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

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4

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## 1 **Abstract**

2

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

10

11 Key words: CMAS system, 3D, projection.

12

## 13 **1-Introduction**

14

15 Major element chemical data of rocks and minerals are of great use in the study of the origins  
16 and evolution of magmatic and metamorphic rocks. Petrologists mostly use binary plots to  
17 evaluate correlation between chemical elements or oxides, but some reduced systems have  
18 been developed to take into account more than 2 elements in the same diagram. For example  
19 some software packages such as MinPet (Richard, 1997), IgPet (Carr, 1995), NewPet (Clarke,  
20 1993), Petrograph (Petrelli, 2003) or GeoPlot (Zhou and Li, 2006) have been developed for  
21 better data visualization and interpretation. Smith and Beermann (2006) proposed to use  
22 multivector diagrams to represent up to nine components. O'Hara (1968) introduced the use  
23 of the CaO-MgO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> (CMAS) system allowing representation of 13 oxides in a four  
24 dimension representation. This pseudo-quaternary projection has been largely used as it is the  
25 simplest way to represent the major element composition of mafic and ultramafic rocks

1 (Garrido and Bodinier, 1999), as well as the main crustal and mantle minerals (Kornprobst,  
2 1970; Kornprobst and Conqu  r  , 1972) or extraterrestrial objects (Grossman and Fedkin,  
3 2003; Grossman et al., 2002; Yoneda and Grossman, 1995) and serves as a good model for  
4 dry basaltic melts (Schiano et al., 2000; Schiano et al., 2004). It is also largely used in  
5 experimental petrology (Hirschmann et al., 2003; Kogiso et al., 2003; Kogiso et al., 2004).  
6 Here we present CMAS 3D, a program written in MATLAB 6.5   . It converts oxide data to  
7 CMAS coordinates and allows visualization of these data in 3 dimensions, and projects the  
8 data onto two dimensional plots. Using CMAS 3D does not require MATLAB programming  
9 expertise. It reads data from a Microsoft Excel<sup>TM</sup> spreadsheet. The visualization uses the  
10 VRML (Virtual Reality Modeling Language) allowing the rotation of the CMAS tetrahedron  
11 in all directions in order to evaluate the different correlations and reactions. CMAS 3D also  
12 permits the addition of lines or planes between the analyzed rocks or minerals for the  
13 purposes of testing for metamorphic reactions or exsolutions, or to illustrate specific chemical  
14 trends. The proportion of the mineral phases that are involved in a reaction as reagents or as  
15 products is represented by the balanced centroid on a line (for two reagents or products), on a  
16 plane (for three reagents or products) or in a polyhedron (for more than three reagents or  
17 products). The intersection between the geometric form formed by the reagents and the one  
18 formed by the products in CMAS space is a test of the chemical feasibility of the reaction.

19

## 20 **2-Program philosophy and projection system**

21

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

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

$$3 \quad C_0 = 100(\text{CaO} - (3 + 1/3)\text{P}_2\text{O}_5 + 2\text{Na}_2\text{O} + 2\text{K}_2\text{O}) * 56.08$$

$$4 \quad M_0 = 100(\text{MgO} + \text{FeO} + \text{MnO} + \text{NiO} - \text{TiO}_2) * 40.32$$

$$5 \quad A_0 = 100(\text{Al}_2\text{O}_3 + \text{Fe}_2\text{O}_3 + \text{Cr}_2\text{O}_3 + \text{TiO}_2 + \text{Na}_2\text{O} + \text{K}_2\text{O}) * 101.96$$

$$6 \quad S_0 = 100(\text{SiO}_2 - 2\text{Na}_2\text{O} - 2\text{K}_2\text{O}) * 60.085$$

7 and:

$$8 \quad \text{Sum} = C_0 + M_0 + A_0 + S_0$$

9 with:

$$10 \quad C = C_0 / \text{Sum}$$

$$11 \quad M = M_0 / \text{Sum}$$

$$12 \quad A = A_0 / \text{Sum}$$

$$13 \quad S = S_0 / \text{Sum}$$

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

15 tetrahedron.

16 Four different types of representations are possible with CMAS 3D: (i) the projection in  
17 moles presented above from O'Hara (1968), (ii) the same projection but in weight percent,  
18 (iii) a modified version proposed in the Basaltic Volcanism Study Project (1981) (hereafter  
19 BVSP\_81) in moles and (iv) the same modified version in weight percent.

20 To use CMAS 3D, data should be compiled in a Microsoft Excel<sup>TM</sup> spreadsheet (\*.xls) that  
21 should have the format depicted in the table 1 (this file is called hereafter data.xls). A first  
22 column contains the sample name (only one word), the 3 following ones contain the symbol  
23 (1 for a sphere and 2 for a cube), the size (8 for a medium size) and the color (between 1 and  
24 12, see the file "C:\CMAS\_1.2\colors&symbols.jpg") selected for the representation. The next  
25 columns contain the oxides organized in 13 columns in the same order as presented in the

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

3

### 4 **3-Starting the program**

5

6 On a PC the folder “CMAS\_1.2” should be copied on the “C:\” directory, no installation is  
7 necessary. A version of Matlab 6.5 ® or younger is required to use CMAS 3D. When  
8 MATLAB is open “C:\CMAS\_1.2” should be written in the “Current Directory” (No.1, Fig. 1)  
9 and then the program is loaded by writing “cmas” in the “Command Window” (No.2, Fig. 1).  
10 Once the interface of CMAS 3D is open (Fig. 2), it is ready to be used, as described in the  
11 next section.

12

### 13 **4-Functionalities**

#### 14 **4.1-CMAS tetrahedron**

15

16 First of all empty CMAS tetrahedrons could be generated by selecting a file name and  
17 pressing the associated button (No.1, Fig. 2), files are stored in the folder  
18 “CMAS\_1.2\Resultats”. Before loading the data file (data.xls), a projection system  
19 (O’Hara\_moles; O’Hara\_wt%; BVSP\_81\_moles or BVSP\_81\_wt%) must be chosen from the  
20 interface illustrated in Figure 2 (No.1). Then the option “Probe file loading” is selected (No.2,  
21 Fig. 2). This opens a new window that allows the data file (e.g. data.xls) to be chosen; a final  
22 window is then opened and an output-file has to be chosen. When the data.xls type file is  
23 loaded, the size of the file is written in the central frame (No.3, Fig. 2). Two different  
24 numbers are present: the first one is the number of samples and the second one, the number of

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

3            cmas= C<sub>1</sub>    M<sub>1</sub>    A<sub>1</sub>    S<sub>1</sub>  
4                    C<sub>2</sub>    M<sub>2</sub>    A<sub>2</sub>    S<sub>2</sub>  
5                    ...    ...    ...    ...  
6                    C<sub>n-1</sub>    M<sub>n-1</sub>    A<sub>n-1</sub>    S<sub>n-1</sub>  
7                    C<sub>n</sub>    M<sub>n</sub>    A<sub>n</sub>    S<sub>n</sub>

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

10

## 11 **4.2-Adding Points or Minerals**

12

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

21

## 22 **4.3-Adding Lines and Planes**

23

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

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

12

#### 13 **4.4-Projections**

14

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

22 To make projections, the line “Projections” should be selected (No.2, Fig. 2). Then  
23 there are two choices in the menu (No.7, Fig. 2): making a projection on a predefined plane  
24 (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  
25 plane. In the first case, the line of the chosen plane should be selected (No.7, Fig. 2) whereas,



1 for the second case, the 3 boxes should be completed with either the number of the line of a  
2 sample (from the data.xls type file, Table 1) or with the abbreviation of a mineral (Table 2).  
3 The “projection pole” definition should be completed in the same way. An output filename  
4 should be written in the box “name of the projection output file here”. The projection will be  
5 activated by pressing the “export” button. The coordinates of the projected samples are  
6 written in the “Command Window” (No.2, Fig. 1). The fourth column indicates the quality of  
7 the projection. The bigger the number is, the closer from the projection pole is the projected  
8 point, and the poorer the quality of the projection. A negative value indicates that the pole is  
9 between the plane and the projected point. Projection results are stored in the folder  
10 “CMAS\_1.2\triangle”  
11

## 12 **5-Visualization of results**

13

14 The visualization of results should be made with a VRML reader (to read the \*.wrl)  
15 because the visualization in MATLAB is not so convenient. The files in  
16 C:\CMAS\_1.2\Results and C:\CMAS\_1.2\triangle should be opened with this type of reader.  
17 Some free VRML readers are available on the web; we propose to use “Flux Player” freely  
18 downloadable at <http://www.mediamachines.com> (also provided with the supplementary  
19 material). The mouse commands to move the tetrahedron are: left button: rotation, right  
20 button: displacement, rolling button: zoom.

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

25

## 1 **6-Example**

2

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

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

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

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

8

## 9 **7-Conclusion**

10

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

18

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20

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22 Alexei Fedkin and James Kelly Russell. We are also grateful to Eric Grunsky, Editor-in-Chief  
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24

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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	Description
triangle	Folder	22-juin-2006 03:17	
interface	Folder	11-mai-2006 05:27	
Resultats	Folder	11-mai-2006 05:27	
cmass.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 Window

Using Toolbox Path Cache. Type "help toolbox\_path\_cache" for more info.

To get started, select "MATLAB Help" from the Help menu.

```
>> cmass
```

2

Command History

Start

BVSP\_81 Moles

1

Create a new empty tetrahedron

enter here tetrahedron name

BVSP (1981) Moles

BVSP (1981) Moles

BVSP (1981) Wt%

BVSP (1981) Wt%

O'Hara (1968) Moles

O'Hara (1968) Moles

O'Hara (1968) Wt%

O'Hara (1968) Wt%

Aegytine aeg

Name:

4 Add a point knowing C M A S coordinates (sum=100) AND SELECT A COLOR

Export



5

CMAS 3D tetrahedron drawing

no file

3

6

Export

CHOOSE A COLOR. Note the corresponding line in the \*.xls loaded file or a mineral name

name of the projection output file here

7

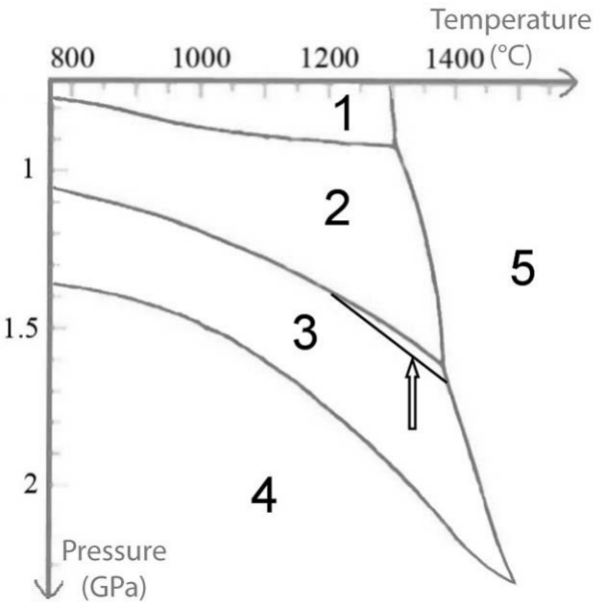
Export

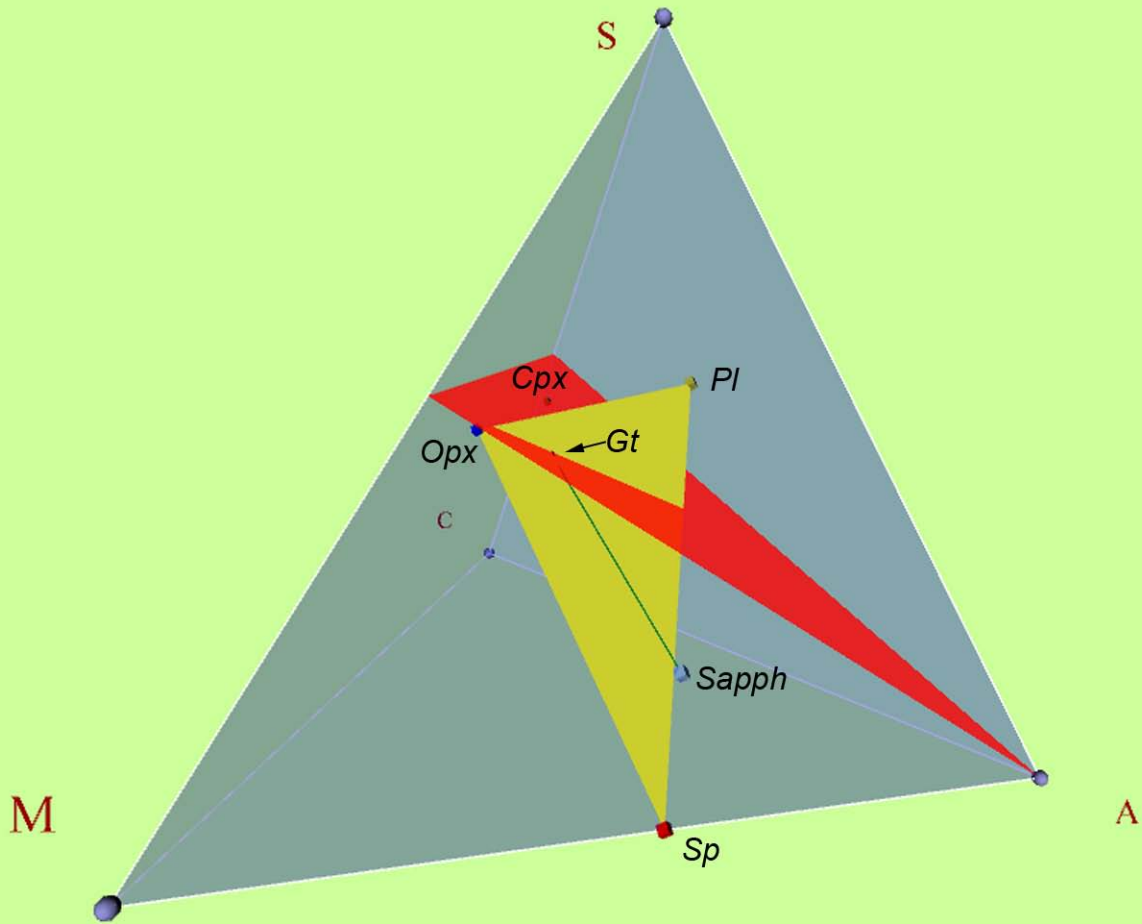
Projection pole

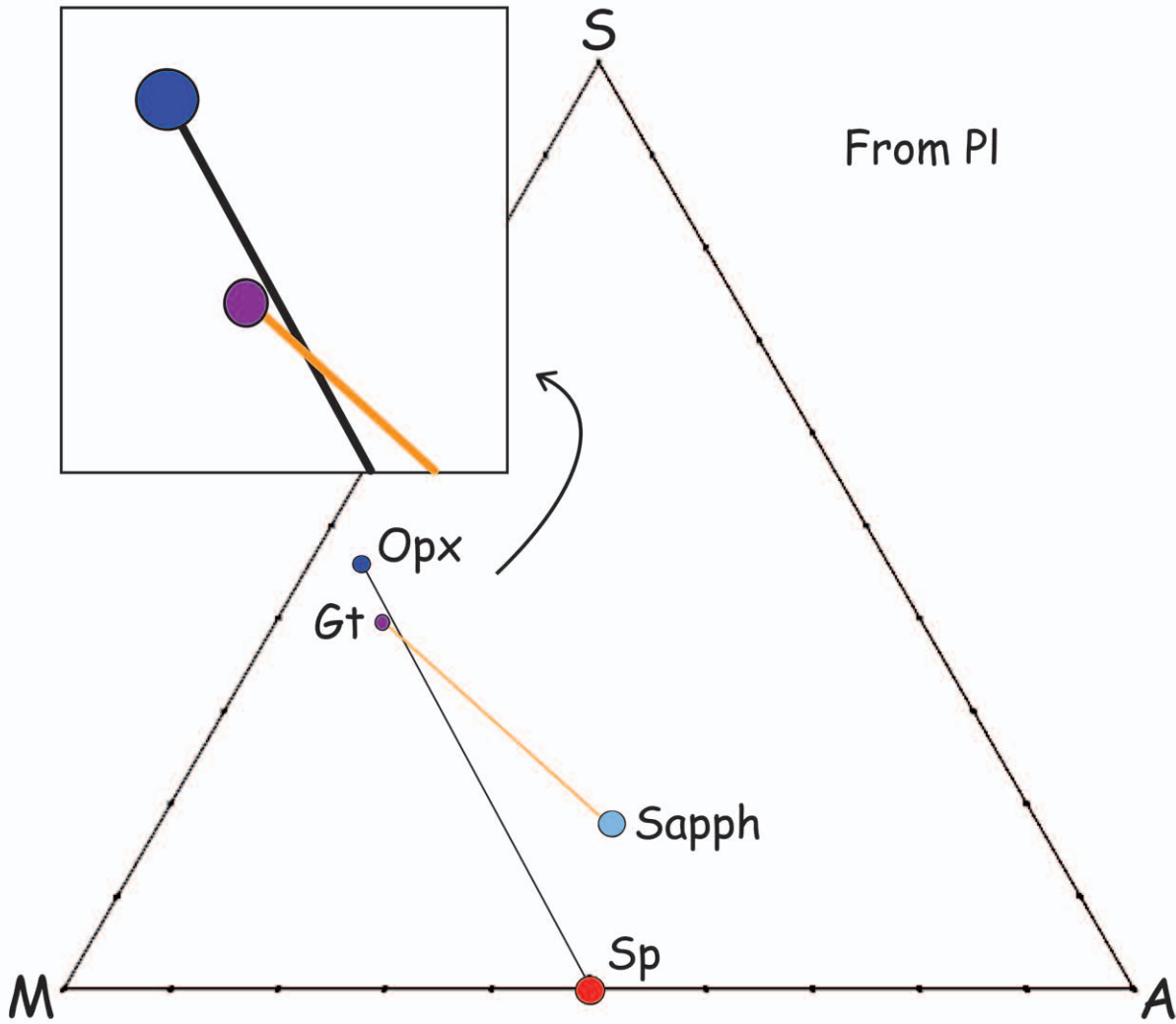
Note the corresponding line in the \*.xls loaded file or a mineral name

To use CMAS 3D, you need an Excel file with the data in oxides 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 oxides (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 WDN'T WORKS









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

<b>Mineral/Pole</b>	<b>To write</b>
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-Tschemmack	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-Tschemmack	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, tschemakite, Ts, ts
hornblende	Hornblende, hornblende, Hbl, hbl
chlorites	Chlorite, chlorite, Clinochlore, clinochlore, Chamosite, chamosite, Chl, chl