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WinClastour—a Visual Basic program for tourmaline formula calculation and classification ☆

Fuat Yavuz[a,*], Vural Yavuz[a], Ahmet Sasmaz[b]

[a] *İstanbul Teknik Üniversitesi, Maden Fakültesi, Jeoloji Mühendisliği Bölümü, 34469, Maslak, İstanbul, Turkey*
[b] *Fırat Üniversitesi, Mühendislik Fakültesi, Jeoloji Mühendisliği Bölümü, 23119, Elazığ, Turkey*

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Abstract

WinClastour is a Microsoft® Visual Basic 6.0 program that enables the user to enter and calculate structural formulae of tourmaline analyses obtained both by the electron-microprobe or wet-chemical analyses. It is developed to predict cation site-allocations at the different structural positions, as well as to estimate mole percent of the end-members of the calcic-, alkali-, and *X*-site vacant group tourmalines. Using the different normalization schemes, such as 24.5 oxygens, 31 anions, 15 cations ($T+Z+Y$), and 6 silicons, the present program classifies tourmaline data based on the classification scheme proposed by Hawthorne and Henry [1999. Classification of the minerals of the tourmaline group. European Journal of Mineralogy 11, 201–215]. The present program also enables the user Al–Mg disorder between *Y* and *Z* sites. WinClastour stores all the calculated results in a comma-delimited ASCII file format. Hence, output of the program can be displayed and processed by any other software for general data manipulation and graphing purposes. The compiled program code together with a test data file and related graphic files, which are designed to produce a high-quality printout from the Grapher program of Golden Software, is approximately 3 Mb as a self-extracting setup file.

Keywords: Tourmaline; Electron-microprobe; Wet-chemical; Normalization; Classification; Al–Mg disorder

1. Introduction

Tourmaline is the most important and common accessory borosilicate mineral in granitic rocks and their pegmatites, associated metallic hydrothermal deposits, and metamorphic and sedimentary rocks. The common occurrence and large stability of tourmaline in different geological environments made it important to understand the physical and chemical conditions of rock formation, as well as the ore-forming processes and hydrothermal ore deposits. Occurrence of tourmaline in earth crust is generally controlled by the amount of boron in the system, the pressure and temperature conditions, and the composition of circulating fluids. The general formula of tourmaline can be expressed as $XY_3Z_6T_6O_{18}(BO_3)V_3W$, where the major and minor substitutions exist in the *X* (Ca, Na, K, vacancy), *Y* (Li, Mg, Fe^{2+}, Mn^{2+}, Al, Cr^{3+}, V^{3+}, Fe^{3+}, Ti^{4+}), *Z* (Mg, Al, Fe^{3+}, V^{3+}, Cr^{3+}), *T* (Si, Al, B), *V* (OH,

☆ Code available from server at http://www.iamg.org/CGEditor/index.htm.

*Corresponding author. P.K. 90, 34711, Kadıköy, İstanbul, Turkey.

E-mail address: yavuz@itu.edu.tr (F. Yavuz).

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O), and *W* (OH, O, F) sites. Currently valid tourmaline species include 13 end-member compositions (dravite, schorl, chromdravite, povondraite, buergerite, elbaite, olenite, magnesiofoititte, foitite, rossmanite, uvite, feruvite, and liddicoatite). Hawthorne (1999) discussed the possible tourmaline minerals taking into account the bond-valence constraints on the chemical composition of tourmaline. Recent studies on tourmaline have shown that this chemically complex borosilicate can be used to illuminate the petrogenesis of magmatic and metamorphic rocks (Henry and Guidotti, 1985; Henry and Dutrow, 1996; Fuchs et al., 1998).

The International Mineralogical Association (IMA) has not currently approved a classification scheme for tourmaline group minerals as in the case of amphibole group minerals (Leake, 1978; Leake et al., 1997, 2004). However, Hawthorne and Henry (1999) proposed a classification scheme for the tourmaline group minerals based on the chemical composition and ordering at the different sites of the tourmaline structure. Consequently, limited computer programs written in Microsoft® QuickBasic (Yavuz 1997; Yavuz et al., 2002) appeared in literature to calculate and classify the tourmaline group minerals. However, Tindle et al. (2002) referenced tourmaline calculation program under Microsoft® Excel based on 31 anions. In this paper, the original program of Clastour (Yavuz et al., 2002) was re-written as WinClastour in Windows operating system to get a better graphical user interface and interaction as the Visual Basic programming environment contains programming tools to develop user-friendly software. WinClastour permits the user to calculate his or her own electron-microprobe or wet-chemical tourmaline data for different normalization procedures such as 31 anion, 24.5 oxygens, 15 cations ($T+Z+Y$), and 6 silicons.

2. Program description

2.1. Data entry

Following the installation process, the start-up view of main program appears on the screen (Fig. 1). Alternatively, upon successful installation, once the user clicks the WinClastour icon, which is the executable form of the main program, this initial program segment is also displayed. At this part of the program, the new tourmaline chemical data can be entered by clicking the *New* icon on the tool bar or by selecting the *File* ⇒ *New File* (Ctrl + N) options from the pull-down menu of *File*. The 24 variables are defined by the program for tourmaline data entry in the following order:

Sample No, SiO_2, TiO_2, Al_2O_3, V_2O_3, Cr_2O_3, Fe_2O_3, FeO, MnO, NiO, CoO, ZnO, MgO, CaO, BaO, Na_2O, K_2O, Rb_2O, Cs_2O, Li_2O, F, Cl, H_2O, B_2O_3.

Microprobe or wet-chemical tourmaline analyses, which are entered or saved as ASCII format in different spreadsheet program, such as Excel™, can be directly imported into to the WinClastour's data entry section by using the Copy–Paste options. In this case, the user must enter his or her own tourmaline data as in the order cited above to obtain the correct output from the clipboard. Additional knowledge on data entry or similar topics can be accessed by pressing the *F1* function key. This key is used to display the Winclastour.hlp file on screen. For example, by selecting the *Data Entry* section from the *Index* of Winclastour.hlp file and clicking the *Display* button during the help file is activated, it opens the necessary documents about the tourmaline *Data Entry* on screen.

2.2. Program details

Once the data entry is completed and saved under a user-defined file name, the program output is provided by clicking the *Calculate* icon on the tool bar or selecting *Calculate* ⇒ *Open File to Calculate* (Ctrl + F) options (Figs. 2A and B). Converting from wt% oxide values to atomic proportions (*apfu*) used in mineral formula estimation is customarily carried out by normalizing on the basis of the number of oxygens or anions. WinClastour calculates the structural formulae of tourmaline on the basis of 24.5 atoms of oxygen as a default. Nevertheless, the program allows the user to select the normalization parameter for the calculation of structural formulae on the basis of 31 anions, $T+Z+Y=15$ oxygens, and 6 silicons. During the program run, selected normalization scheme from *Normalization* ⇒ *Structural formulae* of pull-down menu is displayed at the second base panel (see Figs. 2A and B). In the case of tourmaline, 31 anions normalization seems to be the best-case scenario for samples, which have been fully analyzed for H_2O, B_2O_3, and Li_2O. While the electron-microprobe study of rock-forming minerals is valid for many major and minor elements, the ability to analyze H, B and Li is beyond its capabilities yet. For that reason, electron-microprobe analysis of tourmaline

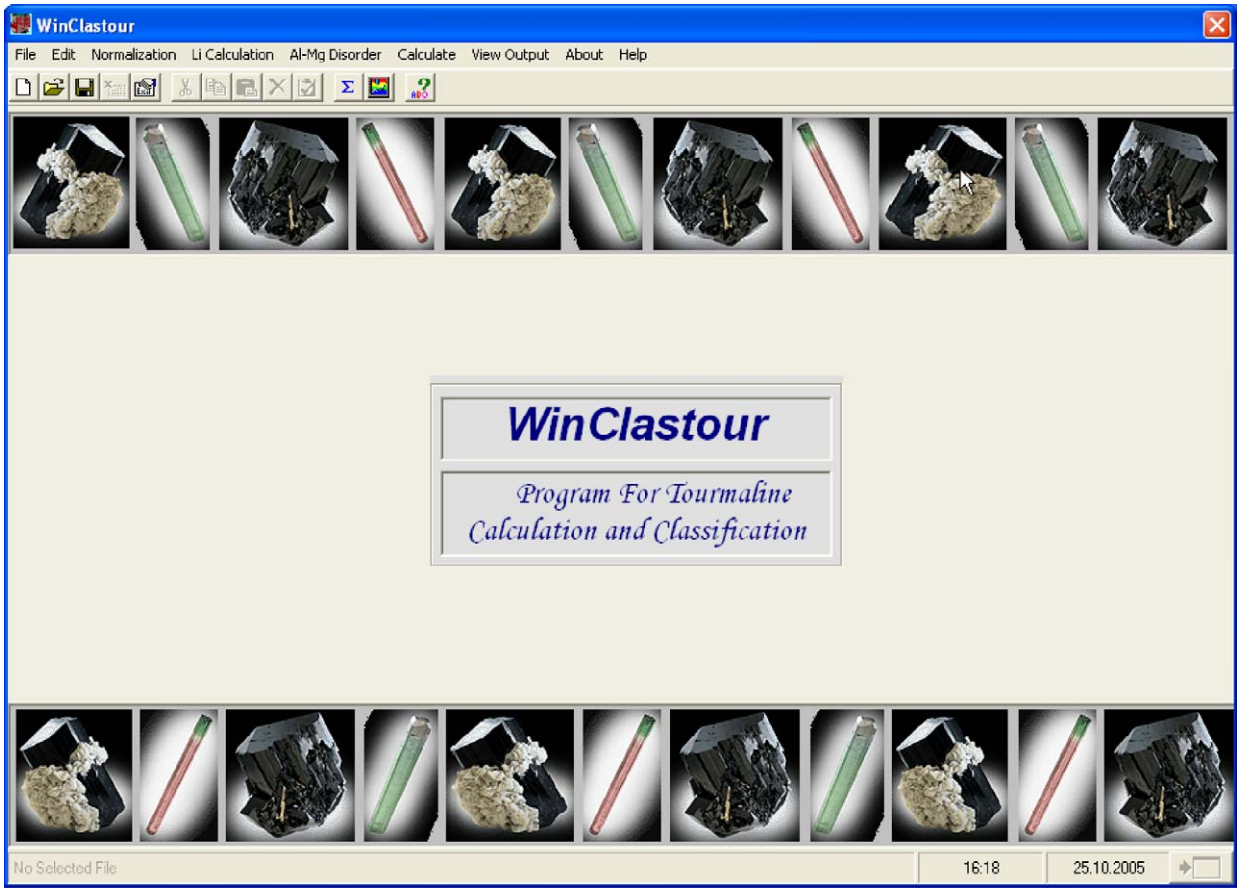


Fig. 1. Start-up window for WinClastour program. User can enter or edit his or her own tourmaline data, select normalization procedure and Li estimation option, and display all calculated output in different window forms.

should be supplemented by light element data either from different analytical techniques or calculations based on tourmaline stoichiometry.

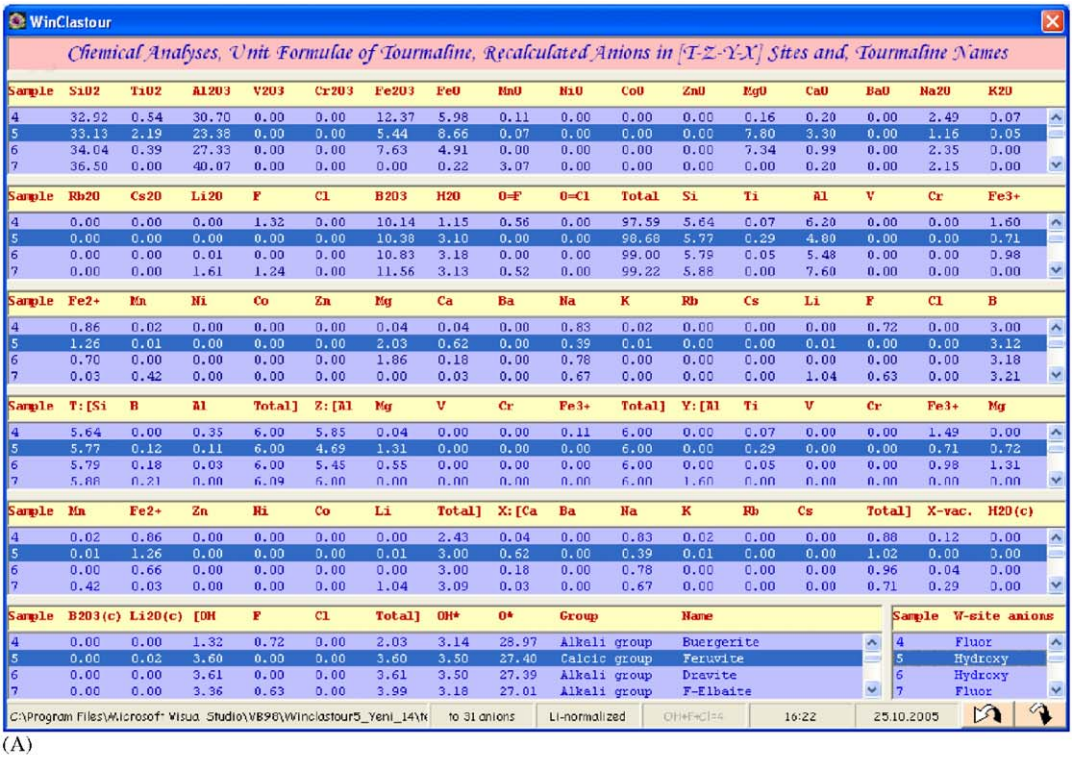
Tourmalines from Li-pegmatites may contain significant amount of lithium at Y site. In these situations, Li content of tourmaline can be calculated stoichiometrically by initially normalizing to 29 oxygens basis (with B calculation) or 24.5 oxygens basis (without B calculation), and then estimating Li by the expression: Li = 3-(Σ Y site) (Henry and Dutrow, 1996). By selecting the *Estimate Li from 3-(Total Y)* and checking *Yes* option in the pull-down menu of *Li Estimation* the present program calculates the stoichiometric amounts of Li_2O except for 15 cations ($T+Z+Y$) option. The allocation of ions to T, Z, Y, and X sites is sequentially carried out by WinClastour as follows:

(1) Sum T to 6 using Si, then B (if B > 3), then Al.
(2) Sum Z to 6 using excess Al from (1) and then successively, Mg, V^{3+}, Cr^{3+}, Fe^{3+}.
(3) Sum Y to 3 using excess Al from (2), then Ti, then successively V^{3+}, Cr^{3+}, Fe^{3+}, Mg from (2) and then Mn^{2+}, Fe^{2+}, Zn, Ni, Co and Li.
(4) Sum X to 1 using Ca, then Ba, Na, K, Rb, and Cs.

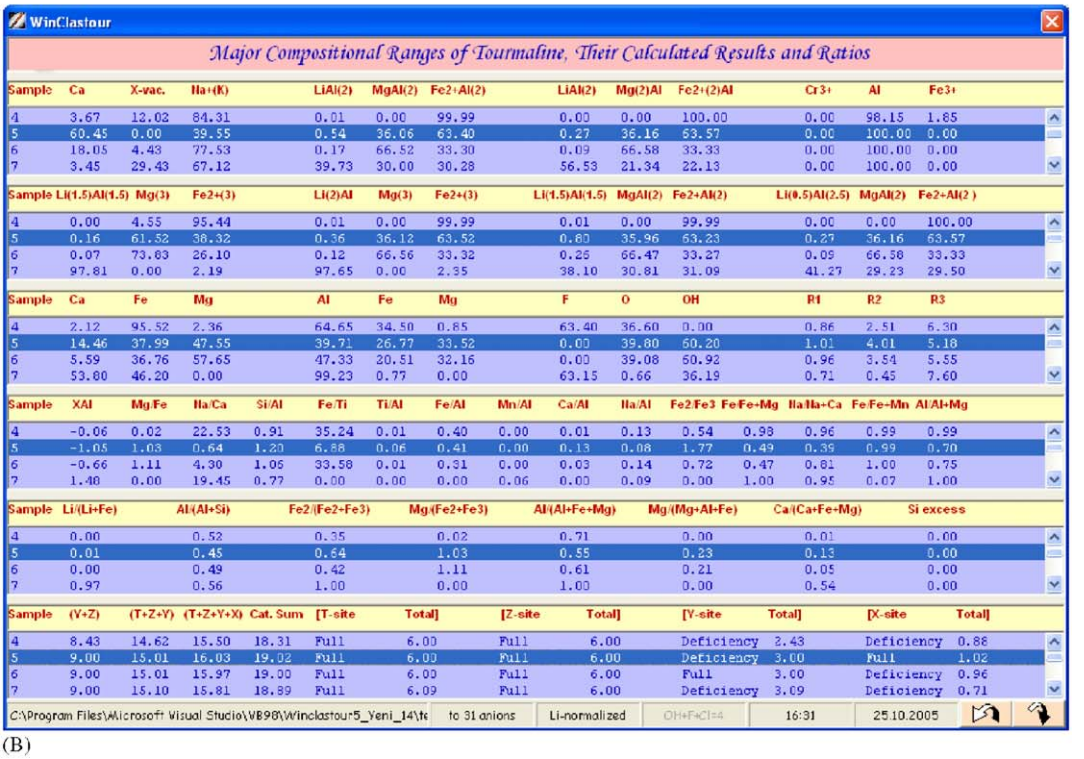
The Al–Mg disorder between the Y and Z sites require measured unit cell volume and Mg/(Mg + Al) ratio in the Z site (Henry and Dutrow, 1996). However, Grice and Ercit (1993) proposed that in the absence of a cell volume measurement, Mg in the Y and Z sites can be estimated for tourmalines with more than 7 wt% FeO by the following expressions:

$$^{Y}Mg = 3[1 - Fe/(Fe + Mg)] \quad (1)$$

$$^{Z}Mg = (\Sigma\ Mg) - {}^{Y}Mg \quad (2)$$

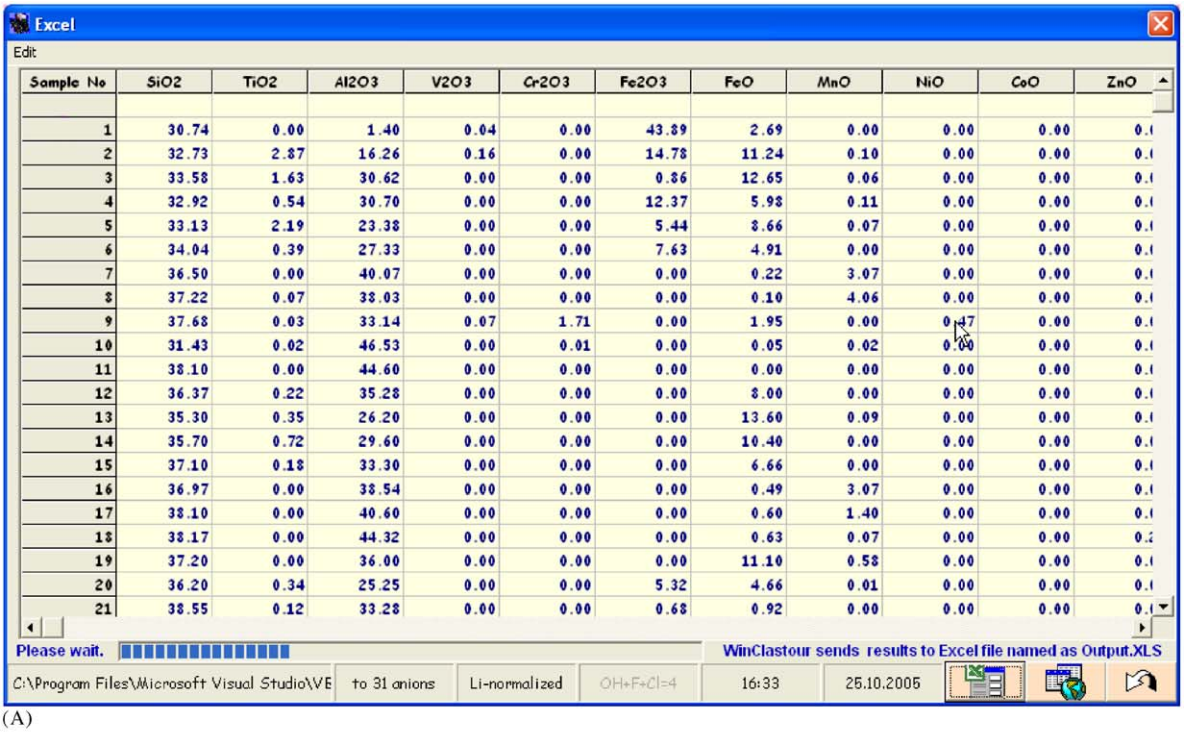


(A)



(B)

Fig. 2. (A) Screen output with recalculation, site-allocation, and classification of tourmaline chemical data. (B) Window displaying end-member fractions of calculated data and selected element ratios for tourmaline data.



Excel

Edit

Sample No	SiO2	TiO2	Al2O3	V2O3	Cr2O3	Fe2O3	FeO	MnO	NiO	CoO	ZnO
1	30.74	0.00	1.40	0.04	0.00	43.89	2.69	0.00	0.00	0.00	0.(
2	32.73	2.87	16.26	0.16	0.00	14.78	11.24	0.10	0.00	0.00	0.(
3	33.58	1.63	30.62	0.00	0.00	0.86	12.65	0.06	0.00	0.00	0.(
4	32.92	0.54	30.70	0.00	0.00	12.37	5.98	0.11	0.00	0.00	0.(
5	33.13	2.19	23.38	0.00	0.00	5.44	8.66	0.07	0.00	0.00	0.(
6	34.04	0.39	27.33	0.00	0.00	7.63	4.91	0.00	0.00	0.00	0.(
7	36.50	0.00	40.07	0.00	0.00	0.00	0.22	3.07	0.00	0.00	0.(
8	37.22	0.07	38.03	0.00	0.00	0.00	0.10	4.06	0.00	0.00	0.(
9	37.68	0.03	33.14	0.07	1.71	0.00	1.95	0.00	0.47	0.00	0.(
10	31.43	0.02	46.53	0.00	0.01	0.00	0.05	0.02	0.00	0.00	0.(
11	38.10	0.00	44.60	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.(
12	36.37	0.22	35.28	0.00	0.00	0.00	8.00	0.00	0.00	0.00	0.(
13	35.30	0.35	26.20	0.00	0.00	0.00	13.60	0.09	0.00	0.00	0.(
14	35.70	0.72	29.60	0.00	0.00	0.00	10.40	0.00	0.00	0.00	0.(
15	37.10	0.18	33.30	0.00	0.00	0.00	6.66	0.00	0.00	0.00	0.(
16	36.97	0.00	38.54	0.00	0.00	0.00	0.49	3.07	0.00	0.00	0.(
17	38.10	0.00	40.60	0.00	0.00	0.00	0.60	1.40	0.00	0.00	0.(
18	38.17	0.00	44.32	0.00	0.00	0.00	0.63	0.07	0.00	0.00	0.2
19	37.20	0.00	36.00	0.00	0.00	0.00	11.10	0.58	0.00	0.00	0.(
20	36.20	0.34	25.25	0.00	0.00	5.32	4.66	0.01	0.00	0.00	0.(
21	38.55	0.12	33.28	0.00	0.00	0.68	0.92	0.00	0.00	0.00	0.(

Please wait.

WinClastour sends results to Excel file named as Output.XLS

C:\Program Files\Microsoft Visual Studio\VB | to 31 anions | Li-normalized | OH+F+Cl=4 | 16:33 | 25.10.2005

(A)

	A	AX	AY	AZ	BA	BB	BC	BD	BE	BF	BG	BH	BI	BJ	BK	BL	BM	BN	BO
91																			
1	Sample No	Si(T)	B(T)	Al(T)	Total(T)	Al(Z)	Mg(Z)	V(Z)	Cr(Z)	Fe3+(Z)	Total(Z)	Al(Y)	Ti(Y)	V(Y)	Cr(Y)	Fe3+(Y)	Mg(Y)	Mn(Y)	Fe2+(Y
2																			
3	1	5.88	0.03	0.10	6.00	0.22	1.84	0.01	0.00	3.94	6.00	0.00	0.00	0.00	0.00	2.38	0.00	0.00	0.43
4	2	5.96	0.00	0.04	6.00	3.44	1.26	0.02	0.00	1.27	6.00	0.00	0.39	0.00	0.00	0.76	0.00	0.02	1.71
5	3	5.79	0.08	0.13	6.00	6.00	0.00	0.00	0.00	0.00	6.00	0.08	0.21	0.00	0.00	0.11	0.69	0.01	1.82
6	4	5.64	0.00	0.35	6.00	5.85	0.04	0.00	0.00	0.11	6.00	0.00	0.07	0.00	0.00	1.49	0.00	0.02	0.86
7	5	5.77	0.12	0.11	6.00	4.69	1.31	0.00	0.00	0.00	6.00	0.00	0.29	0.00	0.00	0.71	0.72	0.01	1.26
8	6	5.79	0.18	0.03	6.00	5.45	0.55	0.00	0.00	0.00	6.00	0.00	0.05	0.00	0.00	0.98	1.31	0.00	0.66
9	7	5.88	0.21	0.00	6.09	6.00	0.00	0.00	0.00	0.00	6.00	1.60	0.00	0.00	0.00	0.00	0.00	0.42	0.03
10	8	5.94	0.00	0.06	6.00	6.00	0.00	0.00	0.00	0.00	6.00	1.09	0.01	0.00	0.00	0.00	0.04	0.55	0.01
11	9	6.05	0.00	0.00	6.05	6.00	0.00	0.00	0.00	0.00	6.00	0.27	0.00	0.01	0.22	0.00	2.32	0.00	0.18
12	10	5.15	1.58	0.00	6.73	6.00	0.00	0.00	0.00	0.00	6.00	2.98	0.00	0.00	0.00	0.00	0.00	0.00	0.01
13	11	5.88	0.00	0.12	6.00	6.00	0.00	0.00	0.00	0.00	6.00	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	12	5.97	0.00	0.03	6.00	6.00	0.00	0.00	0.00	0.00	6.00	0.80	0.03	0.00	0.00	0.00	1.00	0.00	1.10
15	13	6.03	0.00	0.00	6.03	5.27	0.73	0.00	0.00	0.00	6.00	0.00	0.04	0.00	0.00	0.00	0.76	0.01	1.94
16	14	5.94	0.00	0.06	6.00	5.74	0.26	0.00	0.00	0.00	6.00	0.00	0.09	0.00	0.00	0.00	1.18	0.00	1.45
17	15	6.01	0.00	0.00	6.01	6.00	0.00	0.00	0.00	0.00	6.00	0.36	0.02	0.00	0.00	0.00	1.09	0.00	0.90
18	16	5.91	0.00	0.09	6.00	6.00	0.00	0.00	0.00	0.00	6.00	1.18	0.00	0.00	0.00	0.00	0.00	0.42	0.07
19	17	6.02	0.00	0.00	6.02	6.00	0.00	0.00	0.00	0.00	6.00	1.57	0.00	0.00	0.00	0.00	0.00	0.19	0.08
20	18	5.95	0.00	0.05	6.00	6.00	0.00	0.00	0.00	0.00	6.00	2.08	0.00	0.00	0.00	0.00	0.00	0.01	0.08
21	19	6.12	0.00	0.00	6.12	6.00	0.00	0.00	0.00	0.00	6.00	0.98	0.00	0.00	0.00	0.00	0.00	0.08	1.53
22	20	5.97	0.00	0.03	6.00	4.88	1.12	0.00	0.00	0.00	6.00	0.00	0.04	0.00	0.00	0.66	1.34	0.00	0.64
23	21	5.96	0.00	0.04	6.00	6.00	0.00	0.00	0.00	0.00	6.00	0.02	0.01	0.00	0.00	0.08	2.43	0.00	0.12
24	22	5.76	0.00	0.24	6.00	5.93	0.07	0.00	0.00	0.00	6.00	0.00	0.09	0.00	0.00	0.00	2.55	0.00	0.35
25	23	5.79	0.00	0.21	6.00	1.83	2.21	0.36	1.60	0.00	6.00	0.00	0.00	0.00	2.75	0.00	0.00	0.00	0.05
26	24	5.73	0.00	0.27	6.00	2.07	2.18	0.24	1.52	0.00	6.00	0.00	0.03	0.00	2.60	0.00	0.00	0.00	0.03
27	25	5.87	0.00	0.13	6.00	6.00	0.00	0.00	0.00	0.00	6.00	0.39	0.10	0.00	0.00	0.06	1.57	0.01	0.73
28	26	6.16	0.00	0.00	6.16	6.00	0.00	0.00	0.00	0.00	6.00	1.50	0.00	0.00	0.00	0.00	0.00	0.06	0.00
29	27	5.55	0.00	0.45	6.00	4.57	1.43	0.00	0.00	0.00	6.00	0.00	0.00	0.00	0.00	0.23	2.02	0.00	0.44
30	28	5.59	0.00	0.41	6.00	5.25	0.75	0.00	0.00	0.00	6.00	0.00	0.33	0.00	0.00	0.00	0.82	0.00	1.79
31	29	5.94	0.00	0.06	6.00	6.00	0.00	0.00	0.00	0.00	6.00	1.10	0.01	0.00	0.00	0.00	0.04	0.55	0.01
32	30	5.93	0.00	0.07	6.00	6.00	0.00	0.00	0.00	0.00	6.00	1.26	0.00	0.00	0.00	0.00	1.42	0.00	0.13
33	31	6.01	0.00	0.00	6.01	6.00	0.00	0.00	0.00	0.00	6.00	1.47	0.00	0.00	0.00	0.00	0.00	0.08	0.00

(B)

Fig. 3. (A) Screenshot of sending all calculated result to Excel spreadsheet by selecting "View All" option in pull-down menu of "View Output". (B) Typical screen output of "Output.xls" file under Microsoft® Excel spreadsheet by clicking "Display excel file" icon in Excel window.

Despite the practical approach, these types of expressions may overestimate Mg especially in the *Y* site. Ordering of Mg between the *Z* and *Y* sites can be assigned from different solutions. By selecting one of these options from *Al–Mg Disorder* menu, WinClastour allocates Mg contents of tourmaline in *Z* and *Y* sites based on the linear regression lines and correlation coefficients that calculated from the original data by Grice and Ercit (1993), Eqs. (3) and (4), Bloodaxe et al. (1999), Eq. (5), and Bosi et al. (2004a), Eq. (6) as follows:

$$^{Y}Mg = -2.76[Fe/(Fe + Mg)] + 2.63 \quad (3)$$

$$^{Z}Mg = (\Sigma\ Mg) - {}^{Y}Mg \quad (4)$$

$$^{Y}Fe^{2+} = -1.84\,{}^{Z}Mg + 2.09 \quad (5)$$

$$^{Y}Mg = -1.00\,{}^{Y}Fe^{2+} + 1.57 \quad (6)$$

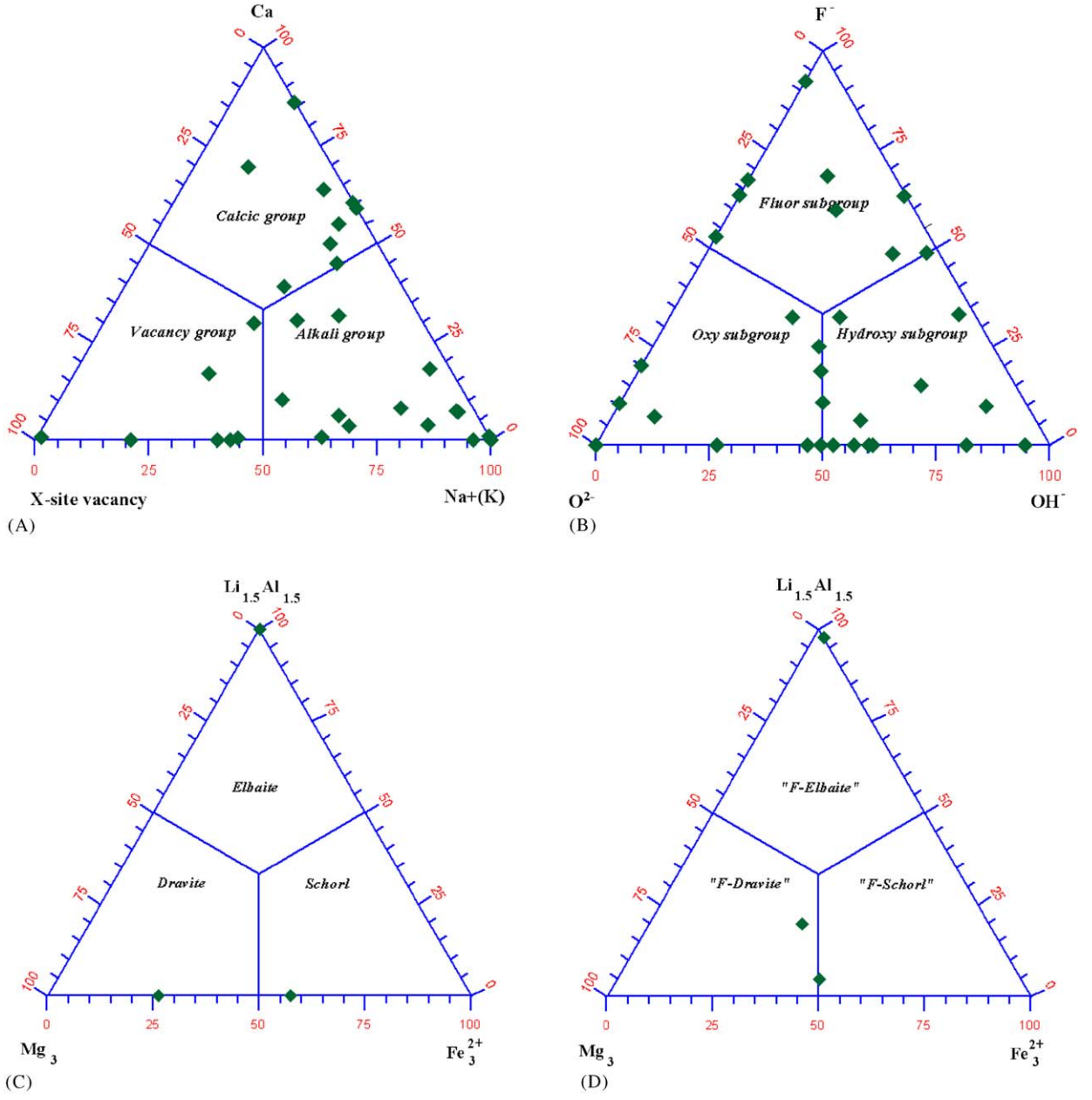


Fig. 4. (A–J) Classification of tourmaline data (i.e., Test1.tou file in Table A.1) into major compositional groups of tourmaline minerals.

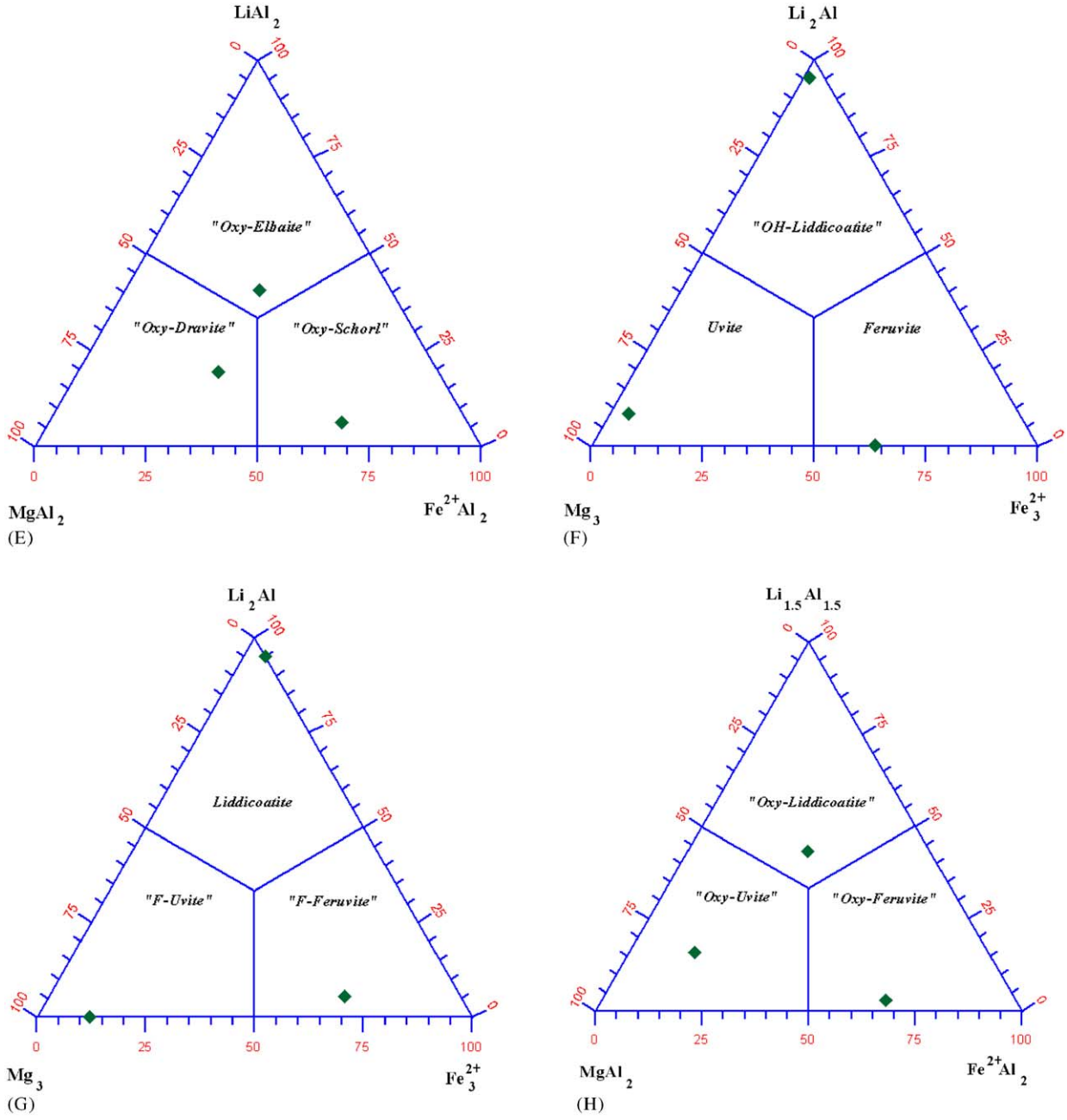


Fig. 4. (*Continued*)

The *(OH+F+Cl) = 4* option under the *Structural formulae* pull-down menu may be used to normalize the sum of OH, F, and Cl to 4. WinClastour also automatically assumes stoichiometric amounts of B_2O_3 (i.e., B = 3 *apfu*) and H_2O if tourmaline data was obtained from electron-microprobe study. Many olenites, elbaites, and rossmanites contain significant amounts of tetrahedrally coordinated B (Ertl et al., 1997, 2005; Tagg et al., 1999; Schreyer et al., 2002; Hughes et al., 2000, 2001, 2004). This program finds tetrahedrally coordinated B, if tourmaline has analytically excess B in its crystal structure (i.e., B > 3; see Fig. 3B).

Electron-microprobe technique is unable to establish ferric iron content from any mineral analysis. Although empirical calculation procedure

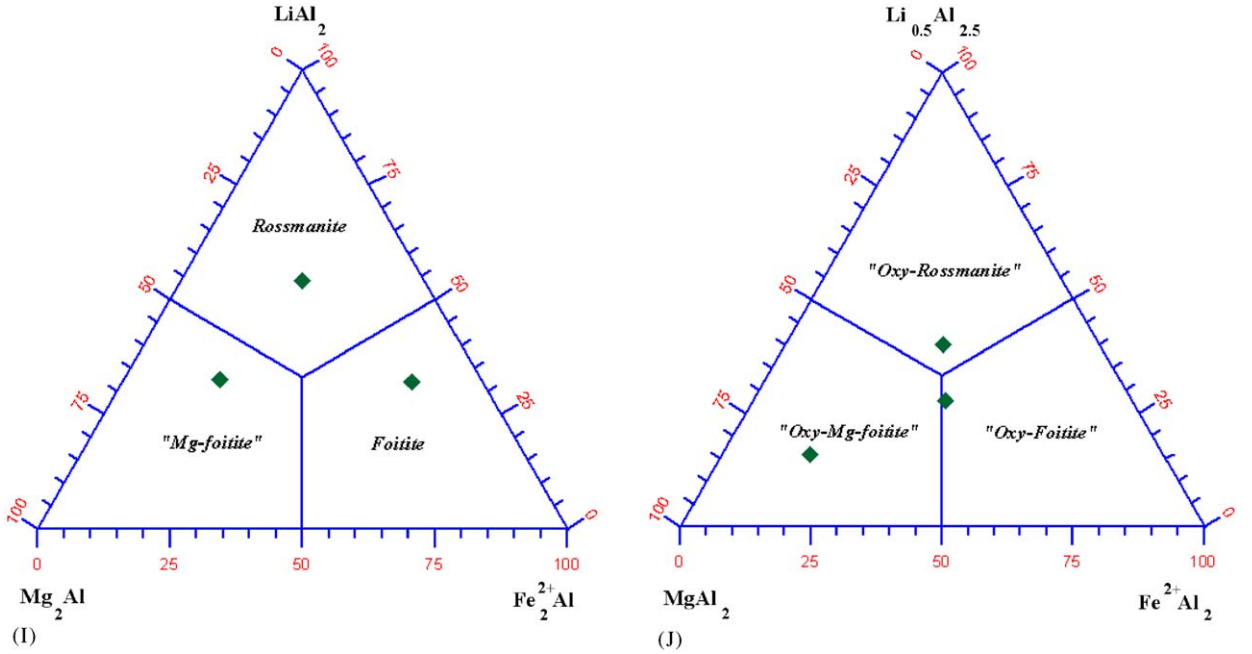


Fig. 4. (*Continued*)

of ferric iron state in *Y*-site from microprobe-derived tourmaline analysis was proposed based on the 24.5 oxygens (Lynch and Ortega, 1997), it is not possible to allocate *Y* and *Z* sites without taking into account the Mössbauer effect spectroscopy (Fuchs et al., 1995). However, taking into consideration, the 24.5 oxygens option was selected from the *Structural formulae* pull-down menu, WinClastour tries to estimate the ferric iron content of microprobe-derived tourmaline analysis on the basis of criteria (i.e., $Fe^{3+} = Fe_{total} - (3 - Mg) - Ca$) given by Lynch and Ortega (1997). Total Fe is assumed to be FeO by WinClastour in dealing with electron-microprobe data.

Calculated tourmaline data can be tabulated in different forms by clicking the *View Output* ⇒ *Output* ⇒ *Tourmaline Analyses* and/or *Calculated Cations* and/or *Cell Contents*, and/or *Classification Parameters*. Data files with the extension of "dat", are created during each program run. Graphic files with the same name of "dat" but the extension of "grf" were created by using the commercial software Grapher to plot ternary classification diagrams. In the case of clicking *View Output* ⇒ *View All* from the pull-down menu, one can display all the calculated results in a separate window called Excel (Fig. 3A). At this part of the program, by clicking *Send to Excel* icon, all the output obtained from the program is sent to Excel file entitled Output.xls. Here, by clicking the *Show Excel File* icon, the results are displayed under the Excel environment (Fig. 3B). Thus, the user of WinClastour may prepare his or her own tourmaline data plots by using the capabilities of Excel™. Thirteen ternary plot types were created under the Grapher software for tourmaline-related classification graphics after Hawthorne and Henry (1999). The complete list of these diagrams together with types and reference list is given by Yavuz et al. (2002). By clicking the *Graph* icon on the tool bar, WinClastour starts up the Grapher software provided that this program is installed on the computer. Selecting the *File* ⇒ *Open* & Grapher files (i.e., "grf" files), the user can display any of the graphic output on the screen under the Grapher software. From here, using the Select All–Copy–Paste options, the user sends the prepared plot to any of the Microsoft product, such as Word, in order to obtain a high-quality print out.

To test the program's correct execution with the original tourmaline data, a list of test data (i.e., "Test1.tou") including most of the tourmaline data types has been selected from the literature and given in Appendix A. The numerical output, including tourmaline groups and names, by WinClastour on this data set is shown in Figs. 2 and 3. Following the

evaluation of "Test1.tou" file by program, the graphical classification of some tourmaline data is given in Fig. 4 based on the classification scheme proposed by Hawthorne and Henry (1999). These types of classification graphics can be plotted by using the Grapher software for 13 diagram types.

2.3. Program requirements and installation

This software is available on the CD-ROM as a self-extracting installation file. Considering that the Microsoft® Visual Studio is not installed on the target system, all the necessary support files used by the WinClastour are added into the installation file (i.e., Setup file) by using the Inno setup compiler (version 5.0). The program and its associated files are installed into the directory of "C:\Program Files\WinClastour" during the installation process. However, the user-specified directory is accepted by the setup program. The Inno setup installer has created uninstalling application from the target computer by using the following "*Start* ⇒ *Programs* ⇒ *WinClastour* ⇒ *Uninstall WinClastour*" options. However, WinClastour can be uninstalled by selecting first "*Add/Remove Programs*" option in the Windows control panel and selecting "*Install/Uninstall*" tab, then highlighting "*WinClastour*" and pressing "*Add/Remove*" button. WinClastour, in its self-extracting setup file, is approximately 3 Mb and can be obtained by anonymous FTP from the server IAMG.ORG.

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Appendix A

A list of test data (i.e., "Test1.tou") including most of the tourmaline data types to test the program's correct execution has been selected from the literature and given in Table A.1.

Table A.1
Calculated results of test data (Test1.tou) by WinClastour program

	1	2	3	4	5	6	7	8	9	10	11
SiO_2	30.74	32.73	33.58	32.92	33.13	34.04	36.50	37.22	37.68	31.43	38.10
TiO_2	0.00	2.87	1.63	0.54	2.19	0.39	0.00	0.07	0.03	0.02	0.00
Al_2O_3	1.40	16.26	30.62	30.70	23.38	27.33	40.07	38.03	33.14	46.53	44.60
V_2O_3	0.04	0.16	0.00	0.00	0.00	0.00	0.00	0.00	0.07	0.00	0.00
Cr_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.71	0.00	0.00
Fe_2O_3	43.89	14.78	0.86	12.37	5.44	7.63	0.00	0.00	0.00	0.00	0.00
FeO	2.69	11.24	12.65	5.98	8.66	4.91	0.22	0.10	1.95	0.05	0.00
MnO	0.00	0.10	0.06	0.11	0.07	0.00	3.07	4.06	0.00	0.02	0.00
NiO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.47	0.00	0.00
ZnO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.08	0.00
MgO	6.45	4.66	2.69	0.16	7.80	7.34	0.00	0.18	9.71	0.00	0.00
CaO	0.00	0.04	0.00	0.20	3.30	0.99	0.20	2.63	0.03	1.74	0.00
Na_2O	2.12	2.71	2.84	2.49	1.16	2.35	2.15	1.40	1.42	1.33	1.43
K_2O	1.04	0.19	0.06	0.07	0.05	0.00	0.00	0.02	0.00	0.00	0.00
Li_2O	0.25[a]	0.005	0.032	0.00	0.015[a]	0.005	1.61	1.86	0.00	0.56	1.13
F	0.00	0.00	0.34	1.32	0.00	0.00	1.24	0.64	0.00	0.12	0.20
B_2O_3	9.17	9.47	10.36	10.14	10.38	10.83	11.56	10.89[a]	10.92[a]	16.20	10.88
H_2O	2.56	2.94	2.96	1.15	3.10	3.18	3.13	3.17	3.29[a]	3.25	3.70
O=F	0.00	0.00	0.14	0.56	0.00	0.00	0.52	0.27	0.00	0.05	0.08
Total	100.35	98.16	98.54	97.59	98.68	99.00	99.22	100.00	100.43	101.29	99.96
Unit formula normalized to 31 *anions*											
Si	5.87	5.96	5.79	5.65	5.77	5.79	5.88	5.94	6.05	4.74	5.88
$^{[4]}B$	0.03	0.00	0.08	0.00	0.12	0.18	0.21	0.00	0.00	1.18	0.00
^{T}Al	0.10	0.04	0.13	0.35	0.11	0.03	0.00	0.06	0.00	0.08	0.12
Sum *T* site	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.05	6.00	6.00
$^{[3]}B$	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00
^{Z}Al	0.22	3.45	6.00	5.85	4.69	5.45	6.00	6.00	6.00	6.00	6.00
Mg	1.84	1.26	0.00	0.04	1.31	0.55	0.00	0.00	0.00	0.00	0.00
V	0.01	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Fe^{3+}	3.93	1.27	0.00	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table A.1 (*continued*)

	1	2	3	4	5	6	7	8	9	10	11
Sum *Z* site	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00
^{Y}Al	0.00	0.00	0.08	0.00	0.00	0.00	1.60	1.09	0.27	2.13	2.00
Ti	0.00	0.39	0.21	0.07	0.29	0.05	0.00	0.01	0.00	0.00	0.00
V	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00
Cr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.22	0.00	0.00
Fe^{3+}	2.38	0.76	0.11	1.49	0.71	0.98	0.00	0.00	0.00	0.00	0.00
Mg	0.00	0.00	0.69	0.00	0.72	1.31	0.00	0.04	2.32	0.00	0.00
Mn	0.00	0.02	0.01	0.02	0.01	0.00	0.42	0.55	0.00	0.00	0.00
Fe^{2+}	0.43	1.70	1.83	0.86	1.26	0.66	0.03	0.01	0.18	0.01	0.00
Zn	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ni	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Li	0.19	0.13	0.07	0.57	0.01	0.03	1.04	1.19	0.00	0.34	0.70
Sum *Y* site	3.00	3.00	3.00	3.00	3.00	3.00	3.09	2.90	3.00	2.48	2.70
Ca	0.00	0.01	0.00	0.04	0.62	0.18	0.03	0.45	0.01	0.31	0.00
Na	0.79	0.96	0.95	0.83	0.39	0.78	0.67	0.43	0.44	0.42	0.43
K	0.25	0.04	0.01	0.02	0.01	0.00	0.00	0.00	0.00	0.00	0.00
Sum *X* site	1.04	1.01	0.96	0.89	1.02	0.96	0.71	0.88	0.45	0.73	0.43
OH	3.27	3.57	3.40	1.32	3.60	3.61	3.36	3.38	3.50	3.55	3.81
F	0.00	0.00	0.19	0.72	0.00	0.00	0.63	0.32	0.00	0.06	0.10
Group	Alkali	Alkali	Alkali	Alkali	Calcic	Alkali	Alkali	Calcic	Vacancy	Alkali	Vacancy
Species	Povondraite	Schorl	Schorl	Buergerite	Feruvite	Dravite	Elbaite	Liddicoatite	Mg-foitite	Olenite	Rossmanite
Reference[b]	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)
Species by WinClastour	Povondraite	Schorl	"Oxy schorl"	Buergerite	Feruvite	Dravite	"Fluor elbaite"	"Hydroxy liddicoatite"	"Oxy-Mg-foitite"	Olenite	Rossmanite

	12	13	14	15	16	17	18	19	20	21	22
SiO_2	36.37	35.30	35.70	37.10	36.97	38.10	38.17	37.20	36.20	36.51	36.01
TiO_2	0.22	0.35	0.72	0.18	0.00	0.00	0.00	0.00	0.34	0.00	0.77
Al_2O_3	35.28	26.20	29.60	33.30	38.54	40.60	44.32	36.00	25.25	30.00	32.70
V_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cr_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Fe_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	5.32	0.00	0.00
FeO	8.00	13.60	10.40	6.66	0.49	0.60	0.69	11.10	4.66	0.74	2.59
MnO	0.00	0.09	0.00	0.00	3.07	1.40	0.01	0.58	0.01	0.00	0.03
NiO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ZnO	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00
MgO	4.08	5.84	5.82	4.53	0.00	0.00	0.00	0.00	10.01	12.84	10.99
CaO	0.96	3.01	1.77	0.46	2.92	0.60	0.04	0.00	5.33	3.91	2.28
Na_2O	0.88	1.18	1.58	2.43	1.28	1.60	0.02	1.25	0.36	0.72	1.09
K_2O	0.08	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.18	0.54	0.06
Li_2O	0.26[a]	0.21[a]	0.17[a]	0.71[a]	1.61[a]	1.55[a]	1.03[a]	0.63[a]	0.47[a]	0.21[a]	0.01[a]
F	0.00	0.90	1.13	1.33	0.96	0.50	0.09	0.00	0.23	0.00	0.41
B_2O_3	10.65[a]	10.07[a]	10.33[a]	10.54	10.60[a]	10.77[a]	11.03[a]	10.57	10.54[a]	10.72[a]	10.86[a]
H_2O	3.11[a]	3.03[a]	2.88[a]	2.88[a]	3.12[a]	3.13[a]	2.83[a]	3.21[a]	1.99	4.17	2.72
O=F	0.00	0.38	0.48	0.56	0.40	0.21	0.04	0.00	0.1	0.00	0.17
Total	99.89	99.40	99.62	99.55	99.16	98.64	98.41	100.55	100.80	100.36	100.34
Unit formula normalized to 31 *anions*											
Si	5.97	6.03	5.94	6.01	5.91	6.02	5.95	6.12	5.97	5.92	5.76
$^{[4]}$B	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
^{T}Al	0.03	0.00	0.06	0.00	0.09	0.00	0.05	0.00	0.03	0.08	0.24
Sum *T* site	6.00	6.03	6.00	6.01	6.00	6.02	6.00	6.12	6.00	6.00	6.00
$^{[3]}$B	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00
^{Z}Al	6.00	5.27	5.74	6.00	6.00	6.00	6.00	6.00	4.88	5.66	5.93
Mg	0.00	0.73	0.26	0.00	0.00	0.00	0.00	0.00	1.12	0.34	0.07
V	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Fe^{3+}	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Sum *Z* site	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00
^{Y}Al	0.80	0.00	0.00	0.36	1.18	1.57	2.08	0.98	0.00	0.00	0.00
Ti	0.03	0.04	0.09	0.02	0.00	0.00	0.00	0.00	0.04	0.00	0.09
V	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Fe^{3+}	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.66	0.00	0.00
Mg	1.00	0.76	1.18	1.09	0.00	0.00	0.00	0.00	1.34	2.76	2.55
Mn	0.00	0.01	0.00	0.00	0.42	0.19	0.01	0.08	0.00	0.00	0.00
Fe^{2+}	1.10	1.94	1.45	0.90	0.07	0.08	0.08	1.53	0.64	0.10	0.35

Table A.1 (*continued*)

	12	13	14	15	16	17	18	19	20	21	22
Zn	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00
Ni	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Li	0.08	0.24	0.28	0.63	1.34	1.17	0.80	0.41	0.31	0.14	0.01
Sum *Y* site	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00
Ca	0.17	0.55	0.32	0.08	0.50	0.10	0.01	0.00	0.94	0.68	0.39
Na	0.28	0.39	0.50	0.76	0.40	0.49	0.01	0.40	0.12	0.23	0.34
K	0.02	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.04	0.11	0.01
Sum *X* site	0.47	0.94	0.82	0.84	0.90	0.59	0.03	0.40	1.10	1.02	0.74
OH	3.47	3.49	3.23	3.17	3.41	3.37	2.97	3.52	2.19	4.51	2.89
F	0.00	0.49	0.59	0.68	0.49	0.25	0.04	0.00	0.12	0.00	0.21
Group	Vacanvy	Calcic	Alkali	Alkali	Calcic	Alkali	Vacancy	Vacancy	Calcic	Calcic	Calcic
Species		"F-feruvite"	"F-schorl"	"F-dravite"	Liddicoatite	Elbaite	Rossmanite	Foitite	Uvite	Uvite	Uvite
Reference[b]	(12)	(13)	(14)	(15)	(16)	(17)	(18)	(19)	(20)	(21)	(22)
Species by WinClastour	"Oxy foitite"	"Fluor feruvite"	"Fluor schorl"	"Fluor dravite"	Liddicoatite	"Oxy elbaite"	"Oxy rossmanite"	Foitite	"Ferri uvite"	Uvite	"Fluor uvite"

	23	24	25	26	27	28	29	30	31
SiO_2	32.50	33.00	36.45	38.81	33.72	32.81	37.22	38.27	38.42
TiO_2	0.03	0.24	0.81	0.00	0.00	2.61	0.07	0.00	0.00
Al_2O_3	9.70	11.40	34.38	40.13	25.88	28.19	38.03	40.17	40.53
V_2O_3	2.50	1.70	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cr_2O_3	30.90	30.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Fe_2O_3	0.00	0.00	0.53	0.00	1.82	0.00	0.00	0.00	0.00
FeO	0.32	0.21	5.39	1.36	3.23	12.58	0.10	0.97	0.00
MnO	0.00	0.00	0.11	0.46	0.00	0.00	4.06	0.00	0.64
NiO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ZnO	0.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MgO	8.33	8.40	6.53	0.00	14.07	6.16	0.18	6.15	0.00
CaO	0.38	0.35	0.36	0.04	6.92	3.50	2.63	0.00	1.78
Na_2O	2.52	2.60	1.99	2.03	2.52	0.95	1.40	0.70	1.09
K_2O	0.07	0.08	0.07	0.01	0.20	0.00	0.02	0.00	0.00
Li_2O	0.26[a]	0.30[a]	0.22[a]	1.93[a]	0.47[a]	0.08[a]	1.81	0.32[a]	1.87[a]
F	0.67	0.60	0.14	0.30	0.00	0.20	0.64	0.00	1.30
B_2O_3	9.76[a]	9.92[a]	10.80[a]	10.71[a]	10.56[a]	10.20[a]	10.88[a]	11.22[a]	10.78[a]
H_2O	2.50	3.11[a]	2.88	3.36[a]	1.80	3.03	3.07	3.82	2.79[a]
O = F	0.28	0.25	0.06	0.13	0.00	0.08	0.27	0.00	0.55
Total	100.28	101.68	100.59	97.68	101.20	100.22	99.84	101.62	98.65
Unit formula normalized to 31 *anions*									
Si	5.79	5.73	5.87	6.16	5.55	5.59	5.94	5.93	6.01
$^{[4]}B$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
^{T}Al	0.21	0.27	0.13	0.00	0.45	0.41	0.06	0.07	0.00
Sum *T* site	6.00	6.00	6.00	6.16	6.00	6.00	6.00	6.00	6.01
$^{[3]}B$	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00
^{Z}Al	1.83	2.07	6.00	6.00	4.57	5.25	6.00	6.00	6.00
Mg	2.21	2.18	0.00	0.00	1.43	0.75	0.00	0.00	0.00
V	0.36	0.24	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cr	1.60	1.52	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Fe^{3+}	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Sum *Z* site	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00
^{Y}Al	0.00	0.00	0.39	1.50	0.00	0.00	1.10	1.26	1.47
Ti	0.00	0.03	0.10	0.00	0.00	0.33	0.01	0.00	0.00
V	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cr	2.75	2.60	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Fe^{3+}	0.00	0.00	0.06	0.00	0.23	0.00	0.00	0.00	0.00
Mg	0.00	0.00	1.57	0.00	2.02	0.82	0.04	1.42	0.00
Mn	0.00	0.00	0.01	0.06	0.00	0.00	0.55	0.00	0.08
Fe^{2+}	0.05	0.03	0.73	0.00	0.44	1.79	0.01	0.13	0.00
Zn	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ni	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Li	0.18	0.34	0.14	1.43	0.31	0.05	1.16	0.20	1.44
Sum *Y* site	3.00	3.00	3.00	3.00	3.00	3.00	2.88	3.00	3.00
Ca	0.07	0.07	0.06	0.01	1.22	0.64	0.45	0.00	0.30
Na	0.87	0.88	0.62	0.62	0.80	0.31	0.43	0.21	0.33
K	0.02	0.02	0.01	0.00	0.04	0.00	0.00	0.00	0.00
Sum *X* site	0.96	0.97	0.69	0.63	2.06	0.95	0.88	0.21	0.63
OH	2.97	3.63	3.09	3.64	1.98	3.44	3.27	3.95	3.00
F	0.38	0.33	0.07	0.15	0.00	0.11	0.32	0.00	0.64
Group	Alkali	Alkali	Alkali	Alkali	Calcic	Calcic	Calcic	Vacancy	Vacancy
Species	Chromdravite	Chromdravite"	"Oxy dravite"	Elbaite	Uvite	Feruvite	Liddicoatite	Magnesiofoitite	"Fluor rossmanite"

Table A.1 (*continued*)

	23	24	25	26	27	28	29	30	31
Reference[b] Species by WinClastour	(23) "Fluor chromdravite"	(24) Chromdravite"	(25) "Oxy dravite"	(26) Elbaite	(27) "Oxy uvite"	(28) "Oxy feruvite"	(29) "Oxy liddicoatite"	(30) Magnesiofoitite	(31) "Fluor rossmanite"

[a]Calculated by WinClastour based on stoichiometry.

[b](7) Grice and Ercit, 1993; (8, 29) Aurisicchio et al., 1999; (9) Baksheev and Kudryavtseva, 2004; (10) Hughes et al., 2000; (11) Selway et al., 1998a; (12) Jiang et al., 1997; (13) Selway et al., 1998b; (14, 15) Selway et al., 2000; (16–17) Teertstra et al., 1999; (18) Zhang et al., 2004; (19) Selway et al., 1999; (20) Kornetova, 1975; (21) Wulfing and Becht, 1913; (22) Jacob, 1938; (23, 24) Bosi et al., 2004b; (25) Novák et al., 2004; (26) Novák and Taylor, 2000; (27) Sargent, 1901; (28) Jiang et al., 1996; (30) Hawthorne et al., 1999; (31) Giller, 2003.

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