Original paper

WinMIgob: A Windows program for magnetite–ilmenite geothermometer and oxygen barometer†

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A Microsoft® Visual Basic software, called WinMIgob, has been developed for wet-chemical and electron-microprobe compositions of coexisting magnetite–ulvöspinel and ilmenite–hematite solid solutions to calculate the temperature (*T*, °C) and oxygen fugacity (fO_2) conditions of magmatic and metamorphic rocks. The program allows the users to enter total of 34 input variables, including Sample No, SiO_2, TiO_2, Al_2O_3, V_2O_3, Cr_2O_3, Nb_2O_3, Fe_2O_3, FeO, MnO, NiO, ZnO, MgO, CaO, Na_2O, K_2O, BaO (wt. %) for each magnetite and ilmenite compositional data. WinMIgob enables to enter and load multiple magnetite and ilmenite analyses in the program's data entry section. Alternatively, the composition of magnetite–ilmenite pairs can be typed in a blank Excel file as in the above order and then loaded into the program's data entry screen for data processing. The ferric and ferrous iron contents from microprobe-derived total FeO (wt. %) of magnetite–ilmenite compositions are estimated by stoichiometric constraints based on three different approaches. Using the calculated multiple magnetite and ilmenite analyses, WinMIgob estimates molecular (%) and mole fractions of magnetite, uvöspinel, ilmenite and hematite amounts. The program evaluates fourteen magnetite–ilmenite geothermometers, thirteen oxygen barometers and six relative to the nickel–nickel oxide (NNO) buffer values based on the different calibrations with various calculation methods. WinMIgob also allows the users to check if their magnetite–ilmenite pairs taken from rocks are within or departure from the Bacon–Hirschmann Mg/Mn exchange equilibrium line ± 2σ level. 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, test data files and graphic files, which are intended to produce a high-quality printout.

Keywords: magnetite, ilmenite, geothermometer, oxygen fugacity, Bacon–Hirschmann, software
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1. Introduction

The two most common Fe–Ti oxide minerals with magnetite–ulvöspinel (mt_{ss}) and ilmenite–hematite (ilm_{ss}) solid solutions, hereafter referred to as magnetite and ilmenite, respectively, in a variety of rocks and mineral deposits provide the earth scientists valuable information about the temperature of equilibration and corresponding oxygen fugacity conditions (Misra 2012). Consequently, magnetite–ilmenite geothermometry and oxygen barometry have been studied and used widely in igneous and metamorphic petrology with numerous refinements to model the exchange and oxidation reactions since its conception was established in the early 1960s to estimate temperature and oxygen fugacity values, especially for extrusive and hypabyssal igneous rocks that were subjected to the relatively rapid cooling process (Buddington and Lindsley 1964; Carmichael 1967; Anderson 1968; Powell and Powell 1977; Spencer and Lindsley 1981; Lindsley and Spencer 1982; Stormer 1983; Andersen and Lindsley 1988; Ghiorso and Sack 1991; Lattard et al. 2005; Ghiorso and Evans 2008; Sauerzapf et al. 2008). However, at relatively temperature conditions of slow cooling of magmatic rocks or hydrothermal alteration, these minerals tend to display oxide–oxide, intraoxide and oxide–silicate re-equilibration processes after their crystallization history (Venezky and Rutherford 1999). Accordingly, Fe–Ti oxide minerals used in magnetite–ilmenite geothermometry and oxygen barometry studies rarely preserve their magmatic compositions in slowly cooled plutonic or hydrothermal rocks. Therefore, their application to plutonic igneous rocks and mineral deposits should be considered with caution (Misra 2012; Wang et al. 2014). On the other hand, in many natural magmas, magnetite and ilmenite may not have coprecipitated. Thus, an absence of ilmenite in these rocks prevents the application of magnetite–ilmenite oxygen barometry technique but allows to estimate it based on Fe and Ti's partitioning between magnetite and silicate melt (Arató and Audétat 2017).

The magnetite–ilmenite geothermometer and oxygen barometer model, on a graphical solution, by Buddington and Lindsley (1964), was one of the first calibrated study based on temperature and redox-sensitive equilibria between magnetite–ulvöspinel and ilmenite–hematite solid solutions in the $FeO–Fe_2O_3–TiO_2$ system. Ghiorso and Carmichael (1981) developed a Fortran IV program for the calculation of temperature and oxygen fugacity using the mole fractions of ulvöspinel (Fe_2TiO_4) and hematite (Fe_2O_3) from compositions of coexisting Fe–Ti oxide pairs in rocks. Their approach depends essentially on the graphical interpolation from published smoothed calibration curves by Buddington and Lindsley (1964). Rao et al. (1991) presented an interactive Basic program of Fe–Ti oxide thermometry, called ITHERM, to calculate temperatures of equilibrium using the methods of Powell and Powell (1977), Spencer and Lindsley (1981), and Andersen and Lindsley (1985). Lepage (2003) developed an Excel spreadsheet (ILMAT) solely on the magnetite–ilmenite geothermometry, but also calculating oxygen fugacity based on the empirical approach proposed by several authors (e.g., Spencer and Lindsley 1981; Andersen and Lindsley 1985). The logic of ILMAT was taken from ITHERM (Rao et al. 1991) with revision and correction on magnetite–ilmenite geothermometry estimations. Hora et al. (2013) presented three Excel spreadsheets for two mineral pairs, including magnetite–ilmenite (Ghiorso and Evans 2008), amphibole–plagioclase (Holland and Blundy 1994) and two feldspar (Putirka 2008) geothermometers with a technique facilitating geothermobarometry estimations on a large number of analyses. When compared to the other two amphibole–plagioclase and two feldspar geothermometers, magnetite–ilmenite geothermometer approach uses an AppleScript to transfer input magnetite and ilmenite analyses from Mac OSX Excel to the standalone application and to receive the calculated results back to the Excel platform (Hora et al. 2013).

In this paper, a new computer program, called WinMIgob, is developed using the Microsoft® Visual Basic programming language to calculate multiple magnetite and ilmenite mineral oxides, up to 350 analyses in each program execution, obtained by both wet-chemical and electron-microprobe techniques. The logic of WinMIgob is based on ILMAT, an Excel spreadsheet developed by Lepage (2003), with additional recent magnetite–ilmenite geothermometers and oxygen barometers (e.g., Sauerzapf et al. 2008). The program recalculates magnetite mineral analyses to four oxygens and three total cations and ilmenite analyses to three oxygens and two total cations. WinMIgob is capable of estimating the Fe^{3+} and Fe^{2+} contents from electron microprobe-derived total FeO (wt. %) analysis based on stoichiometric considerations using different procedures outlined by Carmichael (1967), Stormer (1983) and Droop (1987). Using the recalculated magnetite and ilmenite compositions, the program provides users various geothermometer (T, °C), oxygen fugacity (log fO_2) and relative to the nickel–nickel oxide (NNO) buffer (ΔNNO) estimations (e.g., Powell and Powell 1977; Spencer and Lindsley 1981; Andersen and Lindsley 1985; Sauerzapf et al. 2008). WinMIgob also calculates magnetite–ilmenite geothermometer and ΔNNO developed by Ghiorso and Evans (2008) based on the selected magnetite–ilmenite analyses from literature through linear regression equations between the Andersen and Linsdley (1985) and Sauerzapf et al. (2008) calibrations. WinMIgob provides the user to display magnetite–ilmenite compositions in various binary (e.g., T (°C)–log fO_2) and ternary (e.g., $Ti–R^{2+}–R^{3+}$) diagrams by using the Golden Software's Grapher program. Compared to the previously published computer programs and Excel spreadsheets on Fe–Ti oxides, the current version of program presents of the quick evaluation and comparison of multiple magnetite–ilmenite analyses for numerous geothermometry and oxygen fugacity calculations.

2. Program description

In comparison of executable computer programs and Excel spreadsheets solely based on the calculation and classification of rock-forming silicate group minerals, a limited number of studies appeared in literature for geothermobarometry estimations (e.g., Yavuz 1998; Putirka 2008; Hora et al. 2013; Yavuz 2013; Lanari et al. 2014; Yavuz and Döner 2017; Li et al. 2019; Yavuz and Yıldırım 2020).

WinMIgob is a compiled program presented for running in the Microsoft® Windows platform to estimate the different Fe–Ti oxide geothermometer and oxygen fugacity calibrations. The program comes up with a self–extracting setup file (≈20 Mb), which is created by the Inno Setup Compiler (https://jrsoftware.org/isinfo.php). It runs as a single executable file, WinMIgob.exe (3.17 Mb), on the condition that 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 WinMIgob 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. A list of the calculation steps in the program's *Calculation Screen* and in an Excel output file is given in Tab. 1. The current version of the program presents ten binary and ternary magnetite–ilmenite–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 WinMIgob.

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

Row	Explanation	Column numbers
1	Major oxide magnetite mineral analyses (wt. %)	1–17
2	Stoichiometric Fe_2O_3 and FeO (wt. %) contents from microprobe magnetite analyses	18–19
3	Recalculated cations of magnetite mineral analyses (*apfu*)	20–36
4	Blank	37
5	Major oxide ilmenite mineral analyses (wt. %)	38–55
6	Stoichiometric Fe_2O_3 and FeO (wt. %) contents from microprobe ilmenite analyses	56–57
7	Recalculated cations of ilmenite mineral analyses (*apfu*)	58–74
8	Blank	75
9	Sum of atomic mole proportion of magnetite and ilmenite analyses	76–77
10	Molecular ulvöspinel and magnetite amounts (%) by Carmichael (1967)	78–79
11	Molecular ilmenite and hematite amounts (%) by Carmichael (1967)	80–81
12	Molecular ulvöspinel and ilmenite amounts (%) by Anderson (1968)	82–83
13	Molecular ulvöspinel and ilmenite amounts (%) by Lindsley and Spencer (1982)	84–85
14	Molecular ulvöspinel and ilmenite amounts (%) by Stormer (1983)	86–87
15	Mole fraction of ulvöspinel and magnetite amounts by Spencer and Lindsley (1981)	88–89
16	Mole fraction of ilmenite and hematite amounts by Spencer and Lindsley (1981)	90–91
17	Mole fraction of ulvöspinel and magnetite amounts by Sauerzapf et al. (2008)	92–93
18	Mole fraction of ilmenite and hematite amounts by Sauerzapf et al. (2008)	94–95
19	Blank	96
20	Magnetite–ilmenite geothermometer (°C) by Powell and Powell (1977) using the Carmichael (1967) calculation method	97
21	Magnetite–ilmenite geothermometer (°C) by Powell and Powell (1977) using the Anderson (1968) calculation method	98
22	Magnetite–ilmenite geothermometer (°C) by Powell and Powell (1977) using the Lindsley and Spencer (1982) calculation method	99
23	Magnetite–ilmenite geothermometer (°C) by Powell and Powell (1977) using the Stormer (1983) calculation method	100
24	Magnetite–ilmenite geothermometer (°C) by Spencer and Lindsley (1981) using the Carmichael (1967) calculation method	101
25	Magnetite–ilmenite geothermometer (°C) by Spencer and Lindsley (1981) using the Anderson (1968) calculation method	102
26	Magnetite–ilmenite geothermometer (°C) by Spencer and Lindsley (1981) using the Lindsley and Spencer (1982) calculation method	103
27	Magnetite–ilmenite geothermometer (°C) by Spencer and Lindsley (1981) using the Stormer (1983) calculation method	104
28	Magnetite–ilmenite geothermometer (°C) by Andersen and Lindsley (1985) using the Carmichael (1967) calculation method	105
29	Magnetite–ilmenite geothermometer (°C) by Andersen and Lindsley (1985) using the Anderson (1968) calculation method	106
30	Magnetite–ilmenite geothermometer (°C) by Andersen and Lindsley (1985) using the Lindsley and Spencer (1982) calculation method	107
31	Magnetite–ilmenite geothermometer (°C) by Andersen and Lindsley (1985) using the Stormer (1983) calculation method	108
32	Magnetite–ilmenite geothermometer (°C) by Sauerzapf et al. (2008)	109
33	Magnetite–ilmenite geothermometer (°C) by Ghiorso and Evans (2008) based on the linear regression equation [T_{GE08} (°C) = $1.09826 \times T_{S08} - 67.18938$]	110
34	Blank	111
35	Log oxygen fugacity (fO_2) by Powell and Powell (1977) using the Carmichael (1967) calculation method	112
36	Log oxygen fugacity (fO_2) by Powell and Powell (1977) using the Anderson (1968) calculation method	113
37	Log oxygen fugacity (fO_2) by Powell and Powell (1977) using the Lindsley and Spencer (1982) calculation method	114
38	Log oxygen fugacity (fO_2) by Powell and Powell (1977) using the Stormer (1983) calculation method	115
39	Log oxygen fugacity (fO_2) by Spencer and Lindsley (1981) using the Carmichael (1967) calculation method	116
40	Log oxygen fugacity (fO_2) by Spencer and Lindsley (1981) using the Anderson (1968) calculation method	117
41	Log oxygen fugacity (fO_2) by Spencer and Lindsley (1981) using the Lindsley and Spencer (1982) calculation method	118
42	Log oxygen fugacity (fO_2) by Spencer and Lindsley (1981) using the Stormer (1983) calculation method	119
43	Log oxygen fugacity (fO_2) by Andersen and Lindsley (1985) using the Carmichael (1967) calculation method	120
44	Log oxygen fugacity (fO_2) by Andersen and Lindsley (1985) using the Anderson (1968) calculation method	121
45	Log oxygen fugacity (fO_2) by Andersen and Lindsley (1985) using the Lindsley and Spencer (1982) calculation method	122
46	Log oxygen fugacity (fO_2) by Andersen and Lindsley (1985) using the Stormer (1968) calculation method	123
47	Log oxygen fugacity (fO_2) by Sauerzapf et al. (2008)	124
48	Blank	125
49	Log oxygen fugacity (fO_2, relative to buffer) by Andersen and Lindsley (1985) using the Carmichael (1967) calculation method	126
50	Log oxygen fugacity (fO_2, relative to buffer) by Andersen and Lindsley (1985) using the Anderson (1968) calculation method	127
51	Log oxygen fugacity (fO_2, relative to buffer) by Andersen and Lindsley (1985) using the Stormer (1983) calculation method	128
52	Log oxygen fugacity (fO_2, relative to buffer) by Andersen and Lindsley (1985) using the Stormer (1983) calculation method	129

Tab. 1 Continued

53	Log oxygen fugacity (fO_2, relative to buffer) by Sauerzapf et al. (2008)	130
54	Log oxygen fugacity (fO_2, relative to buffer) by Ghiorso and Evans (2008)	131
55	Blank	132
56	Bacon and Hirschmann (1988) test for titanomagnetite–ilmenite equilibrium	133

apfu – atoms per formula unit; T_{GE08} – (row 33) from Ghiorso and Evans (2008) calculated by online link [http://melts.ofm–research.org/CORBA_CTserver/OxideGeothrm/OxideGeothrm.php]; T_{S08} – (row 33) from Excel spreadsheet estimation developed by Sauerzapf et al. (2008)

2.1. Data entry

This program's users can type both magnetite and ilmenite 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. The standard 17 variables are defined by WinMIgob for calculation of magnetite–ilmenite pairs in the following order:
Sample No[M], SiO_2[M], TiO_2[M], Al_2O_3[M], V_2O_3[M], Cr_2O_3[M], Nb_2O_3[M], Fe_2O_3[M], FeO[M], MnO[M], NiO[M], ZnO[M], MgO[M], CaO[M], Na_2O[M], K_2O[M], BaO[M] and
Sample No[I], SiO_2[I], TiO_2[I], Al_2O_3[I], V_2O_3[I], Cr_2O_3[I], Nb_2O_3[I], Fe_2O_3[I], FeO[I], MnO[I], NiO[I], ZnO[I], MgO[I], CaO[I], Na_2O[I], K_2O[I], BaO[I],
where M and I show the abbreviations of magnetite and ilmenite, respectively. In the data entry section, WinMIgob thus permits the user to enter a total of 34 variables. Magnetite and ilmenite 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*. However, using the copy–paste options, these data in the above order from a Microsoft® Excel spreadsheet can be included in the data entry section of WinMIgob more quickly. By selecting the *Edit Excel File* option from the pull-down menu of *File*, magnetite and ilmenite compositions can be typed in a blank Excel file (i.e., MyMI) in the (C:\Program Files\WinMIgob) folder, stored in a different file name with the extension of "`.xls`" or "`.xlsx`", and then loaded into the WinMIgob's data entry section by clicking the *Open Excel File* option from the pull-down menu of *File* for further data evaluations. Once the analyses in an Excel file are displayed on the screen by using the *Open Excel File* option, they can be stored with the extension of "`.mi`" by clicking the *Save As* option from the pull-down menu of *File*. Additional information about data entry or similar topics can be accessed by pressing the F1 function key to display the program's help file on the screen. For example, selecting the *File* menu section from the index of WinMIgob.chm file, it displays the necessary information concerning the magnetite–ilmenite file operations on the screen.

2.2. Normalization, ferric iron estimation, geothermometer, oxygen barometer and Bacon–Hirschmann equilibrium test

Once the program is executed, WinMIgob calculates magnetite analyses to four oxygens and three total cations and ilmenite to three oxygens and two total cations. Magnetite–ilmenite analyses with measured Fe_2O_3 (wt. %) and FeO (wt. %) contents (e.g., wet-chemical) are calculated by program as Fe^{3+} (*apfu*) and Fe^{2+} (*apfu*) separately. However, if these analyses are given as Fe_2O_3 (wt. %) = 0 and FeO (wt. %) > 0, then the program considers FeO (wt. %) content as FeO_{tot} (wt. %) and estimates the ferric and ferrous iron contents stoichiometrically based on the procedure proposed by Stormer (1983) (Fig. 1a). The ferric iron estimation (Fe^{3+}, *apfu*) from a total iron content (FeO_{tot}, wt. %) of electron-microprobe magnetite–ilmenite analysis is also carried out using two other different empirical equations (e.g., Carmichael 1967; Droop 1987) by selecting one of these from the pull-down menu of *Ferric iron estimation* option in the *Data Entry Screen* of WinMIgob.

In the estimation of log fO_2, the program assumes input pressure as 2000 bars. However, WinMIgob provides the user to select 1, 1000, 3000 and 5000 bars options from the pull-down menu of *Buffer* in the *Data Entry Screen* (Fig. 1b). The program displays T (°C)–log fO_2 graph based on the Andersen and Lindley (1985) calibration using the calculation model by Stormer (1983) as default (Fig. 1c). By selecting other calibrations (e.g., Powell and Powell 1977; Spencer and Lindsley 1981) using different calculation methods (e.g., Carmichael 1967; Anderson 1968; Lindsley and Spencer 1982) from the pull-down menu of *Method*, WinMIgob displays the corresponding graph on screen with the help of Golden Software's Grapher program. The program provides various geothermometers based on different calibrations (e.g., Powell and Powell 1977; Spencer and Lindsley 1981; Andersen and Lindsley 1985; Sauerzapf et al. 2008). On the other hand, by selecting the second option from the pull-down menu of *Geothermometer* (see Fig. 1d) in the *Data Entry Screen* window, WinMIgob also presents the user to estimate Ghiorso and Evans (2008) geothermometer with a high correlation coefficient (r = 0.98) based on the linear regression equation [T_{GE08} (°C) = $1.53448 \times T_{Al85} - 458.13356$] using the model by

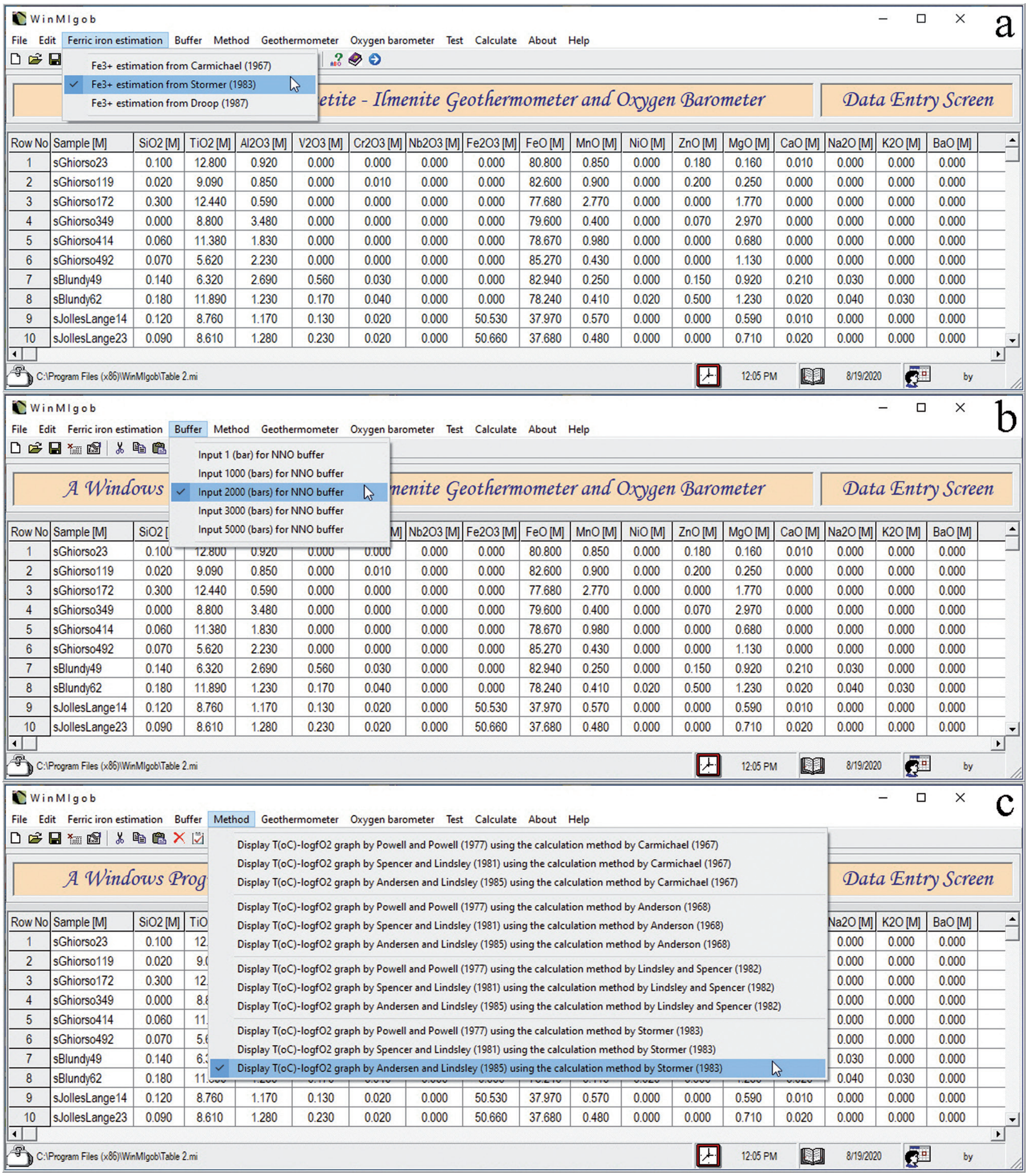


Fig. 1 Screenshots showing the WinMIgob's pull-down menu options for magnetite–ilmenite geothermometer and oxygen barometer estimations. **a** – Selecting stoichiometric ferric and ferrous iron calculation procedure. **b** – Selecting input pressure (bars) value for relative oxygen fugacity (the nickel–nickel oxide buffer, ΔNNO) estimation. **c** – Selecting calibration model to display T (°C)–log fO_2 graph.

Andersen and Lindsley (1985) for 450 magnetite–ilmenite pairs from the literature following the Bacon and Hirschmann's (1988) Mg/Mn exchange test. Similarly, by selecting the second option from the pull-down menu of *Oxygen barometer* in the *Start-up Screen* window (Fig. 1e), WinMIgob calculates the ΔNNO values with a high correlation (r = 0.95) through a linear regression equation [$\Delta NNO_{GE08} = 0.99157 \times \Delta NNO_{AL85} - 0.04250$] using the Andersen and Lindsley's (1985) and Ghiorso and Evans's (2008) calibrations.

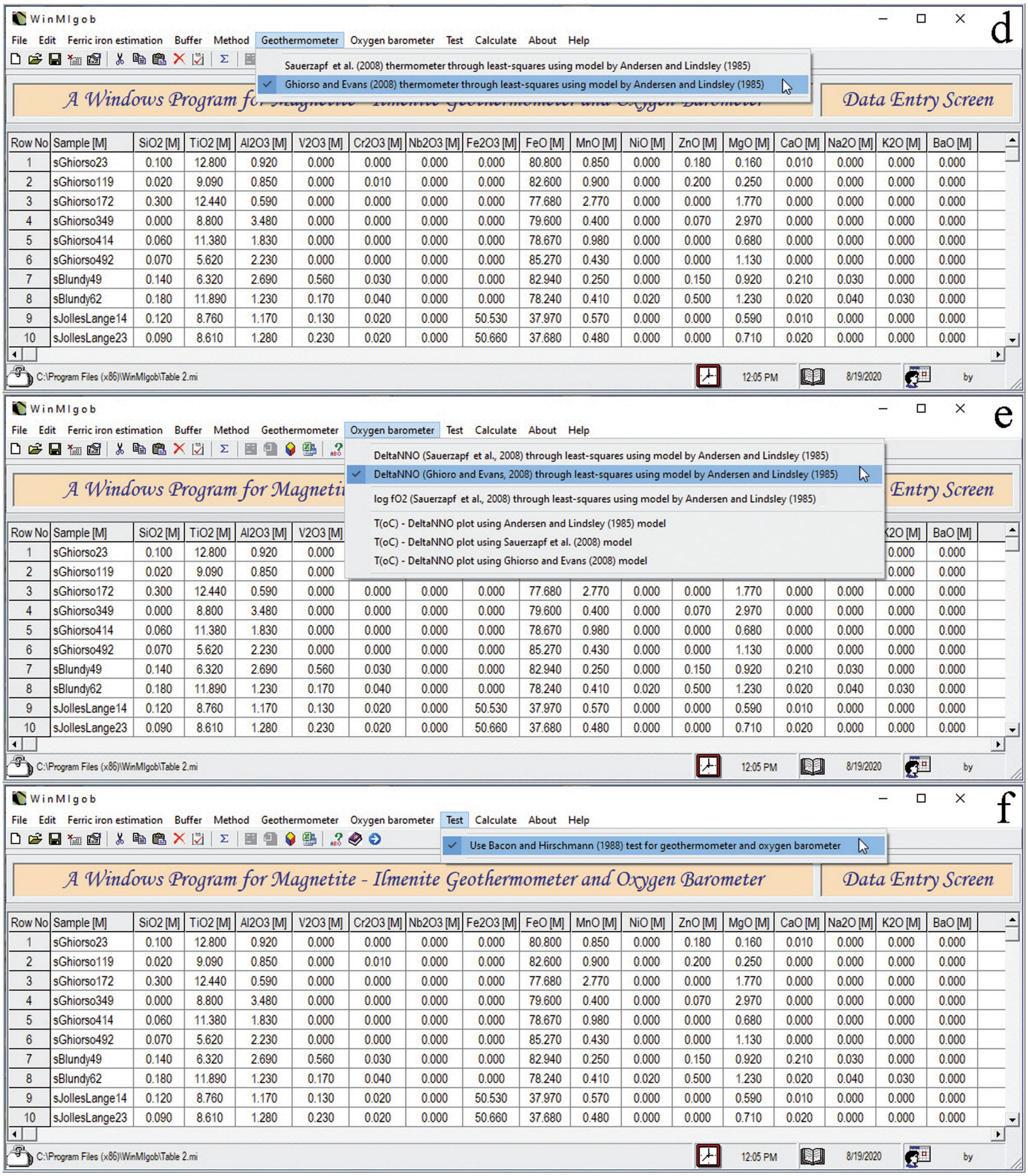


Fig. 1 Screenshots showing the WinMIgob's pull-down menu options for magnetite–ilmenite geothermometer and oxygen barometer estimations. **d** – Selecting magnetite–ilmenite geothermometer through least–squares using the model by Andersen and Lindsley (1985) (rows 15–16 in Tab. 3). **e** – Selecting magnetite–ilmenite relative oxygen barometer (the nickel–nickel oxide buffer, ΔNNO) (rows 40–41 in Tab. 3) and log oxygen fugacity (row 32 in Tab. 3) options using the model by Andersen and Lindsley (1985). **f** – Selecting the Bacon and Hirscmann (1988) equilibrium test for magnetite–ilmenite pairs. By clicking this option, magnetite–ilmenite geothermometer and oxygen barometer estimations are ignored, if any of sample does not pass the test.

WinMIgob allows the user to test the coexistence of analyzed magnetite–ilmenite pairs by clicking the *Use Bacon and Hirschmann (1988) test for geothermometer and oxygen barometer* option from the pull-down menu of *Test* in the *Data Entry Screen* window (Fig. 1f). If coexisting oxides successfully pass the test, the program warns the user in column number 133 of the *Calculation Screen* window with “Passed”, otherwise “Failed” statements. If the Bacon–Hirschmann test option is clicked (see Fig. 1f), but “Failed” statement is encountered for any sample, then WinMIgob does not list the calculated Fe–Ti oxide geothermometers and oxygen barometers in the *Calculation Screen*. Bacon and Hirschmann (1988) proposed that partitioning of Mg and Mn between titanomagnetite and ferrian ilmenite of volcanic rocks can be used as a test for equilibrium between coexisting phases. According to Bacon and Hirschmann (1988), the Mg/Mn magnetite–ilmenite partitioning test appears to be valid for fresh volcanic rocks but inapplicable to pairs in metamorphic, plutonic, and altered volcanic rocks due to these minerals typically have oxidized or exsolved at subsolidus temperatures. The logic of test, in a plot of ilmenite log (Mg/Mn) versus magnetite log (Mg/Mn) plot (Fig. 2), is based on to define the quality of analytical data and whether Fe–Ti oxide pairs have had their compositions altered by post-eruptive processes. Departures from the Bacon–Hirschmann line [$\log (\mathrm{Mg/Mn})_{\mathrm{Mag}} = 0.9317 \times \log (\mathrm{Mg/Mn})_{\mathrm{Ilm}} - 0.0909$] within two standard deviations of the equilibrium line ($\pm 2\sigma$) provide an empirical evaluation of the extent to which Fe–Ti oxide pairs are out of Mg/Mn exchange equilibrium. Thus, we can assume that if the Fe–Ti oxides are in Mg/Mn exchange equilibrium, then it is more likely that their bulk compositions reflect equilibration under the pre-eruptive temperature and oxygen fugacity conditions (Ghiorso and Evans 2008).

3. Worked examples

Using the selected dataset from literature (see Electronic Supplementary Material, ESM 1), the following examples show how WinMIgob can be used for magnetite and ilmenite calculations, molecular ulvöspinel–magnetite and ilmenite–hematite amounts by different approaches, magnetite–ilmenite geothermometers, log oxygen fugacity, as well as in estimation of ΔNNO (Carmichael 1967; Anderson 1968; Powell and Powell 1977; Spencer and Lindsley 1981; Lindsley and Spencer 1982; Stormer 1983; Andersen and Lindsley 1985; Sauerzapf et al. 2008). Once the typed or loaded magnetite–ilmenite pairs 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 1–133 (see Tab. 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 “`.mi`”. Representative Fe–Ti oxides with their stoichiometric Fe_2O_3 and FeO contents (wt. %), structural formulae (*apfu*), the sum of atomic molecular proportions, as well as molecular ulvöspinel, magnetite, ilmenite and hematite amounts by WinMIgob program are given in Tab. 2 (see Fig. 3). 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*

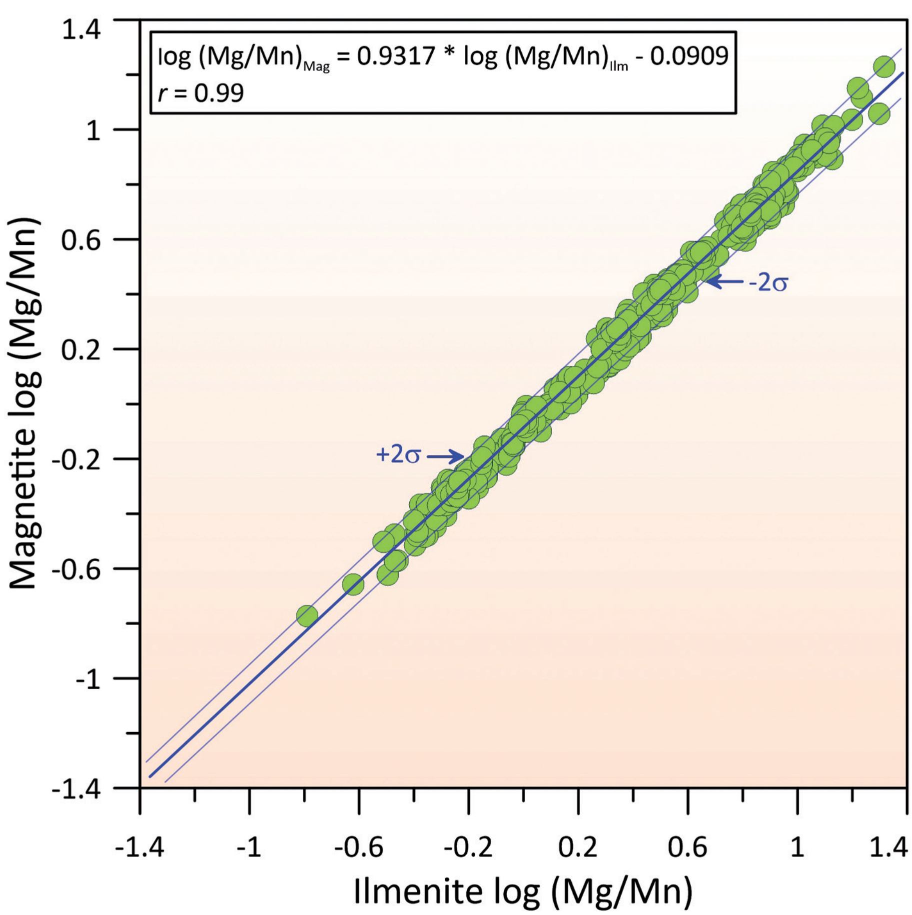


Fig. 2 An application of Mg/Mn exchange test (Bacon and Hirschmann 1988) for magnetite–ilmenite pairs selected from the literature (Ghiorso 2008; Blundy et al. 2008; Jolles and Lange 2019). Only 450 magnetite–ilmenite compositions that passed the test are displayed. Heavy (middle) and other two lines represent the mean linear regression and error envelope (± 2σ), respectively.

Tab. 2a Selected magnetite analyses (wt. %) with their stoichiometric Fe_2O_3 and FeO contents (wt. %), structural formulae (*apfu*), sum of atomic molecular proportions and molecular ulvöspinel and magnetite amounts by WinMIgob program

Row	Magnetite	Mt1	Mt2	Mt3	Mt4	Mt5	Mt6	Mt7	Mt8	Mt9	Mt10
1	SiO_2	0.10	0.02	0.30	0.00	0.06	0.07	0.14	0.18	0.12	0.09
2	TiO_2	12.80	9.09	12.44	8.80	11.38	5.62	6.32	11.89	8.76	8.61
3	Al_2O_3	0.92	0.85	0.59	3.48	1.83	2.23	2.69	1.23	1.17	1.28
4	V_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.56	0.17	0.13	0.23
5	Cr_2O_3	0.00	0.01	0.00	0.00	0.00	0.00	0.03	0.04	0.02	0.02
6	Fe_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	50.53	50.66
7	FeO	80.80	82.60	77.68	79.60	78.67	85.27	82.94	78.24	37.97	37.68
8	MnO	0.85	0.90	2.77	0.40	0.98	0.43	0.25	0.41	0.57	0.48
9	NiO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00
10	ZnO	0.18	0.20	0.00	0.07	0.00	0.00	0.15	0.50	0.00	0.00
11	MgO	0.16	0.25	1.77	2.97	0.68	1.13	0.92	1.23	0.59	0.71
12	CaO	0.01	0.00	0.00	0.00	0.00	0.00	0.21	0.02	0.01	0.02
13	Na_2O	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.04	0.00	0.00
14	K_2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.00
15	∑ (wt. %)	95.82	93.92	95.55	95.32	93.60	94.75	94.24	94.00	99.87	99.78
16	Fe_2O_3(calculated)	43.120	49.733	44.545	49.695	43.687	56.210	52.926	43.502	0.000	0.000
17	FeO(calculated)	41.999	37.848	37.596	34.882	39.358	34.690	35.315	39.095	0.000	0.000
18	Si	0.004	0.001	0.011	0.000	0.002	0.003	0.005	0.007	0.005	0.003
19	Ti	0.363	0.262	0.350	0.242	0.328	0.158	0.179	0.340	0.249	0.245
20	V	0.041	0.038	0.026	0.150	0.083	0.098	0.119	0.055	0.052	0.057
21	Cr	0.000	0.000	0.000	0.000	0.000	0.000	0.017	0.005	0.004	0.007
22	As	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.001	0.001
23	Fe^{3+}	1.225	1.435	1.252	1.366	1.258	1.581	1.496	1.246	1.437	1.440
24	Fe^{2+}	1.326	1.214	1.175	1.066	1.259	1.084	1.110	1.244	1.200	1.191
25	Mn	0.027	0.029	0.088	0.012	0.032	0.014	0.008	0.013	0.018	0.015
26	Ni	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000
27	Zn	0.005	0.006	0.000	0.002	0.000	0.000	0.004	0.014	0.000	0.000
28	Mg	0.009	0.014	0.099	0.162	0.039	0.063	0.052	0.070	0.033	0.040
29	Ca	0.000	0.000	0.000	0.000	0.000	0.000	0.008	0.001	0.000	0.001
30	Na	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000
31	K	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000
32	∑ (*apfu*)	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
33	Usp_{SAMP}	2.27	2.30	2.24	2.20	2.30	2.25	2.26	2.29	2.27	2.27
34	Usp (mol. %)	36.72	26.30	36.08	24.19	32.98	16.06	18.39	34.73	25.37	24.81
35	Mag (mol. %)	63.28	73.70	63.92	75.81	67.02	83.94	81.61	65.27	74.63	75.19
36	X'_{Usp}	0.37	0.27	0.36	0.26	0.34	0.17	0.19	0.35	0.26	0.25
37	X'_{Mag}	0.63	0.73	0.64	0.74	0.66	0.83	0.81	0.65	0.74	0.75

Mt1–Il1 to Mt6–Il6 pairs from Ghiorso (2008); Mt7–Il7 and Mt8–Il8 from Blundy et al. (2008); Mt9–Il9 and Mt10–Il10 from Jolles and Lange (2019); Usp – ulvöspinel, Mag – magnetite, Ilm – ilmenite, Hem – hematite (molecular ulvöspinel, magnetite, ilmenite and hematite amounts by the method of Carmichael 1967); SAMP – sum of atomic molecular proportion (from Lepage 2003); X_i'– mol fraction amount of *i* (formulation from Sauerzapf et al. 2008)

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 (i.e., Output.xlsx) 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. The validity of WinMIgob outputs in terms of magnetite–ilmenite geothermometer and oxygen barometer has been tested with 689 magnetite–ilmenite pairs selected from literature (Ghiorso 2008; Blundy et al. 2008; Jolles and Lange 2019). However, only 450 of the total 689 magnetite and ilmenite compositions passed the Bacon and Hirschmann (1988) equilibrium test (Fig. 2).

3.1. Magnetite–ilmenite geothermometer calbrations and oxygen barometers

Buddington and Lindsley (1964) presented a graphical solution for the Fe–Ti oxide geothermometer and oxygen barometer using the earlier experimental studies carried on cubic and rhombohedral Fe–Ti oxides. The technique takes into account the compositions of coexisting mag-

Tab. 2b Selected ilmenite analyses (wt. %) with their stoichiometric Fe_2O_3 and FeO contents (wt. %), structural formulae (*apfu*), sum of atomic molecular proportions and molecular ilmenite and hematite amounts by WinMIgob program

	Ilmenite	Il1	Il2	Il3	Il4	Il5	Il6	Il7	Il8	Il9	Il10
38	SiO_2	0.02	0.03	0.31	0.00	0.04	0.01	0.03	0.05	0.03	0.04
39	TiO_2	48.30	49.34	47.22	38.50	48.49	41.35	46.40	43.12	45.84	45.27
40	Al_2O_3	0.04	0.06	0.00	0.50	0.11	0.24	0.24	0.15	0.08	0.12
41	V_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.37	0.08	0.12	0.28
42	Cr_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.01	0.01	0.01
43	Fe_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	13.77	15.20
44	FeO	49.10	48.43	44.69	53.60	47.09	53.80	47.44	50.12	37.01	35.85
45	MnO	1.58	1.84	3.81	0.37	1.59	0.60	0.39	0.54	1.10	0.86
46	NiO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
47	ZnO	0.00	0.10	0.00	0.00	0.00	0.00	0.07	0.40	0.00	0.00
48	MgO	0.40	0.63	3.02	3.61	1.31	1.86	1.76	2.21	1.31	1.51
49	CaO	0.02	0.01	0.00	0.00	0.00	0.00	0.04	0.03	0.07	0.02
50	Na_2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00
51	K_2O	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.03	0.00	0.00
52	∑ (wt. %)	99.46	100.44	99.05	96.58	98.63	97.86	96.77	96.76	99.34	99.16
53	Fe_2O_3 (calculated)	8.853	7.887	12.318	28.645	8.188	22.798	10.363	18.049	0.000	0.000
54	FeO (calculated)	41.134	41.333	33.606	27.823	39.722	33.286	38.115	33.879	0.000	0.000
55	Si	0.001	0.001	0.008	0.000	0.001	0.000	0.001	0.001	0.001	0.001
56	Ti	0.915	0.924	0.878	0.723	0.920	0.781	0.892	0.824	0.873	0.863
57	V	0.001	0.002	0.000	0.015	0.003	0.007	0.007	0.004	0.002	0.004
58	Cr	0.000	0.000	0.000	0.000	0.000	0.000	0.008	0.002	0.002	0.006
59	As	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
60	Fe^{3+}	0.168	0.148	0.229	0.538	0.155	0.431	0.199	0.345	0.262	0.290
61	Fe^{2+}	0.866	0.861	0.694	0.581	0.838	0.699	0.815	0.719	0.784	0.760
62	Mn	0.034	0.039	0.080	0.008	0.034	0.013	0.008	0.012	0.024	0.018
63	Ni	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
64	Zn	0.000	0.002	0.000	0.000	0.000	0.000	0.001	0.007	0.000	0.000
65	Mg	0.015	0.023	0.111	0.134	0.049	0.070	0.067	0.084	0.049	0.057
66	Ca	0.001	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.002	0.001
67	Na	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
68	K	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
69	∑ (*apfu*)	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
70	Ilm_{SAMP}	1.51	1.50	1.48	1.50	1.51	1.51	1.54	1.53	1.52	1.52
71	Ilm (mol. %)	91.55	92.52	88.55	72.34	92.07	78.11	89.28	82.49	87.40	86.44
72	Hem (mol. %)	8.45	7.48	11.45	27.66	7.93	21.89	10.72	17.51	12.60	13.56
73	X'_{Ilm}	0.91	0.92	0.86	0.68	0.92	0.76	0.89	0.81	0.86	0.84
74	X'_{Hem}	0.09	0.08	0.14	0.32	0.08	0.24	0.11	0.19	0.14	0.16

Mt1–Il1 to Mt6–Il6 pairs from Ghiorso (2008); Mt7–Il7 and Mt8–Il8 from Blundy et al. (2008); Mt9–Il9 and Mt10–Il10 from Jolles and Lange (2019); Usp – ulvöspinel, Mag – magnetite, Ilm – ilmenite, Hem – hematite (molecular ulvöspinel, magnetite, ilmenite and hematite amounts by the method of Carmichael 1967); SAMP – sum of atomic molecular proportion (from Lepage 2003); X_i'– mol fraction amount of *i* (formulation from Sauerzapf et al. 2008)

netite–ulvöspinel (spinel phase) and ilmenite–hematite solid solution (rhombohedral phase) phases, defined as a mole fraction of ulvöspinel and a mole fraction of hematite, respectively. The magnetite–ilmenite geothermometer is based on the temperature-dependent exchange of Fe^{2+}+Ti^{4+} for $2Fe^{3+}$ between magnetite–ulvöspinel and ilmenite–hematite endmembers, whereas the oxygen barometer considers an iron redox equilibrium, which may be formulated by the magnetite–hematite oxygen buffer equilibrium or by an equilibrium involving the Ti-rich endmembers of the two Fe–Ti oxide series (Sauerzapf et al. 2008).

The geothermometer and oxygen barometer within the concept of a graphical solution later have been reformulated on a thermodynamic basis using the earlier experimental data of Buddington and Lindsley (1964). For example, Powell and Powell (1977) used equilibrium thermodynamic methods to develop an independent Fe–Ti oxide geothermometer and oxygen barometer (Fig. 4), differently, based on the experimental data of Buddington and Lindsley (1964). They presented Fe–Ti geothermometer and oxygen barometer both as graphically and with defined equations for coexisting magnetite and ilmenite solid solutions in $FeO–Fe_2O_3–TiO_2$ system.

a

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
1	WinMIgob	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
2	Sample	[SiO2	TiO2	Al2O3	V2O3	Cr2O3	Nb2O3	Fe2O3	FeO	MnO	NiO	ZnO	MgO	CaO	Na2O	K2O	BaO	Total](M)	[Fe2O3(cal.)	FeO(cal.)](M)
3	sGhiorso23	0.10	12.80	0.92	0.00	0.00	0.00	0.00	80.80	0.85	0.00	0.18	0.16	0.01	0.00	0.00	0.00	95.82	43.120	41.999
4	sGhiorso119	0.02	9.09	0.85	0.00	0.01	0.00	0.00	82.60	0.90	0.00	0.20	0.25	0.00	0.00	0.00	0.00	93.92	49.733	37.848
5	sGhiorso172	0.30	12.44	0.59	0.00	0.00	0.00	0.00	77.68	2.77	0.00	0.00	1.77	0.00	0.00	0.00	0.00	95.55	44.545	37.596
6	sGhiorso349	0.00	8.80	3.48	0.00	0.00	0.00	0.00	79.60	0.40	0.00	0.07	2.97	0.00	0.00	0.00	0.00	95.32	49.695	34.882
7	sGhiorso414	0.06	11.38	1.83	0.00	0.00	0.00	0.00	78.67	0.98	0.00	0.00	0.68	0.00	0.00	0.00	0.00	93.60	43.687	39.358
8	sGhiorso492	0.07	5.62	2.23	0.00	0.00	0.00	0.00	85.27	0.43	0.00	0.00	1.13	0.00	0.00	0.00	0.00	94.75	56.210	34.690
9	sBlundy49	0.14	6.32	2.69	0.56	0.03	0.00	0.00	82.94	0.25	0.00	0.15	0.92	0.21	0.03	0.00	0.00	94.24	52.926	35.315
10	sBlundy62	0.18	11.89	1.23	0.17	0.04	0.00	0.00	78.24	0.41	0.02	0.50	1.23	0.02	0.04	0.03	0.00	94.00	43.502	39.095
11	sJollesLange14	0.12	8.76	1.17	0.13	0.02	0.00	50.53	37.97	0.57	0.00	0.00	0.59	0.01	0.00	0.00	0.00	99.87	0.000	0.000
12	sJollesLange23	0.09	8.61	1.28	0.23	0.02	0.00	50.66	37.68	0.48	0.00	0.00	0.71	0.02	0.00	0.00	0.00	99.78	0.000	0.000

b

	A	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG	AH	AI	AJ	AK
1	WinMIgob	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
2	Sample	[Si	Ti	Al	V	Cr	Nb	Fe3+	Fe2+	Mn	Ni	Zn	Mg	Ca	Na	K	Ba	Total](M)
3	sGhiorso23	0.004	0.363	0.041	0.000	0.000	0.000	1.225	1.326	0.027	0.000	0.005	0.009	0.000	0.000	0.000	0.000	3.000
4	sGhiorso119	0.001	0.262	0.038	0.000	0.000	0.000	1.435	1.214	0.029	0.000	0.006	0.014	0.000	0.000	0.000	0.000	3.000
5	sGhiorso172	0.011	0.350	0.026	0.000	0.000	0.000	1.252	1.175	0.088	0.000	0.000	0.099	0.000	0.000	0.000	0.000	3.000
6	sGhiorso349	0.000	0.242	0.150	0.000	0.000	0.000	1.366	1.066	0.012	0.000	0.002	0.162	0.000	0.000	0.000	0.000	3.000
7	sGhiorso414	0.002	0.328	0.083	0.000	0.000	0.000	1.258	1.259	0.032	0.000	0.000	0.039	0.000	0.000	0.000	0.000	3.000
8	sGhiorso492	0.003	0.158	0.098	0.000	0.000	0.000	1.581	1.084	0.014	0.000	0.000	0.063	0.000	0.000	0.000	0.000	3.000
9	sBlundy49	0.005	0.179	0.119	0.017	0.001	0.000	1.496	1.110	0.008	0.000	0.004	0.052	0.008	0.001	0.000	0.000	3.000
10	sBlundy62	0.007	0.340	0.055	0.005	0.001	0.000	1.246	1.244	0.013	0.001	0.014	0.070	0.001	0.001	0.001	0.000	3.000
11	sJollesLange14	0.005	0.249	0.052	0.004	0.001	0.000	1.437	1.200	0.018	0.000	0.000	0.033	0.000	0.000	0.000	0.000	3.000
12	sJollesLange23	0.003	0.245	0.057	0.007	0.001	0.000	1.440	1.191	0.015	0.000	0.000	0.040	0.001	0.000	0.000	0.000	3.000

c

	A	AN	AO	AP	AQ	AR	AS	AT	AU	AV	AW	AX	AY	AZ	BA	BB	BC	BD	BE	BF
1	WinMIgob	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57
2	Sample	[SiO2	TiO2	Al2O3	V2O3	Cr2O3	Nb2O3	Fe2O3	FeO	MnO	NiO	ZnO	MgO	CaO	Na2O	K2O	BaO	Total](I)	[Fe2O3(cal.)	FeO(cal.)](I)
3	sGhiorso23	0.02	48.30	0.04	0.00	0.00	0.00	0.00	49.10	1.58	0.00	0.00	0.40	0.02	0.00	0.00	0.00	99.46	8.853	41.134
4	sGhiorso119	0.03	49.34	0.06	0.00	0.00	0.00	0.00	48.43	1.84	0.00	0.10	0.63	0.01	0.00	0.00	0.00	100.44	7.887	41.333
5	sGhiorso172	0.31	47.22	0.00	0.00	0.00	0.00	0.00	44.69	3.81	0.00	0.00	3.02	0.00	0.00	0.00	0.00	99.05	12.318	33.606
6	sGhiorso349	0.00	38.50	0.50	0.00	0.00	0.00	0.00	53.60	0.37	0.00	0.00	3.61	0.00	0.00	0.00	0.00	96.58	28.645	27.823
7	sGhiorso414	0.04	48.49	0.11	0.00	0.00	0.00	0.00	47.09	1.59	0.00	0.00	1.31	0.00	0.00	0.00	0.00	98.63	8.188	39.722
8	sGhiorso492	0.01	41.35	0.24	0.00	0.00	0.00	0.00	53.80	0.60	0.00	0.00	1.86	0.00	0.00	0.00	0.00	97.86	22.798	33.286
9	sBlundy49	0.03	46.40	0.24	0.37	0.02	0.00	0.00	47.44	0.39	0.00	0.07	1.76	0.04	0.00	0.01	0.00	96.77	10.363	38.115
10	sBlundy62	0.05	43.12	0.15	0.08	0.01	0.00	0.00	50.12	0.54	0.00	0.40	2.21	0.03	0.02	0.03	0.00	96.76	18.049	33.879
11	sJollesLange14	0.03	45.84	0.08	0.12	0.01	0.00	13.77	37.01	1.10	0.00	0.00	1.31	0.07	0.00	0.00	0.00	99.34	0.000	0.000
12	sJollesLange23	0.04	45.27	0.12	0.28	0.01	0.00	15.20	35.85	0.86	0.00	0.00	1.51	0.02	0.00	0.00	0.00	99.16	0.000	0.000

d

	A	BG	BH	BI	BJ	BK	BL	BM	BN	BO	BP	BQ	BR	BS	BT	BU	BV	BW
1	WinMIgob	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74
2	Sample	[Si	Ti	Al	V	Cr	Nb	Fe3+	Fe2+	Mn	Ni	Zn	Mg	Ca	Na	K	Ba	Total](I)
3	sGhiorso23	0.001	0.915	0.001	0.000	0.000	0.000	0.168	0.866	0.034	0.000	0.000	0.015	0.001	0.000	0.000	0.000	2.000
4	sGhiorso119	0.001	0.924	0.002	0.000	0.000	0.000	0.148	0.861	0.039	0.000	0.002	0.023	0.000	0.000	0.000	0.000	2.000
5	sGhiorso172	0.008	0.878	0.000	0.000	0.000	0.000	0.229	0.694	0.080	0.000	0.000	0.111	0.000	0.000	0.000	0.000	2.000
6	sGhiorso349	0.000	0.723	0.015	0.000	0.000	0.000	0.538	0.581	0.008	0.000	0.000	0.134	0.000	0.000	0.000	0.000	2.000
7	sGhiorso414	0.001	0.920	0.003	0.000	0.000	0.000	0.155	0.838	0.034	0.000	0.000	0.049	0.000	0.000	0.000	0.000	2.000
8	sGhiorso492	0.000	0.781	0.007	0.000	0.000	0.000	0.431	0.699	0.013	0.000	0.000	0.070	0.000	0.000	0.000	0.000	2.000
9	sBlundy49	0.001	0.892	0.007	0.008	0.000	0.000	0.199	0.815	0.008	0.000	0.001	0.067	0.001	0.000	0.000	0.000	2.000
10	sBlundy62	0.001	0.824	0.004	0.002	0.000	0.000	0.345	0.719	0.012	0.000	0.007	0.084	0.001	0.000	0.000	0.000	2.000
11	sJollesLange14	0.001	0.873	0.002	0.002	0.000	0.000	0.262	0.784	0.024	0.000	0.000	0.049	0.002	0.000	0.000	0.000	2.000
12	sJollesLange23	0.001	0.863	0.004	0.006	0.000	0.000	0.290	0.760	0.018	0.000	0.000	0.057	0.001	0.000	0.000	0.000	2.000

e

	A	BY	BZ	CA	CB	CC	CD	CE	CF	CG	CH
1	WinMIgob	76	77	78	79	80	81	82	83	84	85
2	Sample	[Ulvöspinel	Ilmenite](SAMP)	[Ulvöspinel	Magnetite](Mol%)	[Ilmenite	Hematite](Mol%)	[Ulvöspinel	Ilmenite](Mol%)	[Ulvöspinel	Ilmenite](Mol%)
3	sGhiorso23	2.27	1.51	36.72	63.28	91.55	8.45	36.24	91.17	37.30	91.32
4	sGhiorso119	2.30	1.50	26.30	73.70	92.52	7.48	25.70	92.17	26.89	92.37
5	sGhiorso172	2.24	1.48	36.08	63.92	88.55	11.45	28.68	85.30	36.48	87.08
6	sGhiorso349	2.20	1.50	24.19	75.81	72.34	27.66	17.95	68.34	25.59	72.87
7	sGhiorso414	2.30	1.51	32.98	67.02	92.07	7.93	33.25	91.45	34.08	91.90
8	sGhiorso492	2.25	1.51	16.06	83.94	78.11	21.89	16.26	76.43	16.42	78.17
9	sBlundy49	2.26	1.54	18.39	81.61	89.28	10.72	18.99	89.22	18.90	89.99
10	sBlundy62	2.29	1.53	34.73	65.27	82.49	17.51	32.15	81.26	35.21	82.90
11	sJollesLange14	2.27	1.52	25.37	74.63	87.40	12.60	25.14	86.68	25.59	87.37
12	sJollesLange23	2.27	1.52	24.81	75.19	86.44	13.56	22.86	85.73	25.18	86.59

f

	A	CI	CJ	CK	CL	CM	CN	CO	CP	CQ	CR
1	WinMIgob	86	87	88	89	90	91	92	93	94	95
2	Sample	[Ulvöspinel	Ilmenite](Mol%)	[Xusp	Xmt]	[Xilm	Xhem]	[X'usp	X'mag	X'ilm	X'hem]
3	sGhiorso23	37.29	91.39	0.38	0.62	0.91	0.09	0.37	0.63	0.91	0.09
4	sGhiorso119	26.51	92.35	0.27	0.73	0.92	0.08	0.27	0.73	0.92	0.08
5	sGhiorso172	32.97	87.21	0.34	0.66	0.87	0.13	0.36	0.64	0.86	0.14
6	sGhiorso349	25.22	70.66	0.25	0.75	0.71	0.29	0.26	0.74	0.68	0.32
7	sGhiorso414	34.45	91.87	0.35	0.65	0.92	0.08	0.34	0.66	0.92	0.08
8	sGhiorso492	16.55	77.43	0.17	0.83	0.77	0.23	0.17	0.83	0.76	0.24
9	sBlundy49	19.50	89.53	0.20	0.80	0.90	0.10	0.19	0.81	0.89	0.11
10	sBlundy62	34.61	81.70	0.35	0.65	0.82	0.18	0.35	0.65	0.81	0.19
11	sJollesLange14	25.62	86.31	0.26	0.74	0.86	0.14	0.26	0.74	0.86	0.14
12	sJollesLange23	25.23	84.82	0.26	0.74	0.85	0.15	0.25	0.75	0.84	0.16

Fig. 3 Screenshots of an output Excel file (Output.xlsx) created by WinMIgob program showing all input and output parameters of magnetite–ilmenite compositions. **a** – Magnetite analyses with stoichiometric estimation of Fe_2O_3 and FeO (wt. %) contents. **b** – Recalculated cations of magnetite mineral analyses (*apfu*). **c** – Ilmenite analyses with stoichiometric estimation of Fe_2O_3 and FeO (wt. %) contents. **d** – Recalculated cations of ilmenite mineral analyses (*apfu*). **e** and **f** – Molecular ulvöspinel, magnetite, ilmenite and hematite amounts calculated by different methods (Carmichael 1967; Anderson 1968; Lindsley and Spencer 1982; Stormer 1983).

Although their model may fit for the NNO and the fayalite–magnetite–quartz (FMQ) buffer assemblages, it does not predict the results of experiments reflecting the more reducing buffer conditions such as the cobalt–co-a

	A	CT	CU	CV	CW	CX	CY	CZ	DA	DB	DC	DD	DE	DF	DG
1	*WinMIgob*	97	98	99	100	101	102	103	104	105	106	107	108	109	110
2	Sample	[TP77C67	TP77A68	TP77LS82	TP77S83](oC)	[TSL81C67	TSL81A68	TSL81LS82	TSL81S83](oC)	[TAL85C67	TAL85A68	TAL85LS82	TAL85S83](oC)	[TS08](oC)	[TGE08](oC)
3	sGhiorso23	812	816	820	818	787	794	796	794	796	802	803	802	795	806
4	sGhiorso119	729	731	736	734	718	724	724	723	740	744	744	744	706	709
5	sGhiorso172	858	850	883	857	848	844	877	849	842	839	861	842	849	865
6	sGhiorso349	945	912	954	971	908	869	919	928	878	852	884	889	905	927
7	sGhiorso414	779	792	789	792	756	771	765	767	771	784	779	781	769	777
8	sGhiorso492	812	828	815	823	812	822	815	819	813	820	815	819	757	764
9	sBlundy49	721	727	716	727	739	742	732	741	757	760	751	759	690	691
10	sBlundy62	931	925	930	940	927	916	926	935	891	885	891	896	896	917
11	sJollesLange14	799	806	801	815	798	806	800	813	806	811	807	817	771	779
12	sJollesLange23	807	800	808	829	806	802	807	827	812	809	812	827	785	795

b

	A	DI	DJ	DK	DL	DM	DN	DO	DP	DQ	DR	DS	DT	DU
1	*WinMIgob*	112	113	114	115	116	117	118	119	120	121	122	123	124
2	Sample	[fO2PP77C67	fO2PP77A68	fO2PP77LS82	fO2PP77S83]	[fO2SL81C67	fO2SL81A68	fO2SL81LS82	fO2SL81S83]	[fO2AL85C67	fO2AL85A68	fO2AL85LS82	fO2AL85S83]	[fO2S08]
3	sGhiorso23	-12.10	-12.18	-12.04	-12.04	-14.45	-14.21	-14.21	-14.27	-14.37	-14.18	-14.19	-14.23	-13.79
4	sGhiorso119	-13.63	-13.77	-13.53	-13.60	-16.04	-15.80	-15.88	-15.89	-15.66	-15.45	-15.52	-15.53	-15.32
5	sGhiorso172	-12.38	-13.69	-12.43	-12.89	-12.63	-12.08	-11.91	-12.35	-12.97	-12.52	-12.45	-12.74	-12.18
6	sGhiorso349	-15.53	-17.41	-15.20	-15.46	-9.95	-10.23	-9.85	-9.61	-11.12	-11.25	-11.07	-10.92	-10.09
7	sGhiorso414	-12.56	-12.56	-12.42	-12.37	-15.19	-14.69	-14.97	-14.91	-14.95	-14.54	-14.77	-14.73	-14.24
8	sGhiorso492	-17.20	-17.26	-17.08	-17.09	-11.62	-11.35	-11.60	-11.47	-12.17	-11.99	-12.16	-12.07	-12.72
9	sBlundy49	-15.68	-15.52	-15.49	-15.36	-14.52	-14.45	-14.85	-14.57	-14.37	-14.31	-14.64	-14.41	-14.92
10	sBlundy62	-12.98	-13.43	-12.88	-13.05	-10.56	-10.57	-10.61	-10.36	-11.54	-11.53	-11.58	-11.42	-11.03
11	sJollesLange14	-14.16	-14.25	-14.11	-14.18	-13.15	-12.89	-13.12	-12.72	-13.29	-13.09	-13.26	-12.96	-13.35
12	sJollesLange23	-14.33	-14.80	-14.25	-14.36	-12.83	-12.76	-12.86	-12.26	-13.05	-12.98	-13.06	-12.63	-12.88

c

	A	DW	DX	DY	DZ	EA	EB	EC	ED
1	*WinMIgob*	126	127	128	129	130	131	132	133
2	Sample	[DeltaNNO_AL85C67	DeltaNNO_AL85A68	DeltaNNO_AL85LS82	DeltaNNO_AL85S83]	[DeltaNNO_S08]	[DeltaNNO_GE08]		[Bacon and Hirschmann (1988) Test]
3	sGhiorso23	-0.51	-0.43	-0.48	-0.49	0.10	-0.48		Passed
4	sGhiorso119	-0.49	-0.39	-0.47	-0.46	0.68	0.11		Passed
5	sGhiorso172	-0.05	0.45	0.08	0.17	0.61	0.04		Passed
6	sGhiorso349	1.10	1.45	1.03	1.09	1.63	0.92		Passed
7	sGhiorso414	-0.54	-0.41	-0.52	-0.52	0.24	-0.32		Passed
8	sGhiorso492	1.33	1.37	1.30	1.32	2.03	1.20		Passed
9	sBlundy49	0.39	0.37	0.25	0.31	1.50	0.82		Passed
10	sBlundy62	0.43	0.56	0.39	0.46	0.86	0.27		Passed
11	sJollesLange14	0.38	0.45	0.37	0.47	1.10	0.48		Passed
12	sJollesLange23	0.49	0.61	0.46	0.60	1.23	0.60		Passed

Fig. 4 Screenshots of an output Excel file (Output.xlsx) created by WinMIgob program for a various of magnetite–ilmenite; **a** – geothermometer, **b** – oxygen barometer and **c** – oxygen barometer relative to the nickel–nickel oxide buffer estimations.

balt oxide (Co–CoO) and the wustite–magnetite (WM) at low temperatures (~600–800 °C) due to the increasing non-ideality of the solutions. Hence, Powell and Powell's (1977) calibration is only valid for a limited range of temperature and oxygen fugacity conditions (Spencer and Lindsley 1981). Powell and Powell (1977) also pointed out that significant departures in composition from the system $FeO–Fe_2O_3–TiO_2$ may show large uncertainties in the calculated temperature and activity of oxygen.

Spencer and Lindsley (1981) developed a solution model for coexisting magnetite–ulvöspinel and ilmenite–hematite solid solutions based on a least-squares fit of thermodynamic parameters to experimental data obtained at temperatures from 550 to 1200 °C. They applied their solution approach to Buddington and Lindsley's (1964) geothermometer and oxygen barometer model for coexisting magnetite–ilmenite pairs in a temperature–oxygen fugacity (T–fO_2) grid (Fig. 4). According to Spencer and Lindsley (1981), uncertainties in their model are approximately 40–80 °C and 0.5–1.0 log units fO_2 in ulvöspinel and ilmenite compositions. Taking into account the most analyses of natural Fe–Ti oxides that include small but significant amounts of minor components, Stormer (1983) proposed a new recalculation scheme, apart from the Carmichael's (1967) and Anderson's (1968) approach, based on the models of ionic substitution which is consistent with a thermodynamic model for the pure Fe–Ti system recommended by Spencer and Lindsley (1981). However, the Stormer's (1983) scheme is more consistent with the model used by Spencer and Lindsley (1981) for fitting the experimental data and gives temperature and oxygen fugacity values falling in the middle of the range of variation with respect to the Carmichael's (1967) and Anderson's (1968) models.

Considering the inconsistent results, in addition to the compositional departures from the system Fe–Ti–O, Andersen and Lindsley (1988) presented new experimental data on the compositions of coexisting magnetite–ilmenite pairs to revise the solution model for magnetite and ilmenite solid solutions by including the effects of Mg and Mn, as well as examining the effects of order-disorder on the solution properties of spinels. An internally consistent solution model by Andersen and Lindsley (1988) applies the linear programming based on a multicomponent Margules-type solution for ilmenite and an assumed Akimoto-type and available cation-distribution for magnetite solid solutions. They reported that in terms of the system Fe–Ti–O, T (°C) between 600 and 1200 °C and fO_2 between the NNO and WM buffers, there is little difference between these two models in calculated temperature and oxygen fugacity values.

Ghiorso and Sack (1991) developed a new thermodynamic formulation for the Fe–Ti oxides which is calibrated models for spinel solid–solutions in the quinary system $(Fe^{2+}, Mg)(Al, Fe^{3+}, Cr)_2O_4–(Fe^{2+}, Mg)_2TiO_4$ and rhombohedral oxides in the quaternary system $(Fe^{2+},$

Mg, Mn)TiO_3–Fe_2O_3 that can be applied to the estimation of temperature and oxygen fugacity values for intermediate to silicic volcanic rocks to investigate the systematic of T–log fO_2 trends for various magmatic ferromagnesian–silicate assemblages. However, application of both the Andersen and Lindsley (1988) and Ghiorso and Sack (1991) formulations to Fe–Ti oxides in more oxidized magmas, such as in magmatic arcs, may give too high estimates of oxygen fugacity and temperatures, both too high and too low values depending on the range of log fO_2 (Evans and Scaillet 1997; Evans et al. 2006). For example, Lindsley and Frost (1992) noticed the users for Andersen and Lindsley's (1988) formulation at oxygen fugacities higher than two log bar units above those of the FMQ (i.e., at ΔFMQ>2 or ΔNNO>1.3). Lattard et al. (2005) synthesized assemblages of titanomagnetite–ilmenite, ilmenite–pseudobrookite and single-phase samples under a wide range of fO_2 (in the range ΔNNO–5 to +5) in sub–solidus conditions, at 1 bar and at temperatures between 1000 and 1300 °C, in the Fe–Ti–O system.

Considering unsatisfactory results of previous calibrations, especially at high temperature and low to moderate oxygen fugacity conditions that point out the crystallization of basic and intermediate rocks, Sauerzapf et al. (2008) presented a new version of magnetite–ilmenite geothermometer and oxygen barometer (Fig. 4) based on the numerical fits of a large experimental dataset, nearly 200, in the Fe–Ti–Al–Mg–O system and those of literature studies. Sauerzapf et al. (2008) recognized that their subsolidus experimental results at temperatures in the range 1100–1300 °C and under low to moderate fO_2 (i.e., –4 < ΔNNO < +2) conditions with the addition of Mg and/or Al in the concentration ranges can be accommodated by simple projections. Thus, by applying numerical fits to those cited projections, they generated empirical formulations to retrieve temperature values from X'_{usp} and X'_{ilm} (i.e., projected mole fractions) of titanomagnetite–ilmenite solid solution pairs and oxygen fugacity values from X'_{usp} and T (°C) relationship. According to Sauerzapf et al. (2008), tests carried on the independent experimental results indicate that their model reproduces the experimental temperatures generally within ±70 °C, and in most cases within ±50 °C, as well as the oxygen fugacity values usually within ±0.4 log units. When compared to the Andersen and Lindsley (1988) and Ghiorso and Sack (1991) models, their formulations yield substantial temperature underestimates for assemblages equilibrated at temperatures > 950 °C under moderate to low fO_2 values (i.e., ΔNNO ≤0). Thus, the Sauerzapf et al. (2008) formulations may give reliable results in estimating the magmatic temperature and oxygen fugacity conditions for rapidly cooled intermediate to basic igneous systems.

WinMIgob calculates the temperatures of Sauerzapf et al. (2008) model ($X'_{ilm} = f(X'_{usp}, T)$) through least–squares method using a series of third–order polynomial functions (Fig. 5a). Formulations used in the program's structure indicate that the calculated temperature values, in the range 700–1300 °C, by WinMIgob reproduce the Sauerzapf et al. (2008) model within ±19 °C for 450 magnetite–ilmenite pairs reported in the literature from volcanic rocks that are primarily dacitic and rhyolitic composition. Consequently, WinMIgob calculates the Fe–Ti oxide geothermometer of Sauerzapf et al. (2008) model with a high correlation (r = 0.99) coefficient (Fig. 5b). On the other hand, the estimates of oxygen fugacity relative to the NNO (ΔNNO) by program are mostly within ±0.06 units (Fig. 5c), and there also exists a high correlation coefficient (r = 0.99) between the Sauerzapf et al. (2008) calibration and WinMIgob outputs (Fig. 5d).

Because of the magnetite–ilmenite geothermobarometer of Ghiorso and Sack (1991) has been found to overestimate the temperature and oxygen fugacity in most moderate- to highly-oxidized calc-alkaline magma series (e.g., Mt. Pinatubo dacitic magma), as well as collected high-quality cation-ordering data for hematite–ilmenite solid solutions along the Fe_2O_3–$FeTiO_3$ join since then, a new thermodynamic model for rhombohedral oxide solid solutions in the system Fe_2O_3–$FeTiO_3$–$MgTiO_3$–$MnTiO_3$ containing minor amounts of Al_2O_3 was developed by Ghiorso and Evans (2008) to revise and correct the earlier Fe–Ti oxides geothermometer and oxygen barometer calibration. The model was applied by Ghiorso and Evans (2008) to a newly compiled dataset of natural Fe–Ti oxide pairs from silicic volcanic rocks, and results were compared to previous formulations. The general conclusion is that their current model gives a better estimate of the oxidation state for magmas that equilibrated under conditions more oxidizing than the NNO buffer. On the other hand, temperatures obtained from the Ghiorso and Evans (2008) model are also found to be consistent with experimental phase relations for the stability of cummingtonite in silicic volcanic rocks. According to Ghiorso and Evans (2008), the results of their geothermometer and oxygen barometer differ from previously calibrated Fe–Ti oxide pairs formulations (e.g., Andersen and Lindsley 1988; Ghiorso and Sack 1991), most notably in the estimation of oxidation state under relatively oxidized conditions (> NNO + 1).

WinMIgob provides the users to estimate Ghiorso and Evans (2008) Fe–Ti oxides geothermometer by using a linear regression equation [T_{GE08} (°C) = 1.098258692 × T_{S08} – 67.18937519] correlating the Sauerzapf et al. (2008) and Ghiorso and Evans (2008) calibrations (Fig. 6a). Although a high correlation (r = 0.99) exists between these two calibrations, the users should be careful when using

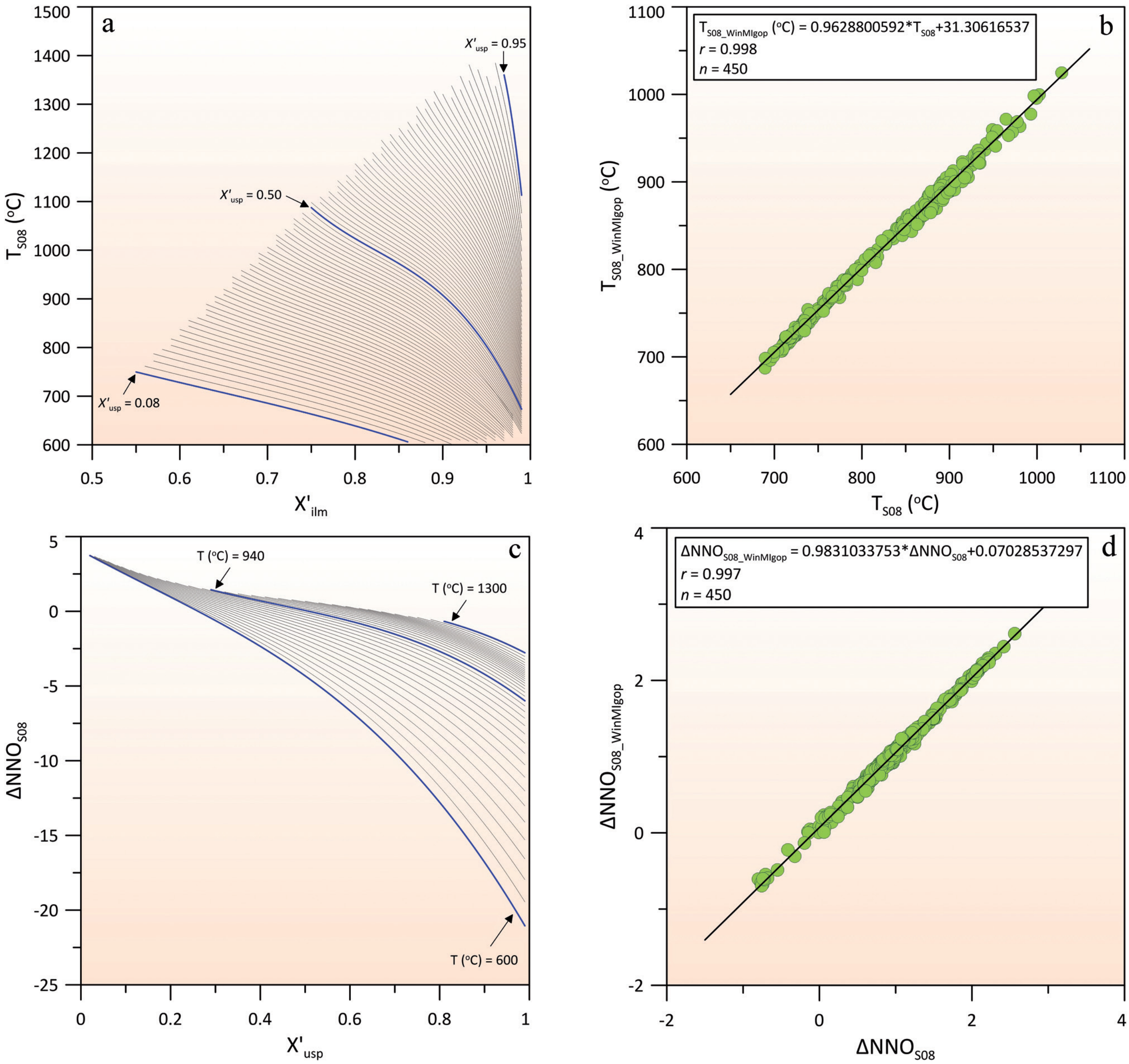
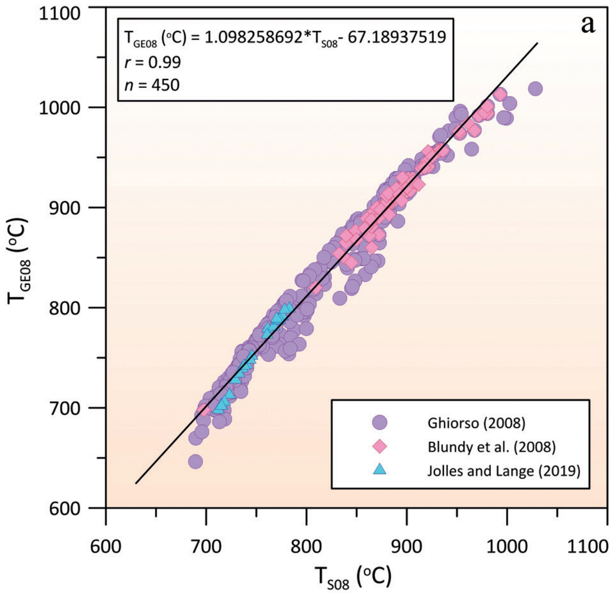
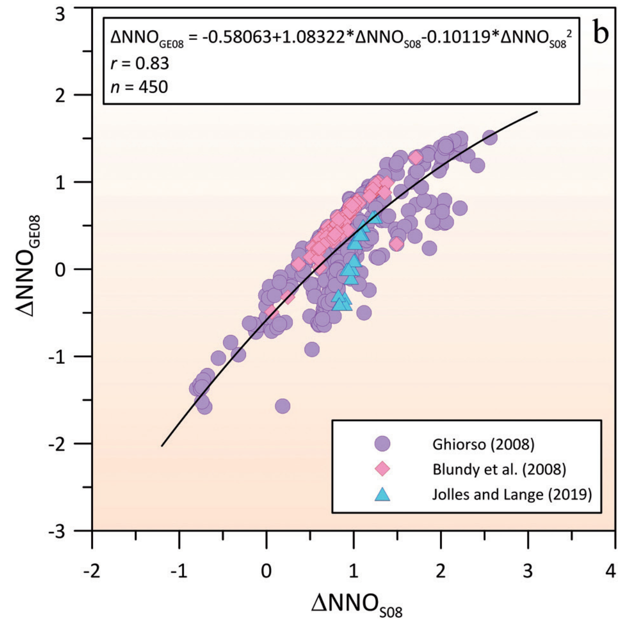


Fig. 5 a – X'_{ilm}–T (°C) relationship for X'_{usp} values between 0.08 and 0.95 using the third-order polynomial functions to estimate the temperature of Sauerzapf et al. (2008) model. **b** – Temperature relationship between the Sauerzapf et al. (2008) model and WinMIgob program. **c** – X'_{usp}–ΔNNO relationship for temperature values between 600 and 1300 °C using the third–order polynomial functions to estimate ΔNNO of the Sauerzapf et al. (2008) model. **d** – ΔNNO relationship between the Sauerzapf et al. (2008) model and WinMIgob program.

WinMIgob's output for the Ghiorso and Evans (2008) geothermometer in their own studies especially for temperatures <700 °C and >950 °C. When compared to the magnetite–ilmenite geothermometer, the ΔNNO values in these two calibrations show much more variations, with a lower correlation (r = 0.83) coefficient (Fig. 6b) and should also be used with caution by the WinMIgob's users. In terms of the ΔNNO values, there is a high correlation coefficient (r = 0.95) between the Andersen and Lindsley (1985) and Ghiorso and Evans (2008) calibrations (Fig. 6c). Thus, by selecting the second option from the pull-down menu of *Oxygen barometer* (see Fig. 1e) this relationship may be used by the program's users in the estimation of the ΔNNO values by Ghiorso and Evans (2008). The current version of WinMIgop provides the users to display ten diagrams by using the Grapher program for coexisting magnetite–ilmenite compositions. Some of selected diagram types from the pull-down menu of *Graph* in the *Calculation Screen* are given in Fig. 7.

In this study, magnetite–ilmenite analyses that present both Fe_2O_3 and FeO (wt. %) were tested with FeO_{tot} (wt. %) contents, estimated from FeO + 0.8998Fe_2O_3, to obtain T (°C) and fO_2 values using different calibrations. Magnetite–ilmenite analyses with Fe_2O_3 and FeO (wt. %)





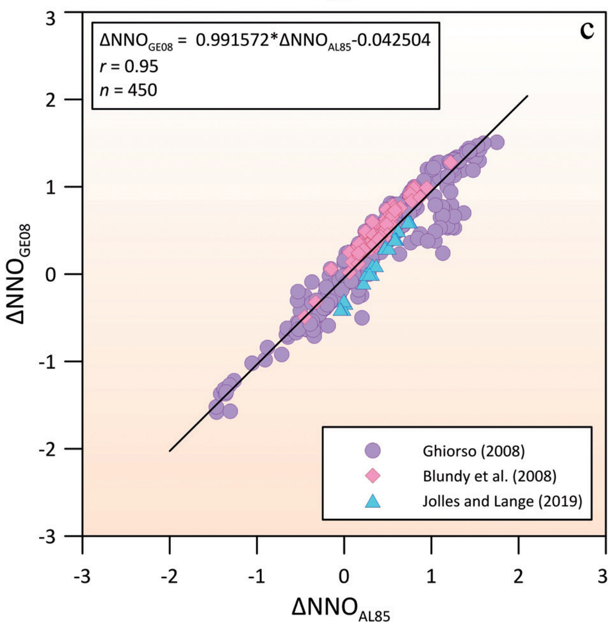


Fig. 6a – T_{S08}–T_{GE08} (°C) relationship between the magnetite–ilmenite geothermometer calibrations by Sauerzapf et al. (2008) and Ghiorso and Evans (2008) for the selected 450 magnetite and ilmenite analyses from the literature. **b** – ΔNNO_{S08}–ΔNNO_{GE08} relationship between magnetite–ilmenite ΔNNO estimations by the Sauerzapf et al. (2008) and Ghiorso and Evans (2008) models. **c** – ΔNNO_{AL85}–ΔNNO_{GE08} relationship between magnetite–ilmenite ΔNNO estimations by the Andersen and Lindsley (1985) and Ghiorso and Evans (2008) models.

compositions from the literature (Himmelberg and Ford 1977; Stormer (1983); Honjo et al. 1992; Venezky and Rutherford 1999; Mullen and McCallum 2013; Ondrejka et al. 2015) were first checked for the Bacon–Hirschmann equilibrium test by WinMIgop program. Then magnetite–ilmenite pairs that passed the test were subjected to both ferric and ferrous and total iron calculations to estimate T (°C) and fO_2 values for different calibration methods (e.g., Anderson and Lindsley (1985); Sauerzapf et al. 2008). Finally, a comparison indicates that the resultant values of T (°C) and fO_2 show no important variations, at least selected for magnetite–ilmenite analyses from the literature, in terms of allocation of ferric and ferrous electron-probe data in which total iron content is available (ESM 2).

4. Summary and availability of the program

WinMIgob is a user-friendly package for compositions of magnetite–ilmenite pairs, which is developed for personal computers running in the Windows operating system. The program calculates structural formulae of multiple magnetite and ilmenite analyses, obtained both from wet-chemical and electron-microprobe techniques, based on different ferric iron estimation methods. WinMIgob generates 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 magnetite and ilmenite analyses into the data entry section and make necessary arrangements for a

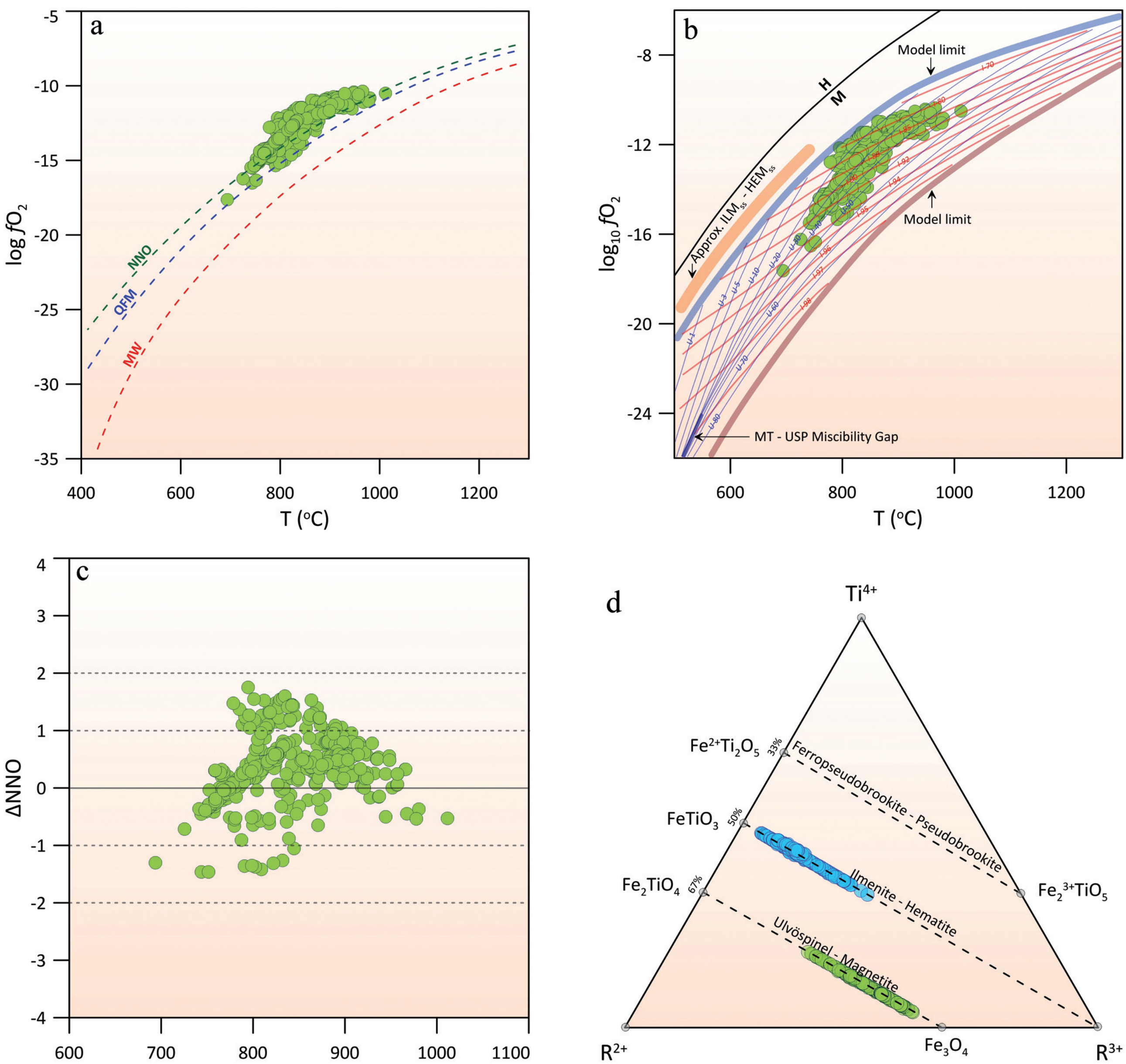


Fig. 7 a – Distribution of selected Fe–Ti oxides from the literature (n = 450; Ghiorso 2008; Blundy et al. 2008; Jolles and Lange 2019) in T (°C)–fO_2 plot using the calibration of Andersen and Lindsley (1985). Oxygen buffer curves are taken from Himmelberg and Ford (1977). NNO = nickel–nickel oxide, QFM = quartz–fayalite–magnetite, MW = magnetite–wüstite. **b** – Distribution of selected Fe–Ti oxides in Spencer and Lindsley (1981) T (°C)–fO_2 grid. **c** – T (°C)–ΔNNO plot using the calibration of Andersen and Lindsley (1985) and calculation method by Stormer (1983) for Fe–Ti oxides dataset. **d** – Compositions of Fe–Ti oxides in Ti–R^{2+}–R^{3+} ternary diagram. $R^{2+} = Fe^{2+} + Mg + Mn + (\pm Zn \pm Ni \pm Ca \pm Ba)$, $R^{3+} = Fe^{3+} + Cr + V + Al$. Dashed lines show high-temperature solid-solutions (magnetite–ulvöspine, hematite–ilmenite, pseudobrookite–ferropseudobrookite).

desired calculation scheme on the toolbar. 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*) allows the user to display all the input and results of cations (*apfu*) with stoichiometric ferric and ferrous iron contents, molecular magnetite–ulvöspinel and ilmenite–hematite amounts, magnetite–ilmenite geothermometers, oxygen barometers, oxygen fugacities relative to the NNO buffer and Bacon–Hirschmann equilibrium test. WinMIgob reports the output in a tabulated form with columns numbered from 1 to 133 in the *Calculation Screen* window, as well as in an Excel file. All the estimated magnetite and ilmenite 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. WinMIgob displays calculated magnetite and ilmenite compositions in binary and ternary diagrams, which can be viewed

Tab. 3 Magnetite–ilmenite geothermometer and oxygen barometer estimations by WinMIgob program

Row		Mt1	Mt2	Mt3	Mt4	Mt5	Mt6	Mt7	Mt8	Mt9	Mt10
	Magnetite–ilmenite geothermometers (T, °C)										
1	T_{P77_C67}	812	729	858	945	779	812	721	931	799	807
2	T_{P77_A68}	816	731	850	912	792	828	727	925	806	800
3	T_{P77_LS82}	820	736	883	954	789	815	716	930	801	808
4	T_{P77_S83}	818	734	857	971	792	823	727	940	815	829
5	T_{SL81_C67}	787	718	848	908	756	812	739	927	798	806
6	T_{SL81_A68}	794	724	844	869	771	822	742	916	806	802
7	T_{SL81_LS82}	796	724	877	919	765	815	732	926	800	807
8	T_{SL81_S83}	794	723	849	928	767	819	741	935	813	827
9	T_{AL85_C67}	796	740	842	878	771	813	757	891	806	812
10	T_{AL85_A68}	802	744	839	852	784	820	760	885	811	809
11	T_{AL85_LS82}	803	744	861	884	779	815	751	891	807	812
12	T_{AL85_S83}	802	744	842	889	781	819	759	896	817	827
13	T_{S08_A}	795	706	849	905	769	757	690	896	771	785
14	T_{GE08_A}	806	709	865	927	777	764	691	917	779	795
15	$T_{S08\_A\_AL85}$	771	693	825	888	743	793	713	896	791	804
16	$T_{GE08\_A\_AL85}$	774	687	835	904	743	799	710	914	796	811
17	T_{S08_B}	790	708	847	896	766	753	698	890	761	772
18	T_{GE08_B}	804	698	849	927	772	763	698	919	779	787
	Log oxygen fugacity (fO_2) values										
19	$fO_{2\ PP77\_C67}$	–12.10	–13.63	–12.38	–15.53	–12.56	–17.20	–15.68	–12.98	–14.16	–14.33
20	$fO_{2\ PP77\_A68}$	–12.18	–13.77	–13.69	–17.41	–12.56	–17.26	–15.52	–13.43	–14.25	–14.80
21	$fO_{2\ PP77\_LS82}$	–12.04	–13.53	–12.43	–15.20	–12.42	–17.08	–15.49	–12.88	–14.11	–14.25
22	$fO_{2\ PP77\_S83}$	–12.04	–13.60	–12.89	–15.46	–12.37	–17.09	–15.36	–13.05	–14.18	–14.36
23	$fO_{2\ SL81\_C67}$	–14.45	–16.04	–12.63	–9.95	–15.19	–11.62	–14.52	–10.56	–13.15	–12.83
24	$fO_{2\ SL81\_A68}$	–14.21	–15.80	–12.08	–10.23	–14.69	–11.35	–14.45	–10.57	–12.89	–12.76
25	$fO_{2\ SL81\_LS82}$	–14.21	–15.88	–11.91	–9.85	–14.97	–11.60	–14.85	–10.61	–13.12	–12.86
26	$fO_{2\ SL81\_S83}$	–14.27	–15.89	–12.35	–9.61	–14.91	–11.47	–14.57	–10.36	–12.72	–12.26
27	$fO_{2\ AL85\_C67}$	–14.37	–15.66	–12.97	–11.12	–14.95	–12.17	–14.37	–11.54	–13.29	–13.05
28	$fO_{2\ AL85\_A68}$	–14.18	–15.45	–12.52	–11.25	–14.54	–11.99	–14.31	–11.53	–13.09	–12.98
29	$fO_{2\ AL85\_LS82}$	–14.19	–15.52	–12.45	–11.07	–14.77	–12.16	–14.64	–11.58	–13.26	–13.06
30	$fO_{2\ AL85\_S83}$	–14.23	–15.53	–12.74	–10.92	–14.73	–12.07	–14.41	–11.42	–12.96	–12.63
31	$fO_{2\ S08\_A}$	–13.79	–15.32	–12.18	–10.09	–14.24	–12.72	–14.92	–11.03	–13.35	–12.88
32	$fO_{2\ S08\_A\_AL85}$	–14.45	–15.14	–13.08	–10.33	–14.76	–12.23	–14.56	–11.23	–13.33	–12.95
33	$fO_{2\ S08\_B}$	–13.99	–15.35	–12.33	–10.41	–14.41	–12.85	–14.72	–11.26	–13.66	–13.33
	Log oxygen fugacity values relative to the nickel–nickel oxide buffer (ΔNNO)										
34	ΔNNO_{AL85_C67}	–0.51	–0.49	–0.05	1.10	–0.54	1.33	0.39	0.43	0.38	0.49
35	ΔNNO_{AL85_A68}	–0.43	–0.39	0.45	1.45	–0.41	1.37	0.37	0.56	0.45	0.61
36	ΔNNO_{AL85_LS82}	–0.48	–0.47	0.08	1.03	–0.52	1.30	0.25	0.39	0.37	0.46
37	ΔNNO_{AL85_S83}	–0.49	–0.46	0.17	1.09	–0.52	1.32	0.31	0.46	0.47	0.60
38	ΔNNO_{S08_A}	0.10	0.68	0.61	1.63	0.24	2.03	1.50	0.86	1.10	1.23
39	ΔNNO_{G08_A}	–0.48	0.11	0.04	0.92	–0.32	1.20	0.82	0.27	0.48	0.60
40	$\Delta NNO_{S08\_A\_AL85}$	0.20	0.23	0.74	1.62	0.18	1.86	0.86	1.00	1.01	1.13
41	$\Delta NNO_{GE08\_A\_AL85}$	–0.53	–0.49	0.12	1.04	–0.56	1.27	0.26	0.42	0.42	0.55
42	ΔNNO_{S08_B}	0.03	0.61	0.54	1.54	0.15	2.01	1.49	0.80	1.01	1.10
43	ΔNNO_{GE08_B}	–0.57	–0.63	–0.18	1.28	–0.63	1.30	0.29	0.51	0.32	0.40

and printed by the Grapher, available from the 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.

WinMIgob is a compiled program that consists of a self-extracting setup file 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 "`.mi`", "`.xls`", "`.xlsx`" and plot files with the extension of "`.grf`") are installed into the personal computer's "C:\ Program Files\WinMIgob" folder with the Windows XP or later operating

Tab. 3 Notes:
Mt1–Il1 to Mt6–Il6 pairs from Ghiorso (2008); Mt7–Il7 and Mt8–Il8 from Blundy et al. (2008); Mt9–Il9 and Mt10–Il10 from Jolles and Lange (2019); Magnetite-ilmenite geothermometers of T_{P77_C67} (row 1) from Powell and Powell (1977) using the Carmichael (1967) method, T_{P77_A68} (row 2) from Powell and Powell (1977) using the Anderson (1968) method, T_{P77_LS82} (row 3) from Powell and Powell (1977) using the Lindsley and Spencer (1982) method, T_{P77_S83} (row 4) from Powell and Powell (1977) using the Stormer (1983) method, T_{SL81_C67} (row 5) from Spencer and Lindsley (1981) using the Carmichael (1967) method, T_{SL81_A68} (row 6) from Spencer and Lindsley (1981) using the Anderson (1968) method, T_{SL81_LS82} (row 7) from Spencer and Lindsley (1981) using the Lindsley and Spencer (1982) method, T_{SL81_S83} (row 8) from Spencer and Lindsley (1981) using the Stormer (1983) method, T_{AL85_C67} (row 9) from Andersen and Lindsley (1985) using the Carmichael (1967) method, T_{AL85_A68} (row 10) from Andersen and Lindsley (1985) using the Anderson (1968) method, T_{AL85_LS82} (row 11) from Andersen and Lindsley (1985) using the Lindsley and Spencer (1982) method, T_{AL85_S83} (row 12) from Andersen and Lindsley (1985) using the Stormer (1983) method, T_{S08_A} (row 13) from Sauerzapf et al. (2008) calculated by WinMIgop, T_{GE08_A} (row 14) from Ghiorso and Evans (2008) based on the linear regression equation [T_{GE08} (°C) = 1.098258692×T_{S08}–67.18937519] between Sauerzapf et al. (2008) and Ghiorso and Evans (2008) calibrations calculated by WinMIgop, $T_{S08\_A\_AL85}$ (row 15) from Sauerzapf et al. (2008) by selecting *Sauerzapf et al. (2008) thermometer through least-squares using model by Andersen and Lindsley (1985)* option from the pull-down-menu of *Geothermometer* in the *Start-up Screen* window of program, $T_{GE08\_A\_AL85}$ (row 16) from Ghiorso and Evans (2008) by selecting *Ghiorso and Evans (2008) thermometer through least-squares using model by Andersen and Lindsley (1985)* option from the pull-down-menu of *Geothermometer* in the *Start-up Screen* window of program, T_{S08_B} (row 17) from Excel spreadsheet estimation developed by Sauerzapf et al. (2008), T_{GE08_B} (row 18) from Ghiorso and Evans (2008) calculated by online link [http://melts.ofm--research.org/CORBA_CTserver/OxideGeothrm/OxideGeothrm.php]; Magnetite-ilmenite oxygen barometers of $fO_{2\ PP77\_C67}$ (row 19) from Powell and Powell (1977) using the Carmichael (1967) method, $fO_{2\ PP77\_A68}$ (row 20) from Powell and Powell (1977) using the Anderson (1968) method, $fO_{2\ PP77\_LS82}$ (row 21) from Powell and Powell (1977) using the Lindsley and Spencer (1982) method, $fO_{2\ PP77\_S83}$ (row 22) from Powell and Powell (1977) using the Stormer (1983) method, $fO_{2\ SL81\_C67}$ (row 23) from Spencer and Lindsley (1981) using the Carmichael (1967) method, $fO_{2\ SL81\_A68}$ (row 24) from Spencer and Lindsley (1981) using the Anderson (1968) method, $fO_{2\ SL81\_LS82}$ (row 25) from Spencer and Lindsley (1981) using the Lindsley and Spencer (1982) method, $fO_{2\ SL81\_S83}$ (row 26) from Spencer and Lindsley (1981) using the Stormer (1983) method, $fO_{2\ AL85\_C67}$ (row 27) from Andersen and Lindsley (1985) using the Carmichael (1967) method, $fO_{2\ AL85\_A68}$ (row 28) from Andersen and Lindsley (1985) using the Anderson (1968) method, $fO_{2\ AL85\_LS82}$ (row 29) from Andersen and Lindsley (1985) using the Lindsley and Spencer (1982) method, $fO_{2\ AL85\_S83}$ (row 30) from Andersen and Lindsley (1985) using the Stormer (1983) method, $fO_{2\ S08\_A}$ (row 31) from Sauerzapf et al. (2008) calculated by WinMIgop, $fO_{2\ S08\_A\_AL85}$ (row 32) from Sauerzapf et al. (2008) by selecting *log fO2 (Sauerzapf et al., 2008) through least-squares using model by Andersen and Lindsley (1985)* option from the pull-down-menu of *Oxygen barometer* in the *Start-up Screen* window of program, $fO_{2\ S08\_B}$ (row 33) from Excel spreadsheet estimation developed by Sauerzapf et al. (2008); Log oxygen fugacity values relative to nickel–nickel oxide buffer of ΔNNO_{AL85_C67} (row 34) from Andersen and Lindsley (1985) using the Carmichael (1967) method, ΔNNO_{AL85_A68} (row 35) from Andersen and Lindsley (1985) using the Anderson (1968) method, ΔNNO_{AL85_LS82} (row 36) from Andersen and Lindsley (1985) using the Lindsley and Spencer (1982) method, ΔNNO_{AL85_S83} (row 37) from Andersen and Lindsley (1985) using the Stormer (1983) method, ΔNNO_{S08_A} (row 38) from Sauerzapf et al. (2008) calculated by WinMIgop, ΔNNO_{G08_A} (row 39) from Ghiorso and Evans (2008) based on the polynomial equation [ΔNNO_{G08} = –0.5806296664 + 1.083216766 × ΔNNO_{S08} –0.1011931202 × ΔNNO_{S08}^2] between Sauerzapf et al. (2008) and Ghiorso and Evans (2008) calibrations calculated by WinMIgop, $\Delta NNO_{S08\_A\_AL85}$ (row 40) from Sauerzapf et al. (2008) by selecting *DeltaNNO (Sauerzapf et al., 2008) through least-squares using model by Andersen and Lindsley (1985)* option from the pull-down-menu of *Oxygen barometer* in the *Start-up Screen* window of program, $\Delta NNO_{GE08\_A\_AL85}$ (row 41) from Ghiorso and Evans (2008) by selecting *DeltaNNO (Ghioro and Evans, 2008) through least-squares using model by Andersen and Lindsley (1985)* option from the pull-down-menu of *Oxygen barometer* in the *Start-up Screen* window of program, ΔNNO_{S08_B} (row 42) from Excel spreadsheet estimation developed by Sauerzapf et al. (2008), ΔNNO_{GE08_B} (row 43) from Ghiorso and Evans (2008) calculated by online link [http://melts.ofm-research.org/CORBA_CTserver/OxideGeothrm/OxideGeothrm.php]

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 20 Mb and may be downloaded from the journal server.

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Electronic supplementary material. Examples of magnetite–ilmenite data recalculated and plotted by the WinMIgop program (ESM 1), comparison of Fe_2O_3 and FeO (wt. %) input (e.g., wet-chemical) with FeO_{tot} (wt. %) contents (e.g., electron-microprobe) in the estimation of temperature (°C) and oxygen fugacity (fO_2) values (ESM 2), the steps for WinMIgop program execution (ESM 3) and self-extracting `WinMIgop.exe` setup file are available online at the Journal web site (*http://dx.doi.org/10.3190/jgeosci.319)*.

References

Andersen DJ, Lindsley DH (1985) New (and final!) models for the Ti–magnetite/ilmenite geothermometer and oxygen barometer. Abst AGU 1985 Spring Meeting Eos Transactions. AGU 66 (18), 416.

Andersen DJ, Lindsley DH (1988) Internally consistent solution models for Fe–Mg–Mn–Ti oxides: Fe–Ti oxides. Amer Miner 73: 714–726

Anderson AT (1968) Oxidation of the LaBlache Lake titaniferous magnetite deposit, Quebec. J Geol 76: 528–547

Aratór, Audétat A (2017) FeTiMM–A new oxybarometer for mafic to felsic magmas. Geochem Perspect Lett 5: 19–23

Bacon CR, Hirschmann MM (1988) Mg/Mn partitioning as a test for equilibrium between Fe–Ti oxides: Amer Miner 73: 57–61

Blundy J, Cashman KV, Berlo K (2008) Evolving Magma Storage Conditions Beneath Mount St. Helens Inferred from Chemical Variations in Melt Inclusions from the 1980–1986 and Current (2004–2006) Eruptions. In: Sherrod DR, Scott WE, Stauffer PH (eds) A Volcano Rekindled: The Renewed Eruption of Mount St. Helens, 2004–2006. USGS Prof Pap 1750, pp 755–790

Buddington AF, Lindsley DH (1964) Iron–titanium oxide minerals and synthetic equivalents. J Petrol 5: 310–357

Carmichael ISE (1967) The iron–titanium oxides of salic volcanic rocks and their associated ferromagnesian silicates. Contrib Mineral Petrol 14: 36–64

Droop GTR (1987) A general equation for estimating Fe^{3+} concentrations in ferromagnesian silicates and oxides from microprobe analyses using stoichiometric criteria. Mineral Mag 51: 431–435

Evans BW, Scaillet B (1997) The redox state of Pinatubo dacite and the ilmenite–hematite solvus. Amer Miner 82: 625–629

Evans BW, Scaillet B, Kuehner SM (2006) Experimental determination of coexisting iron–titanium oxides in the systems FeTiAlO, FeTiAlMgO, FeTiAlMnO, and FeTiAlMgMnO at 800 and 900 °C, 1–4 kbar, and relatively high oxygen fugacity. Contrib Mineral Petrol 152: 149–167

Ghiorso MS (2008) The magnetite–ilmenite database (04GhiorsoDataTable.xls). http://earth.geology.yale.edu/~ajs/SupplementaryData/2008/ (accessed 15.08.20)

Ghiorso MS, Carmichael ISE (1981) A Fortran IV computer program for evaluating temperatures and oxygen fugacities from the compositions of coexisting iron–titanium oxides. Comput Geosci 7: 123–129

Ghiorso MS, Evans BW (2008) Thermodynamics of rhombohedral oxide solid solutions and a revision of the Fe–Ti two–oxide geothermometer and oxygen–barometer. Amer J Sci 308: 957–1039

Ghiorso MS, Sack O (1991) Fe–Ti oxide geothermometry: thermodynamic formulation and the estimation of intensive variables in silicic magmas. Contrib Mineral Petrol 108: 485–510

Himmelberg GR, Ford AB (1977) Iron–titanium oxides of the Dufek intrusion, Antarctica. Amer Miner 62: 623–633

Holland T, Blundy J (1994) Nonideal interactions in calcic amphiboles and their bearing on amphibole–plagioclase thermometry. Contrib Mineral Petrol: 116, 433–447

Honjo N, Bonnichesen B, Leeman WP, Stormer JC Jr (1992) Mineralogy and geothermometry of high-temperature rhyolites from the central and western Snake River Plain. Bull Volcanol: 54, 220–237

Hora JM, Kronz A, Möller–Mcnett S, Wörner G (2013) An Excel-based tool for evaluating and visualizing geothermobarometry data. Comput Geosci 56: 178–185

Jolles JSR, Lange RA (2019) High-resolution Fe–Ti oxide thermometry applied to single-clast pumices from the Bishop Tuff: a re-examination of compositional variations in phenocryst phases with temperature. Contrib Mineral Petrol: 174, 1–43

Lanari P, Vidal O, De Andre V, Dubacq B, Lewin E, Grosch EG, Schwartz S (2014) XMapTools: a MATLAB©-based program for electron microprobe X-ray image processing and geothermobarometry. Comput Geosci 62: 227–240

Lattard D, Sauerzapf U, Käsemann M (2005) New calibration data for the Fe–Ti oxide thermo-oxybarometers from experiments in the Fe–Ti–O system at 1 bar, 1,000–1,300 °C and a large range of oxygen fugacities. Contrib Mineral Petrol 149: 735–754

Lepage LD (2003) ILMAT: an Excel worksheet for ilmenite–magnetite geothermometry and geobarometry. Comput Geosci 29: 673–678

Li W, Cheng Y, Yang Z (2019) Geo–fO_2: Integrated software for analysis of magmatic oxygen fugacity. Geochem Geophys Geosyst 20: 2542–2555

Lindsley DH, Frost BR (1992) Equilibria among Fe–Ti oxides, pyroxenes, olivine, and quartz: part I. Theory. Amer Miner 77: 987–1003

Lindsley DH, Spencer KJ (1982) Fe–Ti oxide geothermometry: Reducing analyses of coexisting Ti-magnetite (Mt) and ilmenite (llm). Trans Amer Geophys Un (EOS) 63: 471

Misra KC (2012) Introduction to Geochemistry Principles and Applications. Wiley–Blackwell, UK, pp 1–438

Mullen EK, McCallum IS (2013) Coexisting pseudobrookite, ilmenite, and titanomagnetite in hornblende andesite of the Coleman Pinnacle flow, Mount Baker, Washington: Evidence for a highly oxidized arc magma. Amer Miner 98:417–425

Ondrejka M, Broska I, Uher P (2015) The late magmatic to subsolidus T–fO_2 evolution of the Lower Triassic A-type rhyolites (Silicic Superunit, Western Carpathians, Slovakia): Fe–Ti oxythermometry and petrological implications. Acta Geol Slov 7: 51–61

Powell R, Powell M (1977) Geothermometry and oxygen barometry using coexisting iron–titanium oxides: a reappraisal. Mineral Mag 41: 257–263

Putirka K (2008) Thermometers and barometers for volcanic systems. In: Putirka KD, Tepley III FJ (eds) Minerals, Inclusions And Volcanic Processes. Mineralogical Society of America and Geochemical Society Reviews in Mineralogy and Geochemistry 69, Washington, pp 61–120

Rao DR, Choubey VM, Rao TV (1991) ITHERM: A Basic program for magnetite–ilmenite thermometry. Comput Geosci 17: 307–314

Sauerzapf U, Lattard D, Burchard M, Engelmann R (2008) The titanomagnetite–ilmenite equilibrium: New experimental data and thermo–oxybarometric applica-

tion to the crystallization of basic to intermediate rocks. J Petrol 49: 1161–1185
Spencer KJ, Lindsley DH (1981) A solution model for coexisting iron–titanium oxides. Amer Miner 66: 1189–1201
Stormer JC Jr (1983) The effects of recalculation on estimates of temperature and oxygen fugacity from analyses of multicomponent–iron–titanium oxides. Amer Miner 68: 586–594
Venezky DY, Rutherford MJ (1999) Petrology and Fe–Ti oxide reequilibration of the 1991 Mount Unzen mixed magma. J Volcanol Geotherm Res 89: 213–230
Wang R, Richards JP, Hou ZQ, Yang ZM, Gou ZB, Dufrane SA (2014) Increasing Magmatic Oxidation State from Paleocene to Miocene in the Eastern Gangdese Belt, Tibet: Implication for Collision-Related Porphyry Cu–Mo±Au Mineralization. Econ Geol 109: 1943–1965
Yavuz F (1998) BIOAPAG–PC: Program for an apatite and biotite geothermometer. Comput Geosci 24: 885–891
Yavuz F (2013) WinPyrox: a Windows program for pyroxene calculation classification and thermobarometry. Amer Miner 98: 1338–1359
Yavuz F, Döner Z (2017) WinAmptb: a Windows program for calcic amphibole thermobarometry. Period di Mineral 86: 135–167
Yavuz F, Yildirim DK (2020) WinGrt, a Windows program for garnet supergroup minerals. J Geosci 65: 71–95