



## Article

# 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 at the surface. Each mineral represents the physico-chemical conditions at which various magmatic processes have occurred over a wide range of depths from upper mantle to shallow crustal levels. These processes are cryptically inscribed in the whole-rock and mineral compositions (e.g. major elements, trace elements and isotopic ratios) and textures (equilibrium vs. disequilibrium features), together with intensive variables (e.g. pressure,  $P$ ; temperature,  $T$ ). Therefore, particular attention should be given to igneous minerals to understand better the processes that took place during their journey from the source through magma chambers and conduit systems to the Earth's surface.

*MagMin\_PT* is an Excel<sup>®</sup> based user-friendly program, designed to calculate mineral formulae and end-members, and to estimate pressure and temperature (e.g. geothermobarometry) from electron microprobe analytical data. The program operates using the most common igneous rock-forming minerals (olivine, pyroxene, amphibole, biotite, feldspar, magnetite, ilmenite, apatite and zircon), resulting in various classification diagrams and  $P$ – $T$  diagrams. The program allows for whole-rock or glass composition to be entered together with the EPMA data to evaluate the equilibration status for most  $P$ – $T$  calculation models.  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  estimation is routinely performed in *MagMin\_PT* based on stoichiometric constraints, and to some extent using machine learning methods for different iron-bearing minerals. *MagMin\_PT* is also able to carry calculations of fugacity, magmatic water content and saturation temperature. Graphical and numerical outputs produced by the program can be easily copied to other media for further processing.

**Keywords:** MagMin\_PT, geology and mineralogy, rock-forming minerals in igneous rocks, mineral classification, geothermobarometry

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### Introduction

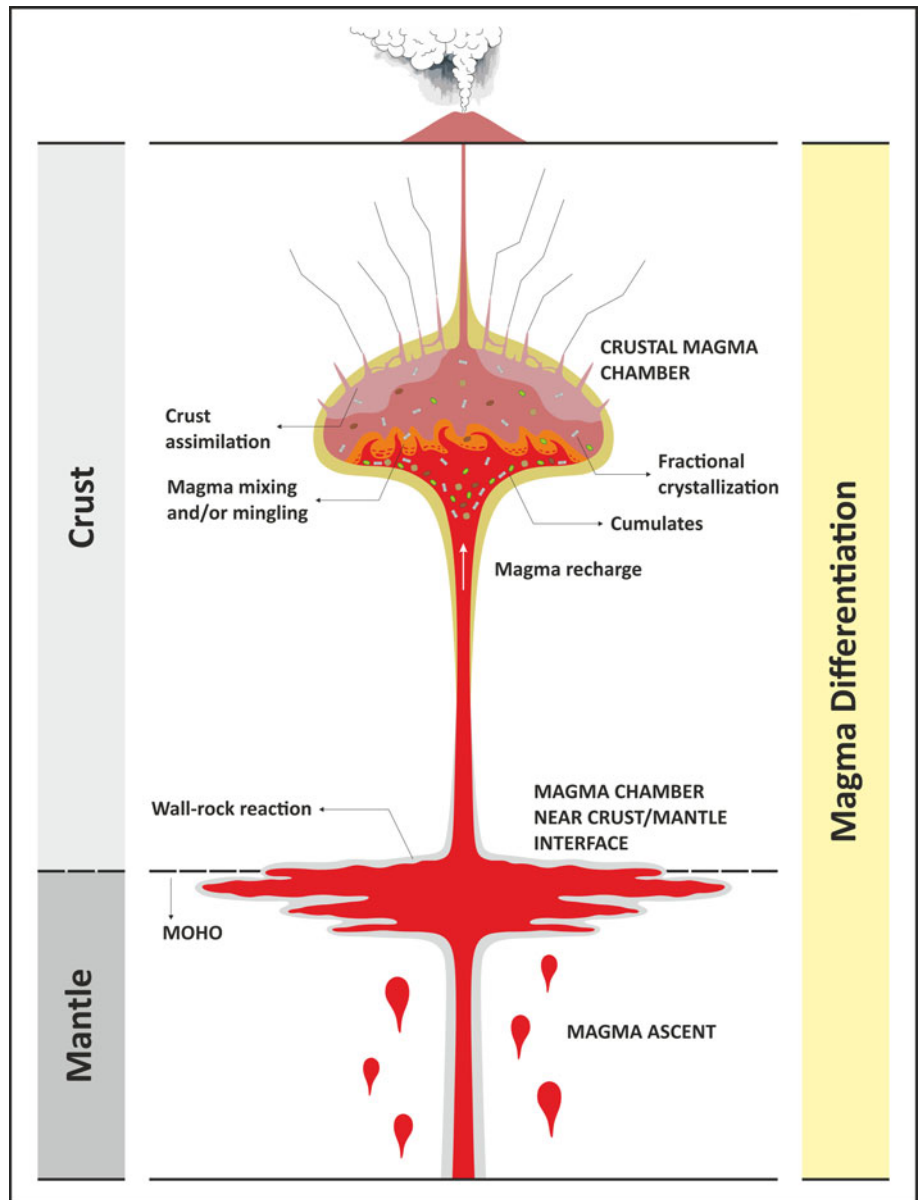
Only a very small number of the thousands of known natural minerals constitute most magmatic rocks. Olivine, pyroxene, amphibole, mica, feldspar, feldspathoids, Fe–Ti oxides (magnetite and ilmenite), and quartz are typically the major constituents in magmatic rocks. Apart from quartz these are all solid solutions. It is a simple task to identify these minerals in hand sample with the aid of a hand lens in the field or in thin section using a polarising microscope in the laboratory. X-ray diffraction and scanning electron microscopy studies are other common options for mineral identification. Electron microprobe analysis (EPMA) is one of the most widely used instruments for compositional analysis of minerals (Best, 2003), and these data are commonly reported in weight percentages of the oxides of the measured elements. These data require calculation of cationic formula and end-member components of each analysed mineral. Such calculations can be easily performed using published mineral

formulae calculation programs that are mainly free Excel-based applications. Most of these programs are mineral-specific formulae calculators with, or without, thermobarometry tools, for example: 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 Yildirim, 2020); tourmaline (Yavuz, 1997); and magnetite–ilmenite (Lepage, 2003; Hora *et al.*, 2013; Yavuz, 2021). A few general mineral formulae calculation programs also included in the literature are: Afifi and Essene (1988); Rock and Carroll (1990); Griffin *et al.* (1991); De Bjerg *et al.* (1992, 1995); Brandelik (2009) etc. In addition, there are many unpublished mineral formula calculators that can be downloaded from web-pages or obtained from their developers. Structural formulae and end-member calculations from mineral compositional analyses are routine intermediate tasks for classification purposes before further petrological calculations can be made (e.g. geothermobarometry, fugacity, magmatic water content, phase equilibria etc.). For the case of geothermobarometry, the programs listed above either include no computations or some only for a specific mineral, implying they are not comprehensive thermobarometry tools.

*MagMin\_PT* is designed mainly as a comprehensive geothermobarometry tool for igneous systems as shown in

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**Fig. 1.** A conceptual diagram showing the ascent of magma and main differentiation processes in a crustal-magma chamber such as fractional crystallization, assimilation, and magma mixing.

**Fig. 1**, which 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. olivine, pyroxene, amphibole, biotite, feldspar, magnetite, ilmenite, apatite and zircon) with minerals and groups defined according to the International Mineralogical Association (IMA).

### Principles of mineral formula calculation

The recasting of compositional data into a mineral formula is a series of mathematical functions based on the atomic weight, charge of cation, etc. of the elements analysed (see Brandelik, 2009) and which depends on the structure of the minerals, and relationships between charge neutrality and crystal chemistry (e.g. 4 oxygens for olivines, 6 oxygens for pyroxenes etc.). Following the scheme of Deer *et al.* (1992), the main steps for

mineral formula calculation are given in **Table 1**, using olivine as an example.

This procedure can be easily used for anhydrous minerals (olivine, pyroxene, feldspar etc.) whose cation-sites are full and the total weight percentage of major oxides are ~100%. However, hydrous minerals such as amphibole and biotite have a more complex mineral chemistry that cannot be fully determined by routine instrumental techniques. The main problem is that electron microprobe analysis cannot directly determine the volatile contents of hydrous minerals and does not differentiate between the valence states of iron ( $\text{Fe}^{2+}$ ,  $\text{Fe}^{3+}$ ), thus requiring additional computations. Such computations can be relatively easily made for anhydrous minerals if it is assumed that they have full-cation sites and perfect charge balance, however 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 science. In the

**Table 1.** Structural formula calculation of an olivine\* composition obtained by electron microprobe analysis.

	Column 1	Column 2	Column 3	Column 4	Column 5	
SiO <sub>2</sub>	40.536	0.675	1.349	1.997	Si	0.998
TiO <sub>2</sub>	0.009	0.000	0.000	0.000	Ti	0.000
Al <sub>2</sub> O <sub>3</sub>	0.019	0.000	0.001	0.001	Al	0.001
Cr <sub>2</sub> O <sub>3</sub>	0.046	0.000	0.001	0.001	Cr	0.001
FeO	10.998	0.153	0.153	0.226	Fe <sup>2+</sup>	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 <sub>2</sub> O	0.009	0.000	0.000	0.000	Na	0.000
Total	100.177		T: 2.70	4.000		3.000

Calculation notes: Column 1: The composition of the olivine as weight percentages of the oxides (wt.%), derived from EPMA.

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.

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).

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 in column 3 by 4/T. For this case the multiplier is 4/2.70 = 1.48.

Column 5: No. of ions in the formula, the number of cations associated with the oxygens in column (4). Thus, for SiO<sub>2</sub> and TiO<sub>2</sub> the column (4) entry is divided by 2, for Al<sub>2</sub>O<sub>3</sub> 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<sub>2</sub>O, Na<sub>2</sub>O) in the analysis, they are doubled in column (5), which is not case in the olivine formula here.

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

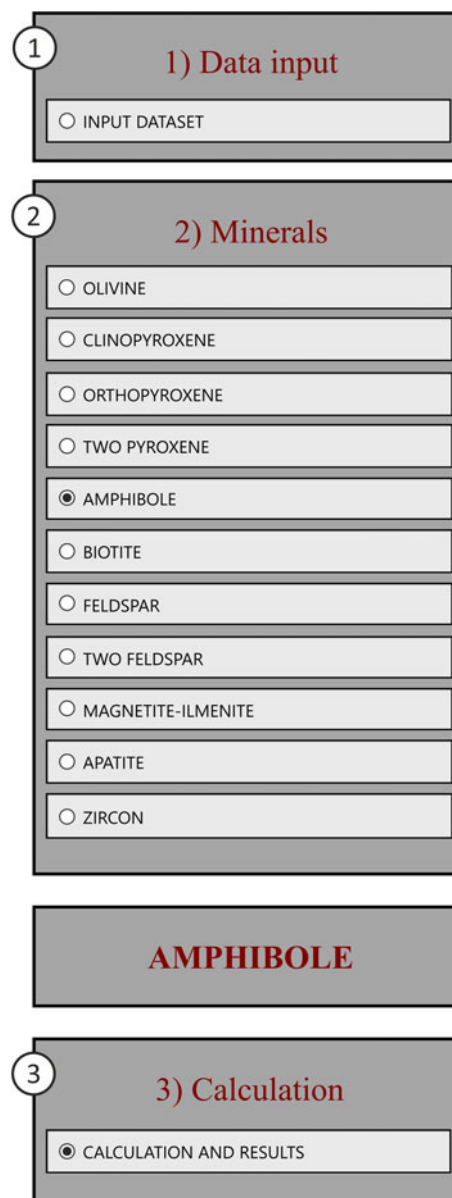
program *MagMin\_PT*, users can find diverse mineral formula calculation methods based on traditional computations, and to some extent machine learning methods which have become popular recently in geothermobarometry (Li *et al.*, 2020a, 2020b; Petrelli *et al.*, 2020; Higgins *et al.*, 2022).

### Tests for liquid equilibria in P–T calculations

The application 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. 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 using polarised-light microscopy or more advanced imaging methods (back-scattered electron (BSE) or cathodoluminescence (CL) petrography) can be first employed to evaluate equilibrium between selected mineral–liquid pairs. The predominant euhedral habit of minerals is generally considered to be evidence of equilibrium with the liquid in which they occur. In contrast, disequilibrium textures in minerals suggest that this condition is not met. Such textural features are diverse, especially in volcanic rocks and include: crystal zoning; resorption and dissolution surfaces; reaction rims; pseudomorphs; overgrowths on existing minerals; crystal clots etc. (Ginibre *et al.*, 2007; Streck, 2008). Therefore, these textures are the best indicators that minerals were out of equilibrium and that they reacted with the enclosing liquid.

Mineral–liquid thermobarometers are imported from Putirka’s equations and are based mostly on iterative equations. Calculation



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

of mineral–liquid partition coefficients is another test for equilibrium that can be automatically made in *MagMin\_PT*. Composition of a glass or whole rock, or some calculated composition can be used as the 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* and is based on the following general equations, originally suggested for olivine by Roeder and Emslie (1970):

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

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

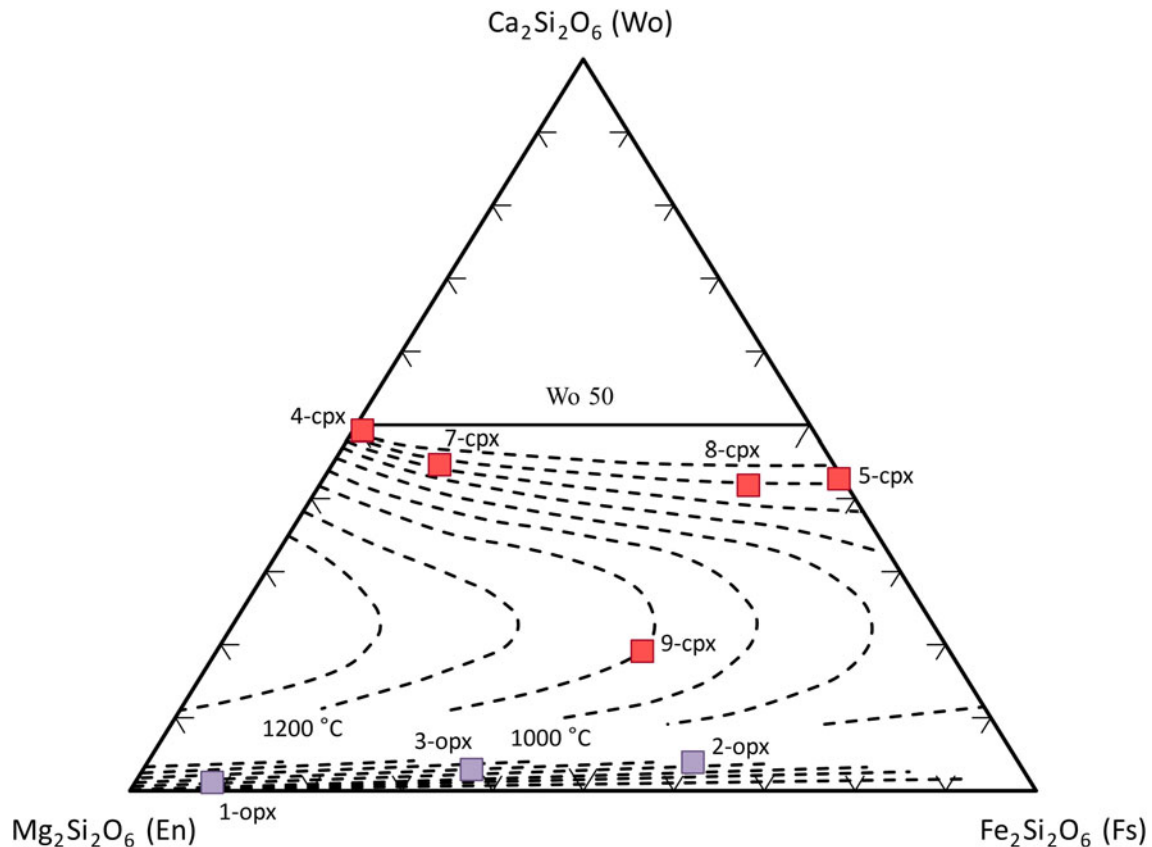


Fig. 3. Plot of ortho- and clinopyroxene compositions (Deer *et al.*, 1992) on the pyroxene isotherm curves (Lindsley and Andersen, 1983).

The acceptable partition coefficient ( $K_D$ ) range for each mineral to be equilibrium with the liquid will be given in the next section.

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 close to each other under equilibrium conditions. This method is only applicable to clinopyroxene in *MagMin\_PT*.

### Program description

*MagMin\_PT* is a Microsoft® Excel® workbook that is specifically designed for the needs and demands of researchers working with mineral compositional data and the geothermobarometry of magmatic rocks. It is divided into eleven Excel sheets: 'Instructions', 'Data Input', 'Olivine', 'Pyroxene', 'Amphibole', 'Biotite', 'Feldspar', 'Magnetite-Ilmenite', 'Apatite', 'Zircon' and 'Conversions'. These sheets are summarised in the following section, based on their principal role in the program.

### Instructions

Instructions are given on this sheet in the program. Note: 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.

### Data Input

'Data Input' contains access to the spreadsheets for user data (i.e. major oxides-wt.% of mineral and glass/whole-rock compositions). First, to enable data entry the check boxes on the 'Data Input' spreadsheet must be clicked in the order: (1) select 'Data input'; (2) select the appropriate 'Mineral' and enter compositions in the appropriate panel on the right; (3) select 'Calculation' to enable the calculation of cation formula and  $P$ - $T$  results – presented in the subsequent sheets (Fig. 2). In the majority of the 'Data Input' sheets, the upper right panel is for mineral compositions, the lower right panel is for 'glass' or 'whole-rock compositions' – the latter should be used if users want to make  $P$ - $T$  calculations based on mineral-liquid geothermobarometry.

### Olivine

Olivine is a ferromagnesian mineral represented by the two end-members of forsterite ( $\text{Mg}_2\text{SiO}_4$ ) and fayalite ( $\text{Fe}_2\text{SiO}_4$ ). Olivine compositions are recalculated on the basis of four oxygens and typically shown as molar percentages of forsterite (Fo) and fayalite (Fa) in the literature and also in *MagMin\_PT*.

*MagMin\_PT* calculates  $T$  (°C) from EPMA data using liquid thermometers (Helz and Thornber, 1987; Beattie, 1993; Sisson and Grove, 1993; Putirka *et al.*, 2007; Putirka, 2008). For the

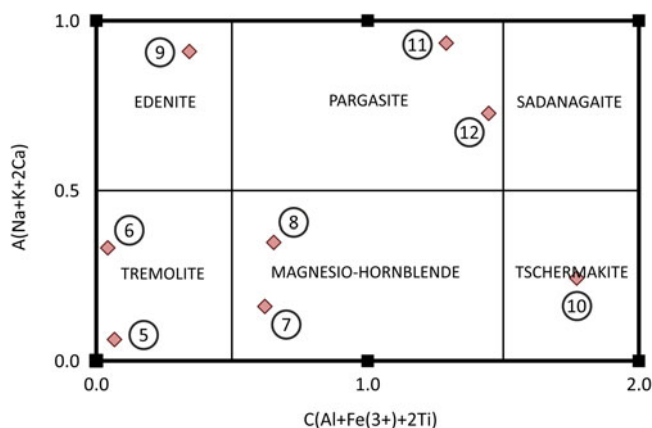


Fig. 4. Classification diagram of calcic-amphibole according to IMA 2012 (Hawthorne *et al.*, 2012). Data set from Deer *et al.* (1992).

olivine–liquid thermometer, the composition of ‘whole rock’ or ‘glass’ needs to be entered in the ‘Data Input’ sheet. Then, the program calculates the Fe–Mg exchange coefficient or  $K_D(\text{Fe–Mg})^{\text{ol-liq}}$  using 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  $K_D = 0.30 \pm 0.03$  (Roeder and Emslie, 1970; Toplis, 2005), which means that the thermometer can be applicable to the volcanic system. The results are presented in the ‘Olivine’ sheet.

### Pyroxene

This sheet designed for pyroxenes whose general chemical formula is  $\text{M}_2\text{M}_1\text{T}_2\text{O}_6$ . They are classified according to the occupancy of the M2 site, though Morimoto *et al.* (1988) assumed the M1 and M2 sites were 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 estimation of  $\text{Fe}^{3+}$  is made using 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  $\text{Fe}^{2+}$ .

In the ‘Data Input’ sheet in *MagMin\_PT*, three different options exist for pyroxene data entry. One option is ‘Two pyroxene’ data under the heading ‘Minerals’, with results appearing in the ‘Pyroxene’ sheet. In this sheet, many classification diagrams (Morimoto and Kitamura, 1983; Morimoto *et al.*, 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 to enter ortho- and clinopyroxene data independently. This is especially useful for mineral–liquid geothermobarometry that requires calculations of the Fe–Mg exchange coefficient for orthopyroxene ( $K_D(\text{Fe–Mg})^{\text{opx-liq}}$ ) and clinopyroxene ( $K_D(\text{Fe–Mg})^{\text{cpx-liq}}$ ) to test for equilibrium between mineral–liquid pairs according to equation 2.  $K_D$  values are expected to be in the range of  $0.29 \pm 0.06$  for opx and  $0.27 \pm 0.03$  for cpx to meet equilibrium conditions. The equilibrium

tests are also graphically portrayed in a ‘Rhodes Diagram’ (Rhodes *et al.*, 1979) in the ‘Pyroxene’ sheet, resulting in a binary plot of  $100 \times \text{Mg}^\# \text{ Liquid}$  vs.  $100 \times \text{Mg}^\# \text{ orthopyroxene}$  or clinopyroxene. On such a plot, the equilibrated mineral–liquid pairs lie between two dashed lines marking error bounds.

*MagMin\_PT* also includes an equilibrium test for clinopyroxene in the ‘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.

### Amphibole

Amphiboles are one of the most complex rock-forming double-chain inosilicates with a wide range of compositions, and are represented by a general formula of  $\text{AB}_2\text{C}_5\text{T}_8\text{O}_{22}\text{W}_2$ . Amphibole classification has not been satisfactory since Leake (1968) presented the first classification for calcic amphiboles. New discoveries of amphibole compositions has led to many classification attempts in parallel with ongoing development in analytical techniques in the intervening years (e.g. IMA reports of Leake, 1978; Leake *et al.*, 1997; Leake *et al.*, 2003; and Hawthorne *et al.*, 2012). These attempts have also been accompanied by the addition of new computer programs and spreadsheets to overcome classification problems resulting from the compositional complexity of amphiboles (e.g. Currie, 1997; Yavuz, 1999; Mogessie *et al.*, 2001; Esawi, 2004; Yavuz, 2007; Locock, 2014).

*MagMin\_PT* converts the entered amphibole microprobe analysis in ‘Data Input’ to formula proportions in atoms per formula unit (apfu) in the ‘Amphibole’ sheet according to the IMA 2012 recommendations (Hawthorne *et al.*, 2012), 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 can compare their formula calculations between this new approach and IMA 2012. The  $\text{Fe}^{3+}/\text{Fe}^{2+}$  ratio cannot be determined routinely by electron microprobe techniques therefore in *MagMin\_PT*  $\text{Fe}^{3+}$  is estimated empirically on the basis of the electroneutrality and stoichiometry rule. Further details on the  $\text{Fe}^{3+}$  calculations for IMA 2012 classification are given 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 the ‘Amphibole’ sheet. Al-in-hornblende calibrations are the most commonly used barometers based on EPMA-derived data. 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) are included in the program. However, these barometers should be used with caution because they are valid only under restricted conditions, and so 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 (lower right panel on Data Input sheet). The Fe–Mg exchange coefficient ( $K_D(\text{Fe–Mg})^{\text{amp-liq}}$ ) is expected to be in the range of  $0.28 \pm 0.11$  for the amphibole–liquid thermobarometer.

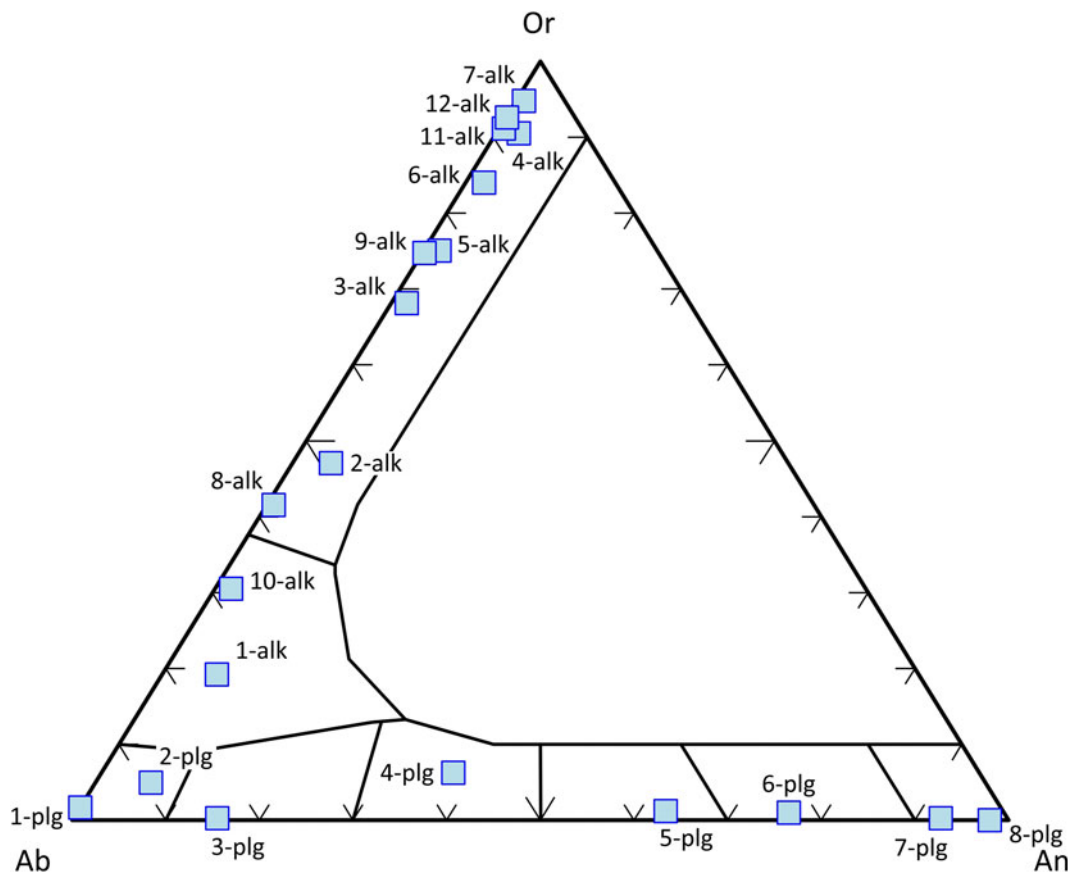


Fig. 5. Classification of feldspars according to the end-members of the Ab–An–Or ternary diagram. Data set from Deer *et al.* (1992).

The program also presents oxygen buffers constraining oxygen fugacity ( $f_{O_2}$ ) as a function of temperature (Fegley, 2012), and water content (%) of melt (Ridolfi *et al.*, 2010; Ridolfi, 2021) calculated from amphibole compositions.

### Biotite

Biotites are trioctahedral micas characterised 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 data (e.g. available of  $H_2O$  analysis) and oxidation state of biotite, etc. Therefore, this can be done traditionally using Rieder *et al.* (1999), and  $Fe^{3+}$  can be calculated on the basis of the equations given by Dymek (1983), though this 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 in the program (Tindle and Webb, 1990; Tischendorf *et al.*, 1997; Tischendorf *et al.*, 1999). Alternatively, *MagMin\_PT* includes a new scheme for the biotite formula calculation and  $Fe^{3+}$  estimation based on a machine learning method by Li *et al.* (2020b). The program includes basic classification diagrams for biotites, and for micas to some extent. *MagMin\_PT* also has options for *P–T* (Lühr *et al.*, 1984; Uchida *et al.*, 2007) calculations and oxygen buffers (Wones and Eugster, 1965; Wones, 1989). Pressure–temperature calculations for biotites do not require whole-rock or glass analysis data because these are not liquid-based thermobarometers.

### 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) solid solution (after Deer *et al.*, 1992). Compositions between Ab and An are referred to as plagioclases and those between Ab and Or as alkali feldspars (Fig. 5).

In *MagMin\_PT*, the feldspar formula is recalculated on the basis of 8, 16 or 32 oxygens depending on user choice, allowing Ab–An–Or components to be calculated 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 the ‘Data Input’ sheet, and then test for equilibrium between pairs on the basis of the Ab–An exchange coefficient ( $K_D$ ) using equation 4. The plagioclase–liquid equilibrium can also be used for a hygrometer, if the temperature is well-defined (Putirka, 2005, 2008). Thus, the program calculates  $H_2O$  (wt.%) content of the liquid using results from the aforementioned hygrometer. *MagMin\_PT* includes another water content ( $H_2O$  wt.%) calculation procedure using 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.

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

### Magnetite–Ilmenite

Ilmenite and magnetite are generally termed as Fe–Ti oxides with the idealised formula of  $\text{FeTiO}_3$  and  $\text{Fe}_3\text{O}_4$ , respectively. Two major solid-solution series occur as ‘ulvöspinel–magnetite’ and ‘ilmenite–hematite’ in the  $\text{FeO–Fe}_2\text{O}_3\text{–TiO}_2$  system. The compositions of coexisting ilmenite and magnetite have been used extensively as a thermobarometer because their compositions are strongly dependent on  $f_{\text{O}_2}$  (oxygen fugacity) and the  $T$  at which they equilibrated.

In natural magmatic systems, there are several buffer reactions that magnetite is involved in that can be used to characterise the oxidation state of magmas, such as the hematite–magnetite (HM), the quartz–fayalite–magnetite (QFM), and the magnetite–wüstite (MW) reactions. The Nickel–Nickel Oxide (NNO) buffer reaction does not occur in natural magmas though 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:

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

where  $T$  is temperature in Kelvin (K),  $P$  is pressure (bar), and  $A$ ,  $B$  and  $C$  are buffers from equilibrium expressions according to 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.  $\text{FeO–Fe}_2\text{O}_3\text{–TiO}_2$  or  $\text{R}^{2+}\text{–R}^{3+}\text{–Ti}^{4+}$ ).  $\text{Fe}^{3+}$  separation is according to the equation of Droop (1987). *MagMin\_PT* calculates  $T$  ( $^{\circ}\text{C}$ ) and  $f_{\text{O}_2}$  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  $T$  ( $^{\circ}\text{C}$ ) vs.  $\Delta\text{NNO}$ , which is the relative oxygen fugacity at given  $T$  for NNO.

A revised Fe–Ti oxide geothermometer and oxygen–barometer has been published by Ghiorso and Evans (2008). This is based on a thermodynamic model that produces different results than older calibrations, most notably in the estimation of oxidation state under relatively oxidised conditions ( $>\text{NNO} + 1$ ). This thermobarometry is not included in *MagMin\_PT*, however users can find an icon in the ‘Magnetite–Ilmenite’ sheet redirecting them to a web-based application designed by these authors for the  $T$  ( $^{\circ}\text{C}$ ) and NNO calculations.

### Apatite

Apatite,  $\text{Ca}_5(\text{PO}_4)_3(\text{F,Cl,OH})$ , 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 calculations. Apatite saturation temperature (Piccoli *et al.*, 1999; Piccoli and Candela, 2002) is calculated from whole-rock geochemical data that must be entered into the ‘Data Input’ sheet in the program.

### Zircon

Zircon is an accessory orthosilicate with the formula of  $\text{ZrSiO}_4$ . It is commonly found as early-formed small crystals enclosed in

later minerals in magmatic rocks. When enclosed, especially in biotite or amphibole, pleochroic haloes resulting from radioactive element content (Th,U) can be observed optically around zircon (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  $M$   $[(\text{Na} + \text{K} + 2\text{Ca})/(\text{Al} \times \text{Si})]$  of Watson and Harrison (1983) and  $\text{FM}$   $[(\text{Na} + \text{K} + (2\text{Ca} + \text{Fe} + \text{Mg})) / (\text{Al} \times \text{Si})]$  of Ryerson and Watson (1987). Additionally, Ti-in-zircon thermometry  $T$  ( $^{\circ}\text{C}$ ) of Watson *et al.* (2006) can be calculated by the program and is included in the ‘Zircon’ spreadsheet.

### Conclusions

*MagMin\_PT* is an Excel<sup>®</sup> based, open, and free mineral classification and geothermobarometry program available in the Supplementary materials. The program processes EPMA data using new and conventional cation recalculation methods, which produces mineral classification diagrams and  $P$ – $T$  data. The objective of this work is to provide a user friendly Excel-based program using the latest developments for those investigating the mineral compositions and petrology of magmatic rocks. Finally, mineral classification diagrams, formulae proportions and geothermobarometry data can easily be exported as ‘gif/jpeg/tiff’ files and tables.

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