

70. HSC Geo

HSC Geo is a program to make mineralogical and petrological calculations and store the results in a database for further analysis with HSC Data.

HSC Geo:

- Prepares a database from the tabulated data
- Performs petrological calculations for rock samples
- Calculates the mineral composition of samples (modal composition) from the chemical analysis
- Calculates the formula of minerals from the mineral analyses
- Includes a mineral database with stoichiometric compositions and extensive data from literature

General procedure

The general procedure of HSC Geo is as follows:

- 1) Prepare the data e.g. in Excel and save using Excel file format.
- 2) Open the files in HscGeo
- 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 in the database
- 8) Launch HSC Data to study the result graphically and statistically

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. E.g. 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/%. For this the following options exist:
 - Place element, method and unit as 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 as its own row and name it UNIT. HSC Geo understands the following units: wt.%, %, ppm, g/t, ppb
 - Place element, method and unit in the first row and separate them with a space or / (e.g. Cr XRF ppm, Cr/XRF/ppm)

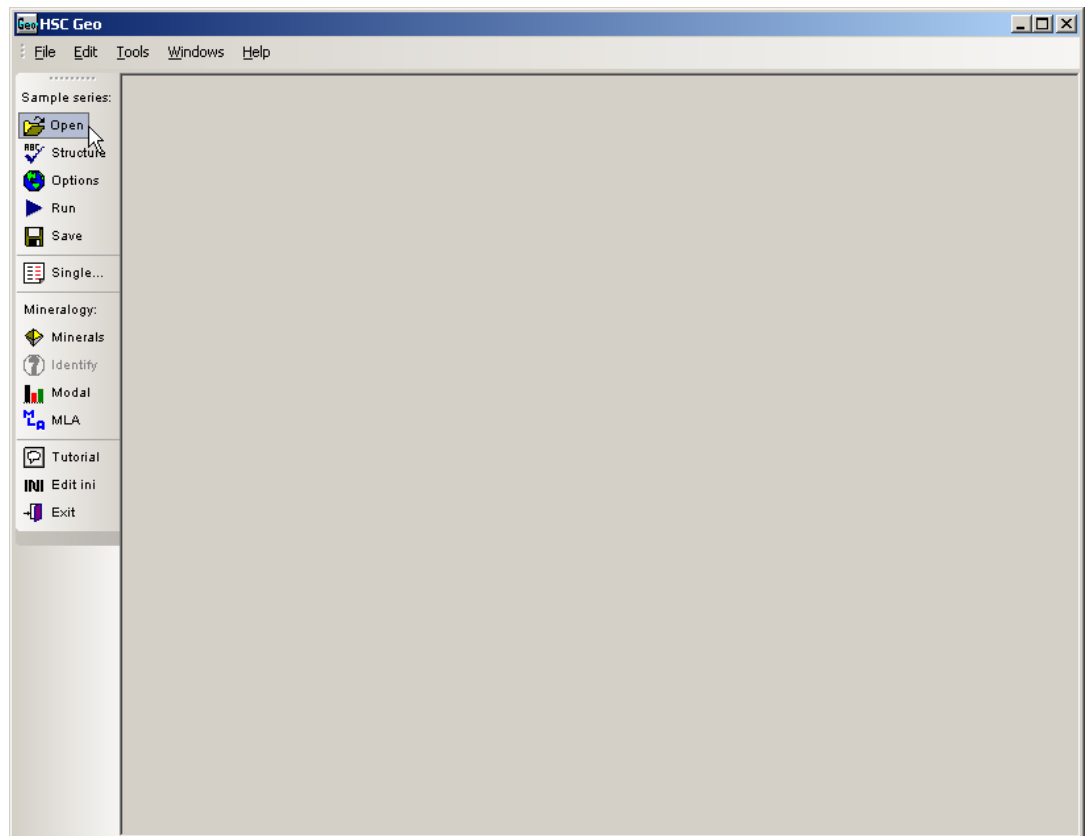
- Name the file or sheet according to the method and then you won't have to repeat it. For example on the sheet called XRF the header gives the element and method, e.g. Cr ppm.

- 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

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

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

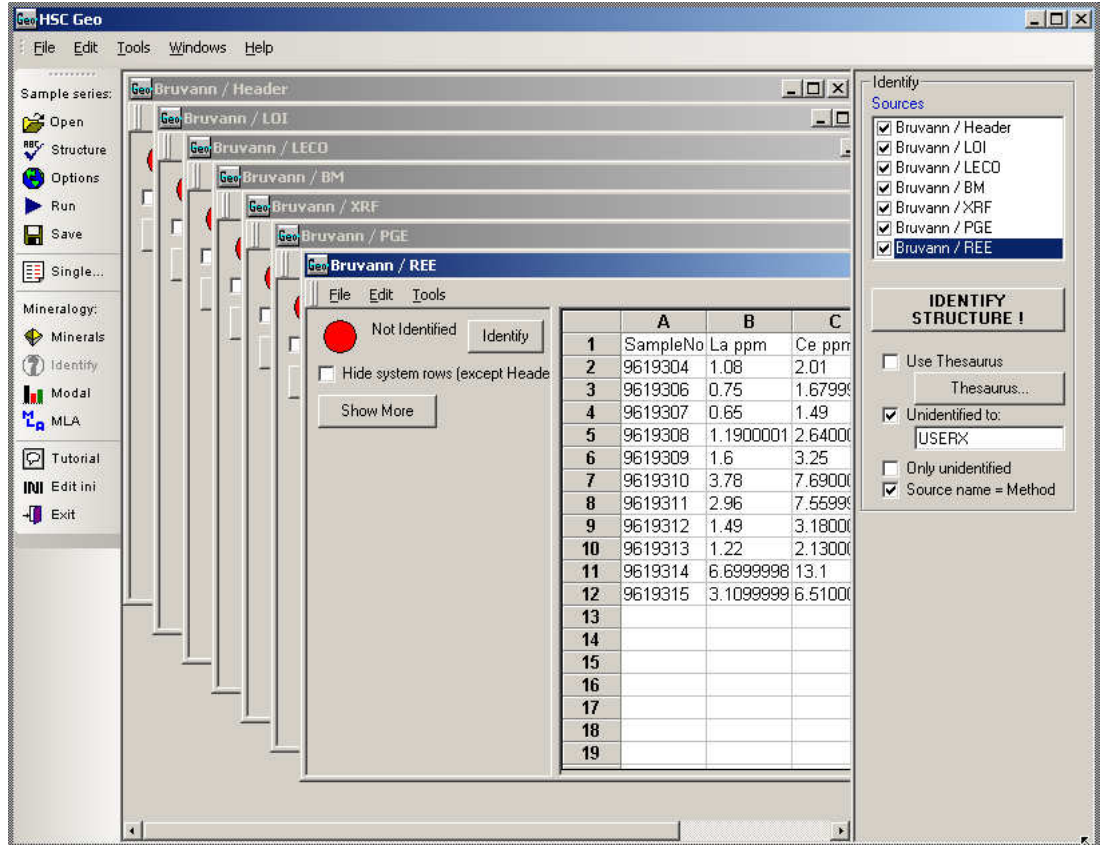
1. Run the HscGeo (Start – All Programs – HSC Chemistry 6.0 – Geo)
2. Select Open from the left button list (or from the HscGeo menu File – Open data)



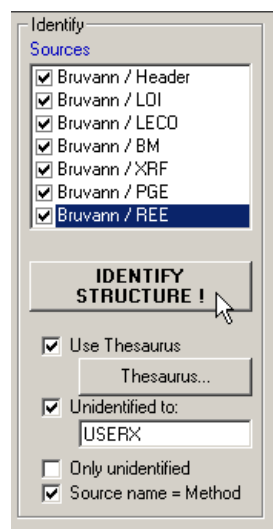
3. Select from the data folder (...\\Geo\\data) example file Bruvann.xls
4. HscGeo opens the Excel file and places each sheet as its own source window. A total of seven sources are visible:
 - Bruvann / Header (header data, location data)
 - Bruvann / LOI (loss of ignition analyses)
 - Bruvann / LECO (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.



- The structure of the sources has to be identified before the calculations. To do this, press the “IDENTIFY STRUCTURE” button. If you want to exclude some of the sources uncheck them before pressing the IDENTIFY button.



- 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 HscGeo 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 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

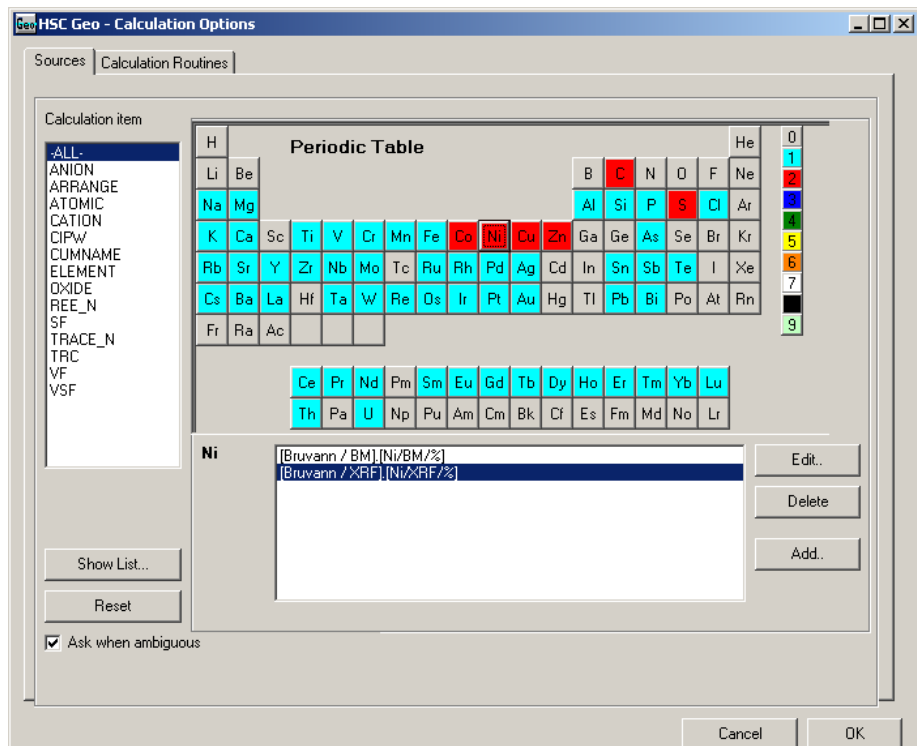
| | A | -ID- | C | D | E | F | G | |
|-------|------------|-----------|-----------|----------|-----------|-----------|----------|------|
| -Hdr- | HEADER | SampleN: | SiO2 % | TiO2 % | Al2O3 % | Cr2O3 % | V2O3 % | Fe |
| -Ele- | ELEMENT | SampleN: | SiO2 | TiO2 | Al2O3 | Cr2O3 | V2O3 | Fe |
| -Met- | METHOD | | XRF | XRF | XRF | XRF | XRF | XR |
| -Uni- | UNIT | | % | % | % | % | % | % |
| -Tab- | TABLE | | ANALYSE | ANALYSE | ANALYSE | ANALYSE | ANALYSE | AN |
| -Fld- | FIELD | SampleN: | SiO2/XRF | TiO2/XRF | Al2O3/XRF | Cr2O3/XRF | V2O3/XRF | Fe |
| -Typ- | TYPE | LONG(U,I) | SINGLE | SINGLE | SINGLE | SINGLE | SINGLE | SIN |
| -Len- | LENGTH | | | | | | | |
| -Dig- | DIGITS | | | | | | | |
| -Idx- | INDEXED | | YES | | | | | |
| -Mul- | MULTIPLIER | | | | | | | |
| -Idf- | IDENTIFIED | | X(Si)1/1 | X(Ti)1/1 | X(Al)1/1 | X(Cr)1/1 | X(V)1/1 | X(F |
| -1- | | 9619251 | 53.200001 | 0.69 | 17.799999 | 0.0226 | 0.0382 | 5.8 |
| 14 | | 9619256 | 47 | 0.725 | 12.1 | 0.143 | 0.0223 | 10.0 |
| 15 | | 9619257 | 45.5 | 0.603 | 11.2 | 0.184 | 0.0223 | 10.0 |
| 16 | | 9619258 | 52.700001 | 0.547 | 13.1 | 0.216 | 0.0478 | 8.10 |
| 17 | | 9619259 | 51 | 0.379 | 12.8 | 0.197 | 0.0564 | 6.90 |
| 18 | | 9619260 | 50.900002 | 0.392 | 13.2 | 0.17 | 0.0504 | 7.10 |
| 19 | | 9619261 | 47.599998 | 0.483 | 11.2 | 0.0874 | 0.0287 | 11.0 |

7. Check the identification. If the “Unidentified to” option was checked, then all the columns that were not identified were marked to be stored in the “USERX” table. The name of the user-table can be changed. If there are errors press “Back” button, correct the contents manually, or make the corrections in the original Excel file and start from the beginning.

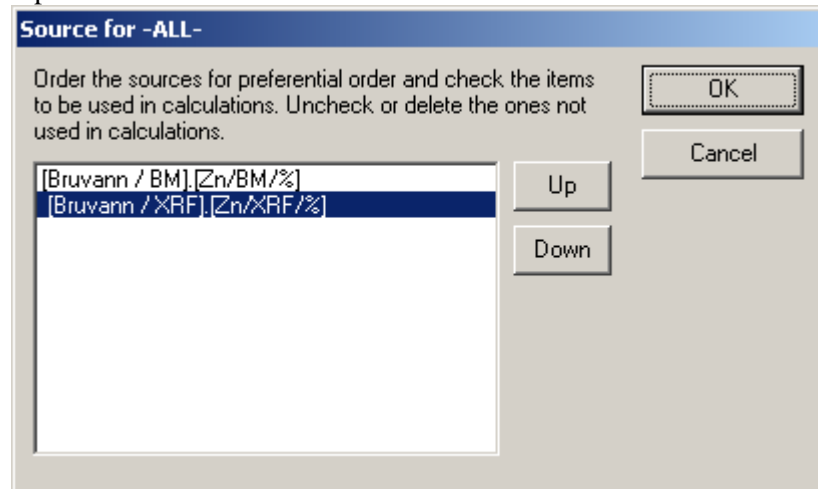
- To check the sources for calculations press Options on the left button list



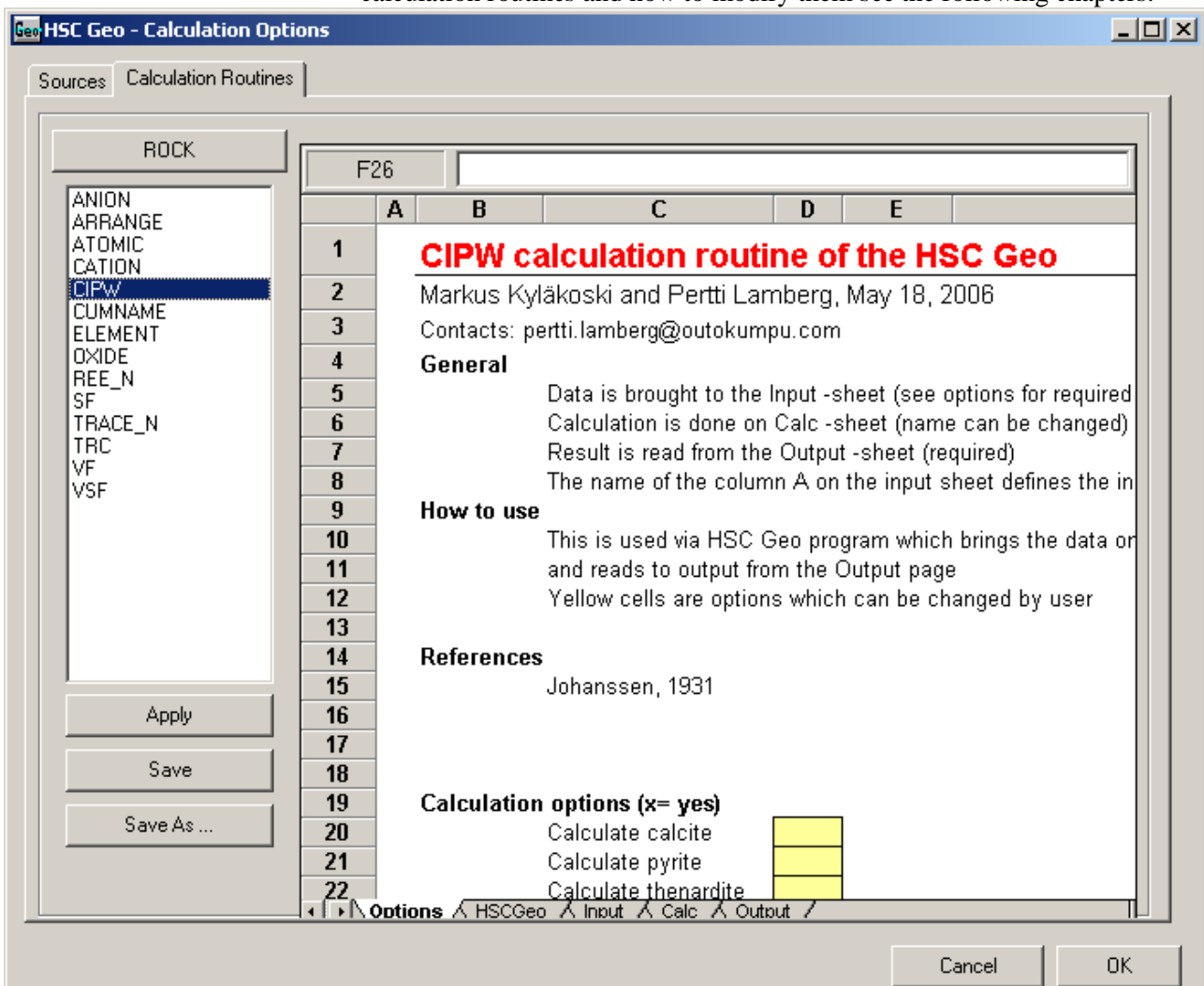
- HscGeo shows a periodic table where the color indicates the number of different assay methods found for an element. If there are several analyses for an element, e.g. for copper, HscGeo will – by default – scan them in alphabetical order. If an assay is found for the sample in question then searching is ended for that sample and the value found is used in the calculations. To exclude some assay press Delete. To add some assay which was not identified press Add. To change the preferential order of the sources, press Edit...



- To edit the window opening, arrange the assays in preferential order with the Up and Down buttons.

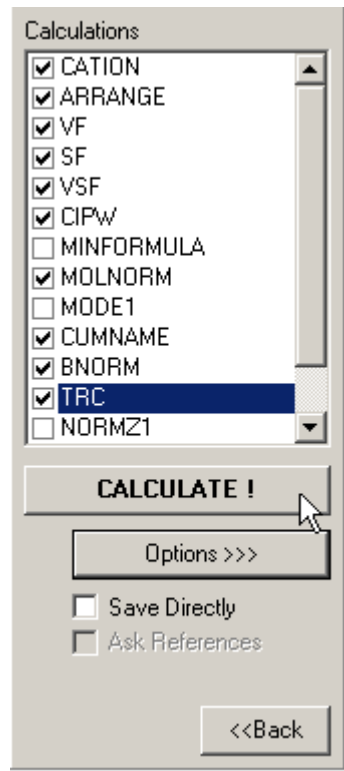


- The calculation options can be edited by selecting the “Calculation Routines” tab and by selecting the appropriate method. For more details on calculation routines and how to modify them see the following chapters.

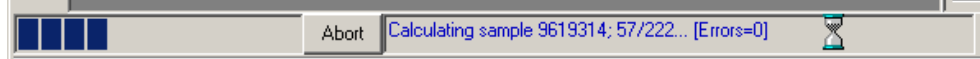


- When the identification is ready, you can progress to calculations. Check the calculations you want to do for the samples by checking and unchecking the

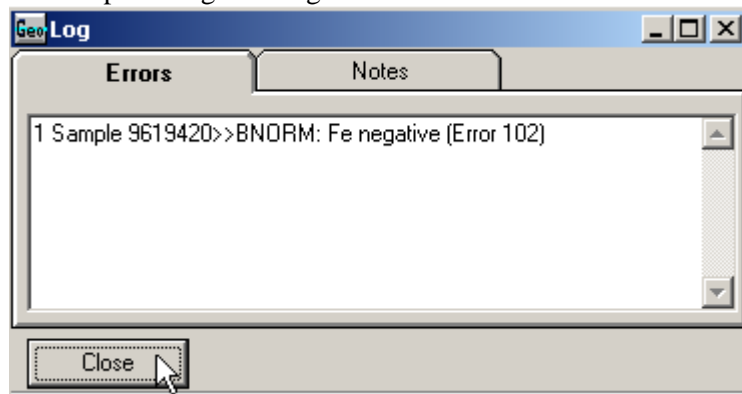
calculations in the list box. The calculations listed below are done by default. When ready press “CALCULATE”



9. The progress bar shows the progress of the calculations. Check the number of errors



10. If there were errors you can see them in the Log- window. In the tutorial Bruvann file, one sample will give a negative Fe in the BNORM calculation.



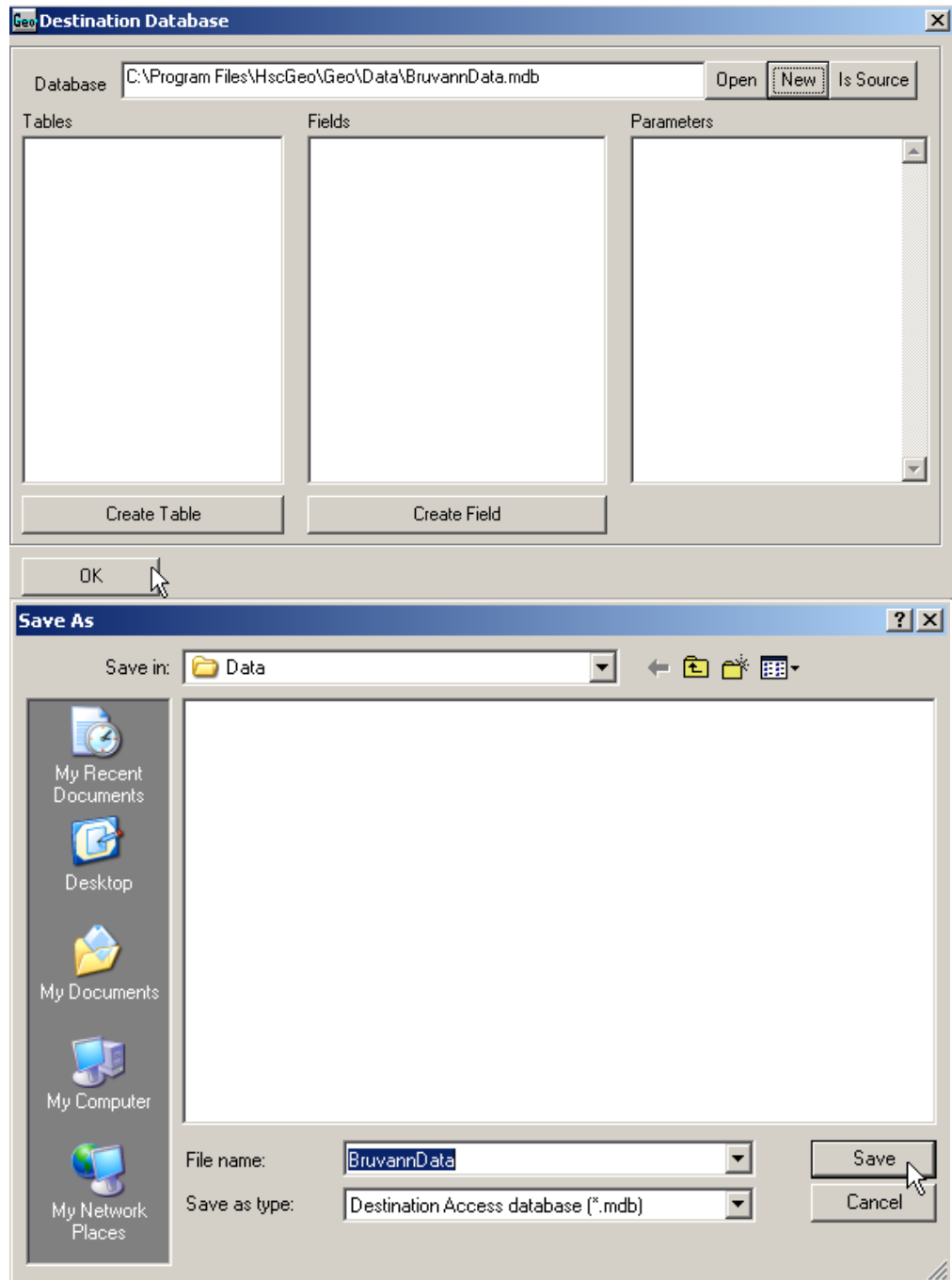
11. Calculation results are calculated in the “Calculation Result” window, which is similar in structure to the input files. The result of each of the calculation routines is shown on its own page.

| -Hdr- | SampleNo | Quartz CIPW % | Orthoclase CIPW % | Albite CIPW % | Anorthite CIPW % | Plagioclase CIPW % | Leucite CIPW % | Neph |
|-------|-----------|---------------|-------------------|---------------|------------------|--------------------|----------------|------|
| -Tab- | CIPW | CIPW | CIPW | CIPW | CIPW | CIPW | CIPW | CIPW |
| -Fld- | SampleNo | Quartz CIPW % | Orthoclase CIPW % | Albite CIPW % | Anorthite CIPW % | Plagioclase CIPW % | Leucite CIPW % | Neph |
| -Typ- | LONG(U,I) | SINGLE | SINGLE | SINGLE | SINGLE | SINGLE | SINGLE | SING |
| -Idx- | YES | | | | | | | |
| .1- | 9619251 | 1.25992635 | 3.40301778 | 25.53990762 | 32.97244946 | 58.51235709 | 0 | |
| 7 | 9619256 | 0 | 6.498850421 | 14.086511 | 22.58988231 | 36.6763933 | 0 | |
| 8 | 9619257 | 0 | 2.971969215 | 14.3837043 | 21.62256511 | 36.00626941 | 0 | |
| 9 | 9619258 | 1.765908384 | 3.060899536 | 13.65433215 | 26.83118787 | 40.48552002 | 0 | |
| 10 | 9619259 | 1.710798834 | 2.720233988 | 9.348181423 | 29.40787251 | 38.75605394 | 0 | |
| 11 | 9619260 | 0.07484059318 | 2.168708273 | 12.76643906 | 28.86002521 | 41.62646427 | 0 | |
| 12 | 9619261 | 0 | 2.490174799 | 15.96055895 | 20.94954697 | 36.91010592 | 0 | |
| 13 | 9619262 | 0 | 2.055783751 | 9.00412144 | 16.25126224 | 25.25538368 | 0 | |
| 14 | 9619263 | 0 | 2.724586694 | 10.60137893 | 16.80740532 | 27.40878426 | 0 | |
| 15 | 9619264 | 0 | 3.936400697 | 18.33963295 | 30.3515182 | 48.69115116 | 0 | |
| 16 | 9619265 | 0 | 2.19711973 | 10.11832281 | 17.66229583 | 27.78061863 | 0 | |
| 17 | 9619266 | 0 | 2.163628329 | 9.122115608 | 15.72470217 | 24.84681778 | 0 | |
| 18 | 9619267 | 0 | 1.617364816 | 8.834683926 | 16.6319138 | 25.46659772 | 0 | |
| 19 | 9619268 | 0 | 1.675378929 | 8.653383392 | 14.74026314 | 23.39364653 | 0 | |
| 20 | 9619269 | 0 | 1.717083286 | 8.732529717 | 15.28686714 | 24.01939686 | 0 | |

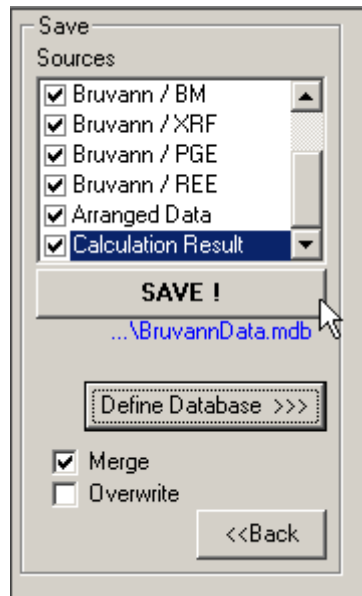
12. To store the results in the database first define the database by pressing the “Define Database >>>” button

The screenshot shows the 'Geo HSC Geo' application window. On the left is a sidebar with menu items like 'Open', 'Structure', 'Options', 'Run', 'Save', 'Single...', 'Mineralogy', 'Minerals', 'Identify', 'Modal', 'MLA', 'Tutorial', 'Edit ini', and 'Exit'. The main window displays the 'Geo Calculation Result' table from the previous screenshot. On the right, a 'Save Sources' dialog box is open, listing several sources with checkboxes: 'Bruvann / BM', 'Bruvann / XRF', 'Bruvann / PGE', 'Bruvann / REE', and 'Calculation Result'. The 'Calculation Result' source is selected. Below the list are buttons for 'Define Database >>>', 'Merge', 'Overwrite', and '<<Back'.

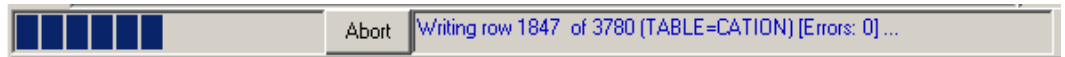
13. In the “Destination Database” window press “New” and give a name to the database (e.g. BruvannData) and press Save. The database has now been created so press “OK” in the “Destination Database” window to accept the database.



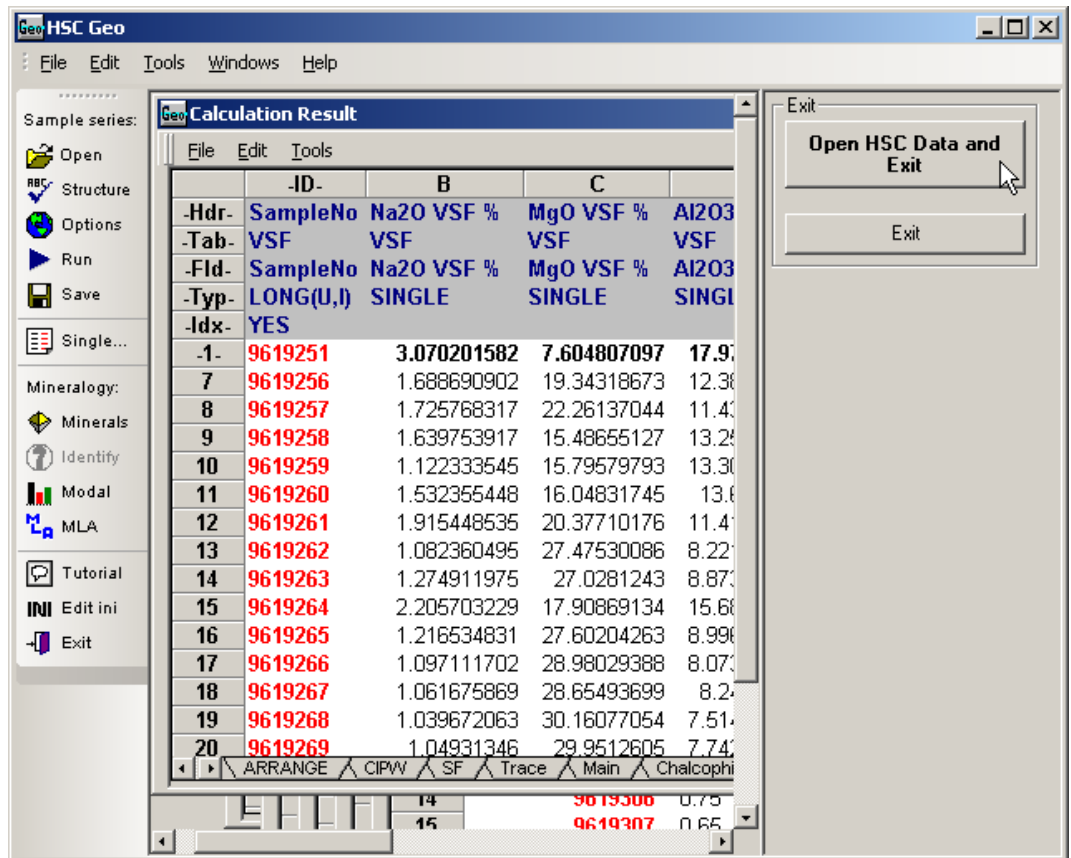
14. Uncheck the sources that you do not want to write in the database. However, it is recommended to write all the source data in the database. It is easier to delete it later or leave it unused than to try to merge it later. When ready press “Save” . The name of the database is given below the “Save!” button in blue.



15. The progress bar at the bottom of the window shows the progress of the saving. Check the number of errors.



16. If there are errors, check them in the Log window after the calculation has been completed.
17. Now the data has been saved in the Microsoft Access database and you are ready to start to study it in HscAux. Press the “Open HSC Data and Exit” button. The created database will be opened in the HSC Data and the HscGeo will be closed.



Calculation routines

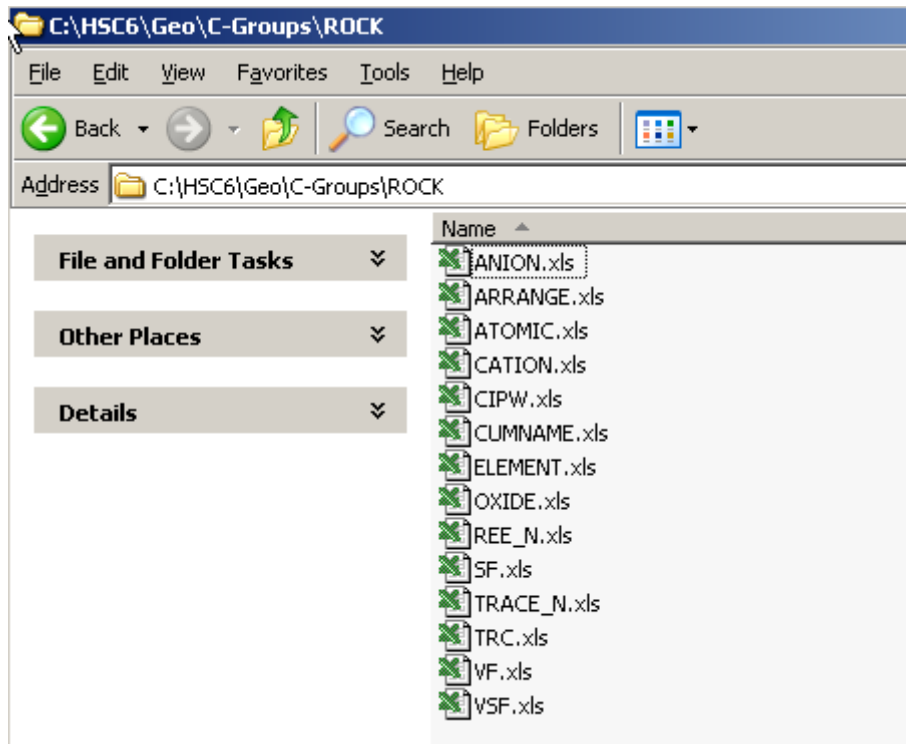
With HSC Geo, it is possible to calculate certain frequently used routines in the same way although the input format may change from one data source to another. HSC Geo includes a number of petrological calculation routines but since the actual calculations are carried out in Microsoft Excel, it is quite easy for the 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 the folders under C:\HSC6\Geo\C-Groups. In the example below there are two different sets of calculations: "ROCK" and "MINERAL".

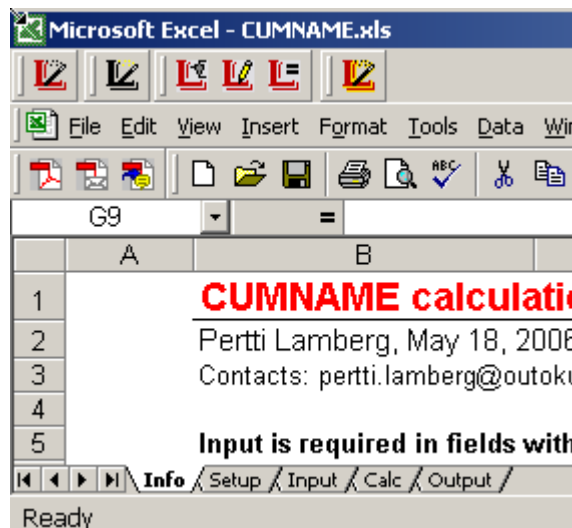


Under the ROCK folder (i.e. C:\HSC6\Geo\C-Groups\ROCK) there are Excel files, all of which have their own individual calculation routines.



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 the 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.

| | A | B | C | D |
|---|-------------------|----|-----------------------|--------|
| 1 | Calculation order | 14 | Calculations required | CIPW |
| 2 | | | | B-NORM |
| 3 | | | | |
| 4 | | | | |

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 |
|----|--------|------|-------|
| 1 | System | User | Input |
| 2 | H | | |
| 3 | He | | |
| 4 | Li | | |
| 5 | Be | | |
| 6 | B | | |
| 7 | C | | |
| 8 | N | | |
| 9 | O | | |
| 10 | F | | |
| 11 | Ne | | |

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 | D |
|----|---------------------------|-------------|--------------|---|
| 1 | System | User | Input | |
| 2 | CIPW.Olivine CIPW % | | 24 | |
| 3 | CIPW.Orthopyroxene CIPW % | | 35 | |
| 4 | CIPW.Clinopyroxene CIPW % | | 10 | |
| 5 | CIPW.Plagioclase CIPW % | | 20 | |
| 6 | CIPW.Magnetite CIPW % | | 1 | |
| 7 | CIPW.Apatite CIPW % | | | |
| 8 | CIPW.Chromite CIPW % | | | |
| 9 | CIPW.Ilmenite CIPW % | | | |
| 10 | CIPW.Quartz % | | | |
| 11 | | | | |

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 B-column. If text appears in the B-column, 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 | Cumname Full | | boOCpa | TEXT(25) | |
| 3 | Cumname Simple | | boOC | TEXT(25) | |
| 4 | C1 | | b | TEXT(25) | |
| 5 | C2 | | o | TEXT(25) | |
| 6 | C3 | | | TEXT(25) | |
| 7 | OMA | | O | TEXT(25) | |
| 8 | CRGN | | C | TEXT(25) | |
| 9 | IC1 | | p | TEXT(25) | |
| 10 | IC2 | | a | TEXT(25) | |
| 11 | IC3 | | | TEXT(25) | |
| 12 | Cums % | | 59 | SINGLE | |
| 13 | I-Cums % | | 30 | SINGLE | |
| 14 | | | | | |

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 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
- 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.

SF – Sulfide fraction

Normative minerals of the SF, i.e. sulfide fraction are: pyrrhotite (FeS), pyrite (FeS₂), pentlandite (Ni_{4.76}Fe_{4.24}S₈), chalcopyrite (CuFeS₂), Co-pentlandite (Co₉S₈), arsenopyrite (FeAsS), sphalerite (ZnS), molybdenite (MoS₂) 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. 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.

Though the sulfides of a sample may also contain other sulfides than those listed in the table below, such as cubanite, gersdorffite, 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: $Po=100 \cdot S/36.48$.
- (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: $Ni_SF\% = Pn_SF\% \cdot 36.16/100$. 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 ₉ S 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 an 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 the element E, in a mineral phase Ma (Bedard 1994). The weight fraction of element E in a sample is

$$W_{E,T} = \sum_{a=1}^n W_{E, Ma} * X_{Ma} \quad ,$$

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%) s=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