MagMin_PT: An Excel-based mineral classification and geothermobarometry program for magmatic rocks

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ABSTRACT

Igneous rock forming minerals carry valuable information from the deep earth that is not directly accessible to the surface. Each phase represents physico-chemical conditions under which various magmatic processes occur at a wide range of depths from upper mantle to shallow crustal levels. These processes are cryptically inscribed in the whole-rock and mineral chemistry (e.g. major elements, trace elements, isotopic ratios) and the mineral textures (equilibrium vs. disequilibrium features), and intensive variables (e.g. pressure, P; temperature, T) as well. Therefore, special attention should be given to igneous minerals to better understand processes operated in their journey from source through magma chamber and conduit system to the earth surface.

MagMin_PT is an Excel© based user-friendly program, designed to calculate mineral formulae and end-members, and to estimate pressure and temperature (e.g. geothermobarometry) from electron microprobe (EPMA) data, from magmatic rocks. The program operates the most common igneous rock-forming minerals (e.g. olivine, pyroxene, amphibole, biotite, feldspar, magnetite, ilmenite, apatite and zircon), resulting in various classification diagrams and P-T plots. Whole-rock or glass composition needs to be entered together with EPMA data into the program to check equilibration status in most P-T calculation models. Fe^{2+} and Fe^{3+} estimation is routinely performed in MagMin_PT based on the stoichiometric constrains, and machine learning method to some extent for different iron-bearing minerals. MagMin_PT is also able to carry out further calculations including fugacity, magmatic water content and saturation-temperature which are useful for igneous petrology studies. Graphical and numerical output produced by the program can be easily copied to further process in another media.

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1. Introduction

Only a very small number of the thousands of known minerals in nature make up most magmatic rocks. Olivine, pyroxene, amphibole, mica, feldspar, feldspathoid, Fe-Ti oxides (mostly magnetite and ilmenite), and quartz are the major constituents in most magmatic rocks, all of which are solid solutions, except the last one. It is a simple first task to identify these minerals in hand sample with the aid of a hand lens in the field and in thin section under a polarizing microscope in the laboratory. XRD (e.g. X-ray diffraction) analysis and SEM (e.g. scanning Electron microscope) studies are the other alternatives for mineral identification, but the electron microprobe is the ultimate tool (e.g. Best, 2003). Electron microprobe analyzer (EPMA) is one of the most widely used instruments for chemical analysis of minerals, and its results are commonly reported in weight percentages of the oxides of the measured elements. This means that researchers need to calculate cationic formula and end-members of each analyzed mineral after taking a large number of data from the instrument. Such calculations can be easily performed by the published mineral formula calculation programs that are mainly free Excel-based applications. Most of these programs are actually mineral-specific formula calculator with or without thermobarometry tools such as amphibole (Yavuz, 1996, 2007; Locock, 2014; Li *et al.*, 2020a), mica (Yavuz and Öztaş, 1997; Yavuz, 2001; Li *et al.*, 2020b), pyroxene (Yavuz, 2013), garnet (Yavuz and Yıldırım, 2020), tourmaline (Yavuz, 1997), magnetite-ilmenite (Lepage, 2003; Hora *et al.*, 2013; Yavuz, 2021). A few general mineral formulae calculation programs are also included in the literature (e.g. Afifi and Essene, 1988; Rock and Caroll, 1990; Griffin *et al.*, 1991; De Bjerg *et al.*, 1992, 1995; Brandelik, 2009 etc.). In addition to the published ones, there are a lot of unpublished mineral formula calculators that can be easily downloaded from web-pages or obtained from their developers with e-mail correspondence. Structural formula and end-members calculations from mineral-chemical analysis are actually routine intermediate task for classification purposes before further petrologic calculations (e.g. geothermobarometry, fugacity, magmatic water content, phase equilibria etc.). Regarding the geothermobarometry, the mentioned programs either don't include any computation or include only for a specific mineral, which means they are not comprehensive thermobarometry tools.

MagMin_PT is mainly designed as a comprehensive geothermobarometry tool of igneous systems (Fig. 1) to fill the gap mentioned above, but it can also be used as a classical mineral classification calculator. Therefore, MagMin_PT includes various classification diagrams and P-T plots for the most common igneous rock-forming minerals (e.g.

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olivine, pyroxene, amphibole, biotite, feldspar, magnetite, ilmenite, apatite and zircon) with the latest approval by the International Mineralogical Association (IMA) and the latest improvements in igneous petrology.

2. Principles of Mineral Formula Calculation

The recasting of chemical analysis into a mineral formula is series of mathematical functions based on the chemical features of atoms such as atomic weight, charge of cation, etc. (see for details; Brandelik, 2009). This depends on the structure of minerals such as relationship between charge neutrality and crystal chemistry (e.g. 4 oxygens for olivines, 6 oxygens for pyroxenes etc.). Based on the scheme by Deer *et al.* (1992), the main steps for mineral formula calculation are following with an example of olivine recalculation (Table 1);

1) "Column 1:" The composition of the olivine as weight percentages of the oxides (wt.%), derived from EPMA.
2) "Column 2:" Molecular proportions of the oxides, derived by dividing each column (1) entry by the molecular weight (Wieser and Berglund, 2009) of the oxide concerned.
3) "Column 3:" Atomic proportion of oxygen from each molecule, derived from column (2) by multiplying by the number of oxygen atoms in the oxide concerned. At the foot of column (3) is its total (T).
4) "Column 4:" No. of anions on the basis of 4 oxygens (e.g. olivine formula based on 4 oxygen atoms), done by multiplying all of the oxides by 4/T.
5) "Column 5:" No. of ions in formula, the number of cations associated with the oxygens in column (4). Thus, for SiO_2 and TiO_2 the column (4) entry is divided by 2, for Al_2O_3 the column (4) entry is multiplied by 2/3. For divalent ions (FeO, MgO, MnO, NiO, CaO) the column (5) value is the same that of column (4). If there are monovalent ions (e.g. K_2O, Na_2O) in the analysis, they are doubled in column (5), which is not case in the olivine formula here.

Above procedure can be simply used for anhydrous minerals (e.g. olivine, pyroxene, feldspar etc.) whose cation-sites are full and total weight percentage of major oxides by electron microprobe are about 100%. However, hydrous minerals such as amphibole and biotite have more complex mineral chemistry that cannot be fully determined by routine instrumental techniques. The main issue is that electron microprobe cannot directly detect volatile contents of hydrous minerals, resulting in lower total weight percentage of major oxides. Another issue arisen from electron microprobe is that this technique does not differentiate among the valence states of iron (Fe^{2+}, Fe^{3+}), requiring

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additional computation. Such a computation can be simply made for anhydrous minerals based on the assumption of their full-cation sites and perfect charge balance, but this is not always straightforward for hydrous minerals. Therefore, many classification schemes and methods have been proposed for hydrous minerals over time, depending on the development of analytical techniques and computer sciences. In MagMin_PT, the users can find various mineral formula calculation methods based on traditional computations, and to some extent machine learning methods which have become recently popular in geothermobarometry (Li *et al.*, 2020a; Li *et al.*, 2020b; Petrelli *et al.*, 2020; Higgins *et al.*, 2022).

3. Tests for liquid equilibria in P-T calculations

The applicable of any geothermobarometry is inevitably related to chemical equilibrium between phases (e.g. liquid-mineral or mineral-mineral). In MagMin_PT, various P-T calculations are based on the application of mineral-liquid thermobarometry, requiring tests for equilibrium before calculations. The users can test equilibrium between mineral-liquid pairs in different ways: (1) petrographic observations, (2) calculation of mineral-liquid partition coefficients, and (3) comparing predicted and calculated mineral components (see Putirka, 2008 for details).

Textural features observed in a polarized light microscopy or more advanced imaging methods (e.g. backscattered electron-BSE- or cathodoluminescence-CL- imaging) can be firstly utilized to test equilibrium between the selected mineral-liquid pairs. The predominant euhedral shape of minerals is mostly considered to be evidence of equilibrium with the liquid in which they occur. In the opposite way, disequilibrium textures in minerals suggest that equilibrium condition is not met. Such textural features are various, especially in volcanic rocks: e.g. crystal zoning, resorption and dissolution surfaces, reaction rims or pseudomorphs, overgrowths on existing minerals, crystal clots etc (Ginibre *et al.*, 2007; Streck, 2008). Therefore, these textures are the best indicator that minerals were out of equilibrium and they reacted with the enclosing liquid.

Mineral-liquid thermobarometers are imported from Putirka's equations and are based mostly on iterative equations. Calculation of mineral-liquid partition coefficients is another test for equilibrium that can be automatically made in MagMin_PT. Composition of a glass or the whole-rock, or some calculated composition can be used as a liquid. The partitioning of Fe-Mg between mineral-liquid pairs (e.g. the Fe-Mg exchange coefficient) is used for mafic minerals (olivine, orthopyroxene, clinopyroxene and amphibole) in MagMin_PT based on the following general equations,

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originally suggested for olivine by Roeder and Emslie (1970). The acceptable partition coefficient (K_D) range for each mineral to be equilibrium with the liquid will be given in the following section.

$$MgO^{min} + FeO^{liq} = MgO^{liq} + FeO^{min} \quad (1)$$

$$K_D(\text{Fe-Mg})^{min\text{-}liq} = \frac{X_{Fe}^{min} X_{Mg}^{liq}}{X_{Mg}^{min} X_{Fe}^{liq}} \quad (2)$$

Comparing predicted and calculated mineral components is a test for equilibrium. The test is to compare predicted and observed values for the clinopyroxene components, producing a bivariate plot. This is based on the idea that predicted and observed values are so close each other under equilibrium conditions. This method is only applicable to clinopyroxene in MagMin_PT.

4. Description of program

MagMin_PT is a Microsoft® Excel© workbook that is specifically designed for the needs and demands of researchers working on mineral chemistry and geothermobarometry of magmatic rocks. It has been divided into eleven Excel sheets: "Instruction", "Data Input", "Olivine", "Pyroxene", "Amphibole", "Biotite", "Feldspar", "Magnetite-Ilmenite", "Apatite", "Zircon", and "Conversions". These sheets are summarized in the following based on their main role in the program.

If users encounter an Excel-Circular Reference problem, they need to go to File > Options > Formulas, and select the "Enable iterative calculation" check box in the Calculation options section. After clicking on the check boxes in the "Data Input" spreadsheet, the output of formula proportions in atoms per formula unit (apfu) and thermobarometry results can take a few seconds due to iterative equations.

4.1. Data Input

"Data Input" is to enter user data (i.e. major oxides-wt.% of mineral and glass/whole-rock) and data set should be entered into the columns and rows within this spreadsheet. First of all, the check boxes on the "Data Input" spreadsheet must be clicked in order of data entry: 1) Input dataset from lefts panels, 2) Select mineral, and 3)

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Calculation for cation formula and P-T results (Fig. 2). In this sheet, users should also enter their "glass" or "whole-rock compositions" if they want to make P-T calculations based on the mineral-liquid geothermobarometry.

4.2. Olivine

Olivine is a ferromagnesian mineral represented by two end-members of forsterite (Mg_2SiO_4) and fayalite (Fe_2SiO_4). Olivine compositions are recalculated on the basis of four oxygens and often shown as molar percentages of forsterite (Fo) and fayalite (Fa) in the literature and MagMin_PT.

MagMin_PT calculates T(°C) from EPMA data based on the liquid thermometers (Helz and Thornber, 1987; Beattie, 1993; Sisson and Grove, 1993; Putirka *et al.*, 2007; Putirka, 2008). For the olivine-liquid thermometer, the composition of "whole rock" or "glass" needs to be entered in "Data Input" sheet. Then, the program calculates the Fe-Mg exchange coefficient *or* $K_D(\text{Fe-Mg})^{ol\text{-}liq}$ based on the equations 1 and 2 to test for equilibrium between olivine and liquid. If the entered liquid is under equilibrium with the olivine composition, this value is expected to be in the range of K_D= 0.30±0.03 (Roeder and Emslie, 1970; Toplis, 2005), which means that the thermometer can be applicable to the volcanic system.

4.3. Pyroxene

This sheet designed for pyroxenes whose general chemical formula is M2M1T2O6. They are classified according to the occupancy of the M2 site, but Morimoto *et al.* (1988) assumed the M1 and M2 sites as a single M site because T, M1, and M2 sites are a function of temperature in pyroxenes (Yavuz, 2013). In MagMin_PT, a pyroxene formula is recalculated on the basis of six oxygens according to the scheme of allocation of cations by Morimoto *et al.* (1988) and the estimating Fe^{3+} is made based on the following equation given by Droop (1987).

$$F = 2X(1 - T/S) \quad (3)$$

where T is the ideal number of cations per formula unit, and S is the observed cation total per X oxygens calculated assuming all iron to be Fe^{2+}.

In Data Input sheet, three different options exist for pyroxene data entry in MagMin_PT. The first option is two pyroxene data under the heading "Minerals" in the left panel of "Data Input" sheet, whose results appear in "Pyroxene" sheet. In this sheet, many classification diagrams (Morimoto and Kitamura, 1983; Morimoto *et al.*,

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1988) and several two pyroxene geothermobarometers (Wood and Banno, 1973; Wells, 1977; Lindsley and Andersen, 1983; Brey and Köhler, 1990; Putirka, 2008) are produced (Fig. 3). Another option for data input is independently to enter chemistry of ortho- and clinopyroxene to make mainly P-T calculations, especially based on the mineral-liquid geothermobarometry which requires calculations of the Fe-Mg exchange coefficient for orthopyroxene (K_D(Fe-Mg)$^{opx\text{-}liq}$) and clinopyroxene (K_D(Fe-Mg)$^{cpx\text{-}liq}$) to test for equilibrium between mineral-liquid pairs according to the equation 2. K_D values are expected to be in the range of 0.29±0.06 for opx and 0.27±0.03 for cpx to meet equilibrium conditions. The equilibrium tests are also graphically portrayed in "Rhodes Diagram" (Rhodes *et al.*, 1979) in the pyroxene sheet, resulting in a binary plot of 100×Mg# Liquid vs. 100×Mg# orthopyroxene or clinopyroxene. On such a plot, the equilibrated mineral-liquid pairs lie along between two dashed lines marking error bounds.

MagMin_PT also includes an equilibrium test for cpx in "pyroxene" sheet, which is a comparison between predicted and observed values for the clinopyroxene components on a binary plot. Under equilibrium conditions, the predicted and observed values plot on or close to the one-to-one regression line.

4.4. Amphibole

Amphiboles are one of the most complex rock-forming double-chain inosilicates with a wide range of chemical compositions, and represented by a general formula of $AB_2C_5T_8O_{22}W_2$. Amphibole classification has not been satisfactory since Leake (1968) presented the first classification for calcic amphiboles. Therefore, new discoveries in amphibole compositions led to many classification attempts in parallel with ongoing development in analytical techniques in the intervening years (e.g. IMA 1978 of Leake, 1978; IMA 1997 of Leake et al 1997; IMA 2004 of Leake et al 2004; IMA 2012 of Hawthorne et al 2012). These attempts have also been accompanied by the addition of new computer programs and spreadsheets to overcome classification problems resulted from the compositional complexity of amphiboles (e.g. Currie, 1997; Yavuz, 1999; Mogessie *et al.*, 2001; Esawi, 2004; Yavuz, 2007; Locock, 2014).

MagMin_PT easily converts the entered amphibole microprobe analysis in "Data Input" to formula proportions in atoms per formula unit (apfu) in "Amphibole" sheet according to the last IMA 2012 recommendations, which results in eight different binary classification diagrams (Fig. 4). MagMin_PT includes an alternative formula calculation scheme based on the machine learning method for Li-free and Li-bearing amphiboles by Li *et al.* (2020a). The users

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can compare their formula calculations between this new approach and IMA 2012. The Fe^{3+}/Fe^{2+} ratio cannot be routinely determined by electron microprobe technique. Fe^{3+} is empirically estimated based on the electroneutrality and stoichiometry rule in MagMin_PT. User can find the detail of Fe^{3+} calculation for IMA 2012 classification in Appendix III of Hawthorne *et al.* (2012).

MagMin_PT includes mineral-mineral (e.g. amphibole-plagioclase), mineral-liquid (e.g.amphibole-liquid) and single-phase amphibole (e.g. Al-in-hornblende) geothermobarometers proposed by different authors in "Amphibole" sheet. Al-in-hornblende calibrations are one of the most-used barometers based on the EPMA-derived data. The users can find several Al-in-hornblende barometers (Hammerstrom and Zen, 1986; Hollister *et al.*, 1987; Johnson and Rutherford, 1989; Blundy and Holland, 1990; Schmidt, 1992; Anderson and Smith, 1995) in the program. However, these barometers should be used with caution because they work under restricted conditions, and so are not generally applicable to igneous systems (Erdmann *et al.*, 2014; Putirka, 2016). Amphibole-plagioclase (Blundy and Holland, 1990; Holland and Blundy, 1994; Molina *et al.*, 2015; Molina *et al.*, 2021) and amphibole-liquid (Molina *et al.*, 2015; Putirka, 2016) geothermobarometers require plagioclase and glass or whole-rock compositions to be entered into the program. The Fe-Mg exchange coefficient ($K_D(\text{Fe-Mg})^{amp\text{-}liq}$) is expected to be in the range of 0.28±0.11 for the amphibole- liquid thermobarometer.

The program also presents oxygen buffers constraining oxygen fugacity (fO_2) as a function of temperature (Fegley, 2012), and water content (%) of melt (Ridolfi *et al.*, 2010; Ridolfi, 2021) calculated from amphibole chemistry.

4.5. Biotite

Biotites are trioctahedral micas characterized by end-members of $KFe_3AlSi_3O_{10}(OH)_2$ (annite), $KMg_3AlSi_3O_{10}(OH)_2$ (phlogopite), $KFe_2AlAl_2Si_2O_{10}(OH)_2$ (siderophyllite) and $KMg_2AlAl_2Si_2O_{10}(OH)_2$ (eastonite) (Rieder *et al.*, 1999). In MagMin_PT, the biotite formula is calculated on the basis of 11, 22 or 24 oxygens depending on user's data (e.g. available of H_2O analysis) and oxidation state of biotite etc. Therefore, this can be traditionally done as suggested by Rieder *et al.* (1999), and Fe^{3+} can be calculated based on the equations given by Dymek (1983) in the program, which may result in large errors in the estimations of $Fe^{3+}/\Sigma Fe$. The concentration of Li_2O in biotites, if essential but not known, can be estimated using the empirical equations (Tindle and Webb, 1990; Tischendorf *et al.*, 1997; Tischendorf *et al.*, 1999). Alternatively, the program includes a new scheme for the biotite formula calculation and Fe^{3+} estimation based on the machine learning method by Li *et al.* (2020b). The program includes basic

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classification diagrams for biotites, and for micas to some extent. MagMin_PT have also options for P-T (Luhr *et al.*, 1984; Uchida *et al.*, 2007) calculations and oxygen buffers (Wones and Eugster, 1965; Wones, 1989). P-T calculations for biotites do not require whole-rock or glass analysis data because these are not liquid-based thermo-barometers.

4.6. Feldspars

Feldspars are classified according to the end members of the $NaAlSi_3O_8$ (albite, Ab)-$CaAl_2Si_2O_8$ (anorthite, An)-$KAlSi_3O_8$ (orthoclase, Or) (after Deer *et al.*, 1992). Compositions between Ab and An are referred as plagioclases and those between Ab and Or as alkali feldspars (Fig. 5).

In MagMin_PT, feldspar formula is recalculated on the basis of 8, 16 or 32 oxygens in terms of user's choice, and then Ab-An-Or components come out and plotted in the feldspar ternary diagram. The program includes several thermobarometers (e.g. plagioclase-liquid, alkali feldspar-liquid, two feldspar etc). For mineral-liquid thermobarometers, users should enter their whole-rock or glass composition into "Data Input" sheet, and then test for equilibrium between pairs on the basis of Ab-An exchange coefficient (K_D) based on the equation 4. The plagioclase-liquid equilibrium can also be used for a hygrometer, if temperature is well-known (Putirka, 2005, 2008). Therefore, the program calculates H_2O (wt.%) content of the liquid based on the aforementioned hygrometer. MagMin_PT includes another water content (H_2O wt.%) calculation procedure based on the Al_2O_3 content of the melt as a hygrometer (P<4 kbar) (Pichavant and Macdonald, 2007), so that users can compare H_2O results from two different calculations.

$$K_D(\text{An-Ab})^{pl\text{-}liq} = \frac{X_{Ab}^{pl} X_{AlO_{1.5}}^{liq} X_{CaO}^{liq}}{X_{An}^{pl} X_{NaO_{0.5}}^{liq} X_{SiO_2}^{liq}} \quad (4)$$

4.7. Magnetite-Ilmenite

Ilmenite and magnetite are chiefly termed as Fe-Ti oxides with the idealized formula of $FeTiO_3$ and Fe_3O_4 respectively. Two major solid-solution series occur as "ulvöspinel-magnetite" and "ilmenite-hematite" solid solutions in the FeO-Fe_2O_3-TiO_2 system. The compositions of coexisting ilmenite and magnetite have been widely used as thermobarometer because their compositions are strongly dependent on fO_2 (oxygen fugacity) and T at which they equilibrated.

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In natural magmatic systems, there are several buffer reactions that magnetite involved in to characterize the oxidation state of magmas such as the hematite-magnetite (HM), the quartz-fayalite-magnetite (QFM), and the magnetite-wüstite (MW). The Nickel-Nickel Oxide (NNO) buffer reaction does not occur in natural magmas but is commonly used for reference. Log oxygen fugacity, an index of the redox state in a magma for each buffer assemblage was compiled by Frost (1991) and calculated from;

$$\log f\mathrm{O}_2 = \frac{\mathrm{A}}{\mathrm{T}} + \mathrm{B} + \frac{\mathrm{C}(\mathrm{P}-1)}{\mathrm{T}} \quad (5)$$

where T is temperature in Kelvin (K), P is pressure (bar), and A, B, and C are buffers from equilibrium expression of Frost (1991).

Magnetite and ilmenite formulae are calculated on the basis of 4 and 3 oxygens, respectively in MagMin_PT. The calculation results are shown on ternary diagrams (e.g. FeO-Fe_2O_3-TiO_2 or R^{2+}-R^{3+}-Ti^{4+}). Fe^{3+} separation is according to the equation of Droop (1987) in MagMin_PT. The program calculates T(°C) and fO_2 values calibrated by different researchers (Powell and Powell, 1977; Spencer and Lindsley, 1981; Andersen and Lindsley, 1985; Sauerzapf *et al.*, 2008), and their results are plotted on a binary diagram with several buffer curves (e.g. MW, QFM, NNO and HM). Users can adjust the buffer curves of the HM and QFM as "low T", "medium T" or "high T" according to their systems. The program presents another binary diagram of T(°C) vs. ΔNNO, which is the relative oxygen fugacity at given T for NNO.

A revised Fe-Ti oxide geothermometer and oxygen-barometer was also given by (Ghiorso and Evans, 2008). It is based on a thermodynamic model which produces different results than older calibrations, most notably in the estimation of oxidation state under relatively oxidized conditions (>NNO+1). This thermobarometry is not included in MagMin_PT, but users can find an icon in "Magnetite-Ilmenite" sheet redirecting them to a web-based application designed by these authors for the T(°C) and NNO calculations.

4.8. Apatite

Apatite-$Ca_5(PO_4)_3(F,Cl,OH)$ is a member of the group of phosphate minerals, and it is very common as an accessory phase in igneous rocks. MagMin_PT includes apatite formula (e.g. 25 or 26 oxygens) and saturation temperature

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calculations. Apatite saturation temperature (Piccoli *et al.*, 1999; Piccoli and Candela, 2002) is calculated from whole-rock geochemical data that must be entered into "Data Input" sheet of the program.

4.9. Zircon

Zircon is an accessory mineral belonging to orthosilicates with the chemical formula of $ZrSiO_4$. It is commonly found early-formed small crystals enclosed in later minerals in magmatic rocks. When enclosed especially in biotite or amphibole, pleochroic haloes may be formed around zircon because of its content of radioactive elements (e.g. U and Th), which can be seen under polarizing microscope (Deer *et al.*, 1992).

MagMin_PT calculates zircon formulae on the basis of 4 oxygens. The program includes options for "zircon saturation temperature" and "Ti-in-zircon thermometry". Therefore, the saturation temperature of zircon (Hanchar and Watson, 2003; Boehnke *et al.*, 2013) can be calculated from the whole-rock chemistry with the parameters M [(Na + K + 2Ca)/(Al × Si)] of Watson and Harrison (1983) and FM [(Na + K + (2Ca + Fe + Mg))/(Al × Si)] of Ryerson and Watson (1987). Additionally, Ti-in-zircon thermometry T(°C) of Watson *et al.* (2006) can be calculated by the program in the "Zircon" spreadsheet.

5. Conclusions

MagMin_PT is an Excel© based, open, and free mineral classification and geothermobarometry program. The program processes EPMA data using new and conventional cations recast methods, and it can produce mineral classification diagrams and P-T results for users. The aim of this study is to provide a user friend Excel-based program under the last developments for researchers and graduate students working on the mineral chemistry and petrology of magmatic rocks. Finally, mineral classification diagrams, formula proportions, and geothermobarometry results can easily be exported as "gif/jpeg/tiff" files and tables.

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The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A: Supplementary data

MagMin_PT.xlsb

Appendix B: Supplementary data

The calibrations used for geothermobarometry and their relevant to igneous system in MagMin_PT.

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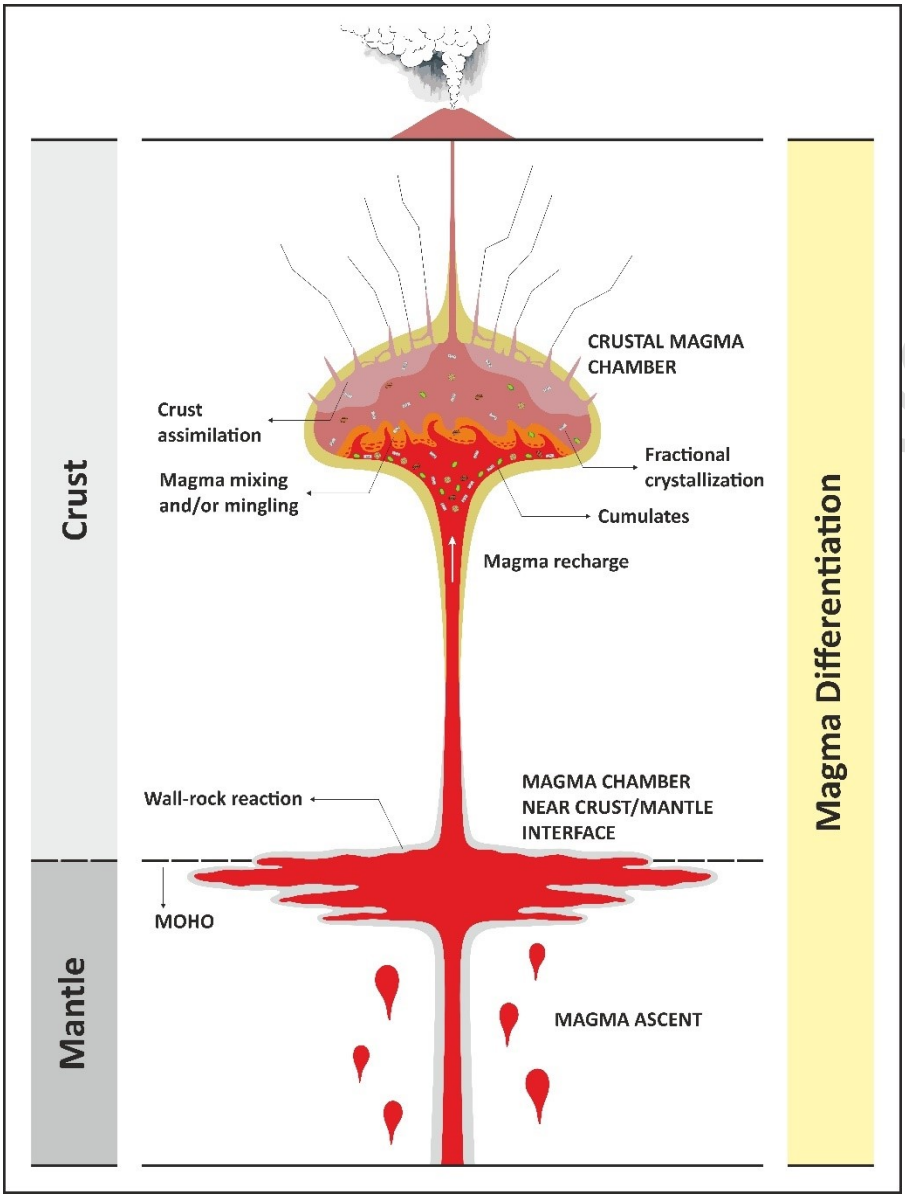

Figure 1: A conceptual section showing the ascent of magma and main differentiation processes in crustal-magma chamber such as fractional crystallization, assimilation, magma mixing, etc.

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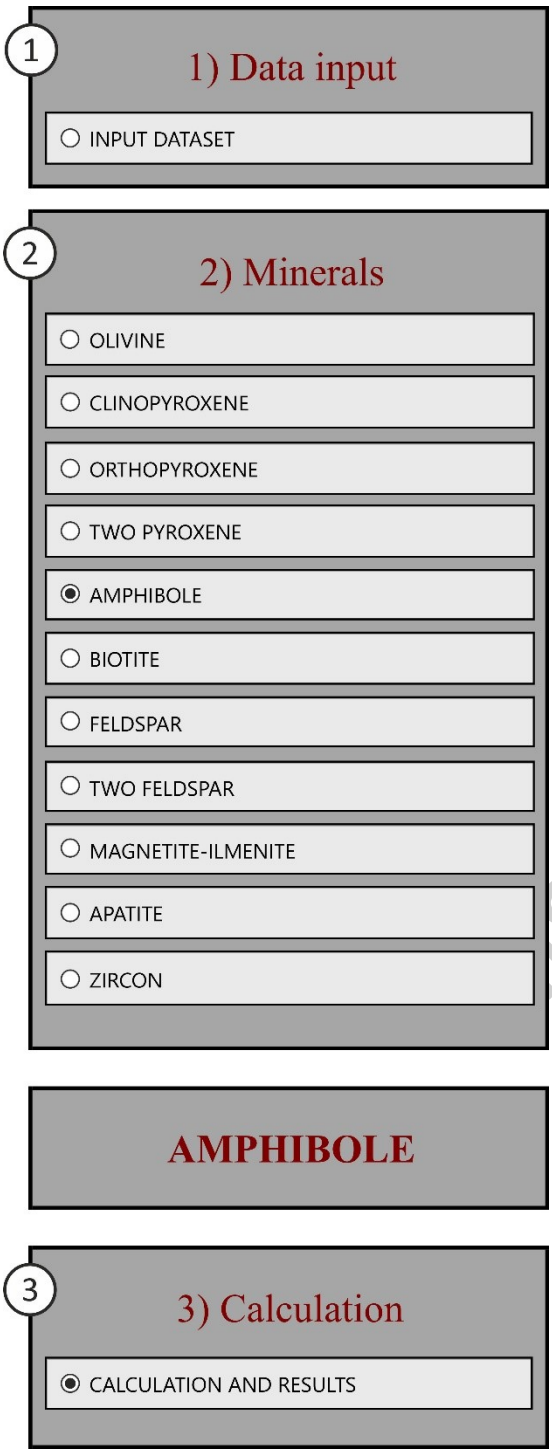

Figure 2: The control panel for data entry which must be in the order of each mineral; 1) Data input, 2) Minerals, and 3) Calculation.

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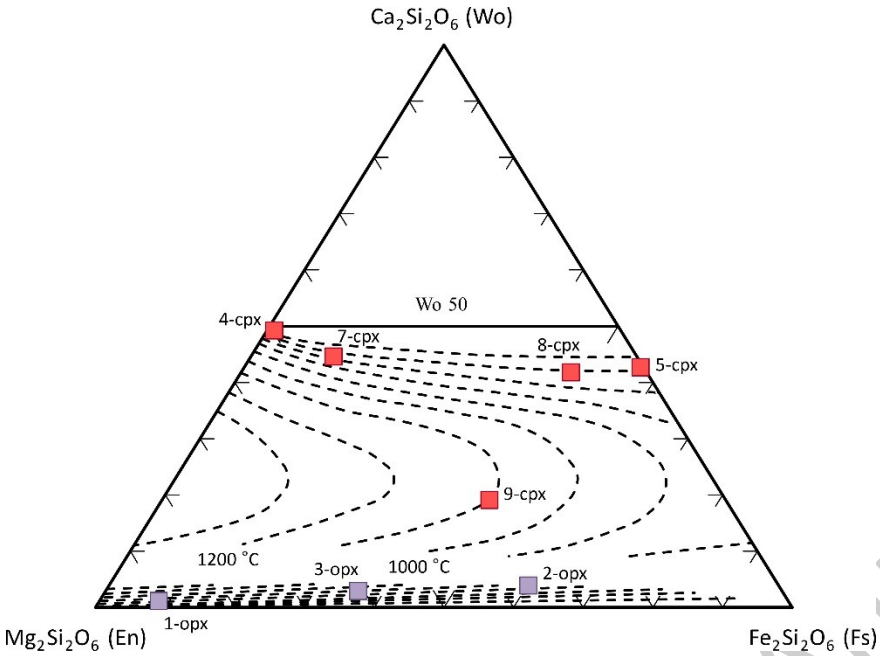

Figure 3: The plot of the ortho- and clinopyroxenes (Deer *et al.*, 1992) on the pyroxene isotherm curves (Lindsley and Andersen, 1983).

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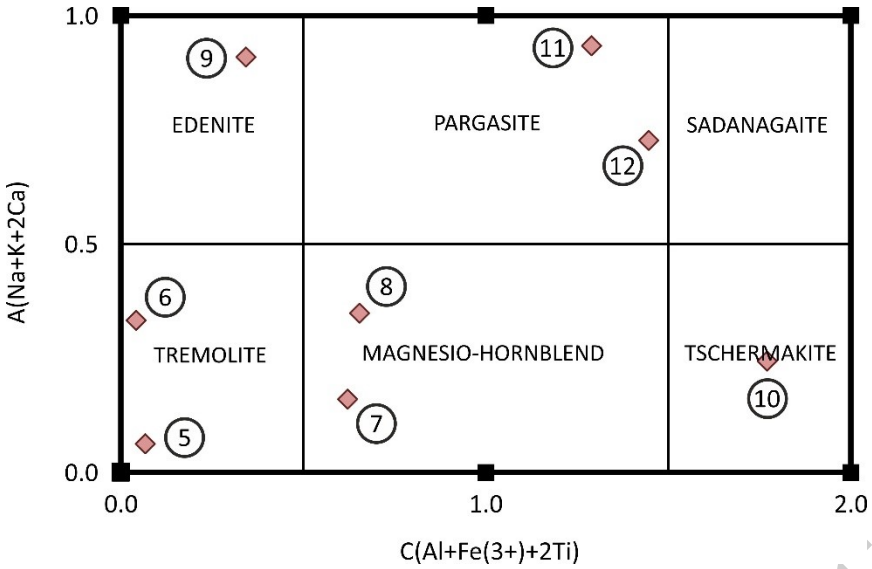

Figure 4: Classification diagram of calcic-amphibole according to IMA 2012 (Hawthorne *et al.*, 2012). Data set from Deer *et al.* (1992).

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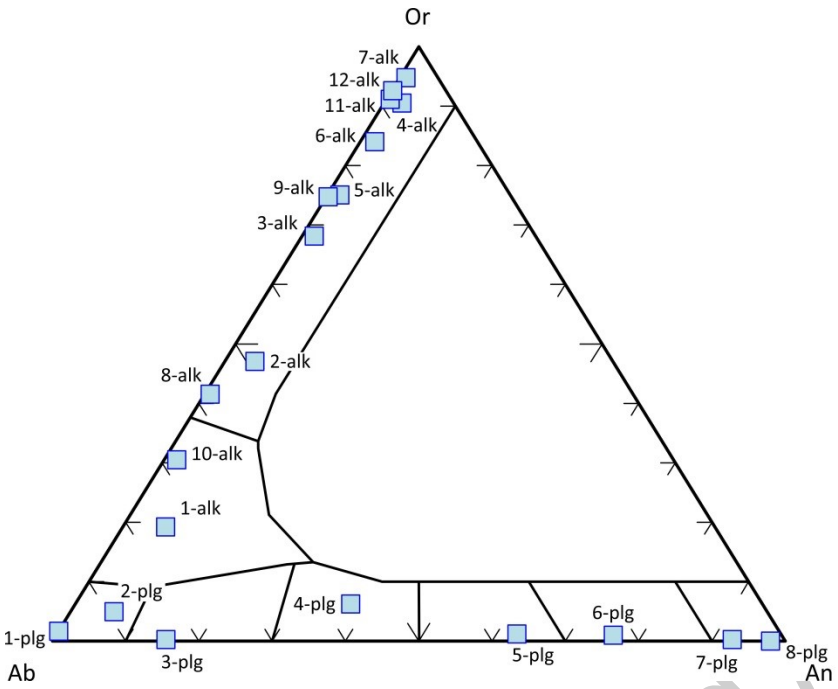

Figure 5: Classification of feldspars according to the end members of the Ab-An-Or ternary diagram. Data set from Deer *et al.* (1992).

List of Tables

Table 1. Chemical formula calculation of an olivine* analysis derived from electron microprobe.

	(1)	(2)	(3)	(4)		(5)
SiO_2	40.536	0.675	1.349	1.997	Si	0.998
TiO_2	0.009	0.000	0.000	0.000	Ti	0.000
Al_2O_3	0.019	0.000	0.001	0.001	Al	0.001
Cr_2O_3	0.046	0.000	0.001	0.001	Cr	0.001
FeO	10.998	0.153	0.153	0.226	Fe^{2+}	0.226
MnO	0.174	0.002	0.002	0.004	Mn	0.004
MgO	47.971	1.190	1.190	1.761	Mg	1.761
NiO	0.292	0.004	0.004	0.006	Ni	0.006
CaO	0.123	0.002	0.002	0.003	Ca	0.003
Na_2O	0.009	0.000	0.000	0.000	Na	0.000
Total	100.177		**T: 2.70**	4.000		3.000

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	4/2.70: 1.48

*Olivine data from Asan *et al.* (2021)

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