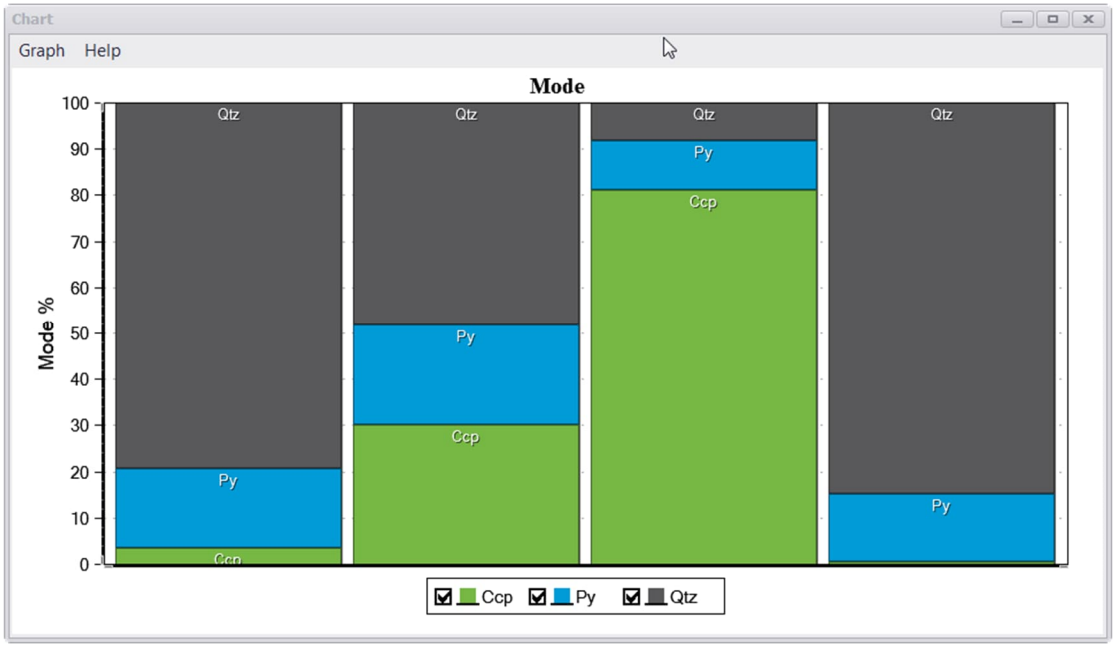
Bulk Chemistry (in the Bulk Ch. Tab) shows the chemical composition of the sample when back-calculated from the modal composition (x) and chemical composition of minerals (A matrix).



	A	B	C	D	E	F	G	H	I
1	ID	Si %	Fe %	O %	Cu %	S %	SG		
2	1	37.175	8.969	42.355	1.200	10.300	2.924		
3	2	22.644	19.158	25.799	10.400	22.000	3.392		
4	3	3.923	29.608	4.470	28.000	34.000	4.184		
5	4	39.701	6.966	45.233	0.100	8.000	2.852		

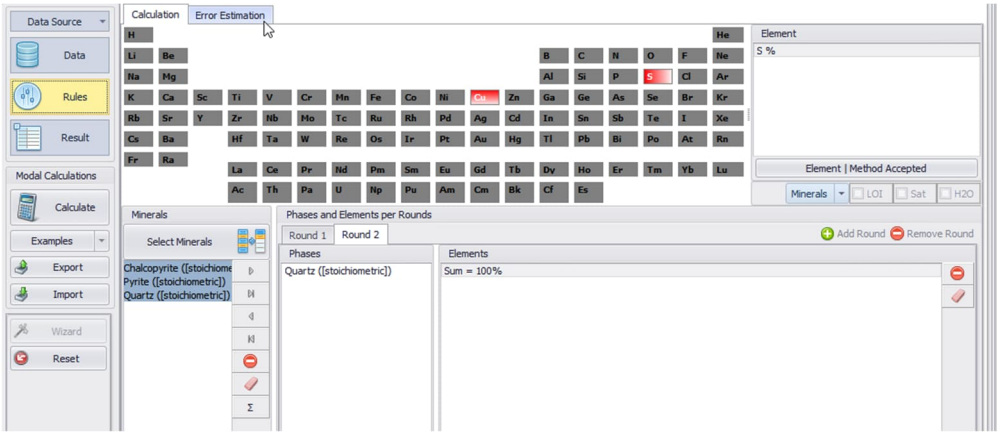
Pressing “Graph” on different sheets (Modal and Distribution sheets) will show the result in a graphical format.

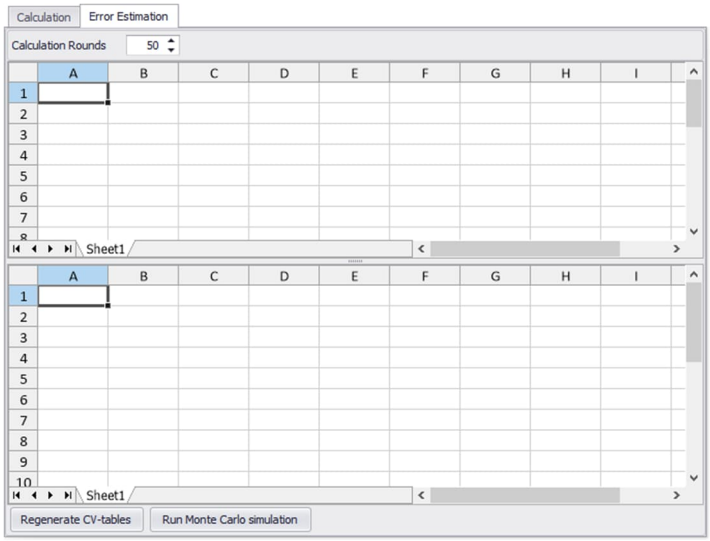




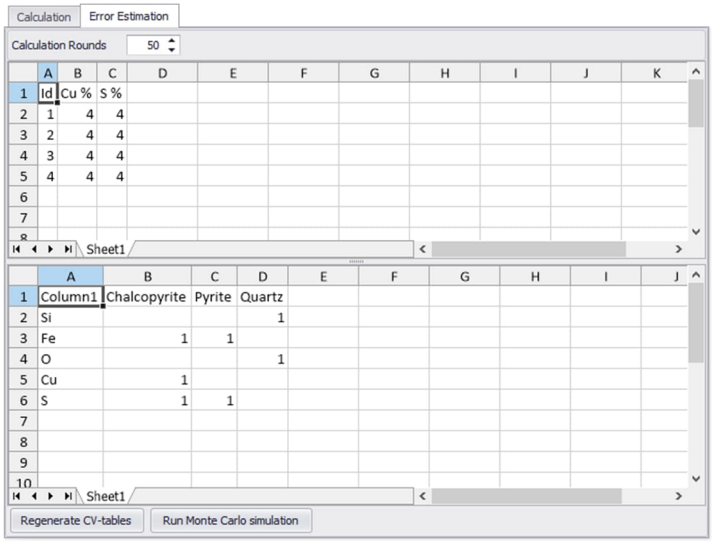
Error Estimation

In the modal calculation, you can also take into account the analytical and sampling errors involved in obtaining the chemical assay. This is done in Error Estimation window under “Rules”. The calculation rules must already be defined before doing error estimation.





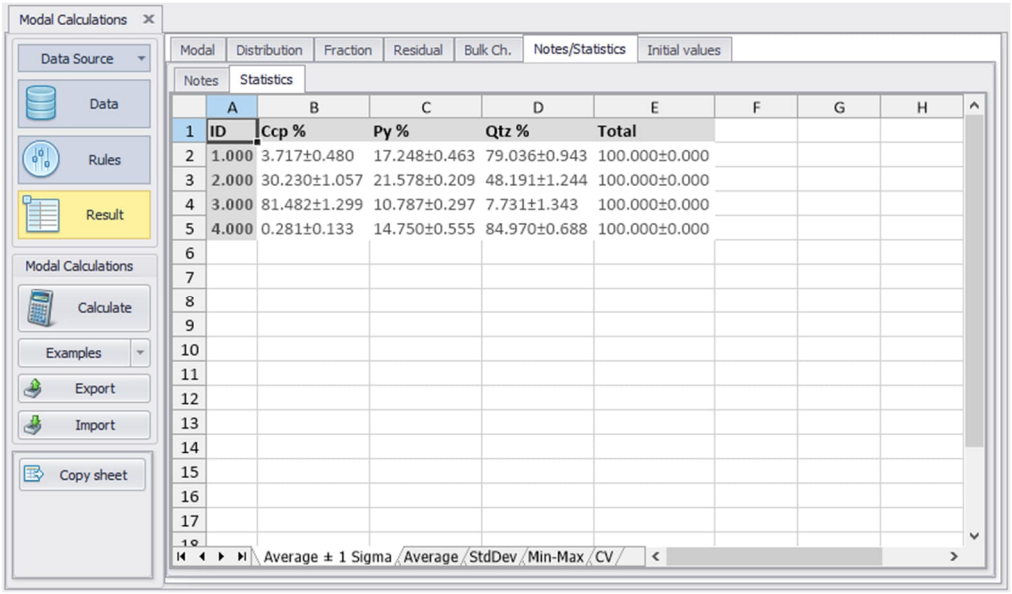
Press “Regenerate CV-tables” to generate the coefficient of variations (CV) for the analyses. CV is also known as relative standard deviation (RSD).



The top sheet refers to the relative standard deviation (RSD) of the chemical analysis of each sample (example: XRF analysis). In this case, we have the chemical analysis of Cu and S respectively for all four samples.

The bottom sheet refers to the relative standard deviation (RSD) of the elemental analysis of each mineral (example: electron microprobe analysis). In this case, we have defined the minerals to be Chalcopyrite, Pyrite, and Quartz. Each elemental analysis for each mineral has its own RSD.

After entering all the RSD values accordingly, you can adjust how many calculation rounds that you want. Then press “Run Monte Carlo Simulation”. The result is available in “Notes/Statistics” tab under “Result”.



The result of the error estimation is given in five tabs:

- Average ± 1 Sigma gives the modal calculation results in the form of average modal mineralogy plus minus the standard deviation.
- Average gives the average modal mineralogy
- StdDev gives the standard deviation of the modal mineralogy

- Min-Max gives the minimum and maximum range of the modal mineralogy.
- CV gives the CV / RSD of the modal mineralogy.

Monte Carlo Simulation for Error Estimation

In principal, the Monte Carlo method simulates a distribution of input data to a model, so that the output of the model can be given as a probability distribution of possible outcomes. The model here is the element to mineral conversion routine; we want to see the modal mineralogy if the chemical assays and elemental analysis of the minerals is not a single value, but rather a distribution of multiple values with a certain variability.

This is very useful since in real life, we would not have just one chemical assay; we usually repeatedly perform chemical assays and in some cases with multiple samples. Since assays costs money, it would be unfeasible to perform a large amount of assaying just to evaluate the variability and its effect to the modal mineralogy calculation. However, if we understand the typical variability of the assays, we can use this knowledge to simulate a large amount of assay to be used for modal mineralogy calculation.

84.8. References

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