Pertti Lamberg, Iikka Ylander, Markus Kyläkoski

GEO MANUAL Partly Demo Version

06120-ORC-T

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.

August 29, 2005

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)



GEO MANUAL Partly Demo Version

Pertti Lamberg, Iikka Ylander, Markus Kyläkoski

August 29, 2005

06120-ORC-T

- 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)

teo HSC Geo	
Eile Edit Tools Windows Help	
Sample series:	
Stucture	
Coptions	
Run	
Save	
E Single	
Mineralogy:	
Interals	
T Identify	
Modal	
M _A MLA	
P Tutorial	
INI Editini	
- Exit	

- 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



GEO MANUAL Partly Demo Version

Pertti Lamberg, Iikka Ylander, Markus Kyläkoski

August 29, 2005

06120-ORC-T

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. 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.

- Identify
Sources
🗹 Bruvann / Header
🗹 Bruvann / LOI
🕑 Bruvann / LECO
🗹 Bruvann / BM
✓ Bruvann / XRF
Bruvann / PGE
Bruvann / REE
Use Thesaurus
Thesaurus
Unidentified to:
USERX
Only unidentified
Source name = Method

- 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

55 - 4(17)

Outotec

Pertti Lamberg, Iikka Ylander, Markus Kyläkoski

GEO MANUAL Partly Demo Version

06120-ORC-T

• -Ele- ELEMENT: is the name of the chemical element if HscGeo has identified the column as a chemical element

August 29, 2005

- -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

🔤 HSC Geo									
Eile Jit I	ools <u>W</u> in	dows <u>H</u> elp							
Sample series:	Geo Bruy	ann / XRF						_	
🎢 Open	Eile	<u>E</u> dit <u>T</u> ools							
Structure		Α	-ID-	С	D	E	F	G	
Options	-Hdr-	HEADER	SampleN	SiO2 %	TiO2 %	AI2O3 %	Cr2O3 %	V203 %	Fet
	-Ele-	ELEMENT	SampleN	Si02	TiO2	AI203	Cr203	V203	Fet
F Kun	-Met-	METHOD		XRF	XRF	XRF	XRF	XRF	XR
🚽 Save	-Uni-	UNIT		%	%	%	%	%	%
E Single	-Tab-	TABLE		ANALYSE	ANALYSE	ANALYSE	ANALYSE	ANALYSE	AN.
E ongre	-Fld-	FIELD	SampleN	SiO2/XRF.	TiO2/XRF/	AI203/XR	Cr203/XR	V203/XRF	Fet
Mineralogy:	-Тур-	TYPE	LONG(U,I)	SINGLE	SINGLE	SINGLE	SINGLE	SINGLE	SIN
< Minerals	-Len-	LENGTH							
() Identify	-Dig-	DIGITS							
	-ldx-	INDEXED	YES						
Modal	-Mul-	MULTIPLI	ER						
MLA	-Idt-	IDENTIFIE	ID	X(Si)1/1	X(1i)1/1	X(AI)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
C I Utonai	14	_	9619256	47	0.725	12.1	0.143	0.0223	10.1
INI Editini	15	_	9619257	45.5	0.603	11.2	0.184	0.0223	10.1
→] E×it	16	-	9619258	52.700001	0.547	13.1	0.216	0.0478	8.11
-	17	-	9619259	51	0.379	12.8	0.197	0.0564	6.9
	18	-	9619260	50.900002	0.392	13.2	0.17	0.0504	7.1
	19	_	9619261	47.599998	0.483	11.2	0.0874	0.0287	11.

- 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

GEO MANUAL Partly Demo Version

Pertti Lamberg, Iikka Ylander, Markus Kyläkoski

August 29, 2005

06120-ORC-T

Sam	ple series:
Ê	Open
	Structure
۲	Options
►	Run 😼
H	Save
	Single
Min	eralogy:
	Minerals
•	
Ò	Identify
	ldentify Modal
() 	ldentify Modal MLA
() 	Identify Modal MLA Tutorial
	ldentify Modal MLA Tutorial Edit ini
	Identify Modal MLA Tutorial Edit ini Exit

- 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...





Pertti Lamberg, Iikka Ylander, Markus Kyläkoski

August 29, 2005

06120-ORC-T

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

Source for -ALL-		
Order the sources for preferential order and check to be used in calculations. Uncheck or delete the used in calculations. [Bruvann / BM].[Zn/BM/%] [Bruvann / XRF].[Zn/XRF/%]	the items ones not Up Down	Cancel

• 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.

Inces Calculation Houtin	es							
ROCK								1
		26						
ANION ABBANGE		Α	В	С	D	E		
	1		CIPW ca	alculation ro	utine o	f the H	SC Ge	0
CIPW	2	'	Markus Ky	läkoski and Pertti I	Lamberg,	May 18,	2006	
CUMNAME FLEMENT	3	1	Contacts: p	ertti.lamberɑ@outok	umpu.com	1		
OXIDE	4	1	General					
REE_N	5		oonordi	Data is brought to t	he Input -s	sheet (see	options for	r required
SF Calculation is done on Calc -sheet (name can be changed in the input of the						sheet (nan	ne can be o	changed)
						/		
VF VSF	8			The name of the co	lumn A on	the input	sheet defir	nes the in
	9		How to use	!				
	10			This is used via HS	IC Geo pro	gram whic	ch brings th	ne data or
	11			and reads to output	t from the I	Output pa	ge	
	12			Yellow cells are op	tions whicl	h can be c	hanged by	user
	13		n - f					
	14		References	i Johanaaan 1021				
Applu	15			Junanssen, 1991				
0990	17							
Save	18							
	19	1	Calculation	n options (x= yes)				
Save As	20	1		Calculate calcite]		
	21			Calculate pyrite				
	22		(Calculate thenardit	e			

8. 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



Pertti Lamberg, Iikka Ylander, Markus Kyläkoski

August 29, 2005

06120-ORC-T

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

Calculations
CATION
ABRANGE
VF
I SF I NOF
VSF
MODE1
CUMNAME
BNORM
✓ TRC
NORMZ1
Options >>>
Save Directly
Ask References
Kack

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

Abort	Calculating sample 9619314; 57/222 [Errors=0]	Z	

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.

Geo Log		
Errors	Notes	
1 Sample 9619420>>I	3NORM: Fe negative (Error 102)	4
Close		

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.

Pertti Lamberg, Iikka Ylander, Markus Kyläkoski

GEO MANUAL Partly Demo Version

August 29, 2005

06120-ORC-T

Geo Calcu	lation Result							
Eile	<u>E</u> dit <u>T</u> ools							
	-ID-	В	С	D	E	F	G	-
-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
-Тур-	LONG(U,I)	SINGLE	SINGLE	SINGLE	SINGLE	SINGLE	SINGLE	SING
-ldx-	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		1.717083286	8.732529717	15,28686714	24.01939686	0	
ТОТ	ARRANGE A	$CIPW \land SF \land Trac$	e 🔨 Main 🔨 Chalcophile	A PGE A REE /				

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

🔤 HSC Geo		
Eile Edit]	<u>[ools W</u> indows <u>H</u> elp	
	Colordation Deput	Save
Sample series:	See Calculation Result	Sources
🚰 Open	<u>Eile E</u> dit <u>T</u> ools	✓ Bruvann / BM
Structure	-ID- B	🗹 Bruvann / XRF
Options	-Hdr- SampleNo Quartz CIPW % Orth	Bruvann / PGE
Run	-Tab- CIPW CIPW CIPI	Bruvann / REE
C Sava	-Fld- SampleNo Quartz CIPW % Urth	
Save	-TYP- LUNG(U,I) SINGLE SING	
📑 Single	-1- 9619251 1.25992635	
Mineralomo	7 9619256 0	
Minorals	8 9619257 O	Define Database
	9 9619258 1.765908384	
T Identity	10 9619259 1.710798834	Merge
Modal	11 9619260 0.07484059318	
<mark>°С</mark> р МLА	12 9619261 0	< <back< td=""></back<>
C Tutorial	13 9619262 U	
	14 9019203 U 15 0610264 O	
	16 9619264 0	
-U Exit	17 9619266	
	18 9619267 0	
	19 9619268 0	
	20 9619269	
	14 5 15 9 16 9 17 9 18 9 19 9	
	I I	

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.

GEO MANUAL Partly Demo Version

55 - 9(17)

Pertti Lamberg, Iikka Ylander, Markus Kyläkoski

August 29, 2005

06120-ORC-T

Geo Destination Dal	tabase				×
Database C:\Pro	gram Files\HscGe	o\Geo\Data\BruvannData.mdb		Open New	Is Source
Database C:\Pro	gram Files\HscGe	eo\Geo\Data\BruvannData.mdb	Parameter	Open New) s	Is Source
Create T	able	Create Field			_
ок 🛵					
Save As					? ×
Save in:	🚞 Data		- + 1) 💣 🎟 -	
My Recent Documents Desktop My Documents My Computer					
My Network Places	File name: Save as type:	BruvannData Destination Access data	base (*.mdb)	• •	Save Cancel

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.

Partly Demo Version

55 - 10(17)

06120-ORC-T



Save
Sources
🗹 Bruvann / BM 🛛 🔺
🗹 Bruvann / XRF 👘 👘
🗹 Bruvann / PGE
🕑 Bruvann / REE
Arranged Data
Calculation Result
SAVE !
\BruvannData.mdb 🖄
Define Database >>>
Merge
Uverwrite
< <back< td=""></back<>

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

GEO MANUAL

August 29, 2005

Abort	Writing row 1847 of 3780 (TABLE=CATION) [Errors: 0]
	j - · · · · ·

- 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.

GEO MANUAL Partly Demo Version

Pertti Lamberg, Iikka Ylander, Markus Kyläkoski

August 29, 2005

06120-ORC-T

ample series:	eo Calcu	lation Result			<u> </u>	Exit
🔆 Open	<u>File</u>	<u>E</u> dit <u>T</u> ools				Open HSC Data and
Structure		-ID-	В	С		
Options	-Hdr-	SampleNo	Na20 VSF %	MgO VSF %	AI203	
	-Tab-	VSF	VSF	VSF	VSF	Exit
Kun	-Fld-	SampleNo	Na2O VSF %	MgO VSF %	AI203	J
Save	-Тур-	LONG(U,I)	SINGLE	SINGLE	SINGL	
Single	-ldx-	YES				
- onigre	-1-	9619251	3.070201582	7.604807097	17.9	
ineralogy:	7	9619256	1.688690902	19.34318673	12.3	
Minerals	8	9619257	1.725768317	22.26137044	11.4	
D 14	9	9619258	1.639753917	15.48655127	13.2	
	10	9619259	1.122333545	15.79579793	13.30	
Modal	11	9619260	1.532355448	16.04831745	13.6	
A MLA	12	9619261	1.915448535	20.37710176	11.4	
	13	9619262	1.082360495	27.47530086	8.22	
P Tutorial	14	9619263	1.274911975	27.0281243	8.871	
U Editini	15	9619264	2.205703229	17.90869134	15.68	
Exit	16	9619265	1.216534831	27.60204263	8.996	
	17	9619266	1.097111702	28.98029388	8.071	
	18	9619267	1.061675869	28.65493699	8.2	
	19	9619268	1.039672063	30.16077054	7.51	
		9619269	1.04931346	29.9512605	7.74	

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".

🔁 C:\HSC6\Geo\C-Group	s
<u>File E</u> dit <u>V</u> iew F <u>a</u> vorit	tes <u>T</u> ools <u>H</u> elp
🚱 Back 🝷 🕥 👻 🏂	🔎 Search 🛛 🎼 Folders 🛛 📔
Address 🛅 C:\HSC6\Geo\C	-Groups
	Name 🔺
File and Folder Tasks	MINERAL
	ROCK
Other Places	*
Details	*

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.

Pertti Lamberg, Iikka Ylander, Markus Kyläkoski

August 29, 2005

06120-ORC-T

😂 C:\HSC6\Geo\C-G	roups\ROCK	
	avorites <u>T</u> ools	Help
🚱 Back 🔹 🕥 🗸	🏂 🔎 Sea	arch 😥 Folders 🛛 🎹 🕶
Address 🛅 C:\HSC6\(Geo\C-Groups\RO	ск
File and Folder Ta	asks ¥	Name A
Other Places	*	ATOMIC.xls
Details	*	CIPW.xls CUMNAME.xls ELEMENT.xls CUIDE.xls CXIDE.xls REE_N.xls SF.xls TRACE_N.xls TRC.xls VF.xls VF.xls

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.

Pertti Lamberg, Iikka Ylander, Markus Kyläkoski

August 29, 2005

Í	<u>F</u> ile <u>E</u> dit	⊻iew	Insert	Fo	rmat <u>T</u> ools	<u>D</u> ata	<u>W</u> indow	<u>H</u> elp	Ado <u>b</u> e F
] 🔁	12 🐔] 🗅 (2 -] e	S 🗟 💞	*	ta 🛍 :	Í	n ⊳≁0
	C1	-		=	Calculatio	ins re	quired		
		А		В		С			D
1	Calcula	tion o	rder	14	Calculatio	ons re	equired	CIP\	N
2								B-N	ORM
3									
4									
-	▶ N\ In	fo 🔪 Set	up / Ir	nput	/ Calc / Outp	out/			
Rea	idy								

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.

12)	<u>File E</u> dit	<u>V</u> iew <u>I</u> nsert	F <u>o</u> rmat <u>T</u> ools I
] 🔁	12 🖏] 🗅 😅 日	i 🖨 🗟 💞
	B8	•	=
	A	В	C
1	System	User	Input
2	Η		
3	He		
4	Li		
5	Be		
6	В		
7	С		
8	N]
9	0		
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).

Pertti Lamberg, Iikka Ylander, Markus Kyläkoski

August 29, 2005

06120-ORC-T

je	<u>File E</u> dit <u>V</u> iew <u>I</u> nsert F <u>o</u> rmat <u>T</u> o	ols <u>D</u> ata <u>W</u> i	indow <u>H</u> elp	Ado <u>b</u> e PDF
	🔁 🐔 🛛 🛥 🖬 🎒 🖎	** 🖻 🖋	KD + 🤮	$\Sigma f_* \left \frac{1}{2} \right $
	D3 💽 =			
	A	В	С	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.IImenite 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.

12	<u>File E</u> dit <u>V</u> iew <u>I</u> nse	rt F <u>o</u> rmat]	[ools <u>D</u> ata	<u>W</u> indow <u>H</u> el	p Ado <u>b</u> e PDF		
] 🔁 🔁] 🗅 😅 🖬 🎒 🖪 🖏 🖤 🛍 🝼 🗠 - 🍓 Σ 🏂 🖢							
	A13 🔹	= I-Cun	ns %				
	Α	В	С	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		0	TEXT(25)			
6	C3			TEXT(25)			
7	OMA		0	TEXT(25)			
8	CRGN		С	TEXT(25)			
9	IC1		р	TEXT(25)			
10	IC2		а	TEXT(25)			
11	IC3			TEXT(25)			
12	Cums %		59	SINGLE			
13	I-Cums %		30	SINGLE			
14							
I	▶ 🕨 \ Info / Setup /	Input / Calc)	Output /		•		
Rea	idy			<u></u>			

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.

55 - 15(17)

Pertti Lamberg, Iikka Ylander, Markus Kyläkoski

)utotec

August 29, 2005

GEO MANUAL

Partly Demo Version

- 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.

<u>SF – Sulfide fraction</u>

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.

GEO MANUAL Partly Demo Version

55 - 16(17)

Pertti Lamberg, Iikka Ylander, Markus Kyläk	toski August 29, 2005	06120-ORC-T
---	-----------------------	-------------

(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: $\begin{bmatrix} 36.48 & 53.45 \\ 63.52 & 0.07 \times 46.55 \end{bmatrix} \bullet \begin{bmatrix} Po \\ Py \end{bmatrix} = \begin{bmatrix} S \\ Fe \end{bmatrix}$, 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.

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.
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 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	Ару	FeAsS	As=	46.01	34.30	19.69	Apy=100*As/46.01
Pyrrhotite	Ро	FeS			63.52	36.48	(3) or (4)
Pyrite	Ру	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

,

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



Pertti Lamberg, Iikka Ylander, Markus Kyläkoski

GEO MANUAL Partly Demo Version

August 29, 2005

06120-ORC-T

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

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