CMAS 3D, a new program to visualize and project major elements compositions in the CMAS system

Lyderic France, N. Ouillon, G. Chazot, J. Kornprobst, Pierre Boivin

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France L.[*], Ouillon N., Chazot G.[**], Kornprobst J., Boivin P.

Laboratoire Magmas et Volcans, OPGC – UBP – CNRS, 5, rue Kessler, 63038 Clermont-Ferrand Cedex, France

*: Present address : Géosciences Montpellier, Université Montpellier 2 - CNRS, 34095 Montpellier cedex 05, France

Corresponding author : **France@gm.univ-montp2.fr**

Equipe Manteau-Noyau

Laboratoire Géosciences Montpellier

CC 060 Université de Montpellier II

Place Eugène Bataillon

34095 Montpellier Cedex 5

FRANCE

Phone : +334 67 14 39 44

Fax: +334 67 14 36 03

** : Present address : UMR 6538 “Domaines Océaniques”, IUEM, Université de Bretagne Occidentale, Place Copernic, 29280 Plouzané, France

Abstract

CMAS 3D, developed in MATLAB ®, is a program to support visualization of major element chemical data in three dimensions. Such projections are used to discuss correlations, metamorphic reactions and the chemical evolution of rocks, melts or minerals. It can also project data into 2D plots. The CMAS 3D interface makes it easy to use, and does not require any knowledge of Matlab ® programming. CMAS 3D uses data compiled in a Microsoft Excel^{TM} spreadsheet. Although useful for scientific research, the program is also a powerful tool for teaching.

Key words: CMAS system, 3D, projection.

1-Introduction

Major element chemical data of rocks and minerals are of great use in the study of the origins and evolution of magmatic and metamorphic rocks. Petrologists mostly use binary plots to evaluate correlation between chemical elements or oxides, but some reduced systems have been developed to take into account more than 2 elements in the same diagram. For example some software packages such as MinPet (Richard, 1997), IgPet (Carr, 1995), NewPet (Clarke, 1993), Petrograph (Petrelli, 2003) or GeoPlot (Zhou and Li, 2006) have been developed for better data visualization and interpretation. Smith and Beermann (2006) proposed to use multivector diagrams to represent up to nine components. O'Hara (1968) introduced the use of the CaO-MgO-Al_2O_3-SiO_2 (CMAS) system allowing representation of 13 oxides in a four dimension representation. This pseudo-quaternary projection has been largely used as it is the simplest way to represent the major element composition of mafic and ultramafic rocks

(Garrido and Bodinier, 1999), as well as the main crustal and mantle minerals (Kornprobst, 1970; Kornprobst and Conquéré, 1972) or extraterrestrial objects (Grossman and Fedkin, 2003; Grossman et al., 2002; Yoneda and Grossman, 1995) and serves as a good model for dry basaltic melts (Schiano et al., 2000; Schiano et al., 2004). It is also largely used in experimental petrology (Hirschmann et al., 2003; Kogiso et al., 2003; Kogiso et al., 2004). Here we present CMAS 3D, a program written in MATLAB 6.5 ®. It converts oxide data to CMAS coordinates and allows visualization of these data in 3 dimensions, and projects the data onto two dimensional plots. Using CMAS 3D does not require MATLAB programming expertise. It reads data from a Microsoft Excel™ spreadsheet. The visualization uses the VRML (Virtual Reality Modeling Language) allowing the rotation of the CMAS tetrahedron in all directions in order to evaluate the different correlations and reactions. CMAS 3D also permits the addition of lines or planes between the analyzed rocks or minerals for the purposes of testing for metamorphic reactions or exsolutions, or to illustrate specific chemical trends. The proportion of the mineral phases that are involved in a reaction as reagents or as products is represented by the balanced centroid on a line (for two reagents or products), on a plane (for three reagents or products) or in a polyhedron (for more than three reagents or products). The intersection between the geometric form formed by the reagents and the one formed by the products in CMAS space is a test of the chemical feasibility of the reaction.

2-Program philosophy and projection system

The CMAS system is a good analog for the main minerals contained in mafic and ultramafic rocks, mainly olivine, magnesian and aluminous pyroxenes (enstatite and polymorphs, pigeonite, diopside), and aluminous phases (plagioclases, spinels, grossular-pyrope solid solutions), as well as for mafic and ultramafic magmas. O'Hara (1968 and 1976) proposed the

pseudo quaternary projection by defining the following CMAS components in terms of mole fractions of the oxides:

$C_0=100(CaO-(3+1/3)P_2O_5+2Na_2O+2K_2O)*56.08$

$M_0=100(MgO+FeO+MnO+NiO-TiO_2)*40.32$

$A_0=100(Al_2O_3+Fe_2O_3+Cr_2O_3+TiO_2+Na_2O+K_2O)*101.96$

$S_0=100(SiO_2-2Na_2O-2K_2O)*60.085$

and:

$Sum=C_0+M_0+A_0+S_0$

with:

$C=C_0/Sum$

$M=C_0/Sum$

$A=C_0/Sum$

$S=C_0/Sum$

The C, M, A and S results are the respective coordinates of the apices in the CMAS tetrahedron.

Four different types of representations are possible with CMAS 3D: *(i)* the projection in moles presented above from O'Hara (1968), *(ii)* the same projection but in weight percent, *(iii)* a modified version proposed in the Basaltic Volcanism Study Project (1981) (hereafter BVSP_81) in moles and *(iv)* the same modified version in weight percent.

To use CMAS 3D, data should be compiled in a Microsoft Excel™ spreadsheet (*.xls) that should have the format depicted in the table 1 (this file is called hereafter data.xls). A first column contains the sample name (only one word), the 3 following ones contain the symbol (1 for a sphere and 2 for a cube), the size (8 for a medium size) and the color (between 1 and 12, see the file "C:\CMAS_1.2\colors&symbols.jpg") selected for the representation. The next columns contain the oxides organized in 13 columns in the same order as presented in the

table 1. The last column contains the total. No cells should be empty, but zero could be written.

3-Starting the program

On a PC the folder “CMAS_1.2” should be copied on the “C:\” directory, no installation is necessary. A version of Matlab 6.5 ® or younger is required to use CMAS 3D. When MATLAB is open “C:\CMAS_1.2” should be writen in the “Current Directory” (No.1, Fig. 1) and then the program is loaded by writing “cmas” in the “Command Window” (No.2, Fig. 1). Once the interface of CMAS 3D is open (Fig. 2), it is ready to be used, as described in the next section.

4-Functionalities

4.1-CMAS tetrahedron

First of all empty CMAS tetrahedrons could be generated by selecting a file name and pressing the associated button (No.1, Fig. 2), files are stored in the folder “CMAS_1.2\Resultats”. Before loading the data file (data.xls), a projection system (O’Hara_moles; O’Hara_wt%; BVSP_81_moles or BVSP_81_wt%) must be chosen from the interface illustrated in Figure 2 (No.1). Then the option “Probe file loading” is selected (No.2, Fig. 2). This opens a new window that allows the data file (e.g. data.xls) to be chosen; a final window is then opened and an output-file has to be chosen. When the data.xls type file is loaded, the size of the file is written in the central frame (No.3, Fig. 2). Two different numbers are present: the first one is the number of samples and the second one, the number of

columns (it should be 17). The CMAS coordinates of the samples are written in the "Command Window" (No.2, Fig. 1) in percent as:

cmas= C_1 M_1 A_1 S_1

C_2 M_2 A_2 S_2

… … … …

C_{n-1} M_{n-1} A_{n-1} S_{n-1}

C_n M_n A_n S_n

These coordinates are also stored at the end of the results file (*.wrl) when it is edited as a text file.

4.2-Adding Points or Minerals

This option allows adding some common minerals or some points if their coordinates in the CMAS space are known. To use this option, the line "Add a point" should be selected (No.2, Fig. 2). To add a common mineral, select it in the drop-down menu (No.4, Fig. 2). Once the mineral is selected, the output-file has to be selected. To add a point from its CMAS coordinates, these coordinates should be written in the four boxes (No.4, Fig. 2) and the sum should be 1. A name could be given in the upper case and a color should be chosen just below (No.5, Fig. 2); to export, the button "export" should be activated. As above, an output-file should be selected.

4.3-Adding Lines and Planes

As discussed above, it can be useful to add lines and planes to the CMAS tetrahedron in order to explore the possibility of subsolidus reactions or exsolutions or to compare whole

rock compositions, or to track the evolution of melt during melting or crystallization. To add lines and planes, the line “Draw lines & planes” should be selected (No.2, Fig. 2). Then there are three choices in the menu (No.6, Fig. 2): *(i)* add the particular plane corindon-enstatite-wollastonite (co-en-wo or A-MS/2-CS-2), *(ii)* add another plane and *(iii)* add a line. For *(ii)* and *(iii)* there are two possibilities to select the apices: *(a)* use some samples that are in the data.xls type file or *(b)* use common minerals. For *(a)*, the number of the line (in the data.xls file, Table 1) of the used sample should be written in the three (for a plane) or two (for a line) boxes. For *(b)*, the abbreviation of the minerals should be used (Table 2). Note that both *(a)* and *(b)* could be simultaneously used. Once the poles of the line or of the plane are selected, select a color, then the button “export” should be activated and the output-file has to be selected.

4.4-Projections

The 3D representations of the CMAS tetrahedron allow the user to visualize the relationships and the correlations between compositions of minerals, rocks or both. Although these 3 dimensional representations are very useful, they are sometimes difficult to use, especially if too many data are plotted at the same time. So, projections on a 2 dimension surface are necessary and widely used. These projections involve a projection pole and 3 apices defining a projection plane. These poles and apices can be mineral, compositions, rock compositions or any combination of compositions.

To make projections, the line “Projections” should be selected (No.2, Fig. 2). Then there are two choices in the menu (No.7, Fig. 2): making a projection on a predefined plane (A-CS/2-MS/2; C-M-A; C-A-S; M-A-S or C-M-S) or making a projection on a user-defined plane. In the first case, the line of the chosen plane should be selected (No.7, Fig. 2) whereas,

for the second case, the 3 boxes should be completed with either the number of the line of a sample (from the data.xls type file, Table 1) or with the abbreviation of a mineral (Table 2). The "projection pole" definition should be completed in the same way. An output filename should be written in the box "name of the projection output file here". The projection will be activated by pressing the "export" button. The coordinates of the projected samples are written in the "Command Window" (No.2, Fig. 1). The fourth column indicates the quality of the projection. The bigger the number is, the closer from the projection pole is the projected point, and the poorer the quality of the projection. A negative value indicates that the pole is between the plane and the projected point. Projection results are stored in the folder "CMAS_1.2\triangle"

5-Visualization of results

The visualization of results should be made with a VRML reader (to read the *.wrl) because the visualization in MATLAB is not so convenient. The files in C:\CMAS_1.2\Results and C:\CMAS_1.2\triangle should be opened with this type of reader. Some free VRML readers are available on the web; we propose to use "Flux Player" freely downloadable at http://www.mediamachines.com (also provided with the supplementary material). The mouse commands to move the tetrahedron are: left button: rotation, right button: displacement, rolling button: zoom.

Note that in order to have an image easily modifiable, the names of the apices are not given in the results of the projection. For the projection, the name of the apices must be in a precise order (No.7, Fig. 2): the first apex name will be the left one, the second one will be the right one and the third one will be the top one.

6-Example

The proportion of the mineral phases that are involved in a reaction as reagents or as products is represented by the balanced centroid on a line (for two reagents or products), on a plane (for three reagents or products) or in a polyhedron (for more than three reagents or products). A metamorphic reaction is chemically supported only if in the composition plots in the chemical space and so in the CMAS chemical reduced space, the balanced centroid of the reagents and the one of the products have the same coordinates.

In mantle conditions, in the subsolidus domain, two reactions separate the Seiland subfacies from the Ariegite one (both subfacies being in the spinel lherzolites facies; Fig.3). These reactions are *Opx+Pl+Sp* ⇔*Gt+Cpx* and *Opx+Pl+Sp* ⇔*Gt+Sapph* (with Opx: orthopyroxene, Pl: plagioclase, Sp: spinel, Gt: garnet, Cpx: clinopyroxene and Sapph: sapphirine) and are located in the P-T space on Figure 3. The reaction involving Cpx is well known from granulites and pyroxenites studies (e.g.: Grégoire et al., 1994) and the one involving the sapphirine has been evidenced by Christy (1989). These reactions are represented in the CMAS tetrahedron by a plane (Opx-Pl-Sp) which is crosscut by a line joining Gt-Cpx and Gt-Sapph, respectively. Cpx and Sapph being situated at the opposite regarding the plane (Opx-Pl-Sp), only one reaction could be effective depending on the position of Gt as regard of the plane. Gt is very close of this plane so precise calculations and graphical representations have to be used to know which reaction is effective. The involvement of Sapph has been reported several times in mantle or in deep crustal domains (Grégoire et al., 1994; Herd et al., 1969; Meyer and Brookins, 1976; Segnit, 1957) and its origin is never very well understood, the use of CMAS 3D allows to resolve such a problem.

A pyroxenite xenolith from Morocco (TAK-4) is made of clinopyroxene, garnet, spinel, plagioclase and sapphirine. Electron microprobe data for these minerals (Table 1) have

been plotted in a CMAS tetrahedron using CMAS 3D and are presented on the Figure 4 as well as the Opx-Pl-Sp plane. On a projection from the plagioclase pole (Fig.5), the Opx-Pl-Sp plane (represented as a line) is crosscut by the Gt-Sapph line, showing that these two minerals are the products of a reaction involving plagioclase, spinel and orthopyroxene. The observation that Gt is close to the Opx-Pl-Sp plane implies that the amount of sapphirine formed during the reaction is very small, which is confirmed by microscopic observations on thin sections.

7-Conclusion

CMAS 3D provides the possibility to project and to visualize chemical data (weight percent of oxides) within the CMAS system in 3 dimensions and to make 2 dimensions projections very easily. Petrologists and geochemists commonly compile their data with Microsoft Excel™ so CMAS 3D uses an Excel source file to make representations and projections. The calculations are made by CMAS 3D with MATLAB ® and the results can be visualized with free downloadable software. The 3D visualizations are very easy to use and provide a very convenient tool for research as well as for teaching igneous and metamorphic petrology.

Acknowledgments

The manuscript has been largely improved thanks to the constructive and patient reviews by Alexei Fedkin and James Kelly Russell. We are also grateful to Eric Grunsky, Editor-in-Chief for his support.

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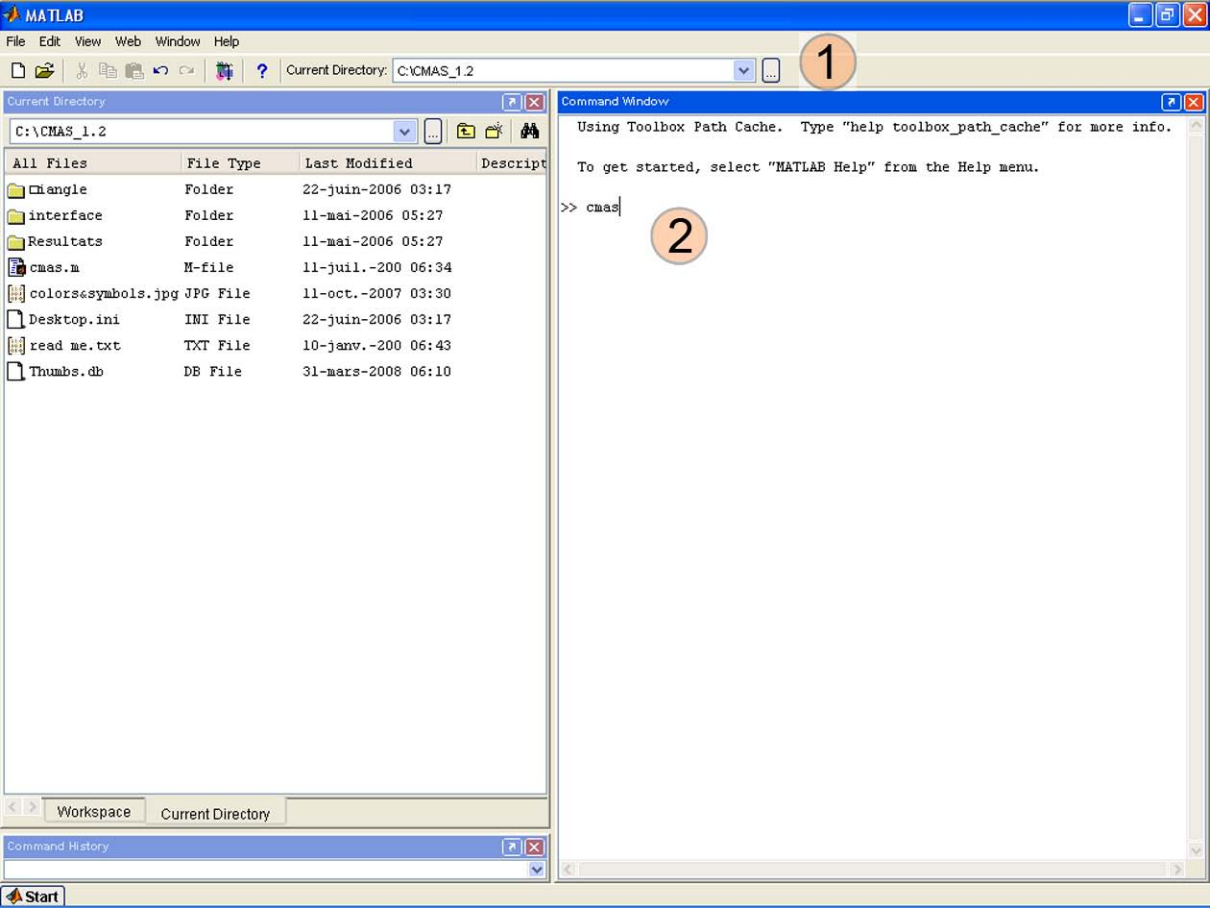

MATLAB
File Edit View Web Window Help
Current Directory: C:\CMAS_1.2
1
Current Directory
C:\CMAS_1.2
All Files File Type Last Modified Descript
Triangle Folder 22-juin-2006 03:17
interface Folder 11-mai-2006 05:27
Resultats Folder 11-mai-2006 05:27
cmas.m M-file 11-juil.-200 06:34
colors&symbols.jpg JPG File 11-oct.-2007 03:30
Desktop.ini INI File 22-juin-2006 03:17
read me.txt TXT File 10-janv.-200 06:43
Thumbs.db DB File 31-mars-2008 06:10
Workspace
Current Directory
Command History
Command Window
Using Toolbox Path Cache. Type "help toolbox_path_cache" for more info.
To get started, select "MATLAB Help" from the Help menu.
>> cmas
2
Start

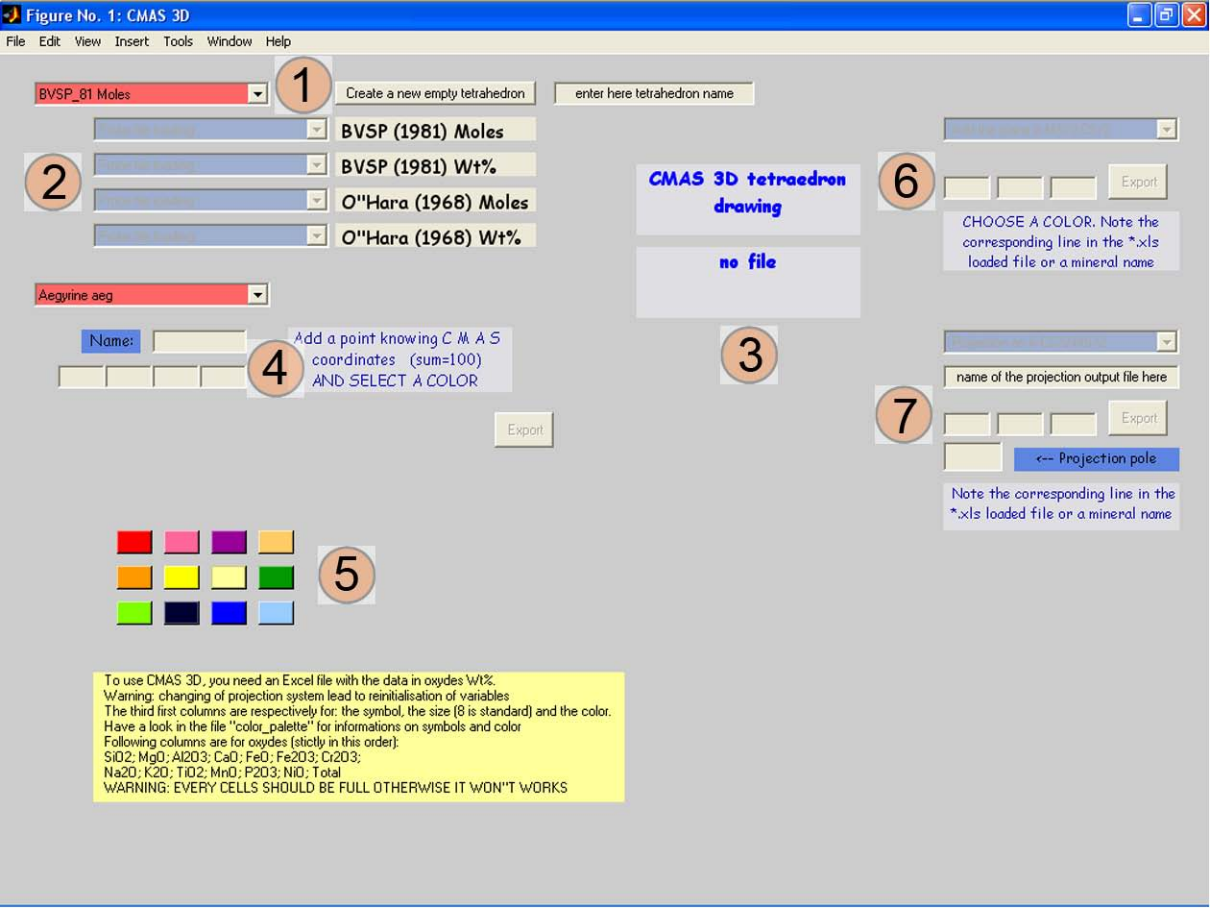
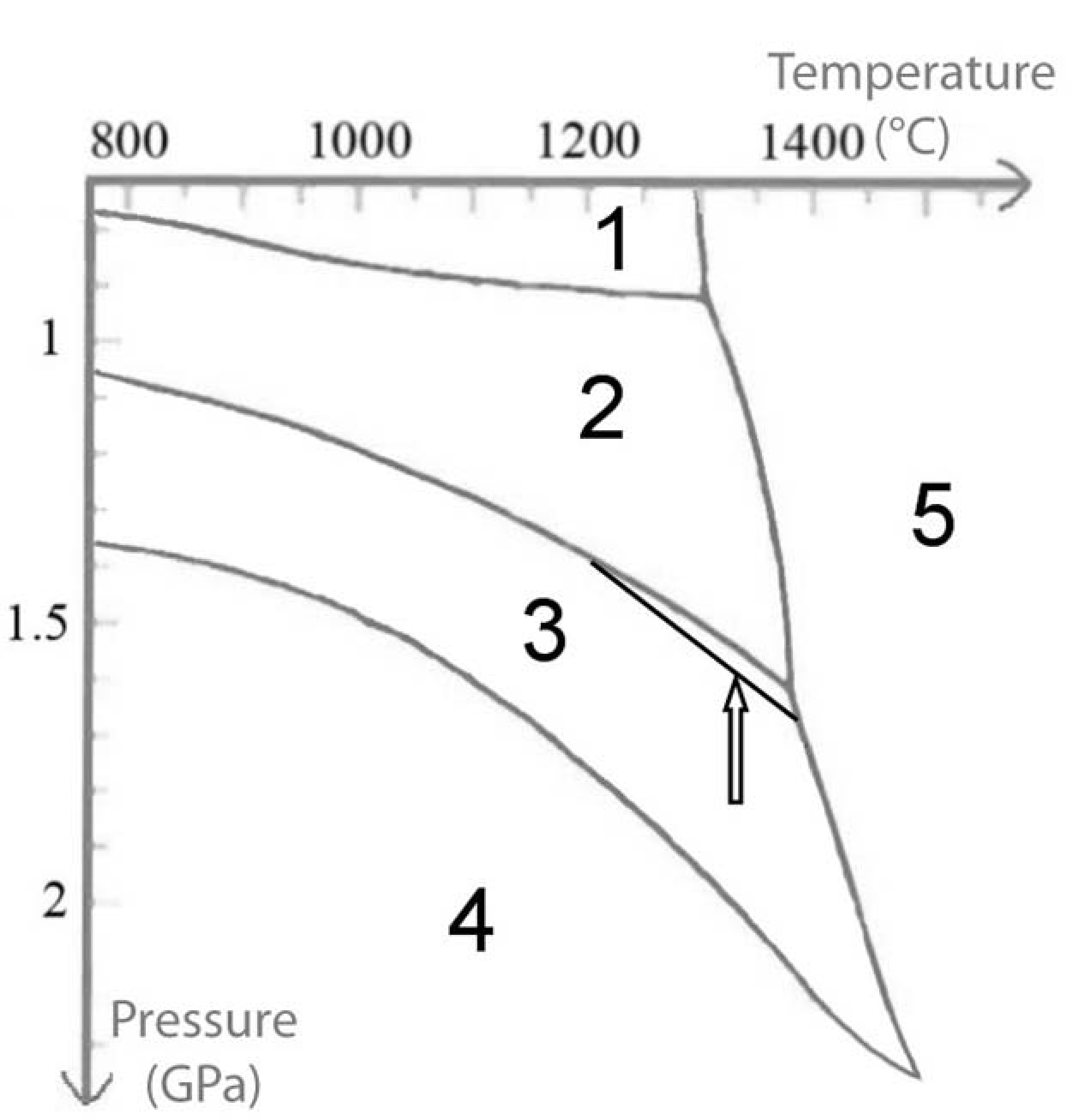


Figure No. 1: CMAS 3D
File Edit View Insert Tools Window Help
BVSP_81 Moles
1
Create a new empty tetrahedron
enter here tetrahedron name
2
BVSP (1981) Moles
BVSP (1981) Wt%
O"Hara (1968) Moles
O"Hara (1968) Wt%
CMAS 3D tetraedron drawing
no file
6
Export
CHOOSE A COLOR. Note the corresponding line in the *.xls loaded file or a mineral name
Aegyrine aeg
Name:
4
Add a point knowing C M A S coordinates (sum=100) AND SELECT A COLOR
Export
3
name of the projection output file here
7
Export
<-- Projection pole
Note the corresponding line in the *.xls loaded file or a mineral name
5
To use CMAS 3D, you need an Excel file with the data in oxydes Wt%.
Warning: changing of projection system lead to reinitialisation of variables
The third first columns are respectively for: the symbol, the size (8 is standard) and the color.
Have a look in the file "color_palette" for informations on symbols and color
Following columns are for oxydes (stictly in this order):
SiO2; MgO; Al2O3; CaO; FeO; Fe2O3; Cr2O3;
Na2O; K2O; TiO2; MnO; P2O3; NiO; Total
WARNING: EVERY CELLS SHOULD BE FULL OTHERWISE IT WON"T WORKS


Temperature
800
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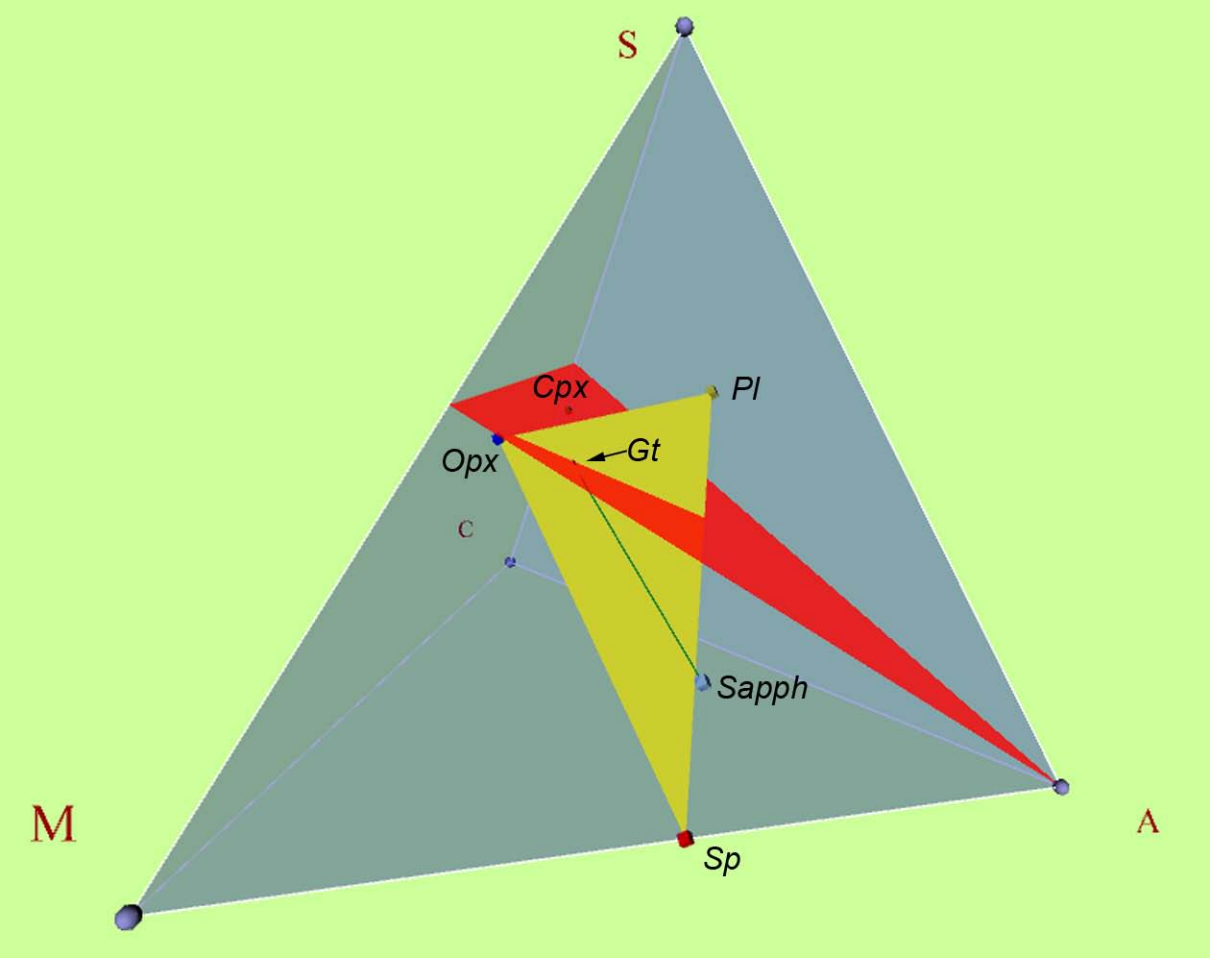
1200
1400 (°C)
1
1
1.5
2
1
2
3
4
5
Pressure
(GPa)


S
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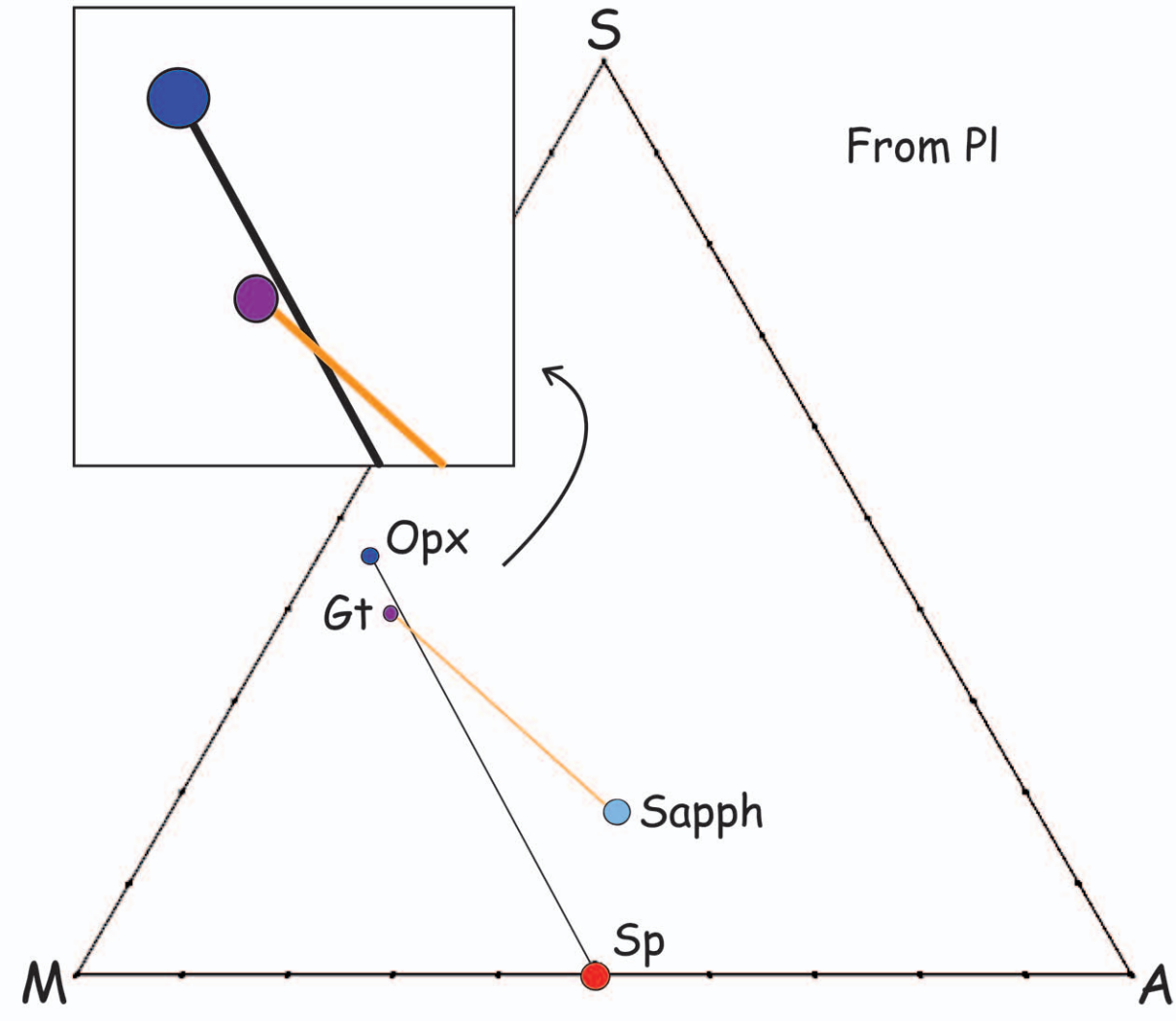
S
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Sapph
Sp
M
A

Samples	Symbol	Size	Color	SiO2	MgO	Al2O3	CaO	FeO	Fe2O3	Cr2O3	Na2O	K2O	TiO2	MnO	P2O5	NiO	Total
Cpx	*2*	*7*	*8*	50.60	13.83	10.31	21.49	2.26	0.00	0.18	1.50	0.01	0.14	0.03	0.00	0.00	100.33
Gt	*2*	*6*	*3*	42.87	20.93	24.12	6.26	6.39	0.00	0.13	0.03	0.01	0.03	0.16	0.00	0.00	100.92
Sp	*2*	*12*	*1*	0.04	23.32	66.18	0.02	7.45	0.00	1.55	0.01	0.00	0.01	0.01	0.00	0.00	98.60
Pl	*2*	*12*	*6*	49.29	0.30	31.68	13.87	0.28	0.00	0.02	2.84	0.29	0.00	0.00	0.00	0.00	98.57
Opx	*2*	*8*	*11*	50.91	30.34	11.19	1.46	6.44	0.00	0.13	0.07	0.02	0.06	0.14	0.00	0.00	100.81
Sapph	*2*	*12*	*12*	15.20	20.56	59.58	0.09	3.11	0.00	0.82	0.03	0.01	0.02	0.02	0.00	0.00	99.43

Mineral/Pole	To write
C	C, c
M	M, m
A	A, a, Crn, crn
S	S, s, Q, q, Qtz, qtz
aegerine	Aegerine, Aeg, aeg, aegerine
albite	Albite, albite, Ab, ab, Pl, pl
almandine	Almandine, almandine, alm, Alm
Alumina silicate	Andalusite, andalusite, And, and, Kyanite, kyanite, Ky, ky, Sillimanite, sillimanite, Sil, sil
anorthite	Anorthite, anorthite, An, an
Ca-Tschermack	CaTs, cats
chromite	Chromite, chromite, chr, Chr
cordierite	Cordierite, cordierite, Crd, crd
diopside	Diopside, diopside, Di, di, Cpx, cpx
enstatite	Enstatite, enstatite, Opx, opx, En, en, MS, ms, MS/2, ms/2
olivine	Olivine, olivine, Ol, ol, Forsterite, forsterite, Fo, fo, Fayalite, fayalite, Fa, fa
ferrosilite	Ferrosilite, ferrosilite, Fs, fs
grossular	Grossular, grossular, Grs, grs
heddenbergite	Heddenbergite, heddenbergite, Hd, hd
hematite	Hematite, hematite, Hem, hem
ilmenite	Ilmenite, ilmenite, Ilm, ilm
jadeite	Jadeite, jadeite, Jd, jd
magnetite	Magnetite, magnetite, Mag, mag
Mg-Tschermack	MgTs, mgts
orthoclase	Orthoclase, orthoclase, Or, or
pleonaste	Pleonaste, pleonaste, Ple, ple
pyrope	Pyrope, pyrope, Prp, prp
sapphirine	Sapphirine, sapphirine, Spr, spr
spinel	Spinel, spinel, Spl, spl
wollastonite	Wollastonite, wollastonite, Wo, wo, CS, cs, CS/2, cs/2
tremolite-actinote	Actinote, Tremolite, actinote, tremolite, act, Act, tr, Tr
anthophyllite-cummingtonite	Anthophyllite, Cummingtonite, Grunerite, anthophyllite, cummingtonite, grunerite, ath, Ath, cum, Cum, gru, Gru
gedrite	Gedrite, gedrite, Ged, ged
edenite	Edenite, edenite, Ed, ed
pargasite-hastingsite	Pargasite, Hastingsite, pargasite, hastingsite, prg, Prg, Hs, hs
tschemakite	Tschemakite, tschermakite, Ts, ts
hornblende	Hornblende, hornblende, Hbl, hbl
chlorites	Chlorite, chlorite, Clinochlore, clinochlore, Chamosite, chamosite, Chl, chl