Computers & Geosciences 63 (2014) 70–87

Contents lists available at ScienceDirect

Computers & Geosciences

journal homepage: www.elsevier.com/locate/cageo

A Windows program for calculation and classification of tourmaline-supergroup (IMA-2011)☆

Fuat Yavuz [a,*], Necati Karakaya [b], Demet K. Yıldırım [a], Muazzez Ç. Karakaya [b], Mustafa Kumral [a]

[a] Department of Geological Engineering, Istanbul Technical University, 34469 Maslak, Istanbul, Turkey
[b] Selçuk Üniversitesi, Mühendislik Fakültesi, Jeoloji Mühendisliği Bölümü, 42079 Konya, Turkey

ARTICLE INFO

Article history:
Received 11 June 2013
Received in revised form
17 October 2013
Accepted 18 October 2013
Available online 6 November 2013

Keywords:
International Mineralogical Association (IMA)
Tourmaline
Classification
Normalization
Software

ABSTRACT

A Microsoft Visual Basic program, WinTcac, has been developed to calculate structural formulae of tourmaline analyses based on the Subcommittee on Tourmaline Nomenclature (STN) of the International Mineralogical Association's Commission on New Minerals, Nomenclature and Classification (IMA-CNMCN) scheme. WinTcac calculates and classifies tourmaline-supergroup minerals based on 31 O atoms for complete tourmaline analyses. For electron-microprobe-derived tourmaline analyses site occupancy can be estimated by using the stoichiometric H_2O (wt%) and B_2O_3 (wt%) contents. This program also allows the user to process tourmaline analyses using 15 cations and 6 silicons normalization schemes. WinTcac provides the user to display tourmaline analyses in a various classification, environmental, substitution, and miscellaneous plots by using the Golden Software's Grapher program. The program is developed to predict cation site-allocations at the different structural positions, including the *T*, *Z*, *Y*, and *X* sites, as well as to estimate the OH^{1-}, F^{1-}, Cl^{1-}, and O^{2-} contents. WinTcac provides editing and loading Microsoft Excel files to calculate multiple tourmaline analyses. This software generates and stores all the calculated results in the output of Microsoft Excel file, which can be displayed and processed by any other software for verification, general data manipulation, 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 designed to produce a high-quality printout of the related plotting software.

1. Introduction

Minerals of the tourmaline-supergroup are the most important and ubiquitous accessory borosilicate minerals in a great diversity of geological settings within the Earth's crust (Dutrow and Henry, 2011; van Hinsberg et al., 2011a, 2011b). Within these settings, tourmalines occur in a wide variety of rock compositions, including as authigenic overgrowths on detrial grains in sedimentary rocks (e.g., Henry et al., 1994; Henry and Dutrow, 1996; Van den Bleeken et al., 2007), as resistant and prograde minerals in different facies of metamorphic rocks (e.g., Henry and Dutrow, 1992, 2012; Kawakami, 2001; Torres-Ruiz et al., 2003; Abu El-Enen and Okrusch, 2007; Ertl et al., 2010; van Hinsberg and Schumacher, 2011), and as a primary phase in intrusive rocks and related pegmatites (e.g., London and Manning, 1995; Roda et al., 1995; Keller et al., 1999; Tindle et al., 2002; Trumbull et al., 2008; Yavuz et al., 2008). Tourmaline is a common mineral in hydrothermal deposits that are formed by epigenetic and syngenetic processes (Slack and Trumbull, 2011). Tourmalines belong to the epigenetic style are composed of porphyry type Cu ± Mo deposits (e.g., Lynch and Ortega, 1997; Yavuz et al., 1999), Cu–Au breccias pipes (e.g., Warnaars et al., 1985; Skewes et al., 2003), and Sn–W veins in or near granites (e.g., Manning, 1986; Mlynarczyk and Williams-Jones, 2006; Neiva et al., 2007; Esmaeily et al., 2009). Tourmaline-supergroup minerals in syngenetic category are mainly found in sedimentary-exhalative (SEDEX) Zn–Pb–Ag deposits (e.g., Bone, 1988; Slack et al., 1993; Jiang et al., 1995) and volcanogenic massive sulfide (VMS) Cu–Zn–Pb–Ag–Au deposits (e.g., Taylor and Slack, 1984; Slack and Coad, 1989; Deb et al., 1997). The presence of tourmaline in such different geological environments made it important to understand the physical and chemical conditions of rock formation, ore-forming processes, and hydrothermal ore deposits. Since the tourmaline-supergroup minerals have an extensive temperature (*T*) and pressure (*P*) stability range, they have been used as a good petrogenetic indicator for P–T–fO_2 conditions (Henry and Guidotti, 1985; van Hinsberg et al., 2011a, 2011b and references therein).

☆The executable code is available in the journal server or from corresponding author on request.

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

0098-3004/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.cageo.2013.10.012

Table 1
Relative site abundances of cations and anions in tourmaline-supergroup minerals (from Henry et al., 2011).

Site	Relative abundance of ions with different valence states	Common cations and anions at each site in order of relative abundance
X	$R^{1+} > R^{2+} >$ vacancy (□)	R^{1+}:**Na^{1+}** $> >$ K^{1+} R^{2+}:**Ca^{2+}**
Y	$R^{2+} > R^{3+} > R^{1+} > R^{4+}$	R^{2+}:**Fe^{2+}** ≈ **Mg^{2+}** > **Mn^{2+}** $> > >$ Zn^{2+}, Ni^{2+}, Co^{2+}, Cu^{2+} R^{3+}:**Al^{3+}** $> >$ **Fe^{3+}** > $Cr^{3+} > > V^{3+}$ R^{1+}:**Li^{1+}** R^{4+}:**Ti^{4+}**
Z	$R^{3+} > > R^{2+}$	R^{3+}:**Al^{3+}** $> >$ **Fe^{3+}** > $Cr^{3+} > V^{3+}$ R^{2+}:**Mg^{2+}** > Fe^{2+}
T	$R^{4+} > > R^{3+}$	R^{4+}:**Si^{4+}** R^{3+}:**Al^{3+}** > B^{3+}
B	R^{3+}	R^{3+}:**B^{3+}**
V	$S^{1-} > > S^{2-}$	S^{1-}:**OH^{1-}** S^{2-}:**O^{2-}**
W	$S^{1-} \approx S^{2-}$	S^{1-}:**OH^{1-}** ≈ **F^{1-}** S^{2-}:**O^{2-}**

Notes: R=cations; S=anions; the bolded cations and anions represent the most common ions at these sites.

Table 2
IMA-accepted and prospective alkali-, calcic-, and vacant-group tourmaline species with their end-member compositions (revised from Henry et al., 2011).

Row	General formula	(*X*)	(Y_3)	(Z_6)	T_6O_{18}	$(BO_3)_3$	V_3	*W*
Alkali group								
1	***Alkali-subgroup* 1**	***R^{1+}***	***R_3^{2+}***	***R_6^{3+}***	***$R_6^{4+}O_{18}$***	***$(BO_3)_3$***	***S_3^{1-}***	***S^{1-}***
2	**Dravite***	Na	Mg_3	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)
3	**Schorl***	Na	Fe_3^{2+}	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)
4	**Chromium-dravite***	Na	Mg_3	Cr_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)
5	**Vanadium-dravite***	Na	Mg_3	V_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)
6	**Fluor-dravite***	Na	Mg_3	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	F
7	**Fluor-schor***	Na	Fe_3^{2+}	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	F
8	"Potassium-dravite"†	K	Mg_3	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)
9	"Tsilaisite"[a]	Na	Mn_3^{2+}	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)
	***Alkali-subgroup* 2**	***R^{1+}***	***$R_{1.5}^{1+}$ $R_{1.5}^{3+}$***	***R_6^{3+}***	***$R_6^{4+}O_{18}$***	***$(BO_3)_3$***	***S_3^{1-}***	***S^{1-}***
10	**Elbaite***	Na	$Li_{1.5}^{1+}Al_{1.5}^{3+}$	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)
11	"Fluor-elbaite"[b]	Na	$Li_{1.5}^{1+}Al_{1.5}^{3+}$	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	F
	***Alkali-subgroup* 3**	***R^{1+}***	***R_3^{3+}***	***R_4^{3+} R_2^{2+}***§	***$R_6^{4+}O_{18}$***	***$(BO_3)_3$***	***S_3^{1-}***	***S^{2-}***
12	**Povondraite***	Na	Fe_3^{3+}	Fe_3^{4+} Mg_2	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	O
13	**Chromo-alumino-povondraite***	Na	Cr_3	Al_4 Mg_2	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	O
14	"Oxy-dravite"[c]	Na	Al_3	Al_4 Mg_2	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	O
15	"Oxy-schorl"[d]	Na	Al_3	Al_4 Fe_2^{2+}	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	O
16	"Na–Cr–O root name (Oxy-chromium-dravite)"[e]	Na	Cr_3	Cr_4 Mg_2	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	O
17	"(Oxy-vanadium-dravite)"[f]	Na	V_3	V_4Mg_2	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	O
18	"Vanadio-oxy-dravite"[g]	Na	V_3	Al_4 Mg_2	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	O
19	"Vanadio-oxy-chromium-dravite"[h]	Na	V_3	Cr_4 Mg_2	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	O
20	"Potassium-povondraite"†	K	Fe_3^{3+}	Fe_3^{4+} Mg_2	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	O
	***Alkali-subgroup* 4**	***R^{1+}***	***R_1^{1+} R_2^{3+}***	***R_6^{3+}***	***$R_6^{4+}O_{18}$***	***$(BO_3)_3$***	***S_3^{1-}***	***S^{2-}***
21	"Na–Li–O root name (Darrellhenryite)"[i]	Na	Li_1 Al_2	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	O
	***Alkali-subgroup* 5**	***R^{1+}***	***R_3^{3+}***	***R_6^{3+}***	***$R_6^{3+}O_{18}$***	***$(BO_3)_3$***	***S_3^{2-}***	***S^{1-}***
22	**Fluor-buergerite***	Na	Fe_3^{3+}	Al_6	Si_6O_{18}	$(BO_3)_3$	$(O)_3$	F
23	**Olenite***	Na	Al_3	Al_6	Si_6O_{18}	$(BO_3)_3$	$(O)_3$	(OH)
24	"Buergerite"‡	Na	Fe_3^{3+}	Al_6	Si_6O_{18}	$(BO_3)_3$	$(O)_3$	(OH)
25	"Fluor-olenite"‡	Na	Al_3	Al_6	Si_6O_{18}	$(BO_3)_3$	$(O)_3$	F
	***Alkali-subgroup* 6**	***R^{1+}***	***R_3^{3+}***	***R_6^{3+}***	***$R_3^{3+}R_3^{4+}O_{18}$***	***$(BO_3)_3$***	***S_3^{1-}***	***S^{1-}***
26	"Na–Al–Al–Al root name"‡	Na	Al_3	Al_6	$Al_3Si_3O_{18}$	$(BO_3)_3$	$(OH)_3$	(OH)
27	"Na–Al–Al–B root name"‡	Na	Al_3	Al_6	$B_3Si_3O_{18}$	$(BO_3)_3$	$(OH)_3$	(OH)
28	"Fluor-Na–Al–Al–Al root name"‡	Na	Al_3	Al_6	$Al_3Si_3O_{18}$	$(BO_3)_3$	$(OH)_3$	F
29	"Fluor-Na–Al–Al–B root name"‡	Na	Al_3	Al_6	$B_3Si_3O_{18}$	$(BO_3)_3$	$(OH)_3$	F
Calcic group								
	***Calcic-subgroup* 1**	***Ca^{2+}***	***R_3^{2+}***	***$R^{2+}R_5^{3+}$***	***$R_6^{4+}O_{18}$***	***$(BO_3)_3$***	***S_3^{1-}***	***S^{1-}***
30	**Fluor-uvite***	Ca	Mg_3	$MgAl_5$	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	F
31	**Feruvite***	Ca	Fe_3^{2+}	$MgAl_5$	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)