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A Windows Program for Feldspar Group Thermometers and Hygrometers

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ABSTRACT

A Microsoft® Visual Basic software, called WinFeldth, has been developed for plagioclase, alkali feldspar and liquid compositions that coexisting as two-feldspar, plagioclase-liquid and alkali feldspar-liquid pairs to calculate the temperature (T, °C) and water contents (H_2O wt%) of igneous rocks. The program allows the users to enter major oxide of each plagioclase and alkali feldspar data and liquid compositions. Alternatively, 10 input variables such as the mole fractions of X_{Ab}^{PF}, X_{Or}^{PF}, X_{An}^{PF}, X_{Cn}^{PF}, X_{Ab}^{AF}, X_{Or}^{AF}, X_{An}^{AF}, X_{Cn}^{AF} as well as pressure (P, kbar) and temperature (T, °C) can be entered to estimate two-feldspar thermometers on the basis of thermodynamic modelling of ternary solid solutions and pressure- and temperature-dependent equations, respectively. WinFeldth enables the users to enter and load multiple two-feldspar and liquid analyses in the program's data entry section. Alternatively, the composition of analyses can be typed in a blank Excel file (i.e., WinPAL.xlsx) and then loaded into the program's data entry screen for data processing. Representative two-feldspar analyses are calculated based on 8 or optionally 32 oxygens by the program. WinFeldth evaluates eleven two-feldspar thermometers, nine two-feldspar thermometers based on the thermodynamic modelling of ternary solid solutions, six plagioclase-liquid thermometers, two alkali feldspar-liquid thermometers, five plagioclase-liquid hygrometers, one alkali feldspar-liquid hygrometer and plagioclase-liquid barometer. This program generates and stores all the calculated results in the Microsoft Excel file (i.e., Output.xlsx), which can be displayed and processed by any other software for further data presentation and graphing purposes. The compiled program code is distributed as a self-extracting setup file, including a help file (i.e., WinFeldth.chm), test data files and various graphic files for binary and ternary plots, which are intended to produce a high-quality printout.

Keywords: Plagioclase; alkali feldspar; two-feldspar thermometer; plagioclase-liquid hygrometer; thermodynamic model; software.

INTRODUCTION

Quantitative estimates of temperature (T, °C), pressure (P, kbar) and water content (H_2O, wt%) from mineral-mineral and mineral-melt assemblages in igneous rocks provide an important basis for the understanding of the condition of magma storage, fractionation, accent, eruption and melt generation processes in any tectonic setting (Putirka, 2008; Humphreys et al., 2016). Thus, igneous thermobarometers and hygrometers are frequently used to predict temperatures and depths of crystallization of natural systems (Mollo et al., 2011). Plagioclase phenocrysts in basalts through rhyolites crystallize over

a wide range of temperature, pressure and melt-water contents. Accordingly, the composition of plagioclase is one of the most promising minerals to be used as either a thermometer or hygrometer in igneous magmatic processes (Zeng et al., 2014; Waters and Lange, 2015). Plagioclase compositions from calc-alkaline rocks can also be used as an exploration indicator tool on a diagram of anorthite (An%) versus Al/(Ca+Na+K) (*apfu*) for porphyry copper deposits to discriminate fertile (excess Al>1) and barren (excess Al<1) systems (Williamson et al., 2016).

Natural feldspars with solid solutions mainly composed of $KAlSi_3O_8$, $NaAlSi_3O_8$ and $CaAl_2Si_2O_8$ form the most common rock-forming minerals in igneous and metamorphic rocks. In these rocks, plagioclase consisting primarily of the albite (Ab) and anorthite (An) components, whereas alkali feldspar consisting essentially of albite and orthoclase (Or) components. In igneous rocks, development of feldspars are observed in three stages; magmatic, post-magmatic (i.e., subsolidus) and hydrothermal (i.e., deuteric). In the magmatic stage, that controls the crystal growth, the ternary phase equilibrium relationships of feldspars predominantly influence rock genesis as well as the fractionation process. On the other hand, at the other two subsolidus and deuteric stages, the crystallographic properties of feldspar control the reactivity and capacity in terms of retaining or losing isotopes (Parsons and Brown, 1983). The major element chemical compositions of feldspars which are used in the classification of igneous rocks plays an important role in fluid-rock interactions, ore genesis at low temperature conditions by their control on hydrothermal fluid compositions and temperature of equilibration estimated from the two-feldspar thermometers. Feldspars in igneous rocks can also be used in the development of ideas on differentiation process (Parsons and Brown, 1983; Brown and Parsons, 1994).

The compositions of coexisting plagioclase and alkali feldspars in igneous and metamorphic rocks strongly depend on the temperature conditions of crystallization. Hence, ternary feldspar solvus relations establish the basis for thermometry of ternary feldspar solid solutions (Nekvasil, 1994). The first analytic two-feldspar thermometer, which is based on the partitioning of the three feldspar components (i.e., Ab, Or and An) between the plagioclase and alkali feldspar phases, was proposed by Barth (1934, 1951) and later his original formulation has been subjected to several modifications and improvements (e.g., Barth 1962, 1968; Stormer, 1975; Whitney and Stormer, 1977; Powell and Powell, 1977). Plagioclase-melt or plagioclase-liquid thermometers are associated with the equilibrium exchange of albite and anorthite components between solid and melt phases. The composition of plagioclase that crystallizing from a melt is controlled by various parameters including temperature, melt composition and melt H_2O concentration (Humphreys et al., 2016). Kudo and Weill (1970) developed the first plagioclase-liquid thermometer; since then plagioclase thermometry has received much attention in numerous earth science applications (Putirka, 2005, 2008, see references therein).

Volatiles in the composition of magma have a significant effect on the physicochemical properties of silicate melts as well as on the eruption style of active volcanoes. The most important volatile H_2O, which is dissolved in a silicate magma is also the most abundant and effective parameter controlling the phase balance and rheological properties of the system. Consequently, the determination of the dissolved H_2O concentration in differentiated magmas provides very important information for resolving a number of geological questions as well as for understanding the mechanisms of silicic magma evolution, the triggering of volcanic eruptions, volcanic hazard assessments as well as even the formation of porphyry copper deposits (Fiedrich et al., 2018; Masotta and Mollo, 2019). Experimental studies show that the anorthite content of plagioclase increases with an increase in H_2O (wt%) content of coexisting melt. This observation has led to develop a variety of empirical and semi-empirical plagioclase phenocryst hygrometers (e.g., Putirka, 2005, 2008; Lange et al., 2009; Waters and Lange, 2015; Masotta and Mollo, 2019) for determining the H_2O concentration in magmas with compositions ranging from basalt to rhyolite and trachyte (Ushioda et al., 2014; Masotta and Mollo, 2019).

Although several computer programs have been developed for thermobarometry calculations of rock-forming silicate minerals (e.g., Putirka, 2008; Hora et al., 2013; Yavuz, 1998, 2013; Lanari et al., 2014; Yavuz et al., 2015; Yavuz and Döner, 2017; Yavuz and Yıldırım, 2018, 2020; Yavuz, 2021), restricted attention was given on two-feldspar thermometers as well as plagioclase-liquid hygrometers. Wen and Nekvasil (1994) developed an interactive Solvcalc program, using C language, for calculating ternary feldspar solvus and two-feldspar thermometry. The Solvcalc program provides the user one user-defined and six selected Margules models for the temperature calculations from 400 to 1300 ^oC and pressure ranges from 1 bar to 15 kbar including graphics options with twelve solvus isotherms and thermometric tie lines. Putirka (2008) developed Excel spreadsheets on thermobarometers for two-feldspar and plagioclase-liquid analyses (see website references). Benisek et al. (2004, 2010) presented an Excel spreadsheet that calculating three temperatures (i.e., T_{Ab}, T_{Or} and T_{An}) from the compositions of two-feldspars based on the thermodynamic model of ternary feldspars with an option using the Kroll et al.

(1993) model for slowly cooled rocks.

In this paper, a Windows program, called WinFeldth, has been developed using the Microsoft® Visual Basic programming language to calculate multiple plagioclase, alkali feldspar and liquid oxides, up to 300 analyses, in each program running for thermometer and hygrometer estimations. The program recalculates plagioclase and alkali feldspar formula proportions of cations based on 8 oxygen atoms as default or 32 oxygen atoms by selecting *Structural formula on the basis of 32 oxygens* option from the pull-down menu of *Normalization in the Data Entry Screen*. Using the recalculated plagioclase and alkali feldspar and liquid compositions, the program allows users to select among various two-feldspar thermometers, plagioclase-liquid thermometers, plagioclase-liquid barometer, alkali feldspar-liquid thermometers and alkali feldspar-liquid hygrometer. WinFeldth displays two-feldspar compositions in various binary (e.g., X_{Ab}^{AF}-X_{Ab}^{PF}) and ternary (e.g., Ab-Or-An) diagrams by using the Golden Software's Grapher program. Compared to the previously published computer programs and Excel spreadsheets on two-feldspar and plagioclase-liquid oxides, the current version of program presents quick evaluation and comparison of multiple plagioclase, feldspar and liquid analyses for numerous thermometer and hygrometer calculations.

PROGRAM DESCRIPTION

WinFeldth is a compiled program developed essentially for running in the Microsoft® Windows platform to estimate various two-feldspar thermometer and plagioclase-liquid calibrations. The program comes up with a self-extracting setup file (≈24 Mb), which is created by the Inno Setup Compiler (https://jrsoftware.org/isinfo.php). It runs as a single executable file, WinFeldth.exe (3.00 Mb), if the Microsoft® Visual Studio package is installed into the same personal computer. On the other hand, with the help of necessary ".ocx" and ".dll" support files, came up with a setup file, the users of this program can execute WinFeldth without requiring the Microsoft® Visual Studio package. Following the successful installation of the program, the start-up screen with various pull-down menus and shortcuts appears on the screen. A list of the calculation steps in the program's *Calculation Screen* and in an Excel output file is given in Table 1. The current version of the program presents total 38 binary and ternary two-feldspar-related plots. These plots are displayed by selecting a desired diagram type from the pull-down menu of *Graph* in the *Calculation* Screen window of WinFeldth.

Data entry

The program's users can type both two-feldspar and liquid analyses by clicking the *New* icon on the toolbar, by selecting *New File* from the pull-down menu of *File* option or pressing the *Ctrl+N* keys in the *Start-up Screen* window. The standard 13 variables are defined by WinFeldth for calculation of plagioclase feldspar and alkali feldspar pairs in the following order: Sample No(PF), SiO_2(PF), TiO_2(PF), Al_2O_3(PF), Cr_2O_3(PF), FeO_{tot}(PF), MnO(PF), NiO(PF), MgO(PF), CaO(PF), BaO(PF), Na_2O(PF), K_2O(PF), and Sample No(AF), SiO_2(AF), TiO_2(AF), Al_2O_3(AF), Cr_2O_3(AF), FeO_{tot}(AF), MnO(AF), NiO(AF), MgO(AF), CaO(AF), BaO(AF), Na_2O(AF), K_2O(AF), where PF and AF show the abbreviations of plagioclase and alkali feldspar, respectively. In the data entry section, WinFeldth thus permits the user to enter 26 variables for two-feldspar compositions. On the other hand, liquid compositions are defined by the program in the following order: Sample No(Liq.), SiO_2(Liq.), TiO_2(Liq.), Al_2O_3(Liq.), Cr_2O_3(Liq.), FeO_{tot}(Liq.), MnO(Liq.), MgO(Liq.), CaO(Liq.), Na_2O(Liq.), K_2O(Liq.), P_2O_5(Liq.) and H_2O(Liq.), where Liq. shows the abbreviation of liquid. The program additionally enables the users to enter mole fractions of X_{Ab}^{PF}, X_{Or}^{PF}, X_{An}^{PF}, X_{Cn}^{PF}, X_{Ab}^{AF}, X_{Or}^{AF}, X_{An}^{AF} and X_{Cn}^{AF}, pressure (P, kbar) and temperature (T, ^oC) values as input for ternary two-feldspar thermometers and pressure- and temperature-dependent equations. Thus, in the data entry section, WinFeldth permits the user to enter up to 49 variables. However, if plagioclase and alkali feldspar compositions were typed in the *Data Entry Screen*, the users of program do not have to enter the mole fraction values in the corresponding columns for ternary feldspar thermometer estimations based on the thermodynamic model. Two-feldspar and liquid compositions typed in Excel files with the extension of ".xls" and ".xlsx" in the above order can be loaded into the program's data entry section (i.e., *Data Entry Screen*) by clicking the *Open Excel File* option from the pull-down menu of *File*. Nevertheless, using the copy-paste options these data as in the above order from a Microsoft® Excel spreadsheet can be included in the data entry section of WinFeldth more quickly. By selecting the *Edit Excel File* option from the pull-down menu of *File*, compositions of analyses can be typed in a blank Excel file (i.e., WinPAL) in the (C:\ Program Files\WinFeldth) folder, stored in a different file name with the extension of ".xls" or ".xlsx", and then loaded into the WinFeldth's data entry section by clicking the *Open Excel File* option from the pull-down menu of *File* for further data evaluations.

Normalization, correction procedure, ternary feldspar thermometry and hygrometers

Once the program is executed, WinFeldth calculates plagioclase and alkali feldspar formula proportions of cations based on eight oxygen atoms. However, selecting

Table 1. Description of column numbers in the *Calculation Screen* window of WinFeldth program and an output Excel file.

Row	Explanation	Column numbers
1	Major oxide plagioclase analyses (wt%)	1-13
2	Blank	14
3	Recalculated cations of plagioclase analyses (*apfu*)	15-27
4	T and M site total contents of plagioclase analyses (*apfu*)	28-29
5	Blank	30
6	Ab, Or, An and Cn components of plagioclase analyses	31-34
7	Blank	35
8	Cation fractions of plagioclase analyses	36-47
9	Blank	48
10	Major oxide alkali feldspar analyses (wt%)	49-62
11	Blank	63
12	Recalculated cations of alkali feldspar analyses (*apfu*)	64-76
13	T and M site total contents of alkali feldspar analyses (*apfu*)	77-78
14	Blank	79
15	Ab, Or, An and Cn components of alkali feldspar analyses	80-83
16	Blank	84
17	Cation fractions of alkali feldspar analyses	85-96
18	Blank	97
19	Two-feldspar thermometer (ºC) by Barth (1951)	98
20	Two-feldspar thermometer (ºC) by Barth (1968; Fig. 3, line a)	99
21	Two-feldspar thermometer (ºC) by Barth (1968; Fig. 3, line b)	100
22	Two-feldspar thermometer (ºC) by Barth (1968; Fig. 3, line c)	101
23	Two-feldspar thermometer (ºC) by Barth (1968; Fig. 3, average of lines a, b and c)	102
24	Two-feldspar thermometer (ºC) by Stormer (1975)	103
25	Two-feldspar thermometer (ºC) by Powell and Powell (1977)	104
26	Two-feldspar thermometer (ºC) by Whitney and Stormer (1977)	105
27	Two-feldspar thermometer (ºC) by Ferry (1978)	106
28	Two-feldspar thermometer (ºC) by Powell (1978)	107
29	Two-feldspar thermometer (ºC) by Haselton et al. (1983)	108
30	Two-feldspar thermometer (ºC) by Putirka (2008; Eq. 27a)	109
31	Two-feldspar thermometer (ºC) by Putirka (2008; Eq. 27b)	110
32	Two-feldspar thermometer (ºC) by Putirka (2008; Global regression)	111
33	Blank	112
34	Two-feldspar thermometer (ºC) based on the thermodynamic model by Ghiorso (1984; including T_{Ab}, T_{Or} and T_{An})	113-115
35	Two-feldspar thermometer (ºC) based on the thermodynamic model by Green and Usdansky (1986; including T_{Ab}, T_{Or} and T_{An})	116-118
36	Two-feldspar thermometer (ºC) based on the thermodynamic model by Nekvasil and Burnham (1987; including T_{Ab}, T_{Or} and T_{An})	119-121
37	Two-feldspar thermometer (ºC) based on the thermodynamic model by Fuhrman and Lindsley (1988; including T_{Ab}, T_{Or} and T_{An})	122-124
38	Two-feldspar thermometer (ºC) based on the thermodynamic model by Lindsley and Nekvasil (1989; including T_{Ab}, T_{Or} and T_{An})	125-127
39	Two-feldspar thermometer (ºC) based on the thermodynamic model by Elkins and Grove (1990; including T_{Ab}, T_{Or} and T_{An})	128-130

apfu = atoms per formula unit; Ab = Albite, Or = Orthoclase, An = Anorthite, Cn = Celsian.

Table 1. ... Continued

Row	Explanation	Column numbers
40	Two-feldspar thermometer (°C) based on the thermodynamic model by Benisek et al. (2004; including T_{Ab}, T_{Or} and T_{An} for molecular mixing model)	131-133
41	Two-feldspar thermometer (°C) based on the thermodynamic model by Benisek et al. (2004; including T_{Ab}, T_{Or} and T_{An} for Al-avoidance model)	134-136
42	Two-feldspar thermometer (°C) based on the thermodynamic model by Benisek et al. (2010; including T_{Ab}, T_{Or} and T_{An})	137-139
43	Blank	140
44	Major oxide liquid analyses (wt%)	141-154
45	Blank	155
46	Cation fractions of liquid analyses	156-166
47	Blank	167
48	Plagioclase-liquid thermometer (°C) by Kudo and Weill (1970)	168
49	Plagioclase-liquid thermometer (°C) by Putirka (2005; Model A)	169
50	Plagioclase-liquid thermometer (°C) by Putirka (2005; Model B)	170
51	Plagioclase-liquid thermometer (°C) by Putirka (2005; Model D)	171
52	Plagioclase-liquid thermometer (°C) by Putirka (2008; Eq. 24a)	172
53	Plagioclase-liquid thermometer (°C) by Putirka (2008; Eq. 26)	173
54	Blank	174
55	Plagioclase-liquid barometer (kbar) by Putirka (2005; Model C)	175
56	Blank	176
57	Plagioclase-liquid hygrometer (H_2O, wt%) by Putirka (2005; Model H)	177
58	Plagioclase-liquid hygrometer (H_2O, wt%) by Putirka (2008; Eq. 25b)	178
59	Plagioclase-liquid hygrometer (H_2O, wt%) by Lange et al. (2009)	179
60	Plagioclase-liquid hygrometer (H_2O, wt%) by Waters and Lange (2015) based on the second- degree polynomial equation using the Masotta and Mollo (2019) model [i.e., $H_2O_{WL15} = 0.7047007288 + 0.3930365565 * H_2O_{MM19} + 0.03203103204 * (H_2O_{MM19})^2$]	180
61	Plagioclase-liquid hygrometer (H_2O, wt%) by Masotta and Mollo (2019)	181
62	Blank	182
63	Alkali feldspar-liquid thermometer (°C) by Putirka (2008; Eq. 24b)	183
64	Alkali feldspar-liquid thermometer (°C) by Putirka (2008; Eq. 24c)	184
65	Blank	185
66	Alkali feldspar-liquid hygrometer (H_2O, wt%) by Mollo et al. (2015)	186
67	Blank	187
68	Input pressure (kbar) values for pressure-dependent equations	188
69	Input temperature (°C) values for temperature-dependent equations	189
70	Blank	190
71	Reference line for calculated analyses	191
72	Sample numbers for plagioclase and feldspar analyses	192
73	Ab, Or, An and Cn components of plagioclase analyses to be used for the Kroll et al. (1993) correction method	193-196
74	Ab, Or, An and Cn components of alkali feldspar analyses to be used for the Kroll et al. (1993) correction method	197-200
75	Input pressure (bar) values	201

apfu = atoms per formula unit; Ab = Albite, Or = Orthoclase, An = Anorthite, Cn = Celsian.

Structural formula based on 32 oxygens option from the pull-down menu of *Normalization*, the program carries out calculation process based on 32 oxygens. Compared to volcanic rocks, two-feldspar pairs from high-grade metamorphic rocks that cooled slowly under dry conditions suffer from a distinct type of retrograde resetting due to the Na and K exchange between phases. Therefore, the two-feldspar thermometer produces three, usually incongruent temperatures including T_{Ab}, T_{Or} and T_{An} (Benisek et al., 2004). As a solution to this situation, Fuhrman and Lindsley (1988) suggested adjusting compositions within assumed chemical uncertainties (e.g., ±2 mol%) so that congruent temperatures, which are approximately 40 ºC of each other, could be obtained. The procedure proposed by Fuhrman and Lindsley (1988) might not show a unique solution owing to the minute variations in the starting compositions could be resulted in several tens of degrees. Taking into account the retrograde resetting in high-grade metamorphic rocks that were dominated by slow cooling under dry conditions, Kroll et al. (1993) modified the Fuhrman and Lindsley (1988) model to reverse the K-Na exchange, also called correction procedure, and derive concordant temperatures. Benisek et al. (2004) advised to use a statistical procedure in which plagioclase and alkali feldspar compositions are randomly generated according to Gaussian distributions with their means at the observed compositions as well as standard errors chosen according to the quality of the chemical analysis. An exact incongruent temperature adjustment, which is developed by Benisek et al. (2010) on the basis of minimum variance of the three temperature values, can be carried out by the users in the *Correction* tab of Output.xlsx file using the Excel's solver option (i.e., Solver Add-ins). WinFeldth calculates the plagioclase and alkali feldspar-liquid hygrometers using the input temperature (T, ºC) values. In case of empty input temperatures in the *Data Entry Screen*, the program estimates water contents (H_2O, wt%) using the temperature estimation equation by Putirka (2008; Eq. 24a). However, by selecting one of three options including the temperature estimations by Putirka (2008, Eq. 26; 2005, Model A and Model B) from the pull-down menu of *Hygrometer*, WinFeldth calculates the water contents based on selected option.

WORKED EXAMPLES

Using the data set from literature (see Electronic Supplementary Material, ESM 1), the following examples show how WinFeldth can be used in various two-feldspar thermometer (e.g., Barth, 1951, 1968; Stormer, 1975; Powell and Powell, 1977; Whitney and Stormer, 1977; Ferry, 1978; Powell, 1978; Haselton et al., 1983; Putirka, 2008), two-feldspar thermometer based on the ternary feldspar solid solutions (e.g., Green and Usdansky, 1986; Fuhrman and Lindsley, 1988; Lindsley and Nekvasil, 1989; Elkins and Grove, 1990; Bensisek et al., 2004, 2010), plagioclase-liquid thermometer (e.g., Kudo and Weill, 1970; Putirka, 2005, 2008) and hygrometer (Putirka, 2005, 2008; Lange et al., 2009; Waters and Lange, 2015; Masotta and Mollo, 2019), plagioclase-liquid barometer (Putirka, 2005), alkali feldspar-liquid thermometer (Putirka, 2008) and hygrometer (Mollo et al., 2015) calculations. The program calculates the Waters and Lange (2015) hygrometer model based on second-degree polynomial equation [H_2O_{WL15} (wt%)=0.7047+0.3930H_2O_{MM19}+0.0320$H_2O_{MM19}^2$] using the water contents (H_2O, wt%) of Masotta and Mollo (2019) approach. The hygrometer model by Masotta and Mollo (2019) has been developed for trachytic lava and trachyandesitic products. Although high correlation coefficient (r=0.96, n=319) exist for H_2O_{WL15} equation, the Waters and Lange (2015) hygrometer estimations by WinFeldth program should be used with cautions for rocks especially those outside the trachytic and trachyandesitic compositions.

Once the typed or loaded two-feldspar and liquid compositions are processed by clicking the *Calculate icon* (i.e., Σ) in the *Data Entry Section* window of program, all output parameters are displayed in columns 1-201 (see Table 1) of the *Calculation Screen* and in an output Excel file. Pressing the *Ctrl + F* keys or clicking the *Open File to Calculate* option from the *Calculate* menu also executes the data processing for a selected data file with the extension of ".pal". Representative two-feldspar oxides with their stoichiometric structural formulae (*apfu*) and mole fractions of albite (Ab), orthoclase (Or), anorthite (An) and celsian (Cn) by WinFeldth program are given in Table 2 (see rows 1-43). By clicking the *Send results to Excel file* icon in the *Calculation Screen*, all outputs can be stored in an Excel file (Output.xlsx) and then displayed by clicking the *Open and edit Excel file* icon or by selecting *Open Excel File (Output.xlsx)* option from the pull-down menu of *Excel* in the *Calculation Screen* window. All input and calculated parameters from an *Output* tab of an Excel file are transposed automatically to the *Transpose* tab. This procedure provides the user to prepare a quick table for direct presentation and publication by using the copy and paste options. For example, representative plagioclase and alkali feldspar analyses (wt%) with their structural formulae (*apfu*), components and cation fraction values by WinFeldth program in the *Transpose* tab of output Excel file are shown in Figure 1 and Figure 2, respectively. The *Correction* tab in an Excel file provides the users to adjust ternary feldspar temperatures (i.e., T_{Ab}, T_{Or} and T_{An}), especially for coexisting plagioclase and alkali feldspar pairs from high-grade metamorphic rocks. Compositions of feldspars in these rocks may be changed by intercrystalline Na-K exchange at a constant

Table 2. Calculation of selected plagioclase and alkali feldspar analyses (wt%) with their structural formulae (*apfu*) and components (Ab, Or, An, Cn), two–feldspar thermometers (°C), two-feldspar thermometers (°C) based on the thermodynamic modeling of ternary feldspars and their application to the Kroll et al. (1993) correction method for coexisting feldspars in slowly cooled rocks by WinFeldth program.

Row	Plagioclase	PF1	PF2	PF3	PF4	PF5	PF6	PF7	PF8	PF9	PF10
1	SiO_2	61.8	64.82	63.44	63.12	65.00	64.47	64.16	64.75	62.32	62.39
2	Al_2O_3	23.97	22.04	22.92	22.80	22.15	22.20	22.45	22.05	22.66	23.59
3	CaO	5.47	2.70	4.15	4.02	4.52	3.49	3.38	3.58	4.39	4.67
4	BaO	0.00	0.52	0.55	0.43	0.00	0.54	0.36	0.15	0.57	0.21
5	Na_2O	7.56	9.03	8.25	8.33	8.20	8.72	9.26	8.69	10.39	8.18
6	K_2O	0.17	0.37	0.22	0.31	0.18	0.24	0.27	0.16	0.20	0.29
7	∑ (wt. %)	98.97	99.48	99.53	99.01	100.05	99.66	99.88	99.38	100.53	99.33
8	Si	2.758	2.870	2.816	2.816	2.856	2.854	2.837	2.863	2.772	2.778
9	Al	1.261	1.150	1.199	1.199	1.147	1.158	1.170	1.149	0.188	1.238
10	Ca	0.262	0.128	0.197	0.192	0.213	0.166	0.160	0.170	0.209	0.223
11	Ba	0.000	0.009	0.010	0.008	0.000	0.009	0.006	0.003	0.010	0.004
12	Na	0.654	0.775	0.710	0.721	0.699	0.748	0.794	0.745	0.896	0.706
13	K	0.010	0.021	0.012	0.018	0.010	0.014	0.015	0.009	0.011	0.016
14	∑ (*apfu*)	4.944	4.953	4.945	4.953	4.925	4.948	4.983	4.939	5.087	4.965
15	∑ T site (*apfu*)	4.018	4.020	4.016	4.015	4.003	4.012	4.007	4.013	3.961	4.016
16	∑ M site (*apfu*)	0.925	0.933	0.930	0.938	0.921	0.937	0.975	0.926	1.127	0.949
17	Ab	0.707	0.831	0.764	0.768	0.758	0.799	0.814	0.804	0.795	0.744
18	Or	0.010	0.022	0.013	0.019	0.011	0.014	0.016	0.010	0.010	0.017
19	An	0.283	0.137	0.212	0.205	0.231	0.177	0.164	0.183	0.186	0.235
20	Cn	0.000	0.010	0.010	0.008	0.000	0.010	0.006	0.003	0.009	0.004
21	Alkali feldspar	AF1	AF2	AF3	AF4	AF5	AF6	AF7	AF8	AF9	AF10
22	SiO_2	63.52	65.02	64.24	65.08	65.38	65.06	65.44	65.34	63.92	63.57
23	Al_2O_3	20.72	19.29	20.96	20.16	20.63	20.40	19.86	19.67	19.74	22.13
24	CaO	2.18	0.85	2.31	1.53	1.63	1.29	1.03	1.34	1.27	2.32
25	BaO	0.00	0.64	0.53	0.49	0.13	1.06	0.40	0.22	0.57	0.52
26	Na_2O	3.75	5.15	5.76	5.06	4.34	5.48	4.26	4.49	4.01	5.67
27	K_2O	9.11	9.22	5.90	8.38	8.96	7.45	10.07	8.92	9.68	5.53
28	∑ (wt%)	99.28	100.17	99.70	100.70	101.07	100.74	101.06	99.98	99.19	99.74
29	Si	2.896	2.952	2.984	2.927	2.923	2.923	2.944	2.953	2.932	2.857
30	Al	1.113	1.032	1.113	1.069	1.087	1.080	1.053	1.048	1.067	1.172
31	Ca	0.107	0.041	0.112	0.074	0.078	0.062	0.050	0.065	0.062	0.112
32	Ba	0.000	0.011	0.009	0.009	0.002	0.019	0.007	0.004	0.010	0.009
33	Na	0.332	0.453	0.503	0.441	0.376	0.477	0.372	0.393	0.357	0.494
34	K	0.530	0.534	0.339	0.481	0.511	0.427	0.578	0.514	0.567	0.317
35	∑ (*apfu*)	4.978	5.025	4.970	5.000	4.977	4.989	5.004	4.977	4.996	4.962
36	∑ T site (*apfu*)	4.010	3.985	4.007	3.995	4.010	4.004	3.998	4.001	4.000	4.030
39	∑ M site (*apfu*)	0.968	1.040	0.963	1.004	0.968	0.985	1.006	0.976	0.996	0.932
40	Ab	0.343	0.436	0.522	0.439	0.389	0.485	0.369	0.403	0.358	0.530
41	Or	0.547	0.513	0.352	0.479	0.528	0.433	0.574	0.527	0.569	0.340
42	An	0.110	0.040	0.116	0.073	0.081	0.063	0.049	0.066	0.063	0.120
43	Cn	0.000	0.011	0.010	0.009	0.002	0.019	0.007	0.004	0.010	0.010

Table 2. ... Continued

Two-feldspar thermometers (°C)											
44	T_{B51}	645	696	913	757	681	804	607	666	603	956
45	T_{B68} (a)	762	798	935	838	787	868	735	777	732	959
46	T_{B68} (b)	747	794	987	850	780	891	712	766	708	1023
47	T_{B68} (c)	690	739	943	797	724	841	654	710	650	982
48	T_{B68} (average)	733	777	955	828	764	867	700	751	696	988
49	T_{S75}	702	666	810	730	699	728	641	669	647	856
50	T_{PP77}	624	664	586	667	652	644	642	638	622	614
51	T_{WS77}	854	883	1254	981	887	1038	795	858	795	1362
52	T_{F78}	340	344	286	345	347	323	345	336	335	299
53	T_{P78}	553	589	518	592	578	571	569	566	551	543
54	T_{H83}	694	702	692	745	719	709	676	682	659	762
55	$T_{P08Eq27a}$	678	810	683	772	760	808	790	782	766	692
56	$T_{P08Eq27b}$	715	834	716	807	785	830	813	799	794	717
57	$T_{P08GlobReg}$	638	763	600	712	715	693	734	736	647	592
Two-feldspar thermometers (°C) based on the thermodynamic modeling of ternary feldspar solid solutions											
58	$T_{Ab\ G84}$	809	795	658	573	821	843	767	762	767	728
59	$T_{Or\ G84}$	454	504	461	346	393	468	469	365	467	453
60	$T_{An\ G84}$	1341	551	1947	4609	953	717	718	1034	929	1350
61	$T_{Ab\ GU86}$	857	875	814	796	874	862	859	856	845	837
62	$T_{Or\ GU86}$	526	512	466	490	499	475	505	471	478	499
63	$T_{An\ GU86}$	504	464	354	375	498	440	504	480	507	364
64	$T_{Ab\ NB87}$	406	613	155	64	491	533	570	498	527	127
65	$T_{Or\ NB87}$	267	419	252	135	261	340	377	265	356	232
66	$T_{An\ NB87}$	1442	1241	1260	1591	1329	1137	1441	1468	1539	1041
67	$T_{Ab\ FL88}$	608	698	560	483	654	692	661	639	640	593
68	$T_{Or\ FL88}$	426	554	466	347	420	508	511	427	495	448
69	$T_{An\ FL88}$	1466	1213	1360	1709	1334	1128	1442	1511	1569	1087
70	$T_{Ab\ LN89}$	625	687	561	503	656	681	656	636	639	595
71	$T_{Or\ LN89}$	388	520	429	311	385	471	477	394	461	409
72	$T_{An\ LN89}$	1138	981	1082	1322	1061	917	1156	1209	1251	865
73	$T_{Ab\ EG90}$	611	682	545	475	647	676	649	625	629	588
74	$T_{Or\ EG90}$	408	532	443	328	402	486	491	408	475	426
75	$T_{An\ EG90}$	1385	1169	1287	1624	1270	1071	1402	1463	1526	998
76	$^{(1)}T_{Ab\ B04}$	628	704	519	416	668	701	665	639	646	568
77	$^{(1)}T_{Or\ B04}$	485	571	511	410	466	539	535	458	525	501
78	$^{(1)}T_{An\ B04}$	1027	957	981	1070	989	915	1046	1058	1087	884
79	$^{(2)}T_{Ab\ B04}$	561	687	461	345	620	664	646	611	620	480
80	$^{(2)}T_{Or\ B04}$	489	573	512	409	467	541	536	458	527	504
81	$^{(2)}T_{An\ B04}$	1227	1073	1149	1279	1158	1048	1189	1216	1249	1049
82	$T_{Ab\ B10}$	363	426	102	102	375	340	441	371	423	75
83	$T_{Or\ B10}$	507	468	476	435	460	475	468	421	477	488
84	$T_{An\ B10}$	1524	1188	1324	1607	1351	1174	1348	1371	1437	1240

Table 2. ... Continued

Two-feldspar thermometers (°C) after the correction procedure by Kroll et al. (1993) for ternary feldspar solid solutions											
85	$T_{Ab, Or, An\ G84}$	1006	656	1144	1354	856	819	695	828	786	1151
86	$T_{Ab, Or, An\ NB87}$	1077	945	1086	1134	1035	1015	971	1009	1006	1102
87	$T_{Ab, Or, An\ FL88}$	1023	883	1038	963	972	948	906	944	940	1050
88	$T_{Ab, Or, An\ LN89}$	917	822	939	882	886	873	839	871	866	945
89	$T_{Ab, Or, An\ EG90}$	990	866	1006	940	948	927	888	923	920	1016
90	$T_{Ab, Or, An\ B04}$ (1)	931	858	954	908	910	902	873	901	895	956
91	$T_{Ab, Or, An\ B04}$ (2)	1016	892	1029	965	973	952	914	949	945	1037
92	$T_{Ab, Or, An\ B10}$ (Ave.)	1011	789	877	878	912	893	869	893	941	886
93	Input P (kbar)	7	7	7	7	7	7	7	7	7	7
94	Input T (°C)	800	800	800	800	800	800	800	800	800	800

PF1-PF10 to AF1-AF10 pairs from Mora and Valley (1985); *apfu* = Atomic per formula unit, Ab = albite, Or = orthoclase, An = anorthite and Cn = celsian; (1) = Calculation on the basis of molecular mixing model; (2) = Calculation on the basis of Al-avoidance model; (Ave.) = Average temperature (°C) of T_{Ab}, T_{Or} and T_{An}; Plagioclase and alkali feldspar analyses are estimated on the basis of 8 oxygens (see rows 8-13 and 29-34); Two-feldspar thermometers of T_{B51} (row 44) from Barth (1951), $T_{B68\ (a)}$ (row 45), $T_{B68\ (b)}$ (row 46), $T_{B68\ (c)}$ (row 47) and $T_{B68\ (average)}$ (row 48) from Barth (1968), T_{S75} (row 49) from Stormer (1975), T_{PP77} (row 50) from Powell and Powell (1977), T_{WS77} (row 51) from Whitney and Stormer (1977), T_{F78} (row 52) from Ferry (1978), T_{P78} (row 53) from Powell (1978), T_{H83} (row 54) from Haselton et al. (1983), $T_{P08Eq27a}$ (row 55), $T_{P08Eq27b}$ (row 56) and $T_{P08GlobReg}$ (row 57) from Putirka (2008); Two-feldspar thermometers (°C) based on the thermodynamic modelling of ternary feldspars of $T_{Ab, Or, An\ G84}$ (rows 58-60) from Ghiorso (1984), $T_{Ab, Or, An\ GU86}$ (rows 61-63) from Green and Usdansky (1986), $T_{Ab, Or, An\ NB87}$ (rows 64-66) from Nekvasil and Burnham (1987), $T_{Ab, Or, An\ FL88}$ (rows 67-69) from Fuhrman and Lindsley (1988), $T_{Ab, Or, An\ LN89}$ (rows 70-72) from Lindsley and Nekvasil (1989), $T_{Ab, Or, An\ EG90}$ (rows 73-75) from Elkins and Grove (1990), $T_{Ab, Or, An\ EG90}$ (rows 77-78) from Benisek et al. (2004) based on the molecular mixing model, $T_{Ab, Or, An\ B04}$ (rows 79-81) from Benisek et al. (2004) based on the Al-avoidance model, $T_{Ab, Or, An\ B10}$ (rows 82-84) from Benisek et al. (2010); Two-feldspar thermometers (°C) following the correction procedure by Kroll et al. (1993) for the models of: $T_{Ab, Or, An\ G84}$ (row 85) from Ghiorso (1984), $T_{Ab, Or, An\ NB87}$ (row 86) from Nekvasil and Burnham (1987), $T_{Ab, Or, An\ FL88}$ (row 87) from Fuhrman and Lindsley (1988), $T_{Ab, Or, An\ LN89}$ (row88) from Lindsley and Nekvasil (1989), $T_{Ab, Or, An\ EG90}$ (row 89) from Elkins and Grove (1990), $T_{Ab, Or, An\ B04}$ (row 90) from Benisek et al. (2004) based on the molecular mixing model, $T_{Ab, Or, An\ B04}$ (row 91) from Benisek et al. (2004) based on the Al-avoidance model, $T_{Ab, Or, An\ B10}$ (row 92) from Benisek et al. (2010); Input pressure (kbar) and temperature (°C) values (from Mora and Valley 1985) in rows 93 and 94 are used in the necessary calculations of pressure- and temperature-dependent equations.

An content. This situation causes shifting in opposite directions parallel to the Ab-Or joins and may be resulted in exsolution texture and intracrystalline exchange within alkali feldspar crystals, while plagioclase crystals continue to exchange K for Na with alkali feldspar crystals (Nekvasil, 1994). Consequently, considering one of nine model interaction parameters in Table 3 (rows 1-21); the users are able to adjust congruent temperature values using the correction procedure by Kroll et al. (1993) for their feldspar analyses. For this, the cells in lines from 193 to 203 of the *Transpose* tab are copied and then pasted into the C2 to C12 cells of the *Correction* tab in values and number formats with a paste special option. Similarly, the Margules parameters for each model within the F14-N37 cells of the *Correction* tab should be used with copy-paste options in estimation of the temperature values for ternary feldspar compositions. To adjust incongruent temperature values in the *Correction* tab, the users first check if the Solver Add-in has been installed in the Excel (i.e., use *File*→Options→*Add-ins*→*Go* options and then click the *Solver Add-in* option). By clicking the *Solver* button in the *Data* tab of Excel, following these steps, brings the *Solver Parameter* window on the screen (Figure 3a). At this stage, by clicking the *Solve* button displays the congruent temperature values of T_{Ab}, T_{Or} and T_{An} in the *Correction* tab of M2-M5 cells using the Benisek et al. (2010) model based on the minimum variance approach (see Figure 3b). Consequently, estimated T_{Ab}=363, T_{Or}=507 and T_{An}=1524 (°C) incongruent temperature values (see Figure 3a) for plagioclase (i.e., PF1 in Table 2) and alkali feldspar (i.e., AF1 in Table 2) compositions have been adjusted to T_{Ab}=1008, T_{Or}=1007 and T_{An}=1008 (°C) based on the ternary feldspar model by Bensisek et al. (2010) using the Kroll et al. (1993) approach (see Figure 3b).

Two-feldspar thermometers

Two-feldspar thermometer is independent of the bulk chemistry of rock due to its dependent on the distribution of three components of Ab, Or and An between the plagioclase and alkali feldspar phases at complete

Row		PF1	PF2	PF3	PF4	PF5	PF6	PF7	PF8	PF9	PF10
1	[SiO_2	59.10	59.00	63.40	64.90	66.10	63.80	64.90	64.90	63.50	64.70
2	TiO_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	Al_2O_3	25.90	26.30	23.10	22.10	20.80	23.20	21.70	22.10	23.10	22.30
4	Cr_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	$FeO_{(tot.)}$	0.06	0.05	0.00	0.07	0.15	0.09	0.00	0.14	0.00	0.06
6	MnO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	NiO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	MgO	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	CaO	6.94	7.68	4.38	3.25	0.97	4.23	2.78	3.18	4.23	3.41
10	BaO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	Na_2O	6.78	6.84	8.44	9.18	8.44	8.42	9.28	9.07	8.26	8.69
12	K_2O	1.13	1.09	1.01	1.15	3.78	1.38	1.19	1.21	1.09	1.03
13	Total (%)] Plagioclase	99.91	100.99	100.33	100.65	100.24	101.12	99.85	100.60	100.18	100.19
14											
15	[Si	2.645	2.620	2.800	2.852	2.926	2.800	2.870	2.853	2.806	2.850
16	Ti	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
17	Al	1.366	1.377	1.202	1.145	1.085	1.200	1.131	1.145	1.203	1.158
18	Cr	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
19	Fe	0.002	0.002	0.000	0.003	0.006	0.003	0.000	0.005	0.000	0.002
20	Mn	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
21	Ni	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
22	Mg	0.000	0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
23	Ca	0.333	0.365	0.207	0.153	0.046	0.199	0.132	0.150	0.200	0.161
24	Ba	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
25	Na	0.588	0.589	0.723	0.782	0.724	0.717	0.796	0.773	0.708	0.742
26	K	0.065	0.062	0.057	0.064	0.213	0.077	0.067	0.068	0.061	0.058
27	Total (*apfu*)] Plagioclase	4.999	5.017	4.989	4.999	5.000	4.997	4.996	4.995	4.978	4.971
28	[T-site$_{(tot.)}$ (*apfu*)	4.013	4.001	4.002	3.999	4.017	4.004	4.001	4.004	4.008	4.010
29	M-site$_{(tot.)}$ (*apfu*)] Plagioclase	0.986	1.016	0.987	1.000	0.984	0.993	0.995	0.991	0.969	0.961
30											
31	[Ab	0.597	0.580	0.732	0.782	0.736	0.722	0.800	0.780	0.730	0.772
32	Or	0.065	0.061	0.058	0.064	0.217	0.078	0.068	0.068	0.063	0.060
33	An	0.338	0.360	0.210	0.153	0.047	0.200	0.132	0.151	0.207	0.167
34	Cn] Plagioclase	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
35											
36	[SiO_2 [Cation Fractions (CF)]	0.52910	0.52229	0.56121	0.57053	0.58514	0.56045	0.57452	0.57130	0.56363	0.57333
37	TiO_2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
38	$AlO_{3/2}$	0.27328	0.27439	0.24099	0.22897	0.21701	0.24019	0.22640	0.22928	0.24165	0.23290
39	$CrO_{3/2}$	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
40	$FeO_{(tot.)}$	0.00045	0.00037	0.00000	0.00051	0.00111	0.00066	0.00000	0.00103	0.00000	0.00044
41	MnO	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
42	NiO	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
43	MgO	0.00000	0.00040	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
44	CaO	0.06657	0.07284	0.04154	0.03061	0.00920	0.03981	0.02637	0.02999	0.04023	0.03238
45	BaO	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
46	$NaO_{0.5}$	0.11769	0.11740	0.14485	0.15647	0.14486	0.14341	0.15928	0.15480	0.14215	0.14930
47	$KO_{0.5}$] (CF) Plagioclase	0.01291	0.01231	0.01141	0.01290	0.04269	0.01547	0.01344	0.01359	0.01234	0.01164

Figure 1. Screenshot of the *Transpose* tab of the Excel output created by program for evaluations of plagioclase analyses. Samples are taken from Elkins and Grove (1990, see rows 1-13).

equilibrium. Natural feldspars, commonly with ternary solid solutions, are of particular importance in high-temperature felsic to intermediate igneous rocks such as syenites and trachytes and high-grade metamorphic rocks including granulite (Nekvasil, 1994). The distribution of Ab component between plagioclase and alkali feldspar compositions has been used to calculate equilibration temperature of these two phases at a particular pressure. Consequently, most versions of two-feldspar thermometers (e.g., Stormer, 1975; Powell and Powell, 1977; Whitney and Stormer, 1977; Haselton et al., 1983) have used a double binary formulation on the basis of thermodynamic properties of limiting An-Ab and Ab-Or binary joins (i.e., a pseudo-thermodynamic formulation) and do not fully account for ternary compositions as well as does not take into account Al-Si ordering (i.e., Al-avoidance) (Green and Usdansky, 1986; Fuhrman and Lindsley, 1988; Elkins and Grove, 1990). On the other hand, thermodynamically based thermometers are principally designed to account for ternary solid solutions both for plagioclase and alkali feldspar phases (Brown and Parsons, 1985). Although three simultaneous equilibria among Ab, Or and An components

Row		AF1	AF2	AF3	AF4	AF5	AF6	AF7	AF8	AF9	AF10
50	[SiO_2	65.00	64.90	64.90	66.00	66.00	65.50	65.30	66.40	66.00	65.90
51	TiO_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
52	Al_2O_3	19.20	19.30	18.60	18.90	19.20	18.90	18.90	18.80	18.70	18.60
53	Cr_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
54	$FeO_{(tot.)}$	0.00	0.06	0.00	0.05	0.00	0.11	0.00	0.12	0.00	0.11
55	MnO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
56	NiO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
57	MgO	0.00	0.03	0.00	0.00	0.00	0.04	0.00	0.00	0.00	0.00
58	CaO	0.35	0.29	0.17	0.18	0.18	0.17	0.20	0.25	0.14	0.10
59	BaO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
60	Na2O	2.51	2.30	3.02	3.73	4.31	2.58	3.54	3.57	2.48	2.54
61	K_2O	12.80	13.30	12.10	11.30	10.40	12.50	10.90	11.30	12.70	12.70
62	Total (%)] Alkali feldspar	99.86	100.18	98.79	100.16	100.09	99.80	98.84	100.44	100.02	99.95
63											
64	[Si	2.973	2.966	2.992	2.992	2.984	2.991	2.992	3.000	3.005	3.005
65	Ti	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
66	Al	1.035	1.040	1.011	1.010	1.023	1.017	1.021	1.001	1.003	1.000
67	Cr	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
68	Fe	0.000	0.002	0.000	0.002	0.000	0.004	0.000	0.005	0.000	0.004
69	Mn	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
70	Ni	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
71	Mg	0.000	0.002	0.000	0.000	0.000	0.003	0.000	0.000	0.000	0.000
72	Ca	0.017	0.014	0.008	0.009	0.009	0.008	0.010	0.012	0.007	0.005
73	Ba	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
74	Na	0.223	0.204	0.270	0.328	0.378	0.228	0.314	0.313	0.219	0.225
75	K	0.747	0.775	0.712	0.654	0.600	0.728	0.637	0.651	0.738	0.739
76	Total (*apfu*)]	4.994	5.004	4.993	4.994	4.993	4.979	4.974	4.982	4.972	4.977
77	[T-site$_{(tot.)}$ (*apfu*)	4.008	4.010	4.003	4.004	4.007	4.014	4.012	4.005	4.008	4.009
78	M-site$_{(tot.)}$ (*apfu*)] Alkali feldspar	0.987	0.993	0.990	0.990	0.986	0.965	0.961	0.976	0.963	0.968
79											
80	[Ab	0.226	0.205	0.273	0.331	0.383	0.237	0.327	0.320	0.227	0.232
81	Or	0.757	0.781	0.719	0.660	0.608	0.755	0.663	0.667	0.766	0.763
82	An	0.017	0.014	0.008	0.009	0.009	0.009	0.010	0.012	0.007	0.005
83	Cn] Alkali Feldspar	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
84											
85	[SiO2 [Cation Fractions [CF]	0.59524	0.59281	0.59929	0.59914	0.59758	0.60060	0.60152	0.60220	0.60440	0.60377
86	TiO_2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
87	$AlO_{3/2}$	0.20722	0.20777	0.20242	0.20221	0.20488	0.20425	0.20519	0.20095	0.20183	0.20084
88	$CrO_{3/2}$	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
89	$FeO_{(tot.)}$	0.00000	0.00046	0.00000	0.00038	0.00000	0.00084	0.00000	0.00091	0.00000	0.00084
90	MnO	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
91	NiO	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
92	MgO	0.00000	0.00041	0.00000	0.00000	0.00000	0.00055	0.00000	0.00000	0.00000	0.00000
93	CaO	0.00343	0.00284	0.00168	0.00175	0.00175	0.00167	0.00197	0.00243	0.00137	0.00098
94	BaO	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
95	$NaO_{0.5}$	0.04457	0.04073	0.05407	0.06565	0.07566	0.04587	0.06322	0.06277	0.04403	0.04512
96	$KO_{0.5}$] Alkali Feldspar	0.14954	0.15498	0.14254	0.13086	0.12013	0.14622	0.12809	0.13074	0.14837	0.14844

Figure 2**.** Screenshot of the *Transpose* tab of the Excel output created by program for evaluations of alkali feldspar analyses. Samples are taken from Elkins and Grove (1990, see rows 50-62).

may provide unnecessary information on temperature, a great advantage of two-feldspar thermometers on the basis of ternary models is that it permits an additional test of equilibrium, provided that one believes the model to be correct (Fuhrman and Lindsley, 1988).

The validity of WinFeldth outputs in terms of two-feldspar thermometers (Figure 4) has been tested using plagioclase and alkali feldspar compositions (Table 2, see rows 44-84) from Mora and Valley (1985). Barth (1934) showed that the relative solution of albite into plagioclase and alkali feldspar could be used as an analytic thermometer. Later, he followed his own idea with several two-feldspar calibrations (Barth, 1951, 1962, 1968). In the *Calculation Screen* of program and an output Excel file, two-feldspar thermometers by Barth (1951, 1968) are displayed in columns from 98 to 102 (see Table 2, rows 44-48).

The first major revision of the two-feldspar thermometer (Figure 5a) was carried out by Stormer (1975) in an illustration of some important deficiencies such as to predict the activity of albite in the Barth (1962) model (see Table 2, row 49). In the following years, various

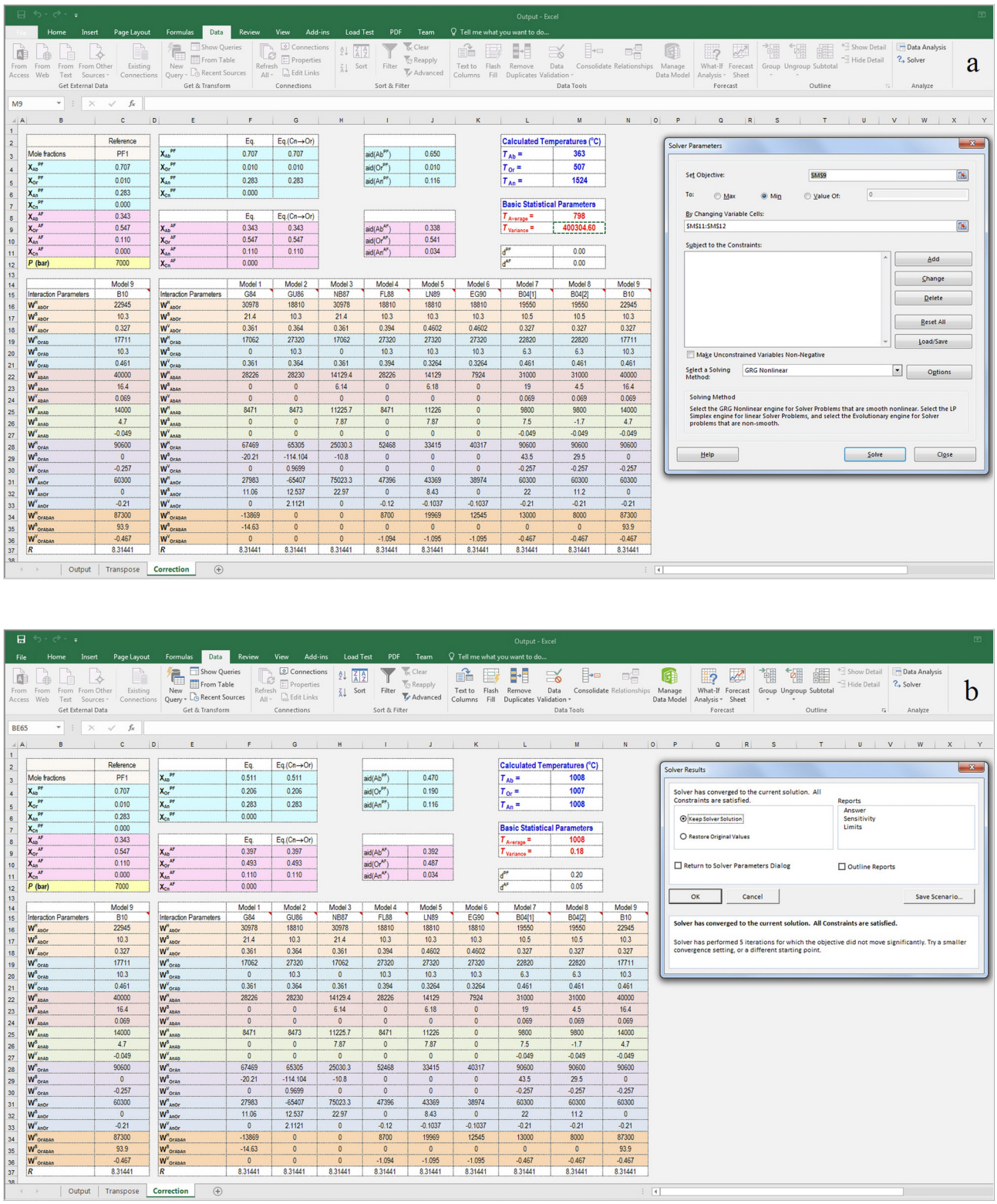

Figure 3. Screenshot of the Kroll et al. (1993) correction method to reverse the K-Na exchange and to derive concordant temperatures for two-feldspar thermometry of slowly cooled rocks using the Excel's solver option. a) Incongruent T_{Ab}, T_{Or} and T_{An} (ºC) temperature values before the correction procedure; b) Congruent temperature values after the correction procedure. Calculation procedure, which is based on the minimum variance estimation approach, is taken from Benisek et al. (2010).

Row		PF1AF1	PF2AF2	PF3AF3	PF4AF4	PF5AF5	PF6AF6	PF7AF7	PF8AF8	PF9AF9	PF10AF10
98	$[T_{B51}$	516	488	510	570	690	458	553	555	439	426
99	$T_{B68\,(a)}$	666	643	660	707	794	618	694	696	602	591
100	$T_{B68\,(b)}$	624	597	618	676	789	566	660	662	547	534
101	$T_{B68\,(c)}$	565	537	558	618	733	507	601	603	488	475
102	$T_{B68\,(average)}$	618	592	612	667	772	564	652	653	545	533
103	T_{S75}	651	634	618	636	714	590	622	629	577	562
104	T_{PP77}	646	633	634	651	730	606	634	639	594	581
105	T_{WS77}	729	703	715	765	902	669	746	751	652	637
106	T_{F78}	436	432	404	401	447	392	391	396	386	376
107	T_{P78}	646	633	621	637	715	593	621	626	582	569
108	T_{H83}	737	713	695	707	841	654	679	692	635	609
109	$T_{P08Ea27a}$	793	773	713	713	689	695	715	738	679	636
110	$T_{P08Ea27b}$	801	784	720	718	692	702	717	739	685	644
111	$T_{P08GlobRes}$] (°C) Two-feldspar	801	783	706	703	711	694	706	728	681	640
112											
113	$[T\,Ab_{G84}$	830	802	743	742	699	702	708	729	684	649
114	$T\,Or_{G84}$	888	896	679	636	694	716	617	647	680	620
115	$T\,An_{G84}$] (°C)	93	82	22	29	74	32	74	81	25	17
116	$[T\,Ab_{GU86}$	982	964	937	944	921	895	916	927	880	854
117	$T\,Or_{GU86}$	798	803	673	651	758	717	648	660	689	661
118	$T\,An_{GU86}$] (°C)	678	692	623	567	429	636	552	567	643	622
119	$[T\,Ab_{N887}$	737	729	686	685	673	650	652	662	639	617
120	$T\,Or_{N887}$	686	675	599	586	716	654	577	596	612	574
121	$T\,An_{N887}$] (°C)	823	797	747	751	1000	811	852	870	781	762
122	$[T\,Ab_{FL88}$	732	711	696	703	681	653	673	684	638	611
123	$T\,Or_{FL88}$	771	763	681	670	725	716	659	676	684	650
124	$T\,An_{FL88}$] (°C)	711	676	602	629	875	654	743	760	619	599
125	$[T\,Ab_{LN89}$	740	724	682	690	674	639	662	672	624	599
126	$T\,Or_{LN89}$	717	706	645	639	706	680	631	645	649	619
127	$T\,An_{LN89}$] (°C)	594	563	516	534	706	555	621	639	527	505
128	$[T\,Ab_{EG90}$	779	767	702	702	677	658	670	683	643	613
129	$T\,Or_{EG90}$	755	746	668	657	717	703	647	663	672	638
130	$T\,An_{EG90}$] (°C)	641	604	573	605	858	628	721	735	595	582
131	$[^{(1)}T_{Ab804}$	780	766	702	701	675	659	667	682	643	611
132	$^{(1)}T_{Or804}$	768	763	687	668	715	717	655	674	689	652
133	$^{(1)}T_{An804}$] (°C)	652	625	599	626	777	630	702	711	606	595
134	$[^{(2)}T_{Ab804}$	708	688	680	689	673	643	659	670	626	601
135	$^{(2)}T\,Or_{804}$	803	800	699	676	718	730	661	681	701	659
136	$^{(2)}T\,An_{804}$] (°C)	766	735	667	684	829	701	766	783	674	651
137	$[T\,Ab_{810}$	675	679	587	542	527	593	518	535	581	549
138	$T\,Or_{810}$	814	827	640	574	548	668	546	579	646	585
139	$T\,An_{810}$] (°C) Two-feldspar	926	899	825	836	975	869	920	938	843	821

Figure 4. Screenshot of two-feldspar thermometer calculations in the *Transpose* tab. Plagioclase and alkali feldspar analyses for two-feldspar thermometers are taken from Elkins and Grove (1990).

two-feldspar thermometers based on the thermodynamic concepts have been developed with increasing complexity (e.g., Powell and Powell, 1977; Whitney and Stormer, 1977; Green and Usdansky, 1986; Fuhrman and Lindsley, 1988; Elkins and Grove, 1990; Benisek et al., 2004, 2010). Comparative results of these calculations are listed in rows 49 to 54 in Table 2. Powell and Powell (1977) reformulated the Stormer (1975) thermometer using ternary regular solution model equations due to the Stormer (1975) model does not take into account the effect of small amounts of Ca in alkali feldspars. According to Powell and Powell (1977), an increasing Ca content in alkali feldspar increases the calculated temperature, as well as the Stormer (1975) thermometer (Table 2, row 50). Whitney and Stormer (1977) modelled the partitioning of Ab between coexisting microcline and plagioclase solid-solutions using the published Margules parameters for microcline-low albite solid solutions and developed two-feldspar thermometer (Figure 5b), which is applicable to low-temperature alkali feldspars for P=3.5 kbar (Table 2, row 51). Ferry (1978) used the compositions of plagioclase-microcline pairs from 53

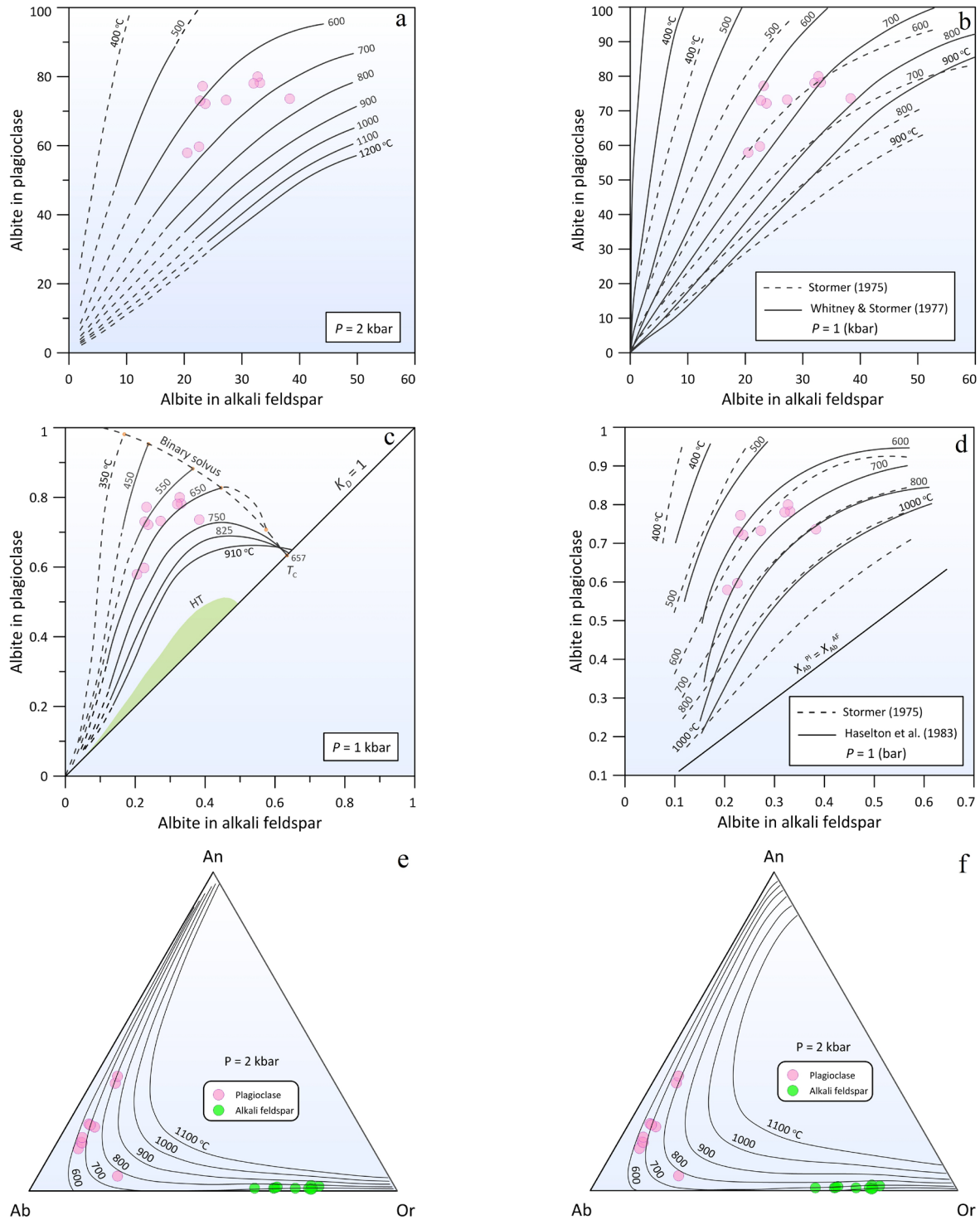

Figure 5. Distribution of feldspar components in temperature based binary and ternary model diagrams. Plot of albite component between coexisting plagioclase and alkali feldspars with determinative temperature curves and corresponding pressure value for the: a) Stormer (1975) model (P=2 kbar), b) Whitney and Stormer (1977) model (P=1 kbar), c) Brown and Parsons (1981) model, where the curve HT is a hypothetical isotherm for a very high temperature, T_c is the critical temperature for An-free solid solutions and K_D is the distribution coefficient (K_D=$N_{Ab}^{\text{Alkali feldspar}}/N_{Ab}^{\text{Plagioclase}}$), d) Haselton et al. (1983) model (P=1 bar). e) Ternary feldspar plot showing the location of the 600-1100 ºC isotherms at 2 kbar pressure condition using the: Fuhrman and Lindsley (1988) model, f) Elkins and Grove (1990) model. Solvus are produced from the Solvcalc program (Wen and Nekvasil, 1994) for each ternary feldspar model. Plagioclase and alkali feldspar analyses are taken from Elkins and Grove (1990).

samples and calculated the Ab fractionation temperatures by a scheme similar to that of the Stormer (1975) approach with the calibration utilizing mixing parameters for microcline-low albite (Table 2, row 52). Taking into account the Stormer (1975) thermometer did not consider the solution of small amounts of Ca in the alkali feldspar, Powell (1978) reformulated the Powel and Powel (1977) model for a pressure of 1 kbar and applied it to the crystallization history of the Igdlerfigssalik nepheline syenite intrusion, Greenland (Table 2, row 53). Brown and Parsons (1981) made several modifications on the Seck's (1971) two-feldspar thermometer and discussed their revised graphical thermometer (Figure 5c) in terms of less misleading than any of the thermodynamic thermometers such as the Stormer (1975), Powell and Powell (1977), Whitney and Stormer (1977) and Ferry (1978) models. Haselton et al. (1983) used the combined alkali feldspar and calorimetric results of high plagioclase data to derive an expression for the two-feldspar thermometer (Figure 5d) based on the thermodynamics of solid solutions. According to Haselton et al. (1983), their thermometer that partially accounts for the ternary solution of each feldspar yields higher temperatures than do the models based on previous thermodynamic descriptions of two-feldspars (Table 2, row 54).

Despite these efforts, expressions that are in the more complex forms showed unable to yield better thermometers (Putirka, 2008). Hence, using 41 experimental data from the literature, Putirka (2008) attempted to propose empirical two-feldspar thermometers (i.e., Eqs. 27a, 27b and global regression in Putirka, 2008) that appear much simpler than the thermodynamic models and lack the systematic errors (see Table 2, rows 55-57). According to Putirka (2008), these thermometers recover temperature for the used calibration data to ±23 ºC and 44 ºC (for Eq. 27a) and ±30 (for Eq. 27b) based on the selected experimental data.

Ghiorso (1984) presented a two-feldspar thermometer (Table 2, rows 58-60) based on the activity/composition relations derived from the solution model (see Table 3, Model 1) that provides somewhat more sensible estimates of crystallization temperature values when compared the temperatures obtained from equations and graphs of earlier studies (e.g., Stormer 1975; Powell and Powell, 1977; Brown and Parsons, 1981; Haselton et al., 1983). The thermometric methodology by Green and Usdansky (1986; see Table 2, rows 61-63) does not require an independent pressure estimate. In their model (see Table 3, Model 2), a pressure at which the differences between temperatures are minimized. Thus, the compositions are not modified during calculations. The thermometric model by Green and Usdansky (1986) generally yields good temperatures within its 650 to 900 ºC calibration range, but inapplicable for strongly ternary feldspar compositions. In the Nekvasil and Burnham (1987) approach (Table 2, rows 64-66), an ideal part of the mixing free energy is based on an ideal single-site model considering three components in the ternary solution of Margules formalism and using an ion-exchange data from Seil and Blencoe (1979) to obtain their values (see Table 3, Model 3).

Fuhrman and Lindsley (1988) proposed a revised thermodynamic model (see Table 3, Model 4) for ternary feldspars and developed a computer program for estimating temperature by adjusting feldspar compositions within analytical uncertainty. They compared their methodology (Table 2, rows 67-69) with those of previous feldspar thermometers and came to the conclusion that their model yielded a significant improvement over the previous two-feldspar thermometers (e.g., Haselton et al., 1983); Ghiorso, 1984; Green and Usdansky, 1986). According to Fuhrman and Lindsley (1988), their model yields nearly concordant temperatures of 900-1000 ºC for strongly ternary feldspar pairs from plutonic igneous rocks when compared to the Green and Usdansky (1986) thermometer. On the other hand, application of their methodology to metamorphic feldspars from granulite-facies rocks shows restricted concordant temperatures (Figure 5e). Using the Lindsley and Nekvasil (1989) Margules parameters (see Table 3 Model 5), which were adopted from Nekvasil and Burnham (1987), the program estimates two-feldspar thermometer (Table 2, rows 70-72) for ternary feldspar solid solutions. Elkins and Grove (1990) reported the results of 20 experiments for coexisting plagioclase and alkali feldspars, which were carried out over the 700-900 ºC and 1-3 kbar under water-saturated conditions. They showed that their thermodynamic model (see Table 3, Model 6) produces slightly higher temperatures than those of the Fuhrman and Lindsley (1988) model for feldspars in volcanic rocks and the difference in temperature among the three equilibria (i.e., T_{Ab}, T_{Or} and T_{An}) are equal to or smaller than the equated thermometer. When compared to the strongly ternary feldspar compositions from plutonic rocks, they also reported that their methodology (Table 2, rows 73-75) predicts temperatures higher than those of the Fuhrman and Lindsley (1988) model (Figure 5f). In terms of coexisting feldspars in granulite-facies metamorphic rocks, both of the Fuhrman and Lindsley (1988) and Elkins and Grove (1990) models, give similar temperature estimations.

Benisek et al. (2004) revised the thermodynamic model of two-feldspar thermometer based on the recent enthalpy (S) and volume (V) measurements in the (Na, Ca)- and (K, Ca)-feldspar binaries, derived new interaction parameters, updated previous ones (see Table 3, Model 7 and 8) and presented Mathematica and Excel files in

Table 3. Interaction parameters of nine ternary solution models in estimation of two-feldspar thermometers (oC) based on the thermodynamic descriptions (in joules).

Row	Parameters	Model 1	Model 2	Model 3	Model 4	Model 5	Model 6	Model 7	Model 8	Model 9
1	W^H_{AbOr}	30978	18810	30978	18810	18810	18810	19550	19550	22945
2	W^S_{AbOr}	21.4	10.3	21.4	10.3	10.3	10.3	10.5	10.5	10.3
3	W^V_{AbOr}	0.361	0.364	0.361	0.394	0.4602	0.4602	0.327	0.327	0.327
4	W^H_{OrAb}	17062	27320	17062	27320	27320	27320	22820	22820	17711
5	W^S_{OrAb}	0	10.3	0	10.3	10.3	10.3	6.3	6.3	10.3
6	W^V_{OrAb}	0.361	0.364	0.361	0.394	0.3264	0.3264	0.461	0.461	0.461
7	W^H_{AbAn}	28226	28230	14129.4	28226	14129	7924	31000	31000	40000
8	W^S_{AbAn}	0	0	6.14	0	6.18	0	19	4.5	16.4
9	W^V_{AbAn}	0	0	0	0	0	0	0.069	0.069	0.069
10	W^H_{AnAb}	8471	8473	11225.7	8471	11226	0	9800	9800	14000
11	W^S_{AnAb}	0	0	7.87	0	7.87	0	7.5	-1.7	4.7
12	W^V_{AnAb}	0	0	0	0	0	0	-0.049	-0.049	-0.049
13	W^H_{OrAn}	67469	65305	25030.3	52468	33415	40317	90600	90600	90600
14	W^S_{OrAn}	-20.21	-114.104	-10.8	0	0	0	43.5	29.5	0
15	W^V_{OrAn}	0	0.9699	0	0	0	0	-0.257	-0.257	-0.257
16	W^H_{AnOr}	27983	-65407	75023.3	47396	43369	38974	60300	60300	60300
17	W^S_{AnOr}	11.06	12.537	22.97	0	8.43	0	22	11.2	0
18	W^V_{AnOr}	0	2.1121	0	-0.12	-0.1037	-0.1037	-0.21	-0.21	-0.21
19	W^H_{OrAbAn}	-13869	0	0	8700	19969	12545	13000	8000	87300
20	W^S_{OrAbAn}	-14.63	0	0	0	0	0	0	0	93.9
21	W^V_{OrAbAn}	0	0	0	-1.094	-1.095	-1.095	-0.467	-0.467	-0.467

Model 1 = Ghiorso (1984), Model 2 = Green and Usdansky (1986), Model 3 = Nekvasil and Burnham (1987), Model 4 = Fuhrman and Lindsley (1988), Model 5 = Lindsley and Nekvasil (1989), Model 6 = Elkins and Grove (1990), Model 7 = Benisek et al. (2004) using molecular mixing, Model 8 = Benisek et al. (2004) using Al-avoidance, Model 9 = Benisek et al. (2010); H = Internal energy, S = Entropy, V = Volume; Margules parameters (W) were taken from Wen and Nekvasil (1994) and Benisek et al. (2004, 2010).

estimation of the two-feldspar thermometer for ternary feldspar solid solutions including the resetting correction calculation procedure. In their new developments in two-feldspar thermometry study, Benisek et al. (2004) presented molecular mixing (Table 2, rows 76-78) and Al-avoidance models (Table 2, rows 79-81) with the new and updated Margules parameters. Comparison of temperature values for feldspar compositions from granulite-facies metamorphic rocks indicate that the Benisek et al. (2004) model range halfway between the Fuhrman and Lindsley (1988) and Elkins and Grove (1990) methodologies because they combined those of authors data sets. Benisek et al. (2004) also reported that their temperature values are about 40 ^{o}C higher than the Lindsley and Nekvasil (1989) model. Benisek et al. (2010) presented a new mixing model (see Table 3, Model 9) for high structural state ternary feldspars in the Ab-Or-An system based particularly on the calorimetric and volumetric measurements, compared their methodology with published models, tested it with natural feldspar assemblages from well-studied magmatic and high-grade metamorphic rocks and finally concluded that the model to a large extent eliminates discrepancies between observed and predicted feldspar compositions. They used the asymmetric ternary Margules methodology in their recent model that contains six interaction parameters for each binary plus three ternary interaction parameters. According to Benisek et al. (2010), their calorimetry-based mixing model presents petrologic relationship in ternary feldspars more reliably than those of other mixing models as a result of tested feldspar compositions from fast- and slowly-cooled magmatic, as well as high-grade metamorphic rocks (Table 2, rows 82-84).

In slowly cooled magmatic and high-grade metamorphic

rocks, plagioclase phenocrysts are frequently observed with exsolved alkali feldspars. Because of exsolved alkali feldspars mostly have a high Ca-content in comparison to the low K content of the plagioclases, two-feldspar compositions, in general, do not plot on a common isotherm as a consequence of the slow cooling of the rock as well as the difference in the ease of Na-K and Al-Si exchanges (Benisek et al. 2010). To reach equilibrium during the slow cooling history of rock, plagioclase and alkali feldspar have to minimize their K- and Ca-contents, respectively. Consequently, alkali feldspars generally decompose into plagioclase and K-rich feldspar and thus, they gave rise to development of perthitic exsolution forms, whereas Na-K exchange in plagioclase rarely causes antiperthitic exsolution textures. Taking into account the whole exchanges and exsolution forms of feldspars in slowly cooled high-grade metamorphic rocks, Kroll et al. (1993) suggested that the original compositions of plagioclase and alkali feldspar could be restored by reversing the Na-K exchange event at a constant anorthite content. Finally, three incongruent temperature values in Table 2 (see rows 58-84, except for rows 61-63) have been subjected to the Kroll et al. (1993) correction procedure and obtained congruent temperatures using the Excel's Solver Add-in are listed in rows 85-92 of Table 2. As the Green and Usdansky (1986) model does not require an input pressure value in temperature estimation, the Kroll et al. (1993) correction procedure has been ignored in rows 85-92 of Table 2. The values in rows 93 and 94 of Table 2 show *P*-*T* values used in the pressure- and temperature-dependent equations.

Plagioclase-liquid and alkali feldspar-liquid thermometers

It can be stated that plagioclase-liquid thermometers are among the earliest thermometers developed for igneous systems (Figure 6). In general, early models put into relationship temperature with coexisting plagioclase and liquid compositions using the calibrations at 1-atmosphere experimental conditions (Putirka, 2005; see references therein). Kudo and Weill (1970) developed an empirical thermometer on the basis of plagioclase-magmatic liquid equilibrium using electron microprobe analyses of quenched samples from the experimental studies of natural granitic rocks at water pressure of 0.5 and 1.0 kbar along with earlier data from the equilibrium experiments (see Table 4, row 47). They reported that an application of their thermometer to natural occurrences provided useful information on temperature of equilibration of coexisting plagioclase and liquid in rocks ranging from basalt to rhyolite compositions. Following studies increased the database on pressure and temperature conditions of coexisting plagioclase and liquid pairs.

Putirka (2005) tested existing plagioclase-liquid equilibria models for their ability to recover crystallization temperature of plagioclase from available calibration data set and proposed a model based on the regression analysis of thermodynamically derived partial melting experiments (Putirka, 2005; Model A) to predict temperature with up to 40 % greater precision (Table 4, row 48). Model A was calibrated on basaltic to rhyolitic liquids that crystallized plagioclase from 0.001-13 kbar, 725-1350 ^{o}C and H_2O concentrations up to 15 wt% (Humphreys et al., 2016). If water (H_2O, wt%) content of liquid is absent, Putirka (2005) presented another plagioclase-liquid thermometer (i.e., Model B) as an alternative to Model A (Table 4, row 49). To calculate a plagioclase composition and saturation temperature when pressure (*P*, kbar) and a liquid composition (wt%) are provided, Putirka (2005) also presented a liquid thermometer (i.e., Model D) that predicts temperature to within ±48 ^{o}C for the global LEPR data set (Table 4, row 50). Putirka (2008; Eq. 24a) revised the earlier plagioclase-liquid Model A with a global regression model that yields an approximately 6 ^{o}C improvement in the SSE at which plagioclase should crystallize from a silicate liquid at a given pressure value (Table 4, row 51). Plagioclase-liquid thermometers developed by Putirka (2005; Model A) and Putirka (2008; Eq. 24a) can be compared to the temperature value that is required for a liquid to reach plagioclase saturation. Hence, using the global LEPR data set, Putirka (2008; Eq. 26) proposed a regression model based on liquid compositions that yield a 10 ^{o}C improvement in precision (Table 4, row 52).

Because all these thermometers are pressure (*P*, kbar) sensitive, Putirka (2005; Model C) developed a temperature-dependent barometer for plagioclase-liquid equilibria (Table 4, row 53) that predicts pressure to within *P* (kbar) < 3 and yields poor results for some experiments (see references therein). For alkali feldspar compositions, Putirka (2008) also proposed two new models (Eq. 24b, 24c) based on the albite-liquid equilibrium. As the first model (i.e., Eq. 24b) is calibrated at temperature <1050 °C, with a calibration error of ±23 °C, it may show strong systematic error at temperature >1050 °C (Table 5, row 47). On the other hand, the second model (i.e., Eq. 24c) yields the saturation temperature for alkali feldspar. Thus, the model is independent of alkali feldspar composition (Table 5, row 48).

Plagioclase-liquid and alkali feldspar-liquid hygrometers

Measuring water contents of magmas is an elementary parameter in understanding a number of geological questions. The pre-eruptive water concentration in the melt as well as magma degassing process influence the crystallizing mineral assemblages from melt, thereby

Row		PF1LIQ1	PF2LIQ2	PF3LIQ3	PF4LIQ4	PF5LIQ5	PF6LIQ6	PF7LIQ7	PF8LIQ8	PF9LIQ9	PF10LIQ10
142	$[SiO_2$	71.70	71.91	72.00	70.94	70.67	69.74	70.14	69.69	68.87	69.00
143	TiO_2	0.67	0.62	0.76	0.66	0.86	0.84	0.80	0.72	0.95	1.23
144	Al_2O_3	13.78	13.77	13.82	13.94	13.89	14.05	13.96	14.08	13.61	12.42
145	Cr_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
146	FeO	3.72	3.50	3.77	3.95	3.88	4.46	4.25	4.62	5.53	6.39
147	MnO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
148	MgO	0.61	0.64	0.72	0.80	0.87	0.99	0.96	1.12	0.89	1.09
149	CaO	2.47	2.42	2.62	2.71	2.85	3.11	3.20	3.25	3.71	3.44
150	Na_2O	4.34	4.35	3.58	4.47	4.41	4.19	4.09	4.00	4.04	3.72
151	K_2O	2.70	2.79	2.73	2.52	2.57	2.61	2.59	2.52	2.39	2.70
152	P_2O_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
153	H_2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
154	Anhydrous Total] (%) Liquid	99.99	100.00	100.00	99.99	100.00	99.99	99.99	100.00	99.99	99.99
155											
156	$[SiO_2$ [Cation Fractions [CF]	0.67028	0.67160	0.67722	0.66208	0.65978	0.65225	0.65648	0.65246	0.64707	0.65171
157	TiO_2 [CF] (Liq.)	0.00471	0.00436	0.00538	0.00463	0.00604	0.00591	0.00563	0.00507	0.00671	0.00874
158	$AlO_{3/2}$	0.15182	0.15157	0.15320	0.15333	0.15283	0.15487	0.15399	0.15536	0.15071	0.13826
159	$CrO_{3/2}$	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
160	FeO	0.02908	0.02734	0.02966	0.03083	0.03029	0.03488	0.03327	0.03617	0.04345	0.05047
161	MnO	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
162	MgO	0.00850	0.00891	0.01010	0.01113	0.01211	0.01380	0.01339	0.01563	0.01247	0.01535
163	CaO	0.02474	0.02422	0.02640	0.02710	0.02851	0.03116	0.03209	0.03260	0.03735	0.03481
164	$NaO_{0.5}$	0.07866	0.07877	0.06529	0.08089	0.07983	0.07598	0.07422	0.07261	0.07360	0.06812
165	$KO_{0.5}$	0.03220	0.03324	0.03276	0.03000	0.03061	0.03114	0.03093	0.03010	0.02865	0.03253
166	$PO_{5/2}$] Liquid	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
167											
168	$[T_{KW70}$	1163	1157	1167	1182	1189	1222	1182	1201	1188	1178
169	$T_{P05ModelA}$	1030	1027	1039	1039	1044	1056	1054	1058	1060	1039
170	$T_{P05ModelB}$	905	904	889	930	929	939	925	936	961	1008
171	$T_{P05ModelD}$	1019	1018	1021	1026	1027	1035	1034	1037	1037	1016
172	$T_{P08Eq24a}$	1011	1006	1016	1024	1031	1045	1040	1046	1051	1032
173	$T_{P08Eq26}$] Plagioclase-Liquid	1016	1014	1011	1028	1030	1037	1035	1039	1047	1036
174											
175	[$P_{P05ModelC}$ (kbar)] Plagioclase-Liquid	3.04	3.27	3.20	2.17	2.33	1.33	2.90	1.82	2.05	0.59
176											
177	$[H_2O_{P05ModelH}$	0.60	0.53	0.74	0.55	0.56	0.27	0.68	0.51	0.95	0.15
178	$H_2O_{P08Eq25b}$	2.66	2.61	3.21	3.18	3.25	2.59	2.54	2.69	2.39	1.72
179	H_2O_{LFH09}	3.42	3.38	3.54	3.68	3.72	3.32	2.92	3.04	2.70	2.47
180	H_2O_{WL15}	2.54	2.45	3.13	2.95	3.15	2.71	2.36	2.53	2.27	2.21
181	H_2O_{UM19}] Plagioclase-Liquid	3.61	3.46	4.52	4.24	4.54	3.87	3.32	3.59	3.17	3.06

Figure 6. Screenshot of liquid compositions, cation fraction values, plagioclase-liquid thermometers, plagioclase-liquid barometer and plagioclase-liquid hygrometers by program in the *Transpose* tab. Plagioclase and liquid analyses are taken from Araya et al. (2019).

controlling both geochemical trends and eruptive styles (Fiedrich et al., 2018). Pre-eruptive concentrations can be determined by measuring melt inclusions or fresh, undegassed glass using different instrumental methods (e.g., Secondary ion mass spectrometry, Raman spectroscopy and Fourier-transform infrared spectroscopy). Alternatively, pre-eruptive water concentrations can be estimated thanks to phase equilibria including various mineral and melt analyses such as plagioclase-liquid and alkali feldspar-liquid compositions. Among plagioclase-liquid hygrometers, the models proposed by Putirka (2008), Lange et al. (2009), Waters and Lange (2015) and Masotta and Mollo (2019) are semi-empirical models derived by global regression analysis of a broad calibration data set, including plagioclase-bearing experiments conducted under variable P-T-H_2O conditions.

Putirka (2005) developed an empirical hygrometer (i.e., Model H) taking into account the effect of water contents on plagioclase-melt equilibria (Table 4, row 54). Because of the Model H tends to over-predict water contents based on the LEPR-derived data set, Putirka (2008; Eq. 25b) proposed a new global calibration that yields within ±1.1 wt% H_2O for 730 hydrous experimental data, and recovers a mean H_2O content of 0.04±1.0 wt% for 825 anhydrous compositions (Table 4, row 55). Lange et al. (2009) presented a hygrometer (Table 4, row 56) which is calibrated on 71 plagioclase-liquid experiments consisting

Table 4. Calculation of selected plagioclase and liquid analyses (wt%) with structural formulae (*apfu*) of plagioclase compositions and components (Ab, Or, An), plagioclase-liquid thermometers (°C), plagioclase-liquid barometer (kbar) and hygrometers (H_2O, wt%) by WinFeldth program.

Row	Plagioclase	PF1	PF2	PF3	PF4	PF5	PF6	PF7	PF8	PF9	PF10
1	SiO_2	58.96	57.47	58.65	54.29	54.24	56.37	54.89	54.08	52.81	49.10
2	TiO_2	0.05	0.08	0.05	0.03	0.04	0.05	0.04	0.19	0.05	0.05
3	Al_2O_3	25.24	26.28	26.02	29.03	28.84	27.61	27.94	27.37	28.60	30.86
4	FeO_{tot}	0.67	0.97	0.51	0.70	0.88	0.57	0.81	1.21	1.04	1.18
5	MnO	0.01	0.02	0.01	0.03	0.02	0.02	0.00	0.00	0.00	0.00
6	MgO	0.05	0.10	0.02	0.06	0.07	0.04	0.09	0.17	0.13	0.13
7	CaO	6.80	7.98	7.07	10.91	10.86	9.56	10.25	10.56	12.04	15.09
8	Na_2O	6.11	5.53	6.05	4.50	4.40	5.17	4.66	4.90	4.48	2.89
9	K_2O	1.98	1.61	1.76	0.81	0.78	1.13	0.98	0.69	0.49	0.20
10	∑ (wt%)	99.87	100.04	100.14	100.36	100.13	100.52	99.66	99.17	99.64	99.50
11	Si	2.654	2.591	2.630	2.451	2.455	2.531	2.493	2.478	2.416	2.269
12	Ti	0.002	0.003	0.002	0.001	0.001	0.002	0.001	0.007	0.002	0.002
13	Al	1.339	1.396	1.375	1.545	1.538	1.461	1.495	1.478	1.542	1.681
14	Fe	0.025	0.037	0.019	0.026	0.033	0.021	0.031	0.046	0.040	0.046
15	Mn	0.000	0.001	0.000	0.001	0.001	0.001	0.000	0.000	0.000	0.000
16	Mg	0.003	0.007	0.001	0.004	0.005	0.003	0.006	0.012	0.009	0.009
17	Ca	0.328	0.386	0.340	0.528	0.527	0.460	0.499	0.518	0.590	0.747
18	Na	0.533	0.483	0.526	0.394	0.386	0.450	0.410	0.435	0.397	0.259
19	K	0.114	0.093	0.101	0.047	0.045	0.065	0.057	0.040	0.029	0.012
20	∑ (*apfu*)	4.998	4.996	4.994	4.996	4.991	4.994	4.992	5.014	5.024	5.024
21	∑ T site (*apfu*)	4.024	4.034	4.028	4.028	4.033	4.019	4.026	4.020	4.008	4.006
22	∑ M site (*apfu*)	0.975	0.962	0.966	0.968	0.958	0.975	0.966	0.994	1.016	1.018
23	Ab	0.547	0.503	0.544	0.407	0.403	0.462	0.425	0.438	0.391	0.254
24	Or	0.117	0.096	0.104	0.048	0.047	0.066	0.059	0.041	0.028	0.012
25	An	0.336	0.401	0.352	0.545	0.550	0.472	0.516	0.522	0.581	0.734
	Liquid	Liq1	Liq2	Liq3	Liq4	Liq 5	Liq 6	Liq 7	Liq 8	Liq 9	Liq 10
26	SiO_2	64.34	63.16	64.45	62.79	62.60	62.22	61.82	63.92	62.81	62.02
27	TiO_2	0.29	0.37	0.28	0.31	0.32	0.43	0.33	0.43	0.58	0.63
28	Al_2O_3	17.99	17.25	18.01	17.32	17.37	16.99	17.42	19.61	19.79	19.18
29	FeO	1.71	2.35	1.73	2.10	2.13	2.64	2.87	1.71	1.98	2.38
30	MnO	0.02	0.11	0.04	0.14	0.05	0.15	0.12	0.00	0.00	0.00
31	MgO	0.47	0.81	0.52	0.72	0.88	1.06	1.21	0.80	0.71	1.28
32	CaO	1.74	1.98	1.91	1.65	2.20	2.62	3.12	2.76	3.53	4.58
33	Na_2O	4.49	4.69	4.41	4.39	4.35	4.29	4.26	5.69	5.83	5.63
34	K_2O	7.54	7.05	7.42	7.27	6.48	6.39	6.09	4.87	4.50	3.94
35	H_2O	1.37	2.20	1.27	2.96	3.50	2.23	2.63	5.75	6.65	6.56
	∑ Anhyd. (wt%)	99.64	97.77	98.77	96.69	96.38	96.79	97.24	99.79	99.73	99.64
36	SiO_2	0.59521	0.58894	0.59563	0.59270	0.59333	0.58832	0.58169	0.58014	0.57042	0.56460
39	TiO_2	0.00202	0.00260	0.00195	0.00220	0.00228	0.00306	0.00234	0.00294	0.00396	0.00431
40	$AlO_{3/2}$	0.19614	0.18957	0.19616	0.19269	0.19403	0.18933	0.19318	0.20976	0.21182	0.20579
41	FeO	0.01323	0.01833	0.01337	0.01658	0.01688	0.02088	0.02258	0.01298	0.01504	0.01812

Table 4. ... Continued

Row	Liquid	Liq1	Liq2	Liq3	Liq4	Liq 5	Liq 6	Liq 7	Liq 8	Liq 9	Liq 10
42	MnO	0.00016	0.00087	0.00031	0.00112	0.00040	0.00120	0.00096	0.00000	0.00000	0.00000
43	MgO	0.00648	0.01126	0.00716	0.01013	0.01243	0.01494	0.01697	0.01082	0.00961	0.01737
44	CaO	0.01725	0.01978	0.01891	0.01669	0.02234	0.02654	0.03146	0.02684	0.03435	0.04467
45	$NaO_{0.5}$	0.08053	0.08479	0.07902	0.08034	0.07994	0.07865	0.07772	0.10013	0.10266	0.09937
46	$KO_{0.5}$	0.08898	0.08386	0.08748	0.08755	0.07835	0.07708	0.07310	0.05639	0.05214	0.04576
Plagioclase-liquid and plagioclase saturation thermometers (°C)											
47	T_{KW70}	1216	1240	1211	1320	1291	1239	1251	1281	1294	1355
48	$T_{P05\ Model\ A}$	1012	986	1020	959	957	1002	1003	907	896	914
49	$T_{P05\ Model\ B}$	854	912	859	972	944	933	939	924	940	939
50	$T_{P05\ Model\ D}$	1043	1008	1049	982	971	1014	1012	926	910	915
51	$T_{P08\ Eq24a}$	965	953	972	928	935	972	979	908	904	928
52	$T_{P08\ Eq26}$	956	947	962	919	920	960	959	897	890	909
Plagioclase–liquid barometer (kbar)											
53	$P_{P05\ Model\ C}$	9.14	6.74	9.46	1.45	3.30	6.66	6.79	3.91	4.59	4.25
Plagioclase-liquid hygrometers (H_2O, wt%)											
54	$H_2O_{P05\ Model\ H}$	2.50	2.11	2.60	1.04	1.94	2.21	2.63	4.42	5.09	4.25
55	$H_2O_{P08\ Eq25b}$	1.22	1.15	1.41	0.58	1.55	1.35	1.83	5.05	5.54	5.19
56	H_2O_{LFH09}	3.73	3.76	3.61	4.67	4.23	3.23	3.28	6.01	6.14	5.73
57	H_2O_{WL15}	1.44	1.68	1.46	2.28	2.35	1.60	1.85	4.44	4.92	4.83
58	H_2O_{MM19}	1.65	2.11	1.70	3.19	3.29	1.96	2.43	6.29	6.87	6.77
59	Input *P* (kbar)	1.50	1.50	1.50	1.50	1.50	1.50	1.50	2.02	2.02	1.70
60	Input *T* (°C)	1000	1000	1000	1000	1000	1020	1020	900	900	950

PF1-PF10 to Liq1-Liq10 pairs from Masotta and Mollo (2019); *apfu* = Atomic per formula unit, Ab = albite, Or = orthoclase and An = anorthite, Anhyd. = Anhydrous; Plagioclase analyses are estimated on the basis of 8 oxygens (see rows 11-19); Rows 36 to 46 show cation fractions of liquid compositions; Plagioclase-liquid thermometers of T_{KW70} (row 47) from Kudo and Weill (1970), $T_{P05\ Model\ A}$ (row 48) from Putirka (2005), $T_{P05\ Model\ B}$ (row 49) from Putirka (2005), Plagioclase saturation of $T_{P05\ Model\ D}$ (row 50) from Putirka (2005), Plagioclase-liquid thermometer of $T_{P08\ Eq24a}$ (row 51) from Putirka (2008), Plagioclase saturation of $T_{P08\ Eq26}$ (row 52) from Putirka (2008); Plagioclase-liquid barometer of $P_{P05\ Model\ C}$ (row 53) from Putirka (2005); Plagioclase-liquid hygrometers of $H_2O_{P05\ Model\ H}$ (row 54) from Putirka (2005); $H_2O_{P08\ Eq25b}$ (row 55) from Putirka (2005); H_2O_{LFH09} (row 56) from Lange et al. (2009); H_2O_{WL15} (row 57) from Waters and Lange (2015) based on the second-degree polynomial equation [H_2O_{WL15} (wt%) = 0.7047 + 0.3930H_2O_{MM19} + 0.0320$H_2O_{MM19}^2$] using the water contents by the Masotta and Mollo (2019) model; H_2O_{MM19} (row 58) from Masotta and Mollo (2019); Input pressure (kbar) and temperature (°C) values (from Masotta and Mollo 2019) in rows 59 and 60 are used in the necessary calculations of pressure- and temperature-dependent equations.

of 45 hydrous and 26 anhydrous data set that spans a wide range of liquid (46-74 wt% SiO_2; i.e., metaluminous basalts through rhyolites in equilibrium with An_{95}-An_{35}) and plagioclase compositions (An_{93}-An_{37}), temperatures (825-1230 °C), pressures (0-3 kbar) and dissolved melt water concentrations (0-7 wt% H_2O). The Lange's thermodynamic model (Lange et al., 2009) also produces the smallest SSE of water content (0.313 H_2O wt%) and the smallest recovered temperature range (±21 °C), if the model is treated as a thermometer (Zeng et al., 2014). Waters and Lange (2015) used expanded data set including 214 plagioclase-liquid equilibrium pairs from 40 experimental studies in the literature and recalibrated the thermodynamic model for the plagioclase-liquid hygrometer of Lange et al. (2009). An updated model is applicable to metaluminous and alkaline magmas that considers all available volumetric and calorimetric data for the pure end-member components. The Waters and Lange (2015) model takes into account a wide range in liquid and (45-80 wt% SiO_2; 1-10 wt% Na_2O+K_2O) plagioclase (An_{17-95}) compositions as well as temperature (750-1244 °C), pressure (0.0-3.5 kbar) and H_2O (0.0-8.3 wt%) contents. The SSE estimate on the hygrometer model is 0.35 wt% H_2O and application of the model as

Table 5. Calculation of selected alkali feldspar and liquid analyses (wt%) with structural formulae (*apfu*) of alkali feldspar compositions and components (Ab, Or, An), alkali feldspar-liquid and alkali feldspar saturation thermometers (°C) together with alkali feldspar-liquid hygrometer (H_2O, wt%) by WinFeldth program.

Row	Alkali feldspar	AF1	AF2	AF3	AF4	AF5	AF6	AF7	AF8	AF9	AF10
1	SiO_2	62.22	60.78	64.48	64.29	66.07	63.82	66.00	64.90	65.20	63.70
2	TiO_2	0.10	0.19	0.00	0.00	0.00	0.00	0.12	0.09	0.38	0.16
3	Al_2O_3	20.07	20.72	19.72	19.02	19.87	18.83	19.07	20.22	19.18	19.32
4	FeO_{tot}	0.31	0.73	0.51	0.43	0.26	0.26	0.67	0.49	1.24	1.07
5	MnO	0.01	0.01	0.06	0.04	0.08	0.03	0.01	0.00	0.00	0.00
6	MgO	0.00	0.05	0.01	0.00	0.01	0.01	0.00	0.01	0.19	0.28
7	CaO	0.99	2.18	1.13	0.87	0.82	0.91	0.28	1.11	1.34	1.71
8	Na_2O	1.82	2.40	5.60	5.76	4.76	1.94	6.26	8.55	7.58	7.69
9	K_2O	12.30	11.02	7.67	7.44	7.84	12.78	8.03	4.47	4.39	4.15
10	∑ (wt%)	97.82	98.08	99.18	97.85	99.71	98.58	100.44	99.84	99.50	98.08
11	Si	2.911	2.846	2.933	2.958	2.968	2.965	2.967	2.910	2.934	2.911
12	Ti	0.004	0.007	0.000	0.000	0.000	0.000	0.004	0.003	0.013	0.006
13	Al	1.107	1.143	1.057	1.031	1.052	1.031	1.010	1.068	1.017	1.041
14	Fe	0.012	0.029	0.019	0.017	0.010	0.010	0.025	0.018	0.047	0.041
15	Mn	0.000	0.000	0.002	0.002	0.003	0.001	0.000	0.000	0.000	0.000
16	Mg	0.000	0.003	0.001	0.000	0.001	0.001	0.000	0.001	0.013	0.019
17	Ca	0.050	0.109	0.055	0.043	0.039	0.045	0.013	0.053	0.065	0.084
18	Na	0.165	0.218	0.494	0.514	0.415	0.175	0.546	0.743	0.661	0.681
19	K	0.734	0.658	0.445	0.437	0.449	0.757	0.461	0.256	0.252	0.242
20	∑ (*apfu*)	4.982	5.014	5.007	5.001	4.938	4.986	5.027	5.052	5.001	5.025
21	∑ T site (*apfu*)	4.033	4.028	4.013	4.008	4.034	4.008	4.007	4.000	4.023	4.017
22	∑ M site (*apfu*)	0.949	0.985	0.994	0.994	0.903	0.978	1.020	1.052	0.978	1.007
23	Ab	0.174	0.221	0.497	0.517	0.459	0.179	0.535	0.706	0.676	0.677
24	Or	0.774	0.668	0.448	0.440	0.497	0.775	0.452	0.243	0.258	0.240
25	An	0.052	0.111	0.055	0.043	0.044	0.046	0.013	0.051	0.066	0.083
	Liquid	Liq1	Liq2	Liq3	Liq4	Liq5	Liq6	Liq7	Liq8	Liq9	Liq10
26	SiO_2	58.82	58.65	60.39	62.19	63.10	64.90	61.41	62.00	61.40	62.10
27	TiO_2	0.40	0.54	0.21	0.34	0.11	0.24	0.50	0.46	0.31	0.45
28	Al_2O_3	20.61	20.16	19.75	19.07	20.15	18.94	19.40	20.60	19.80	20.20
29	FeO	2.46	2.89	2.09	1.77	1.69	1.61	0.14	1.77	2.30	1.86
30	MnO	0.13	0.16	0.27	0.22	0.21	0.15	0.53	0.13	0.14	0.12
31	MgO	0.18	0.21	0.12	0.22	0.06	0.18	0.22	0.20	0.21	0.26
32	CaO	2.88	3.11	1.41	1.59	0.93	1.75	2.70	0.56	0.61	0.71
33	Na_2O	4.71	5.04	9.25	7.82	8.10	5.48	9.80	8.90	9.50	9.10
34	K_2O	9.77	9.18	6.50	6.76	5.64	6.74	5.30	5.40	5.70	5.20
35	P_2O_5	0.04	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
36	∑ (wt%)	100.00	100.00	99.99	99.98	99.99	99.99	100.00	100.02	99.97	100.00
37	SiO_2	0.53201	0.53054	0.53105	0.55327	0.56085	0.58870	0.53774	0.54742	0.54017	0.54796
38	TiO_2	0.00272	0.00367	0.00139	0.00228	0.00074	0.00164	0.00329	0.00306	0.00205	0.00299
39	$AlO_{3/2}$	0.21970	0.21493	0.20469	0.19995	0.21108	0.20248	0.20021	0.21437	0.20530	0.21007
40	FeO	0.01861	0.02186	0.01537	0.01317	0.01256	0.01221	0.00103	0.01307	0.01692	0.01373

Table 5. ... Continued

Row	Liquid	Liq1	Liq2	Liq3	Liq4	Liq5	Liq6	Liq7	Liq8	Liq9	Liq10
41	MnO	0.00100	0.00123	0.00201	0.00166	0.00158	0.00115	0.00393	0.00097	0.00104	0.00090
42	MgO	0.00243	0.00283	0.00157	0.00292	0.00080	0.00243	0.00287	0.00263	0.00275	0.00342
43	CaO	0.02791	0.03014	0.01329	0.01516	0.00886	0.01701	0.02533	0.00530	0.00575	0.00671
44	$NaO_{0.5}$	0.08260	0.08839	0.15771	0.13489	0.13959	0.09638	0.16638	0.15236	0.16204	0.15569
45	$KO_{0.5}$	0.11273	0.10594	0.07292	0.07672	0.06395	0.07800	0.05921	0.06083	0.06397	0.05854
46	$PO_{5/2}$	0.00031	0.00046	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Alkali feldspar-liquid and alkali feldspar saturation thermometers (ºC)											
47	$T_{P08\ Eq24b}$	577	518	996	978	883	768	605	861	914	872
48	$T_{P08\ Eq24c}$	647	581	1014	980	929	938	836	813	850	883
Alkali feldspar-liquid hygrometer (H_2O, wt%)											
49	$H_2O_{M15\ Eq1}$	4.55	3.20	5.84	5.00	8.50	6.55	5.25	4.74	3.60	3.47
50	Input *P* (kbar)	3	3	0.5	0.5	2	1.5	1	1	2	2
51	Input *T* (ºC)	900	900	810	840	745	825	775	850	900	875

AF1-AF10 to Liq1-Liq10 pairs from Mollo et al. (2015); *apfu* = Atomic per formula unit, Ab = albite, Or = orthoclase and An = anorthite; Alkali feldspar analyses are estimated on the basis of 8 oxygens (see rows 11-19); Rows 37 to 46 show cation fractions of liquid compositions; Alkali feldspar-liquid thermometer of $T_{P08\ Eq24b}$ (row 47) from Putirka (2008); Alkali feldspar saturation thermometer of $T_{P08\ Eq24c}$ (row 48) from Putirka (2008); $H_2O_{M15\ Eq1}$ (row 49) from Mollo et al. (2015); Input pressure (kbar) and temperature (ºC) values (from Mollo et al. 2015) in rows 50 and 51 are used in the necessary calculations of pressure- and temperature-dependent equations.

a thermometer recovers temperatures to within ±12 °C. WinFeldth estimates the Waters and Lange (2015) model (Table 4, row 57) based on the second-degree polynomial equation [H_2O_{WL15} (wt%) = 0.7047 + 0.3930H_2O_{MM19} + 0.0320$H_2O_{MM19}^2$] using the water content by the Masotta and Mollo (2019) approach.

Masotta and Mollo (2019) presented a new empirical plagioclase-liquid hygrometer to estimate the H_2O (wt%) content dissolved in trachytic magmas using as the starting composition of trachytic lava from Vulcano Island, Southern Italy (Table 4, row 58). The model takes into account the exchange reaction of the anorthite component between plagioclase and liquid as well as the albite component in plagioclase and the alkali fraction in the melt. An empirical plagioclase-liquid hygrometer is calibrated using crystallization experiments where the concentration of H_2O in quenched glasses has been accurately determined based on Fourier Transform Infrared Spectroscopy (FTIR) analysis. The model, which was obtained at 1.5-2.02 kbar, 850-1020 ºC, 1.17-7.57 wt% H_2O and ΔNNO + 2.5 buffer conditions, considers the exchange reaction of the anorthite component between plagioclase and liquid as well as the albite component in plagioclase and alkali fraction in the melt with a calibration uncertainty of ±0.29 wt% H_2O.

When compared to hygrometers, which are based on the plagioclase-liquid exchange between anorthite and albite components, the alkali feldspar-liquid ones are scarce. Mollo et al. (2015) developed an alkali feldspar-liquid hygrometer (Table 5, row 49) using the calibration of regression analysis of sanidine and anorthoclase crystals coexisting with trachyte and phonolite melts. Content of melt is one of the most important parameters in highly explosive eruptions. Hence, the model presented by Mollo et al. (2015) is applicable particularly to alkaline differentiated magmas. The data set used to calibrate the alkali feldspar-liquid hygrometer comprise experimental data from previous studies that cover 0.5-3.0 kbar, 700-950 ºC, 2-9.5 wt% H_2O, liquid composition (57.8-69 wt% SiO_2; 10.9-16.1 wt% Na_2O+K_2O) and QFM-NNO+1.5 fO_2 conditions.

SUMMARY AND AVAILABILITY OF THE PROGRAM

WinFeldth is a user-friendly package for compositions of plagioclase-alkali feldspar, plagioclase-liquid and alkali feldspar-liquid pairs, which is developed for personal computers running in the Windows operating system. The program calculates structural formulae of multiple two-feldspar analyses based on 8 or optionally 32 oxygens normalization schemes. WinFeldth presents two main windows. The first window (i.e., *Data Entry Screen*) appears on the screen with several pull-down menus and equivalent shortcuts. By selecting options or clicking buttons on the start-up screen, the user can enter or load

plagioclase, alkali feldspar and liquid analyses into the data entry section and make necessary arrangements for a desired calculation scheme on the toolbar. For example, by clicking the *Calculate* icon (i.e., Σ) on the toolbar in the *Data Entry Screen* window, all calculated parameters are displayed in the second window. The second window (i.e., *Calculation Screen*) show all the input and results of cations (*apfu*) and cation fractions of two-feldspars and liquid compositions, feldspar components (Ab, Or, An and Cn), various two-feldspar thermometers as well as thermometers based on the thermodynamic modelling of ternary feldspars, plagioclase-liquid thermometers and hygrometers, plagioclase-liquid barometer, alkali feldspar-liquid thermometers and hygrometer.

The program reports the output in a tabulated form with columns numbered from 1 to 201 in the *Calculation Screen* window as well as in an output Excel file. All the estimated feldspars and liquid data in the *Calculation Screen* can be sent to a Microsoft Excel file (i.e., Output.xlsx) and then this file can be used for further data manipulation, graphing and preparing a quick table for publication and presentation purposes. WinFeldth displays calculated feldspar compositions in binary and ternary diagrams, which can be viewed and printed by the Grapher program of Golden software. These plots appear on the screen by selecting desired diagram type from the pull-down menu of *Graph* in the *Calculation Screen* window. WinFeldth is a compiled program that consists of a self-extracting setup file (Electronic Supplementary Material, ESM 2) including all the necessary support files (i.e., with the extension of ".dll" and ".ocx" files) for the 32-bit system. If the Microsoft® Visual Studio package is not installed on the computer, all these support files are used by the program for proper execution. During the setup procedure, the program and its associated files (i.e., support files, help file, data files with the extensions of ".pal", ".xls", ".xlsx" and plot files with the extension of ".grf") are installed into the personal computer's "C:\Program Files\WinFeldth" folder with the Windows XP or later operating systems. However, an installation of the program into a personal computer with the 64-bit operating system may require the msflexgrd adjustment. This procedure is explained in detail in Electronic Supplementary Material (ESM 3) for the users. The self-extracting setup file is approximately 24 Mb and may be downloaded from the journal server.

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